APPLIED PROBABILITY, STOCHASTIC PROCESSES,
AND SAMPLING THEORY

THE UNIVERSITY OF WESTERN ONTARIO SERIES IN PHILOSOPHY OF SCIENCE

A SERIES OF BOOKS
IN PHILOSOPHY OF SCIENCE, METHODOLOGY,
EPISTEMOLOGY, LOGIC, HISTORY OF SCIENCE
AND RELATED FIELDS

VOLUME 34

ADVANCES IN THE STATISTICAL SCIENCES

Festschrift in Honor of Professor V. M. Joshi's 70th Birthday

VOLUME I

APPLIED PROBABILITY, STOCHASTIC PROCESSES, AND SAMPLING THEORY

Edited by

IAN B. MacNEILL and GARY J. UMPHREY

Department of Statistical and Actuarial Sciences,
The University of Western Ontario

Associate editors:

DAVID R. BELLHOUSE

and

REGINALD J. KULPERGER

Department of Statistical and Actuarial Sciences,
The University of Western Ontario

D. REIDEL PUBLISHING COMPANY

A MEMBER OF THE KLUWER  ACADEMIC PUBLISHERS GROUP

DORDRECHT / BOSTON / LANCASTER / TOKYO

Library of Congress Cataloging in Publication Data

Applied probability, stochastic processes, and sampling theory.

(Advances in the statistical sciences; v. 1)
(The University of Western Ontario series in philosophy of science; v. 34)
Bibliography: p.
1. Probabilities—Congresses. 2. Stochastic processes—Congresses.
3. Sampling (Statistics)—Congresses. I. MacNeill, Ian B., 1931–
II. Umphrey, Gary J., 1953– . III. Series. IV. Series: University
of Western Ontario series in philosophy of science; v. 34.
QA276.A1A39 vol. 1 519.5 s 86–29673
[QA273.A1] [519.2]

ISBN-13: 978-94-010-8622-6 e-ISBN-13: 978-94-009-4786-3
DOI: 10.1007/978-94-009-4786-3

Published by D. Reidel Publishing Company,
P.O. Box 17, 3300 AA Dordrecht, Holland.

Sold and distributed in the U.S.A. and Canada
by Kluwer Academic Publishers,
101 Philip Drive, Assinippi Park, Norwell, MA 02061, U.S.A.

In all other countries, sold and distributed
by Kluwer Academic Publishers Group,
P.O. Box 322, 3300 AH Dordrecht, Holland.

TABLE OF CONTENTS

CONTENTS OF THE OTHER VOLUMES OF THE JOSHI FESTSCHRIFT

VOLUME II

Foundations of Statistical Inference

VOLUME III

Time Series and Econometric Modelling

VOLUME IV

Stochastic Hydrology

VOLUME V

Biostatistics

VOLUME VI

Foundations of Actuarial Science

PREFACE

On May 27–31, 1985, a series of symposia was held at The University of Western Ontario, London, Canada, to celebrate the 70th birthday of Professor V. M. Joshi. These symposia were chosen to reflect Professor Joshi's research interests as well as areas of expertise in statistical science among faculty in the Departments of Statistical and Actuarial Sciences, Economics, Epidemiology and Biostatistics, and Philosophy.

From these symposia, the six volumes which comprise the "Joshi Festschrift" have arisen. The 117 articles in this work reflect the broad interests and high quality of research of those who attended our conference. We would like to thank all of the contributors for their superb cooperation in helping us to complete this project.

Our deepest gratitude must go to the three people who have spent so much of their time in the past year typing these volumes: Jackie Bell, Lise Constant, and Sandy Tamowski. This work has been printed from "camera ready" copy produced by our Vax 785 computer and QMS Lasergraphix printers, using the text processing software TEX. At the initiation of this project, we were neophytes in the use of this system. Thank you, Jackie, Lise, and Sandy, for having the persistence and dedication needed to complete this undertaking.

We would also like to thank Maria Hlawka-Lavdas, our systems analyst, for her aid in the layout design of the papers and for resolving the many difficult technical problems which were encountered. Nancy Nuzum and Elly Pakalnis have also provided much needed aid in the conference arrangements and in handling the correspondence for the Festschrift.

Professor Robert Butts, the Managing Editor of *The University of Western Ontario Series in Philosophy of Science* has provided us with his advice and encouragement. We are confident that the high calibre of the papers in these volumes justifies his faith in our project.

In a Festschrift of this size, a large number of referees were needed. Rather than trying to list all of the individuals involved, we will simply say "thank you" to the many people who undertook this very necessary task for us. Your contributions are greatly appreciated.

Financial support for the symposia and Festschrift was provided by The University of Western Ontario Foundation, Inc., The University of Western Ontario and its Faculties of Arts, Science, and Social Science, The UWO Statistical Laboratory, and a conference grant from the Natural Sciences

and Engineering Research Council of Canada. Their support is gratefully acknowledged.

Finally, we would like to thank Professor Joshi for allowing us to hold the conference and produce this Festschrift in his honor. Professor Joshi is a very modest man who has never sought the limelight. However, his substantial contributions to statistics merit notice (see Volume I for a bibliography of his papers and a very spiffy photo). We hope he will accept this as a tribute to a man of the highest integrity.

INTRODUCTION TO VOLUME I

The areas of applied probability, stochastic processes, sampling theory and the foundations of statistical inference are those to which Professor V. M. Joshi has directed most of his research effort. The twenty-two articles in this volume are devoted to the first three of these areas; another volume in this series is composed of articles on foundations. Articles on modelling of physical and biological systems appear in the first part of this volume, followed by those on more theoretical aspects of probability and stochastic models. The final set of papers is on sampling theory.

Alan Cornish begins this first volume of the Festschrift with a most appropriate paper, "V. M. Joshi and the Markov Oscillation Problem". Cornish considers standard p-functions and reviews some of the contributions of Professor Joshi to this area.

The next seven articles consider important applications of probability and stochastic processes, and give body and flavour to the extreme breadth of usefulness of the discipline. Anderson's paper considers the photographic process and discusses temporal and spatial problems of a probabilistic nature. Aspects of photosynthesis are modelled by Matthews, Minder and McMillan who also fit their models to experimental data. Metal fatigue and the time to failure are the subjects of the paper by Desmond. Todorovic's paper is concerned with stochastic models of soil erosion. Brillinger considers models for sinusoidal data of unknown frequency and discusses a wide range of physical examples including ones from seismology, geophysics, nuclear magnetic resonance and oceanography. Ferland and Giroux also consider applications to physics, in particular to quantum mechanics. Gani continues his work in the development of epidemic behaviour.

Some of the central issues of applied probability and stochastic processes are considered in the next six papers. In particular, queueing theory has been an active and important area of applied probability. A recent development in this area has been the study of networks of queues, which is the subject of the paper by Blais. Limit theorems play an important role in probability, and Kulperger obtains a limit theorem for point processes utilizing a more elementary result. Ramsay obtains limit theorems for sums of random variables defined on a finite Markov chain.

Prakasa Rao describes the theory of estimation for nonlinear regression models in an extensive review paper. McLeish and Small consider the discrimination problem and develop asymptotic results for minimizing mis-

classification. Nguyen's paper considers the problem of determining bounds on the size of the class of bivariate distributions which contains two given marginal distributions.

The remaining papers in this volume are concerned with finite sampling, and it is fitting that the paper by Ghosh is concerned with the concept of admissibility in survey sampling. Professor Joshi's first paper, a 1965 *Annals* paper written jointly with Godambe, generalized some earlier results on the admissibility of the Horvitz-Thompson estimator. Subsequently, Professor Joshi has published about twenty-five articles on the topic of admissibility and was invited to review that topic for the *Encyclopedia of Statistical Sciences*. Ghosh's paper contains a comprehensive review of admissibility and uniform admissibility, much of which has emanated from Professor Joshi's pioneering work. In addition the paper contains a review of a recently developed "Step-wise Bayes" technique, due to Ghosh and Meeden, which can be used to generate new estimates of the finite population mean and variance.

Another area of research that emerged in the sixties and seventies over the controversies surrounding foundational aspects of sampling was that of model-based inference for finite populations. The next two papers by Royall and Thompson address issues in this line of research. Throughout a series of previously published papers Royall has studied the consequences of model breakdown on inference in finite populations and has recommended procedures to deal with the problem. In the current paper he examines the effect of correlation on model-based large sample confidence intervals for the finite population mean when the assumed working model is based on the assumption of independent observations. With the growing use of models in survey research some survey statisticians are examining the parallels between results in sampling and experimental design. Here Thompson has shown how ideas in sampling based on random permutation models or exchangeable prior distributions on the observations may be applied to inference problems in the one-way layout in experimental design.

The analysis of complex surveys is a rapidly developing field of research in survey sampling. Major developments to date have included the examination of the use of regression analysis and categorical data analysis when several stages of sampling and/or clustering is present in the survey design. Fuller, one of the leaders in this field of research, has presented some new research on the application of the factor model to complex surveys. The interest in the general topic of the analysis of complex surveys by large statistical agencies, such as Statistics Canada, is represented by the papers of Binder, Hidiroglou and their co-authors. Binder and his colleagues have reviewed the uses of regression methodology, categorical data analysis and percentile estimation in complex surveys. Hidiroglou and Paton have examined similar topics but from the point of view of computer methods necessary

to implement these analyses.

Amode Sen, along with his co-author Pranab Sen, continues his long interest in sampling animal populations. Here the capture-recapture problem from the point of view of sampling on two occasions is examined. Finally, Warner has presented a model to measure the ability of individuals to process information rationally as opposed to being influenced by sloganeering.

The sampling papers taken together show the broad range of work being done in survey research.

PROFESSOR V. M. JOSHI

CURRENT BIBLIOGRAPHY OF PROFESSOR V. M. JOSHI

The following bibliography gives the statistical papers of Professor Joshi up to August, 1986. We emphasize that this list is by no means complete; Dr. Joshi is still very active in the Department of Statistical and Actuarial Sciences and will have a full teaching load this fall, at the age of 72.

A biography of Professor Joshi was recently published in the *Canadian Journal of Statistics* (**14**, 1–3). Although we do not wish to cover old ground, we might mention that when Professor Joshi's first paper was published, he was in his early 50's. Statistics has been a second career for him, after distinguished service in the civil service in India. The remarkable success he has had in this "second career" is apparent from a perusal of his writings.

1965

Admissibility and Bayes estimation in sampling finite populations. I. (Jointly with V. P. Godambe). *Annals of Mathematical Statistics* **36**, 1707–1722.

Admissibility and Bayes estimation in sampling finite populations. II. *Annals of Mathematical Statistics* **36**, 1723–1729.

Admissibility and Bayes estimation in sampling finite populations. III. *Annals of Mathematical Statistics* **36**, 1730–1742.

1966

Admissibility of confidence intervals. *Annals of Mathematical Statistics* **37**, 629–638.

Admissibility and Bayes estimation in sampling finite populations—IV. *Annals of Mathematical Statistics* **37**, 1658–1670.

1967

Confidence intervals for the mean of a finite population. *Annals of Mathematical Statistics* **38**, 1180–1207.

Inadmissibility of the usual confidence sets for the mean of a multivariate normal population. *Annals of Mathematical Statistics* **38**, 1868–1875.

1968

Note on a minimax design for cluster sampling. *Annals of Mathematical Statistics* **39**, 278–281.

Admissibility of the sample mean as estimate of the mean of a finite population. *Annals of Mathematical Statistics* **39**, 606–620.

Distribution-free sufficiency in sampling finite populations. *Journal of the Royal Statistical Society*, Series B **30**, 551–555.

Asymptotic risk of maximum likelihood estimates. *Journal of the Indian Statistical Association* **6**, 31–42.

The sample mean as a unique minimax estimate of the mean of a normal population with a generalized loss function. *Journal of the Indian Statistical Association* **6**, 57–66.

Admissibility of confidence intervals. *Journal of the Indian Statistical Association* **6**, 127–134.

1969

On a theorem of Karlin regarding admissible estimates for exponential populations. *Annals of Mathematical Statistics* **40**, 216–223.

Admissibility of the usual confidence sets for the mean of a univariate or bivariate normal population. *Annals of Mathematical Statistics* **40**, 1042–1067.

Admissibility of estimates of the mean of a finite population. In *New Developments in Survey Sampling*, edited by N. L. Johnson and H. Smith, Jr. New York: John Wiley and Sons.

1970

Admissibility of invariant confidence procedures for estimating a location parameter. *Annals of Mathematical Statistics* **41**, 1568–1581.

Note on the admissibility of the Sen-Yates-Grundy variance estimator and Murthy's estimator and its variance estimator for samples of size two. *Sankhyā*, Series A **32**, 431–438.

A minimax property of the invariant confidence sets for a multivariate poulation. *Journal of the Indian Statistical Association* **8**, 55–62.

1971

Admissibility of the usual confidence sets for a class of bivariate populations. *Annals of Mathematical Statistics* **42**, 662–679.

Hyperadmissibility of estimators for finite populations. *Annals of Mathematical Statistics* **42**, 680–690.

Admissibility of arbitrary estimates as unbiased estimates of their expectations in a finite population. *Annals of Mathematical Statistics* **42**, 839–841.

A note on admissible sampling designs for a finite population. *Annals of Mathematical Statistics* **42**, 1425–1428.

Inadmissibility of the usual confidence sets for a class of multivariate populations. *Journal of the Indian Statistical Association* **9**, 24–29.

1972

A note on hyperadmissibility of estimators for finite populations. *Annals of Mathematical Statistics* **43**, 1323–1328.

1973

A note on two-sided confidence intervals for linear functions of the normal mean and variance. (Jointly with C. E. Land and B. R. Johnson). *Annals of Statistics* **1**, 940–943.

1974

A note on the incompatibility of one-sided Bayes and frequency confidence intervals. *Journal of the Royal Statistical Society*, Series B **36**, 237–242.

1975

A conjecture of Berry regarding a Bernoulli two-armed bandit. *Annals of Statistics* **3**, 189–202.

Strong admissibility of a set of confidence intervals for the mean of a finite population. *Annals of Statistics* **3**, 483–488.

On the minimax estimation of a random probability with known first N moments. *Annals of Statistics* **3**, 680–687.

A new bound for standard p-functions. *Annals of Probability* **3**, 346–352.

1976

Confidence intervals for linear functions of the normal parameters. *Annals of Statistics* **4**, 413–418.

On the attainment of the Cramér-Rao lower bound. *Annals of Statistics* **4**, 998–1002.

A note on Birnbaum's theory of the likelihood principle. *Journal of the American Statistical Association* **71**, 345–346.

1977

An improved upper bound for standard p-functions. *Annals of Probability* **5**, 999–1003.

A note on estimators in finite populations. *Annals of Statistics* **5**, 1051–1053.

First-passage percolation on the plane square lattice. *Sankhyā*, Series A **39**, 206–209.

An upper bound for exponentially starting standard p-functions. *Sankhyā*, Series A **39**, 334–340.

Estimators of the mean of a finite population. *Journal of the Indian Statistical Association* **15**, 1–9.

1979

The best strategy for estimating the mean of a finite population. *Annals of Statistics* **7**, 531–536.

Joint admissibility of the sample means as estimators of the means of finite populations. *Annals of Statistics* **7**, 995–1002.

1980

Joint admissibility of the sample means as estimators of the means of finite populations under a general loss function. *Sankhyā*, Series C **42**, 118–123.

1981

Multiple three-decision rules for factorial simple effects: Bonferroni wins again! (jointly with Robert Bohrer, Winston Chow, Ray Faith and C.-F. Wu). *Journal of the American Statistical Association* **76**, 119–124.

A generalization of Davidson's upper bound for standard jump p-functions. *Journal of the Indian Statistical Association* **19**, 69–76.

1982

A characterization of the normal population. *Journal of the Indian Statistical Association* **20**, 85–88.

A counter example of Hacking against the long run rule. *British Journal for the Philosophy of Science* **33**, 287–289.

Article on 'Admissibility'. In *Encyclopedia of Statistical Sciences*, Volume 1, edited by S. Kotz and N. L. Johnson, pp. 25–29. New York: John Wiley and Sons.

1983

Nonvalidity of a counter example of Hajek. (Letter to the editor). *American Statistician* **37**, 96.

Article on 'Kingman Inequalities'. In *Encyclopedia of Statistical Sciences*, Volume 4, edited by S. Kotz and N. L. Johnson, pp. 384–386. New York: John Wiley and Sons.

Article on 'Likelihood Principle'. In *Encyclopedia of Statistical Sciences*, Volume 4, edited by S. Kotz and N. L. Johnson, pp. 644–647. New York: John Wiley and Sons.

1984

A conjecture of Chernoff relating to an optimization problem. *Sankhyā*, Series A **46**, 253–266.

On the admissibility of the regression estimator. (Jointly with D. R. Bellhouse). *Journal of the Royal Statistical Society*, Series B **46**, 268–269.

1985

Article on 'Linear Sufficiency'. In *Encyclopedia of Statistical Sciences*, Volume 5, edited by S. Kotz and N. L. Johnson, pp. 64–65. New York: John Wiley and Sons.

Resolution of Godambe's paradox. (Discussion). *Canadian Journal of Statistics* **13**, 299.

A family of probability densities having a complete sufficient statistic for a location parameter. *Journal of the Indian Statistical Association* **23**, 1–18.

1986

Admissibility of the best invariant estimator of a location parameter. *Sankhyā*, Series A **48**, to appear.

Alan Cornish [1]

V. M. JOSHI AND THE MARKOV OSCILLATION PROBLEM

ABSTRACT

In 1968 Davidson posed the following tantilising problem. Suppose $p(t)$ denotes for $t \geq 0$ a p-function or transition function for some state of a Markov chain (with $p(0) = 1$). For any given $t > 0$, put $p(t) = M$. How small is $m = \inf\{p(s) : s \leq t\}$? In other words, what pairs (m, M) can occur?

The problem remains unsolved but substantial contributions to the eventual solution have been made by V. M. Joshi. This paper reviews Joshi's work and outlines the current state of play.

1. THE PROBLEM

In this paper we sketch the fascinating story of the, as yet, unsolved Markov Oscillation Problem (Kendall and Harding, 1973, pp. 32–34). The substantial contributions made by V. M. Joshi are highlighted in Section 5 and some promising new developments are discussed in Section 6 of this paper.

This story begins with the Kingman inequalities for p-functions (Kingman, 1964). Any diagonal transition function $p(t)$ in a Markov chain (with continuous time parameter and denumerable state space) satisfies, for any positive integer n and any $0 < t_1 < t_2 < \cdots < t_n$, the inequalities

$$\begin{aligned} F(t_1, t_2, \ldots, t_n) &\geq 0, \\ G(t_1, t_2, \ldots, t_n) &\geq 0, \end{aligned} \tag{1}$$

[1] Department of Mathematics and Statistics, Memorial University of Newfoundland, St. John's, Newfoundland A1C 5S7

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 1–7.

where

$$G(t_1, t_2, \ldots, t_n) \equiv 1 - \sum_{r=1}^{n} F(t_1, t_2, \ldots, t_r)$$

and

$$F(t_1, t_2, \ldots, t_n) \equiv \sum_{r=0}^{n-1} (-1)^r \sum_{0=j_0<j_1<\cdots<j_{r+1}=n} \prod_{i=0}^{r} p(t_{j_{i+1}} - t_{j_i}).$$

Thus, for instance, the inequalities of orders 1, 2, 3 are:

$$\begin{aligned}
F(t_1) &= p(t_1), \quad G(t_1) = 1 - p(t_1), \\
F(t_1, t_2) &= p(t_2) - p(t_1)p(t_2 - t_1), \\
G(t_1, t_2) &= 1 - p(t_1) - p(t_2) + p(t_1)p(t_2 - t_1), \\
F(t_1, t_2, t_3) &= p(t_3) - p(t_1)p(t_3 - t_1) - p(t_2)p(t_3 - t_2) \\
&\quad + p(t_1)p(t_2 - t_1)p(t_3 - t_2), \\
G(t_1, t_2, t_3) &= 1 - p(t_1) - p(t_2) - p(t_3) + p(t_1)p(t_2 - t_1) \\
&\quad + p(t_1)p(t_3 - t_1) + p(t_2)p(t_3 - t_2) - p(t_1)p(t_2 - t_1)p(t_3 - t_2).
\end{aligned}$$

Any function satisfying (1) is called a *p-function*. We denote by $\mathcal{P}$ the class of all *standard* p-functions with $p(t) \to 1$ as $t \downarrow 0$. A considerable amount is known about the analytical properties of $\mathcal{P}$ (Kingman, 1972). However, it is likely that the solution of our problem will hinge upon a thorough scrutiny of (1) in conjunction with the following four simple truths for any standard function p ($p(t) \to 1$ as $t \downarrow 0$) that satisfies the first and second-order inequalities:

$$\begin{aligned}
&p(t) > 0, \qquad \text{for all } t > 0, \\
&p \text{ is continuous on } [0, \infty), \\
&q = \lim_{t \downarrow 0} \frac{1}{t}(1 - p(t)) \text{ exists in } [0, \infty], \\
&m = \inf \{p(s) : 0 \le s \le t\} > 0 \text{ for any } t > 0.
\end{aligned}$$

The Markov Oscillation Problem (Davidson, 1968; Blackwell and Freedman, 1968) can be stated as follows. Given any $p \in \mathcal{P}$ and any $t > 0$, put $p(t) = M$. Put $\inf \{p(s) : 0 \le s \le t\} = m$. What pairs of values (m, M) can be assumed? Obviously, (m, M) must lie in the triangle $0 < m \le M \le 1$.

2. THE FIRST MOVES

Rollo Davidson's 1968 paper contained two important initial observations. First, Davidson was able to demonstrate that a part of the triangle $0 < m \leq M \leq 1$ is inaccessible to standard p-functions by considering, for any $0 < s < t$, the second-order inequalities

$$0 \leq 1 - p(s) - p(t) + p(s)p(t-s), \tag{2}$$

$$0 \leq 1 - p(t-s) - p(t) + p(t-s)p(s). \tag{3}$$

Taking the positive combination $p(t-s)(2) + [1 - p(t-s)](3)$ yields

$$p(t) \leq 1 - p(s) + p^2(s),$$

whence a simple application of the continuity and standardness of p gives the bounds

$$\begin{aligned} M &\leq 1 - m + m^2 \quad \text{if } m \geq \tfrac{1}{2}, \\ M &\leq \tfrac{3}{4} \qquad\quad \text{if } m \leq \tfrac{1}{2}. \end{aligned} \tag{4}$$

On the other hand, Davidson used a family of so-called 'jump' p-functions to exhibit a region

$$M \leq e^{m-1}, \qquad 0 < m \leq 1$$

of the (M, m) *diagram* which *is* accessible to standard p-functions. His initial (M, m) diagram is shown in Figure 1.

Davidson's final contribution (see Kingman, 1964, pp. 71–72) before his death in 1970 was to use a remarkable inequality (Bloomfield, 1971), obtained by measure-theoretic arguments, to augment the inaccessible region. He showed that

$$M \leq 1 + m \log m, \qquad 0 < m \leq 1.$$

His final (M, m) diagram is shown in Figure 2.

3. THE USE OF INEQUALITIES OF ORDER n

After Davidson's initial substantial success at providing a lower bound to the inaccessible region of the (M, m) diagram using a pair of second-order Kingman inequalities, it is not surprising that further progress (Cornish, 1973) was made using n nth order inequalities and letting $n \to \infty$. The resulting bound

$$\begin{aligned} M &\leq 1 + m \log m \qquad \text{if } 1 \geq m \geq \frac{1}{e}, \\ M &\leq 1 - \frac{1}{e} \qquad\quad \text{if } 0 < m \leq \frac{1}{e}, \end{aligned}$$

is composed of the Bloomfield-Davidson bound for $m \geq 1/e$ and a tangent to that curve for $0 < m \leq 1/e$. The resulting (M, m) situation is shown in Figure 3.

4. A THIRD-ORDER RESULT

Figure 4 shows the last substantial change to the (M, m) diagram (Cornish, 1972), achieved essentially by eliminating variables between six third-order inequalities. The somewhat ugly result is a three-segment curve:

$$\begin{aligned} M &\leq 1 - 2\sqrt{3}/9 \sim 0.615 \quad \text{if } 0 < m \leq \tfrac{1}{3}, \\ M &\leq 1 - m^{1/2} + m^{3/2} \quad \text{if } \tfrac{1}{3} \leq m \leq \tfrac{1}{2}(3 - \sqrt{5}) \\ M &\leq 2m^{1/2} - 2m + m^2 \quad \text{if } 1 \geq m \geq \tfrac{1}{2}(3 - \sqrt{5}). \end{aligned} \tag{5}$$

The result has interesting applications to the special case when consideration is restricted to those p-functions (with $q < +\infty$) that decay exponentially to their minimum value m. The solution of the problem in the 'exponential-start' case (Griffeath, 1976) is obtained by generalising the third-order result to the nth order case in a natural way and letting $n \to \infty$. It is shown that Davidson's curve

$$M = e^{m-1}, \qquad 0 < m \leq 1 \tag{6}$$

does indeed separate the accessible and inaccessible regions for exponentially starting standard p-functions.

5. FOUR PAPERS OF V. M. JOSHI

The use of nth order inequalities to shed light upon the (M, m) diagram was taken up by V. M. Joshi in his first two papers on the problem (Joshi, 1975, 1977a). In the earlier paper Joshi applied an intricate argument to keep a tighter reign on the inequalities than did Cornish (1973), and obtained a bound

$$\begin{aligned} M &\leq (1 - K)^2 \sim 0.590 \quad \text{if } 0 < m \leq K, \\ M &\leq 1 + m^2 - e^{m-1} \quad \text{if } m \geq K, \end{aligned}$$

where $e^{k-1} = 2K$. The 1977 paper is essentially a refinement of the 1974 argument, producing an improved lower bound to the inaccessible region which intersects the M-axis at 0.560. In almost a decade, Joshi's result has not been improved upon.

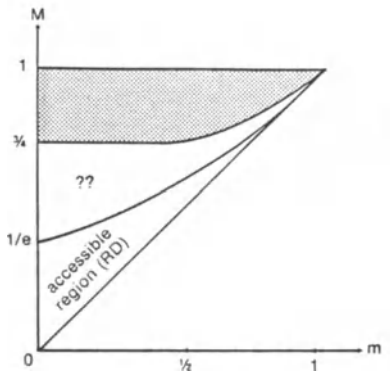

Figure 1. *Davidson's initial (M, m) diagram*

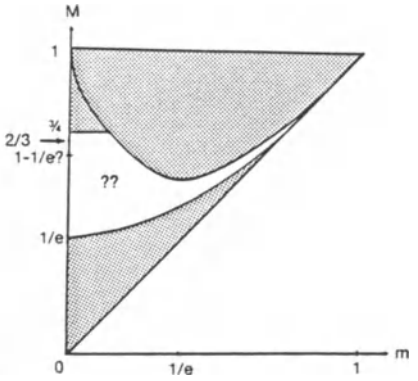

Figure 2. *Davidson's final (M, m) diagram*

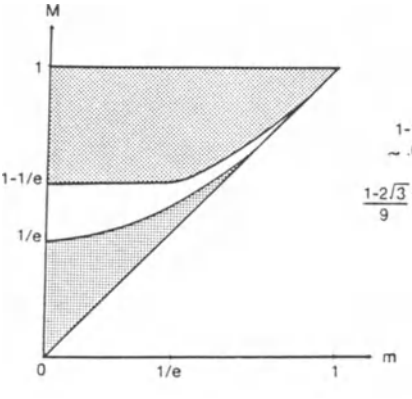

Figure 3. *The (M, m) diagram from the n^{th} order inequalities*

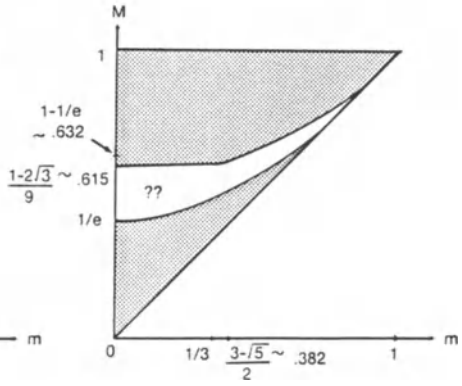

Figure 4. *The (M, m) diagram from equation (5)*

Attacking the Markov Oscillation Problem on a different front, V. M. Joshi extended the class of p-functions for which the problem is solved in two papers (Joshi, 1977b, 1981). In the first of these papers the subclass of $\mathcal{P}$ for which (4) is the solution is extended to those p-functions (with $q < +\infty$) which decay exponentially on a closed interval before reaching the value m. The 1981 paper extended the subclass further to include those p-functions (with $q < +\infty$) with one mass point in $(0, t_0)$, where $p(t_0) = m$, but with arbitrary distribution in $[t_0, \infty)$. The Davidson 'jump' p-functions have a single mass point.

6. TWO WAYS AHEAD?

A great deal of evidence has now accumulated to suggest that Davidson's curve (6) separates the accessible and inaccessible regions of the (M, m) diagram for standard p-functions. The question arises as to whether the technique used to give the third-order bound (5) can be generalised to the nth order case, in much the same way as in the exponential-start case (Griffeath, 1976) but with, presumably, a very considerable increase in the complexity of the computation. Studies currently in progress indicate that a new fourth-order generalisation will be obtained, and this might provide the key to the nth order situation.

On the other hand Griffeath (1973) conjectured that the Markov Oscillation Problem can be solved using *only* third-order inequalities. If this conjecture is correct then, in view of Joshi's results, the bound (5) cannot be the best possible using third-order inequalities. For p-functions that decay exponentially to m this is indeed the case, as can be seen by considering the following simple example. Suppose p is exponential on $[0, t_3]$, where $p(t_3) = m$. For $t > t_3$ put $p(t) = M$. Write $t_3 = 3t_1$, $t_2 = 2t_1$. Then the combination

$$\begin{aligned}\left(m^{1/3} + m^{2/3}\right) G(t_1, t - t_1, t) + mG(t - t_3, t - t_1, t) \\ + \left(1 - m^{1/3} - m^{2/3} - m\right) G(t_1, t - t_2, t) \\ + \left(1 - m^{2/3}\right)\left(1 - m^{1/3} - 2m^{2/3} - m\right) F(t_1, t - t_2)\end{aligned}$$

reduces to

$$1 - m^{1/3} + m^{4/3} - M.$$

Provided that $1 - m^{1/3} - 2m^{2/3} - m \geq 0$, i.e. $m \leq .1009$, all terms in the above combination are non-negative. Thus

$$M \leq 1 - m^{1/3} + m^{4/3}.$$

A simple argument then gives

$$M \leq .5814 \quad \text{if} \quad m \leq .1009.$$

It would be of interest to find a sharp bound for standard functions satisfying inequalities of the first three orders. We note (Griffeath, 1974) that Davidson's bound (4) *is* sharp for functions satisfying the first and second-order inequalities.

REFERENCES

Blackwell, D., and D. Freedman (1968), "On the local behavior of Markov transition probabilities". *Annals of Mathematical Statistics* **39**, 2123–2127.

Bloomfield, P. (1971), "Lower bounds for renewal sequences and p-functions". *Zeitschrift fur Wahrscheinlichkeitstheorie und Verwandte Gebiete* **19**, 271–273.

Cornish, A. G. (1972), unpublished manuscript.

Cornish, A. G. (1973), "Bounds for p-functions". *Bulletin of the London Mathematical Society* **5**, 169–175.

Davidson, R. (1968), "Arithmetic and other properties of certain delphic semigroups". *Zeitschrift fur Wahrscheinlichkeitstheorie und Verwandte Gebiete* **10**, 120–172.

Griffeath, D. (1973), "The maximal oscillation problem for regenerative phenomena". *Annals of Probability* **1**, 405–416.

Griffeath, D. (1974), "Inequalities for oscillating p-functions". *Bulletin of the London Mathematical Society* **6**, 51–56.

Griffeath, D. (1976), "On p-functions with exponential start". *Journal of the London Mathematical Society* **14**, 445–450.

Joshi, V. M. (1975), "A new bound for standard p-functions". *Annals of Probability* **3**, 346–352.

Joshi, V. M. (1977a), "An improved upper bound for standard p-functions". *Annals of Probability* **5**, 999–1003.

Joshi, V. M. (1977b), "An upper bound for exponentially starting standard p-functions". *Sankhya*, Series A **39**, 334–340.

Joshi, V. M. (1981), "A generalization of Davidson's upper bound for standard jump p-functions". *Journal of the Indian Statistical Association* **19**, 69–76.

Kendall, D. G., and E. F. Harding (eds.) (1973), *Stochastic Analysis*. New York: Wiley and Sons.

Kingman, J. F. C. (1964), "The stochastic theory of regenerative events". *Zeitschrift fur Wahrscheinlichkeitstheorie und Verwandte Gebiete* **2**, 180–224.

Kingman, J. F. C. (1972), *Regenerative Phenomena*. New York: Wiley and Sons.

W. J. Anderson [1]

PROBABILISTIC MODELS OF THE PHOTOGRAPHIC PROCESS

ABSTRACT

The photographic process, still not completely understood, is a rich source of temporal and spatial probabilistic processes, to date largely untapped by probabilists. This paper reviews applications of probability to such problems as reciprocity failure, granularity, and adjacency effects in photographic materials, concentrating on developments since 1971.

1. INTRODUCTION AND DESCRIPTION OF THE PHOTOGRAPHIC PROCESS

The photographic process is an interesting source of problems for applied probabilists and, as we shall see, provides realistic applications for a number of well-studied areas of applied probability, such as multidimensional point processes, renewal theory, Gibbsian random fields, and queuing theory. And while the physical and chemical mechanism of the photographic process is relatively well understood, there are a number of fundamental points over which photographic scientists differ; these issues can sometimes be resolved by the study of a well-formulated model of the process.

This article is intended as a review of probability modelling in photographic science, although in order to organize the material, it has been necessary to generalize some of the contributions. We proceed only from 1972, the publication date of a previous review article by Hamilton, Lawton, and Trabka. Among other things, that article contains an interesting account of very early mathematical modelling in photographic science.

We can roughly divide probabilistic applications to photographic science into 'macroscopic' and 'microscopic' applications. The former treat the emul-

[1] Department of Mathematics and Statistics, McGill University, Montreal, Quebec H3A 2K6

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 9–40.

sion as a whole, and the basic probability tools are multidimensional marked point processes and random fields. The microscopic applications treat individual grains in the emulsion, the basic tool being a variant of queuing theory. We examine the microscopic applications, which generally deal with reciprocity failure, in Section 2, and the macroscopic applications, generally subsumed under the title 'random dot model' in Section 3. There are also a very few articles which attempt to combine both aspects, or fall outside this classification; for reasons of length, we only mention these articles or leave them to the bibliography. The bibliography contains a comprehensive listing of pertinent articles since 1972.

What follows now is a description of the photographic process. A readable, more comprehensive account is given by James and Higgins (1968), and the classic reference work in the field is that of James (1977).

All modern photographic materials consist of a photographic emulsion thinly coated on some support medium, such as paper or plastic sheets, or glass plates. The emulsion itself consists of tiny (typically 10^{-6} m. in diameter, generally hexagonally shaped and flat) light sensitive silver halide crystals called *grains*, suspended in a gelatin support medium. Photography would not be possible, but for the fact that these grains contain defects, which may be either dislocations in the crystal structure, or impurities caused by doping with sulphides, or a combination of both. In the unexposed grain, some of these defects have a net positive charge, and are called *traps*. *Deep* traps have a larger charge than *shallow* traps. Grains also contain *interstitial silver ions*, which are positive silver ions liberated from the crystal structure and free to roam throughout the grain. With this background, we now have the *Gurney-Mott Hypothesis*.

(H1) When light strikes a silver halide grain, electron-hole pairs are created which are free to independently drift throughout the grain. Such electrons are called *photoelectrons*.

(H2) A photoelectron may become caught in one of the traps, more likely a deep trap where it is held more tightly. If so, a potential field is set up around the deep trap which repels other photoelectrons, but attracts interstitial silver ions. An ion in the vicinity of the trap will be attracted to the trap, resulting in a silver atom at the trap. The time interval between the trapping of the photoelectron and the arrival of the interstitial silver ion is called the *dead time* τ_d.

(H3) This silver atom is unstable and decays after a time interval of length τ_o, called the *decay time*, into a silver ion and an electron. But if before this silver atom can decay, it is joined by another silver atom formed in the same way at the trap, a more stable two-atom silver speck results.

(H4) Successful repetition of the steps in H2 and H3 above leads eventually

to the formation of a stable silver speck (the minimum number of silver atoms required for stability is a controversial point among photographic scientists, but there is some consensus that a four-atom speck suffices). The aggregate of all the silver specks in all the grains forms the *latent image*. Only those grains which contain a stable silver speck can be reduced to pure silver during subsequent chemical development.

We remark that there seems to be a general consensus over the Gurney-Mott hypothesis, although there are minority divergent opinions over the exact sequence of events.

It is clear that the longer the exposure duration, the more stable silver specks will result. After chemical development, in which grains containing stable silver specks are reduced to pure silver, and clearing, in which unused silver halide is disposed of, the photographic image consists of black particles of pure silver still retaining much of the shape and position of the original grains, randomly distributed throughout the gelatin. Photography is a two-dimensional medium, and what we 'see' are the projections of these developed grains. As such, the 'centres' of the grains form a two-dimensional point process which, for a uniformly exposed and developed emulsion, and in the absence of crowding, has usually in the literature been assumed to be Poisson. The opacity of these grains as opposed to the background, together with their random distribution in space, result in *granularity,* manifested as irregularities in the intensity of the transmitted or reflected light by which the image is viewed.

Two basic observable variables involved in the process are the *exposure* E (= *intensity* I of light, times *duration* t of the exposure) which the emulsion receives, and the resulting *mass density* M (per unit area) of developed silver. However, very early on, photographic scientists observed empirically that M is proportional to the *optical density* D_A, defined by

$$D_A = -\log_{10} T_A, \tag{1.1}$$

where the transmittance $T_A = I_i/I_t$ is the ratio of incident to transmitted intensity of light shone in the region A of the exposed and developed emulsion. T_A is measured with a densitometer (or microdensitometer, if A is small) and A is circular, reflecting the circular aperture of the densitometer. The densitometer actually measures T_A, but has a built-in analog device to convert T_A to D_A via (1.1).

We expect the optical (or mass) density of developed silver to depend on the intensity I and duration t of the exposure $E = It$ that the emulsion receives. What was observed very early in the history of photography, and what every photographer knows, is that density depends on (moderate)

values of I and t only through their product E. This is called the *Law of Reciprocity,* and for a given type of emulsion, the relationship between D_A and E (when I and t are moderate) is graphically portrayed in the *characteristic* (or D-log E) *curve* of the emulsion, an example of which is shown in Figure 1. The location of the characteristic curve along the $\log_{10} E$ axis relates to the 'speed' or 'sensitivity' of the emulsion, while the slope of the middle 'straight line' portion of the curve relates to the 'contrast' of the emulsion.

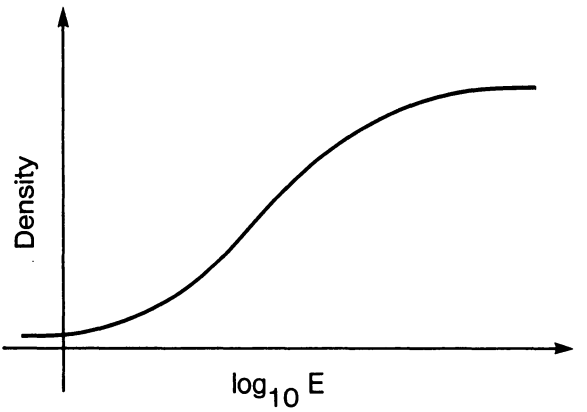

Figure 1. *Characteristic curve of emulsion.*

However, at extreme values of I or t, the law of reciprocity breaks down, and D_A depends on I and t individually. In this case, the graphical tool is the *reciprocity failure diagram,* consisting of a family of sections of a D_A versus $\log_{10} E$ and $\log_{10} I$ surface, each section taken for a fixed value of D_A. The individual sections are called *isodense curves.* An example of a reciprocity failure diagram is shown in Figure 2. Reciprocity failure depends very much on what goes on inside a grain, and therefore on the Gurney-Mott hypothesis. Models which attempt to explain reciprocity failure are discussed in Section 2.

Variations in D_A as a microdensitometer is scanned across a uniformly exposed and developed emulsion are indicative of the granularity of the emulsion, and the *Selwyn granularity*

$$S = \sqrt{|\, A \,|\, \mathrm{Var}(D_A)} \tag{1.2}$$

is the standard measure of granularity. Granularity and the proportionality of optical and mass density, concerning the emulsion as a whole, are the preoccupation of the random dot models of Section 3.

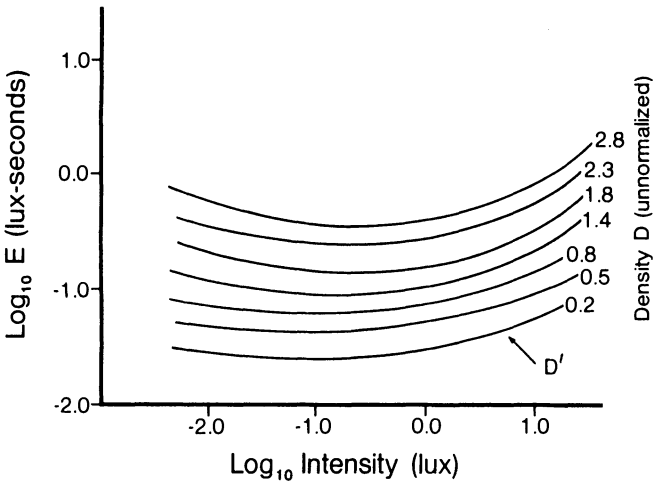

Figure 2. *Reciprocity law failure curves.*

2. RECIPROCITY FAILURE IN THE PHOTOGRAPHIC GRAIN

It has been remarked that the response of the photographic emulsion, as measured by the optical density D_A, depends in general on the intensity I (assumed constant over the duration of the exposure) and the duration t of the light to which the emulsion has been exposed; and that this dependence, for a certain emulsion, is recorded in a family of isodense curves such as the examples in Figure 2. Each isodense curve, such as the one in Figure 2 for density D', records the exposure E required to achieve density D' when the intensity is I. At moderate values of I, the isodense curve is flat, indicating that in this region density depends on I and t only through their product $E = It$. This is the region in which the law of reciprocity holds. But at very low or very high values of I, the law breaks down and the isodense curves bend upwards, indicating that the photographic process is less efficient at these extreme values of I. There are experimental difficulties involved in determining the exact behaviour of isodense curves at very high or low intensities, with the result that different modes of behaviour have been observed in each of these regions. Typically, at high intensities either asymptotic slopes of +1 have been observed, or else some increase in the isodense curve and then an asymptotic slope of zero (called 'bendover'). Both of these situations are portrayed in Figure 2. At low intensities, asymptotic slopes between 0 and −1 are observed (James, 1977). However (Hamilton, 1985), recent data at very extreme intensities indicates that ultimate ben-

dover is characteristic at high intensities, and asymptotic slopes of –1 at low intensities.

There are four mechanisms which are thought to be responsible for high-intensity reciprocity failure (Hamilton, 1966). These are (i) the ionic limitation, (ii) competitive nucleation, (iii) topographic effects, and (iv) recombination effects. The term 'ionic limitation' refers to step (H2) of the Gurney-Mott hypothesis, in which photoelectrons prevented from entering a trap during a dead time may recombine with holes and thus become lost to the photographic process. The general model of reciprocity failure in Section 2.1 is based on the specific sequence of events in (H1) – (H4), and ionic limitation will be seen to be the only actual source of high intensity failure. Competitive nucleation (competition between traps for photoelectrons) and recombination effects appear only as factors affecting the extent of high intensity failure, and cannot be causes. Topographic effects (effects due to spatial and strength distribution of traps) are not included in the models below. Similarily, the only actual cause of low-intensity failure considered below is the thermal decay of silver atoms in step (H3), in which the arrival rate of photoelectrons is so low that it is unlikely a second silver atom can be formed at the trap before the first one decays.

2.1 General Model for Reciprocity Failure

We consider a single grain with N similar deep traps, 'similar' meaning that each deep trap unoccupied by an electron exerts the same attractive force towards photoelectrons. At the beginning of the exposure interval (i.e., at time $t = 0$), all traps are empty. Light incident on the grain creates photoelectrons in the grain which arrive at the trap complex according to a renewal counting process with intensity λ a correlate of the light intensity I. We view the N deep traps as servers and arriving photoelectrons as arriving customers in an N-server queueing system. Let $T_1, T_2, \ldots$ be a sequence of i.i.d. random variables, each with distribution function $F(t)$ and mean λ^{-1}, representing the interarrival times of these photoelectrons (customers) at the trap (server) complex. When a photoelectron arrives at an unoccupied deep trap, it is immediately absorbed into the trap, and the dead time τ_d until an interstitial silver ion arrives to join this photoelectron is assumed to be a random variable with distribution function $P(t)$ and mean β^{-1}. Let $\tau_d^1, \tau_d^2, \ldots$ be a sequence of independent copies of τ_d, representing the dead times (service times) of successive photoelectrons to enter deep traps. Photoelectrons which arrive to find all N deep traps occupied accumulate in temporary shallow traps throughout the grain, forming an electron pool (waiting line) available to the deep traps. The size of this pool fluctuates during, and after, the exposure interval, increasing with the addition of arriving photoelectrons, decreasing when an electron in a shallow trap recombines with a

hole (and is therefore lost to the photographic process), or at the end of a dead time when a temporarily trapped electron enters a deep trap at which a silver atom has just been formed.

So far, we basically have a $GI/GI/N$ queueing system with defections (recombination) allowed from the waiting line. Now let $\tau_o^1, \tau_o^2, \ldots$ be a sequence of i.i.d. random variables, generically represented by τ_o, and representing the decay times of successive silver atoms formed in the deep traps. We assume that interarrival times, dead times, and decay times are always independent of one another, as well as among themselves. In addition, we will assume (for tractability) that a two-atom silver speck at a deep trap is stable, and that the formation of at least one stable silver speck among the N deep traps makes the grain developable. We let T denote the minimum exposure duration required to render the grain developable, and $D(t)$ (or $D(t, \lambda)$, when dependence on λ is to be accentuated) denote the distribution function of T. We interpret $D(t, \lambda)$ as the normalized photographic density resulting from an exposure E of duration t and intensity λ.

This general model, involving as it does the transient behaviour of an N-server queueing system, has so far proved intractable. Below we consider two special cases.

2.2 Multitrap Model for High Intensity Reciprocity Failure

Typical values for the dead time and decay time would appear to be of the order of 10^{-4} seconds and 1 second, respectively (Hamilton and Urbach, 1966). It would therefore seem reasonable (especially in view of some of the results with the model of Section 2.3) to decouple the effects of the dead time and decay time. Hence in the general model described above, we assume, following Anderson (1984), that $\tau_o = +\infty$ a.e., and in addition, for mathematical tractability, that photoelectrons which arrive to find all N traps occupied are lost to the photographic process, so that no pool can form. We therefore have a $GI/GI/N$ loss system in which T is the first time that a server accepts its second customer.

Let X_n denote the number of occupied traps at (i.e., just before) the arrival of the nth photoelectron, Y_n denote the number of traps which have not been occupied before that arrival, and let $Z_n = (X_n, Y_n)$. Then $\{Z_n, n \geq 1\}$ is easily seen to be a Markov chain with state space $S = \{(i, j) \mid i, j \geq 0, i + j \leq N\} \cup A$, where A is the absorbing state which is entered by the chain at the first moment that a trap receives its second photoelectron. T is then the time until absorption in A. If we define the Laplace transforms

$$f_{(i,j)}(s) = E\left(e^{-sT} \mid Z_1 = (i, j)\right),$$
$$P_{(i,j),(k,\ell)}(s) = E\left(e^{-sT_2} I_{\{Z_2 = (k,\ell)\}} \mid Z_1 = (i, j)\right),$$

then

$$f_{(i,0)}(s) = \begin{cases} E(e^{-sT_1}) & \text{if } 0 \le i \le N-1 \\ \sum_{k=0}^{N} P_{(N,0),(k,0)}(s) f_{(k,0)}(s) & \text{if } i = N \end{cases} \tag{2.1}$$

and

$$f_{(i,j)}(s) = \sum_{k=0}^{i+1} P_{(i,j),(k,j-1)}(s) f_{(k,j-1)}(s) + \frac{N-i-j}{N-i} E(e^{-sT_1}), \qquad j \ge 1. \tag{2.2}$$

In (2.2), the sum $\sum_{k=0}^{i+1} P_{(i,j),(k,j-1)}(s) f_{(k,j-1)}(s)$ covers the case where the first photoelectron goes into a previously unoccupied trap at time T_1. But it is then as if we are back at time 0 with new initial conditions $(k, j-1)$ and require T' more time units until absorption in A, where T' is independent of T and has the same distribution as T. The term $\frac{N-i-j}{N-i} E(e^{-sT_1})$ arises from the remaining case where the first electron goes into a previously occupied trap, so that $T = T_1$. Note that $\frac{N-i-j}{N-i}$ is the probability that an electron which enters an unoccupied trap in fact enters one which has previously been occupied. For the case $i = N$ in (2.1), all but the Nth (last) term in the sum are cases in which the first electron arrives to find all traps occupied, so is lost. The time used so far is T_1. Just before the second electron arrives, there are $i < N$ occupied traps, and since all the traps have been previously occupied, this second electron, taking a further T_2 time units, creates a stable silver speck.

Let $D^*(s)$ denote the Laplace-Stieltjes transform $E(e^{-sT} \mid Z_1 = (0, N))$ of $D(t)$. Then $D^*(s) = f_{(0,N)}(s)$. Equation (2.2) can be iterated downwards from $j = N$ to obtain

$$\begin{aligned} D^*(s) = & f_{(N,0)}(s) \prod_{i=0}^{N-1} P_{(i,N-i),(i+1,N-i-1)}(s) \\ & + E(e^{-sT_1}) \sum_{k_2=0}^{1} \sum_{k_3=0}^{k_2+1} \cdots \sum_{k_N=0}^{k_{N-1}+1} \prod_{i=0}^{N-1} P_{(k_i,N-i),(k_{i+1},N-i-1)}(s) \\ & + E(e^{-sT_1}) \sum_{j=1}^{N-1} \sum_{k_1=0}^{1} \cdots \sum_{k_j=0}^{k_{j-1}+1} \left\{ \prod_{i=0}^{j-1} P_{(k_i,N-i),(k_{i+1},N-i-1)}(s) \right\} \frac{j-k_j}{N-k_j} \end{aligned} \tag{2.3}$$

where $k_0 = 0$. $f_{(N,0)}(s)$ is easily obtainable by solving (2.1). Here,

$$\begin{aligned} & P_{(i,j),(k,\ell)}(s) \\ & = \int_0^\infty \int_0^\infty e^{-sv} P[Z_2 = (k,\ell) \mid T_1 = u, T_2 = v, Z_1 = (i,j)] \, dF(v) dF(u) \end{aligned}$$

where, for instance,

$$P[Z_2 = (k,0) \mid T_1 = u, T_2 = v, Z_1 = (N,0)] = \binom{N}{k}(p(v,u))^k(1-p(v,u))^{N-k}$$

with $p(v,u) = P(\tau_d > u+v \mid \tau_d > u)$, $u, v \geq 0$.

Some simplification is possible by making the not unreasonable assumption that interarrival times and dead times are exponential, i.e.,

$$F(t) = 1 - e^{-\lambda t}, \qquad P(t) = 1 - e^{-\beta t}, \qquad t \geq 0. \tag{2.4}$$

Then $D(t)$ is easily obtained from $D^*(s)$ in (2.3) as a sum of convolutions of exponentials. Furthermore, the function $\rho(E) = D(E/\lambda, \lambda)$ can be seen to depend on λ and β only through $r = \lambda/\beta$. For fixed N, a plot of $\rho(E)$ against $\log_{10} E$ gives the characteristic curve for a grain with N deep traps, and examples of characteristic curves computed in this way from (2.3) are shown in Figure 3 for $r = 10$ and $N = 1, 2, 3$. In addition, the expected value $\overline{E} = \lambda E(T)$ and variance $\mathrm{Var}(E) = \lambda^2 \mathrm{Var}(T)$ can be computed from (2.3) as functions of r and N. $\overline{E}$ can be viewed as a measure of the speed of the emulsion (the smaller $\overline{E}$ is, the higher the speed), and $(\mathrm{Var}(E))^{-1/2}$ as a measure of the contrast. The results, reprinted from Anderson (1984), are shown in Figure 4. It can be seen that for each r, there is a value of N for which speed is a maximum (this is straightforward to prove), and there would appear to be an optimal value of N which maximizes the contrast.

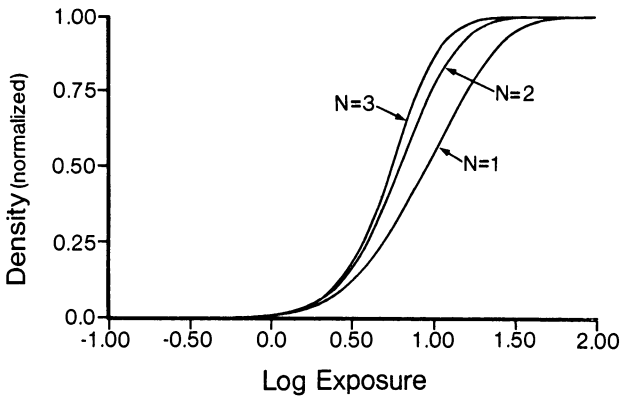

Figure 3. *Normalized characteristic curves for cases* $N = 1, 2$ *and* 3 *and* $r = 10$.

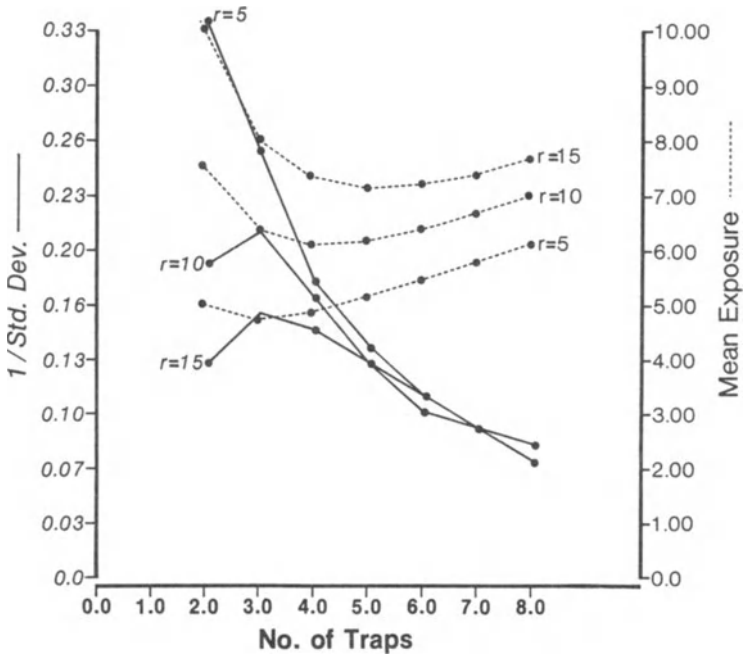

Figure 4. *Dependence of speed and contrast on number of traps N.*

We now turn to the question of reciprocity failure for this model. Given a number ρ with $0 < \rho < 1$, the relation

$$\rho = D(E/\lambda, \lambda), \qquad \lambda > 0 \tag{2.5}$$

defines implicitly a function $E = E_\rho(\lambda)$ of λ. Plotting $\log_{10} E_\rho(\lambda)$ against $\log_{10} \lambda$ then gives the isodense curve corresponding to density ρ. For the model of this section, the isodense curve for $\rho = 0.5$ is plotted in Figure 5 for the values 1, 2 and 3 of N. Again it appears that for each value of r there is a value of N which minimizes the exposure required to achieve density 0.5. Furthermore, the high intensity asymptote of the isodense curve has slope $+1$.

Further investigation of asymptotic slopes of isodense curves is based on the following lemma, which is applicable as well to the model of Section 2.3.

Lemma. Let L denote either 0 or $+\infty$, and let a and ρ be numbers with $0 < \rho < 1$.

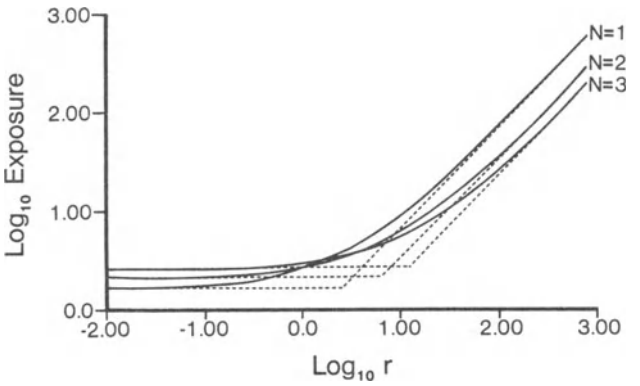

Figure 5. *Exact (solid line) and approximate (dotted line) isodense curves for* $\rho = 0.5$ *and* $N = 1, 2$ *and* 3.

1. The existence of a positive limit

$$x = \lim_{\lambda \to L} \frac{E_\rho(\lambda)}{\lambda^a} \tag{2.6}$$

is equivalent to the existence of the asymptote $\phi(\lambda) = a \log_{10} \lambda + \log_{10} x$ (as $\lambda \to L$) to the isodense curve for density ρ on the log-log plot.

2. Suppose

$$\lim_{\lambda \to L} D(t/\lambda^{1-a}, \lambda) = Z(t), \qquad t > 0$$

or equivalently

$$\lim_{\lambda \to L} D^*(s\lambda^{1-a}, \lambda) = Z^*(s), \qquad s > 0$$

where $Z(t)$ is continuous, strictly increasing, and such that $Z(0+) < \rho < Z(+\infty)$ (and $Z^*(s)$ denotes the Laplace-Stieltjes transform of $Z(t)$). Then the limit x in (2.6) exists and $Z(x) = \rho$.

A proof of this lemma, which requires only that $D(t)$ be increasing in t, is given by Anderson (1984). Returning to the model of this section, again with the exponential assumptions of (2.4), we find via (2.3) that $\lim_{\lambda \to \infty} D(t, \lambda) = 1 - e^{-\beta N t}$, so that by the lemma (with $a = 1$), all isodense curves have asymptotic slope $+1$ as $\lambda \to \infty$, and the equation of the asymptote is

$$\phi(\lambda) = \log_{10} \lambda + \log_{10} \frac{1}{N\beta} \log_e \frac{1}{1-\rho}.$$

2.3 Single Trap Pool Model for Both Low and High Intensity Failure

There is another direction one can take in the general model to achieve tractability. Following Anderson and Mathai (1986), we assume $N = 1$ and examine a model which includes both low and high intensity reciprocity failure. While we lose competitive nucleation (N) as a factor, we can examine the effects of recombination of pool electrons, and obtain a model valid at intermediate intensities.

We shall assume the incoming stream of photoelectrons to be Poisson with intensity λ. Let $W_t(u)$ be the pool size (not including the electron in the deep trap) at time $u \geq 0$ resulting from an exposure during the interval $[0, t]$. We assume that in the time interval between two successive admissions of photoelectrons to the deep trap, $(W_t(u),\ u \geq 0)$ is a birth and death process with birth coefficients

$$\lambda_n(u) = \begin{cases} \lambda & \text{if } u \leq t \\ 0 & \text{if } u \geq t, \end{cases} \qquad n \geq 0, \quad u \geq 0$$

and death coefficients μ_n, $n \geq 1$. The process $(W_t(u),\ t \geq 0)$ can be assumed to have left continuous paths, and the initial pool size $W_t(0)$ will be denoted by W.

In this model, T has a fuzzier meaning since the second silver atom can be formed by an electron from the pool, long after time T Let us write

$$X = \begin{cases} T_1 & \text{if } W = 0 \\ 0 & \text{if } W > 0 \end{cases}$$

and define

$$D_j(t) = P(T \leq t \mid W = j, \text{ no silver atom in the trap at beginning of exposure})$$

so that $D(t) = D_0(t)$, and

$$M_j(t) = P(T \leq t \mid W = j, \text{ one silver atom (just formed) in trap at beginning of exposure})$$

for $j \geq 0$. Using a renewal argument, it can be shown that

$$D_j(t) = H_j^0(t) + \sum_{k=0}^{\infty} \int_0^t M_k(t-u) dK_{jk}^0(u) \tag{2.6}$$

and

$$M_j(t) = H_j^{r_\circ}(t) + \sum_{k=0}^{\infty} \int_0^t M_k(t-u) dK_{jk}^{r_\circ}(u), \tag{2.7}$$

where

$$H_j^{\psi}(t) = P\left(X \le t, X + \tau_d^1 \le \psi \mid W = j\right) + P\left(X \le t < X + \tau_d^1,\ X + \tau_d^1 > \psi,\ W_t\left(X + \tau_d^1 + \ldots + \tau_d^M\right) \ge 1 \mid W = j\right),$$

$$K_{jk}^{\psi} = P\left(\psi < X + \tau_d^1 \le t,\ W_{X+\tau_d^1}(X + \tau_d^1) = k \mid W = j\right),$$

and

$$M = \min\left(n \ge 1 \mid \tau_d^{n+1} \le \tau_o^n\right).$$

The term $H_j^0(t)$ in (2.6) covers the case in which the first silver atom is formed (at time $X + \tau_d^1$) after the end of the exposure interval, so that the second electron in the stable silver speck must come from the pool, and there must be enough (M) electrons in the pool to complete the formation of the two-atom speck from a silver atom. The kth term in the sum in (2.6) arises from the case where the first silver atom is formed at time $u \le t$, and the pool size at time u is k. But then there are $t - u$ time units of exposure remaining to ensure the formation of a stable speck, but with the new initial conditions embodied in $M_k(t - u)$. The derivation of (2.7) is similar.

Equations (2.6) and (2.7) are amenable to easy 'solution' using Laplace-Stieltjes transforms (denoted by $*$). Writing

$$\mathbf{D}(s) = \begin{pmatrix} D_0^*(s) \\ D_1^*(s) \\ \vdots \end{pmatrix}, \mathbf{H}^{\psi}(s) = \begin{pmatrix} H_0^{\psi *}(s) \\ H_1^{\psi *}(s) \\ \vdots \end{pmatrix}, \ \mathbf{K}^{\psi}(s) = \left(K_{jk}^{\psi *}(s)\right)_{j,k=0}^{\infty},$$

the matrix $\mathbf{I} - \mathbf{K}^{r_o}(s)$ can be shown to be invertible and we have

$$\mathbf{D}(s) = \mathbf{H}^0(s) + \mathbf{K}^0(s)\left(\mathbf{I} - \mathbf{K}^{r_o}(s)\right)^{-1}\mathbf{H}^{r_o}(s). \tag{2.8}$$

Some computational results for evaluating $\mathbf{D}(s)$ are given by Anderson and Mathai (1986), but even in the simplest cases (e.g., small finite pool capacity), inversion of (2.8) is a formidable task. Nevertheless, some very interesting results concerning asymptotic slopes of the isodense curves are obtainable from (2.8) and the lemma of Section 2.2.

High Intensity Asymptotes.

It can be shown that if $P(\tau_d = 0) = 0$, then

$$\lim_{\lambda \to \infty} D(t/\lambda, \lambda) = Z_1(t) \stackrel{\text{def}}{=} e^{-t} \sum_{j=0}^{\infty} \frac{t^{j+1}}{(j+1)!} P\left(W_0\left(\tau_d^1 + \ldots + \tau_d^M\right) \ge 1 \mid W = j\right) \tag{2.9}$$

and

$$\lim_{\lambda\to\infty} D(t,\lambda)$$
$$= Z_2(t) \stackrel{\text{def}}{=} 1 - P(\tau_d^1 > t,\ W_0(\tau_d^1 + \ldots + \tau_d^M - t) = 0 \mid W = C), \tag{2.10}$$

where $W_0(u)$, $u \geq 0$ is a pure death process with death parameters μ_n, $n \geq 1$ and unit deletions at times $\tau_d^1, \tau_d^2, \ldots, \tau_d^M$; and C, which may be $+\infty$, is the maximum capacity of the pool. Let

$$\rho_o = P\left(W_0\left(\tau_d^1 + \ldots + \tau_d^M\right) \geq 1 \mid W = C\right). \tag{2.11}$$

The interpretation of (2.10) and (2.11) when $C = +\infty$ is made precise by Anderson and Mathai (1986). But note that if the death parameters are large enough (i.e., $\sum_{n=1}^{\infty} \mu_n^{-1} < +\infty$) there is, for any $u > 0$, a non-zero probability that $W_0(v)$ will experience infinitely many jumps in the interval $[0, u]$. In fact, if $C = +\infty$, then $\rho_o < 1$ if and only if $\sum_{n=1}^{\infty} \mu_n^{-1} < +\infty$.

If $P(\tau_d \leq \tau_o) > 0$, the functions $Z_1(t)$ and $Z_2(t)$ satisfy

$$Z_1(0) = 0, \quad \lim_{t\to\infty} Z_1(t) = \rho_o$$
$$Z_2(0) = \rho_o, \quad \lim_{t\to\infty} Z_2(t) = 1,$$

and the other conditions of the lemma of the last section, and we conclude that ρ_o is a threshold density in the sense that the isodense curve with index ρ (i) exhibits bendover if $0 < \rho < \rho_o$, or (ii) has asymptotic slope $+1$ if $\rho_o < \rho < 1$.

The following examples, in which we assume $\tau_o = +\infty$ a.e. and $P(t) = 1 - e^{-\beta t}$, $t \geq 0$ (i.e., no low intensity failure and exponential dead times) are taken from Anderson (1980).

Example 1. If pool capacity is $C = +\infty$ and death parameters are $\mu_n = n(n+1)\mu$ (proportional to the number of electrons in the pool and the number of holes extant), it can be shown that

$$\rho_o = 1 - \frac{\pi(\beta/\mu)}{\cosh\left(\frac{\pi}{2}\sqrt{4(\beta/\mu) - 1}\right)}.$$

ρ_o is an increasing function of β/μ and ρ_o is already .943 when β/μ is 4.0. Thus, while there appears to be no mention of a threshold effect in the literature, it may be because real values of β/μ are so high that ρ_o is very close to 1 and so far has been beyond experimental detection.

Example 2. If pool capacity is $C = 1$ we find (with $\mu_1 = \mu$)

$$D(t) = \begin{cases} 1 - e^{-\lambda t} + \frac{\lambda^2 \mu}{(\mu+\beta)(\beta-\lambda)^2}(e^{-\lambda t} - e^{-\beta t}) - \frac{\lambda\beta(\mu+\beta-\lambda)}{(\mu+\beta)(\beta-\lambda)} t e^{-\lambda t} & \text{if } \lambda \neq \beta \\ 1 - e^{-\lambda t} - \lambda t e^{-\lambda t} - \frac{\lambda^2 \mu}{2(\lambda+\mu)} t^2 e^{-\lambda t} & \text{if } \lambda = \beta \end{cases}$$

and $\rho_o = \beta/(\beta + \mu)$. A family of isodense curves, with $\mu = \beta = (2/3) \times 10^6$, is shown in Figure 6.

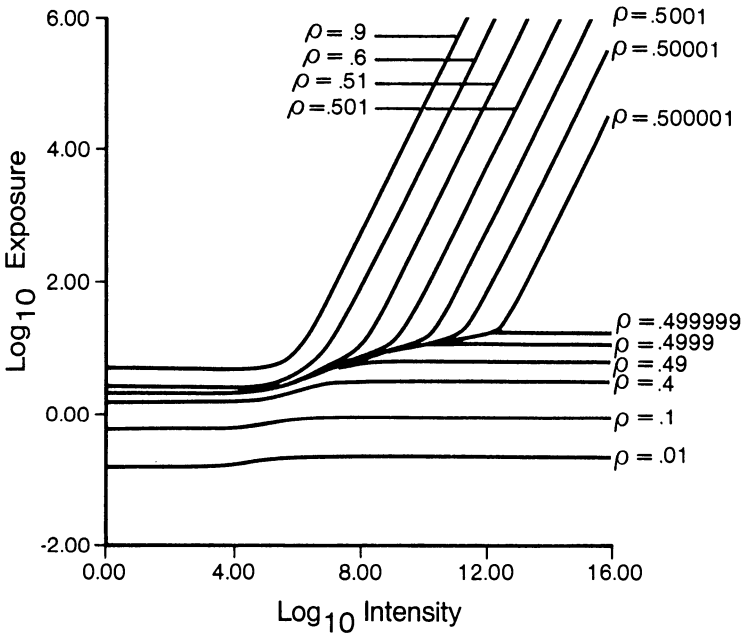

Figure 6. *Family of isodense curves resulting from the model of Example 2, with* $\mu = \beta = (2/3) \times 10^6$ *and maximum pool size* $N = 1$. *The curves exhibit bendover when the index* ρ *is less than the threshold density* $\rho_0 = 0.5$, *and high-intensity asymptotes of* $+1$ *when* ρ *is greater than* ρ_0.

Low Intensity Asymptotes

Returning to the combined reciprocity failure model of this section, the following results concerning low intensity failure may be obtained from (2.8). Assume there is $r > 0$ such that $E[\exp(r\tau_d)] < +\infty$.

(a) If $E(\tau_o) < +\infty$, then $\lim_{\lambda \to 0} D(t/\lambda^2, \lambda) = 1 - e^{-(\varsigma+\eta c)t}$, $t \geq 0$, where

$$c = P(\tau_d \leq \tau_o),$$

$$\varsigma = E\left((\tau_o - \tau_d) I_{\{\tau_d \leq \tau_o\}}\right),$$

and

$$\eta = \begin{cases} E(\tau_d) & \text{if } \mu_1 = 0 \\ E[(1 - \exp(-\mu_1 \tau_d))/\mu_1] & \text{if } \mu_1 > 0. \end{cases}$$

(b) If $P(\tau_o > u) \sim u^a$ as $u \to +\infty$ where $-1 < a < 0$, then $\lim_{\lambda \to 0} D(t/\lambda^{1-a}, \lambda) = 1 - e^{-t\Gamma(1+a)}, t \geq 0$, where $\Gamma(\cdot)$ is the gamma function.

The lemma of Section 2.2 implies that in case (a), we obtain low-intensity asymptotes of slope –1, while in (b) we obtain low intensity asymptotes of 'fractional' slope a.

The special case of the combined model of this section, in which pool capacity is zero, was studied by Anderson (1978). If dead times and decay times are exponential, $D(t)$ is easily determined and isodense curves can readily be plotted, as in Figure 7.

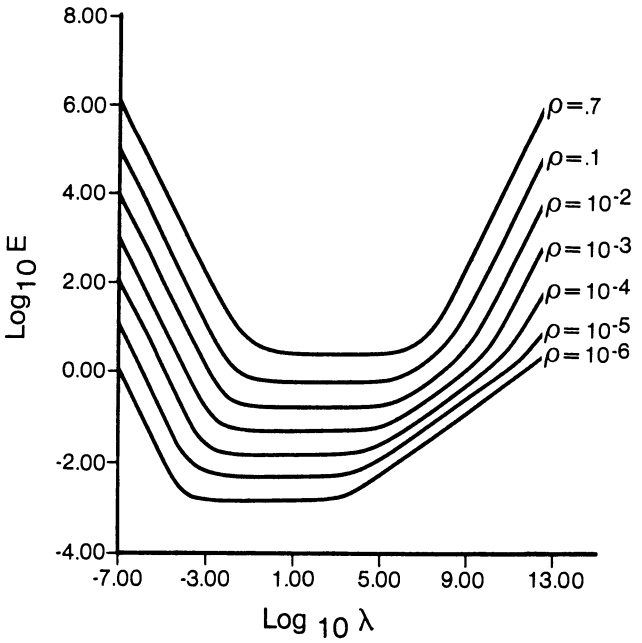

Figure 7. *Family of isodense curves resulting from model when the dead time and decay time are chosen to have exponential distributions with means* 1.5×10^{-6} *seconds and 8 seconds, respectively.*

2.4 Additional Results on Reciprocity Failure

Feedback

It is not clear from the Gurney-Mott hypothesis what happens to the electron produced when a silver atom decays in the trap. Presumably, the electron can be considered a new member of the electron pool, and such 'feedback' of electrons results in increased efficiency, with the resulting isodense curves lying below the corresponding curves of the model of the last section. As high intensity failure is independent of thermal decay, no change in the high intensity asymptotic behaviour is to be expected. But can feedback of decayed photoelectrons change low intensity behaviour, perhaps producing bendover or fractional asymptotic slopes? The answer is no, for the following reason: take $\tau_d \equiv 0$ in the model of the last section, so no pool need form and $C = 0$. Let f be the probability that an electron from a decayed silver atom in the trap feeds (immediately) back to the trap. Then the effective decay time for the first silver atom formed in the trap is $\tau_o' = \tau_o^1 + \sum_{k=1}^{J} \tau_o^{k+1}$, where J (geometric) is the number of times the electron feeds back. If $0 < f < 1$ and $E(\tau_o) < +\infty$, then $E(\tau_o') = E(\tau_o)/1 - f < +\infty$, and the last results of Section 2.3 imply that the low intensity asymptotes have slope -1. Since the isodense curves for this special case lie below the corresponding ones for the feedback version of the model of Section 2.3, the same conclusion must hold for the latter.

The n-Atom Stable Speck

Up to now, we have assumed that a two-atom silver speck is stable and developable, an assumption made for mathematical tractability. The case in which a silver speck requires n (≥ 2) atoms for stability is studied by Anderson (1987). If one assumes that $\tau_o \equiv +\infty$, and therefore examines the high intensity component only of the model of Section 2.3, one obtains results similar to those of Section 2.3, in that there is a threshold density separating high intensity bendover from high intensity asymptotic slopes of $+1$. On the other hand, at low intensities, with τ_d and therefore C assumed zero, one finds, if $E(\tau_o) < +\infty$, that the low intensity asymptotes have slope $-(n-1)$.

3. RANDOM DOT MODELS OF THE PHOTOGRAPHIC EMULSION

The so-called random dot models of the photographic emulsion date from about 1913, and a history of their development is given by Hamilton *et al.*, (1972). Rather than review the contributions since 1971 separately, we follow Kemperman (see Hamilton *et al.*, 1972) in setting up a general framework for the random dot model, from which most of these contributions follow

easily as special cases.

3.1 General Framework for the Random Dot Model

We take the developed emulsion to consist of grains distributed randomly in R^2, in a manner to be made precise below. Each grain in the emulsion is characterized by a reference point x_p (which we shall refer to as the 'centre' of the grain, even though grain shapes might be quite irregular) and an absorptance function $a(s)$, in the sense that the grain with centre x_p and absorptance function $a(s)$ is located at $x_p \in R^2$ and absorbs at the point $x \in R^2$ a fraction $a(x - x_p)$ of the incident light. The reference points x_p are members of a point process in R^2.

More precisely, let $N = \{N_A,\ A \in \mathcal{B}(R^2)\}$ ($\mathcal{B}(R^2)$ = the Borel σ-field of subsets of R^2) be a two-dimensional point process defined on a probability space $(\Omega_1, \mathcal{F}_1, P_1)$. We will identify each $\omega_1 \in \Omega_1$ with a realization of this point process; namely, ω_1 is a countable collection of points in R^2, enumerated so that the pth point of ω_1 is denoted by $x_p = x_p(\omega_1)$.

Let Q be the family of all measurable functions $a(s) : R^2 \to [0,1]$ which vanish on the complement of a bounded set. The members of Q are the absorptance functions mentioned above. Let $\{X_n,\ n \geq 1\}$ be a sequence of independent and identically distributed random variables defined on a second probability space $(\Omega_2, \mathcal{F}_2, P_2)$, with values in Q.

Finally, let $(\Omega, \mathcal{F}, P)$ be the product probability space $(\Omega_1 \times \Omega_2,\ \mathcal{F}_1 \times \mathcal{F}_2,\ P_1 \times P_2)$. If $\omega = (\omega_1, \omega_2) \in \Omega$, then there are grains located at each point x_p of ω_1, and at each such point x_p, the absorptance function $X_p(\omega_2)$ is associated. The grain at x_p absorbs at the point $x \in R^2$ the fraction $X_p(\omega_2)(x - x_p)$ of the incident light. The total effect of all the grains is that at a point $x \in R^2$, the fraction $t(x) = t(x, \omega) = t_b \prod_{x_p \in \omega_1} (1 - X_p(\omega_2)(x - x_p))$ of the incident light is transmitted. Here, t_b is a constant in $[0,1]$, representing the transmittance of the film base. $t(x)$ is called the *point transmittance* at x.

Let $G(\phi) = E(\exp \int \log \phi(S) dN(s))$ be the probability generating functional of the point process N, defined for measurable $\phi : R^2 \to [0,1]$ such that $\phi(s) = 1$ outside a bounded set (see Cox and Isham (1980), Fisher (1972), or Westcott (1972) for background on point processes). Let $y_1, y_2, \ldots, y_n$ be points in R^2 and define $\zeta(x_p, \omega_2) = \prod_{i=1}^n (1 - X_p(\omega_2)(y_i - x_p))^{u_i}$, where $u_i \geq 0$ for all $i = 1, \ldots, n$. Then

$$E\left(\prod_{i=1}^n t(y_i)^{u_i}\right) = t_b^{\sum_{i=1}^n u_i} \int_{\Omega_1} \int_{\Omega_2} \prod_{x_p \in \omega_1} \zeta(x_p, \omega_2) dP_2 dP_1$$

$$= t_b^{\sum_{i=1}^n u_i} \int_{\Omega_1} \prod_{x_p \in \omega_1} E_2(\zeta(x_p, \omega_2)) dP_1 \quad \text{(by independence)}$$

$$= t_b^{\sum_{i=1}^n u_i} G\left(E_2(\zeta(s,\omega_2))\right). \tag{3.1}$$

While (3.1) in theory allows us to determine the joint density of $t(y_1), \ldots, t(y_n)$, in practice we will only be interested in second order properties of the random field $(t(x), x \in R^2)$. Thus

$$E(t(x)) = \psi(1,0), \quad \mathrm{Cov}(t(x), t(y)) = \psi(1,1) - \psi(1,0)\psi(0,1),$$

where

$$\psi(u_1, u_2) = E(t(x)^{u_1} t(y)^{u_2}) = G(E_2(\xi(s,\omega_2))) \tag{3.2}$$

and

$$\xi(s,\omega_2) = (1 - X(\omega_2)(x-s))^{u_1}(1 - X(\omega_2)(y-s))^{u_2},$$

with X identically distributed as X_1, X_2, etc.

Unfortunately, the point transmittances $t(x)$, $x \in R^2$ are not observable. What is observable, with a microdensitometer, is the *average area (or aperture) transmittance*

$$T_A = \frac{1}{|A|} \int_A t(x)dx, \tag{3.3}$$

where $|\cdot|$ denotes Lebesgue measure (area), of a bounded region A ($\in \mathcal{B}(R^2)$) of the emulsion. Note that we have

$$\begin{aligned} E(T_A) &= \frac{1}{|A|} \int_A E(t(x))dx, \\ \mathrm{Var}(T_A) &= \frac{1}{|A|^2} \int_A \int_A \mathrm{Cov}(t(x), t(y))dxdy. \end{aligned} \tag{3.4}$$

Proposition.

1. If the point process N is stationary, then so is the random field $(t(x),\ x \in R^2)$.
2. If N is stationary and rotation invariant, and if Q is rotation invariant (i.e., $a(s) \in Q$ depends only on $|s|$), then $(t(x),\ x \in R^2)$ is stationary and rotation invariant.
3. If N is stationary and mixing (Westcott, 1972), then $\mathrm{Var}(T_A) \to 0$ and so $T_A \to \mu_t = E(t_x)$ in L_2 as $|A| \to +\infty$.

Proof.

1. Let $\phi(z) = E_2\{\prod_{i=1}^n (1 - X(y_i - z))^{u_i}\}$. Since N is stationary, then $G(\phi(s-h)) = G(\phi(s))$. Hence $E(t(y_1+h)^{u_1} \ldots t(y_n+h)^{u_n}) = t_b^{\sum_{i=1}^n u_i} G(\phi(s-h)) = t_b^{\sum_{i=1}^n u_i} G(\phi(s)) = E(t(y_1)^{u_1} \ldots t(y_n)^{u_n})$.
2. Let T be a linear isometry of R^2. Then $G(\phi(Ts)) = G(\phi(s))$ since N is rotation invariant, and $X(\omega_2)(Ts) = X(\omega_2)(s)$ since Q is invariant. It follows that $E(t(0)^{u_1} t(Th)^{u_2}) = E(t(0)^{u_1} t(h)^{u_2})$, so by 1., $E(t(x)^{u_1} t(x+h)^{u_2})$ depends only on $| h |$.
3. From part 1., we have $\mathrm{Cov}(t(x), t(y)) = E(t(0)t(y-x)) - E(t(0))$ $E(t\ (y-x)) = G(E_2((1 - X(-s))\ (1 - X(y-x-s)))) - (G(E_2(1 - X(-s))))^2$. But N mixing is equivalent to $G(\phi(u)\psi(u+v)) \to G(\phi(u))G(\psi(u))$ as $| v | \to +\infty$. Hence $\mathrm{Cov}(t(x), t(y)) \to 0$ as $| y - x | \to +\infty$. Now we show $\mathrm{Var}(T_A) \to 0$ as $| A | \to +\infty$. For $x \in R^2$, define $B_r(x) = \{y : | y - x | \leq r\}$. Given $\varepsilon > 0$, choose r so large that $| \mathrm{Cov}(t(x), t(y)) | \leq \varepsilon/2$ for $| y - x | > r$, and let A be such that $2\pi r^2 / | A | \leq \varepsilon/2$.Then from (3.4), $\mathrm{Var}(T_A) \leq \frac{1}{|A|^2} \int_A \{\int_{A \cap B_r(x)} | \mathrm{Cov}(t(x), t(y)) | \, dy + \int_{A \cap B_r^c(x)} | \mathrm{Cov}(t(x), t(y)) | \, dy\} dx \leq \frac{1}{|A|^2} \int_A \{\int_{A \cap B_r(x)} 2dy + \int_{A \cap B_r^c(x)} (\varepsilon/2) dy\} dx \leq (2\pi r^2 / | A |) + (\varepsilon/2) \leq \varepsilon$.

In the computational examples 1–5 of Section 3.2, the point process N is infinitely divisible. In this case, the probability generating functional G of the process has the canonical form

$$G(\phi) = \exp \int (\exp(\int \log \phi(s) dN(s)) - 1) d\tilde{P}_1,$$

where $\tilde{P}_1$ is the KLM (Kerstan-Lee-Mathes) measure of the point process, and from (3.1) and (3.2) we have

$$\log\ E(t(x)) = \int (\exp(\int \log\ E_2(1 - X(x-s)) dN(s)) - 1) d\tilde{P}_1.$$

The left hand side is the optical density, and as will be seen in the example of Section 3.2, the right hand side is proportional to mass density. The proportionality of optical and mass density has been consistently experimentally observed, and is a fundamental principle among photographic scientists.

Before turning to the examples of Section 3.2, we will narrow down the field of candidates for the underlying point process N, the family Q of absorptance functions, and the shape of the densitometer aperture A. We assume:

(A1) N is stationary and rotation invariant. For a uniformly exposed and developed emulsion, this is reasonable.

(A2) Q is rotation invariant. This is unrealistic, since grains do not have circular shapes, but essential for computational purposes.

(A3) The aperture A is circular.

As a result of (A1) and (A2), the random field $(t(x),\ x \in R^2)$ is isotropic, $E(T_A) = \mu_t$ does not depend on A, and (3.4) becomes

$$\mathrm{Var}(T_A) = \frac{1}{|A|^2} \int_{R^2} C(|z|)k(z)dz, \tag{3.5}$$

where $C(r) = \mathrm{Cov}(t(0), t((r,0)))$, $r \geq 0$ is the autocovariance function of $(t(x), x \in R^2)$ and $k(z) = |A \cap (A - z)|$ is the area of the intersection of A with itself shifted by the amount $-z$. For a circular aperture of radius R,

$$k(z) = |A|\gamma\left(\frac{|z|}{2R}\right), \tag{3.6}$$

where

$$\gamma(r) = \begin{cases} (2/\pi)(\cos^{-1} r - r\sqrt{1-r^2}), & |r| \leq 1 \\ 0, & \text{otherwise.} \end{cases} \tag{3.7}$$

Area intersection functions such as $k(z)$ arise frequently in computations, sometimes involving three or more regions. If A_{ρ_1} and A_{ρ_2} are circular regions with radii $\rho_1 \geq \rho_2$,

$$|A_{\rho_1} \cap (A_{\rho_2} - z)| = \begin{cases} |A_{\rho_2}| & \text{if } 0 \leq |z| \leq \rho_1 - \rho_2 \\ \frac{1}{2}\left(|A_{\rho_1}|\gamma\left(\frac{u}{\rho_1}\right) + |A_{\rho_2}|\gamma\left(\frac{|z|-u}{\rho_2}\right)\right) & \text{if } \rho_1 - \rho_2 \leq |z| \leq \rho_1 + \rho_2 \\ 0 & \text{if } |z| > \rho_1 + \rho_2, \end{cases} \tag{3.8}$$

where

$$u = \frac{|z|^2 + (\rho_1^2 - \rho_2^2)}{2|z|}.$$

Although T_A is the fundamental observable, the meaningful quantity to photographic scientists is optical density, defined as $D_A = -\log_{10} T_A$ (in fact, densitometers have a built in analog device which converts direct readings of T_A to D_A). The traditional measure of granularity, the Selwyn granularity $S = \sqrt{2}\,|A|\,\mathrm{Var}(D_A)$, uses $\mathrm{Var}(D_A)$ rather than $\mathrm{Var}(T_A)$. The

problem here is that the moments of D_A cannot be simply expressed in terms of those of T_A. If $|A|$ is large, however, the approximations

$$E(D_A) \cong -\log_{10} E(T_A) = -\log_{10} \mu_t,$$
$$\mathrm{Var}(D_A) \cong \frac{(\log_{10} e)^2 \mathrm{Var}(T_A)}{\mu_t^2}, \tag{3.9}$$

which result from retaining only the first term in the Taylor series expansion of $\log x$ are valid, and in fact will be used in this paper (as by Hamilton *et al.*, 1972; Trabka and Doerner, 1976) as definitions of $E(D_A)$ and $\mathrm{Var}(D_A)$. The Selwyn granularity becomes, via (3.5)–(3.7) and (3.9),

$$S = \frac{2\log_{10} e}{\mu_t} \sqrt{\pi \int_0^\infty hC(h)\gamma\left(\frac{h}{2R}\right) dh}. \tag{3.10}$$

3.2 Computational Examples

The computational examples to follow below are special cases obtained by specification of (a) the underlying point process N, and (b) the grain absorptance function $X(\rho)$, $\rho \geq 0$. We adopt the following notation:

r = grain radius (in general a random variable),

a = expected grain area = $E(\pi r^2)$,

n = expected number of grain reference points per unit area, and

B_ρ = circular disc with radius ρ, centered at $0 \in R^2$.

Example 1. (Hamilton *et al.*, 1972; Trabka and Doerner, 1976).

Assumptions:

(a) N is stationary Poisson with rate $n > 0$, i.e., $G(\phi) = \exp[n \int (\phi(s) - 1)\, ds]$.

(b) $X(\rho) = g I_{B_r}(\rho)$ where g (grain absorptance) $\in [0, 1]$ is a constant.

This is the basic random dot model. We have from (3.2)

$$\mu_t = E(t(0)) = t_b \exp[-n \int E_2 X(|s|) ds] = t_b \exp(-nga) \tag{3.11}$$

and

$$\begin{aligned} C(|z|) &= t_b^2 e^{n \int E_2((1-X(|s|))(1-X(|z-s|)))-1 ds} - \mu_t^2 \\ &= \mu_t^2 \left(e^{nE_2 \int X(|s|)X(|z-s|) ds} - 1\right) \\ &= \mu_t^2 \left(e^{ng^2 E_2(|B_r \cap (B_r + |z|)|} - 1\right) \\ &= \mu_t^2 \left(e^{ng^2 E_2(\pi r^2 \gamma(|z|/(2r))} - 1\right). \end{aligned} \tag{3.12}$$

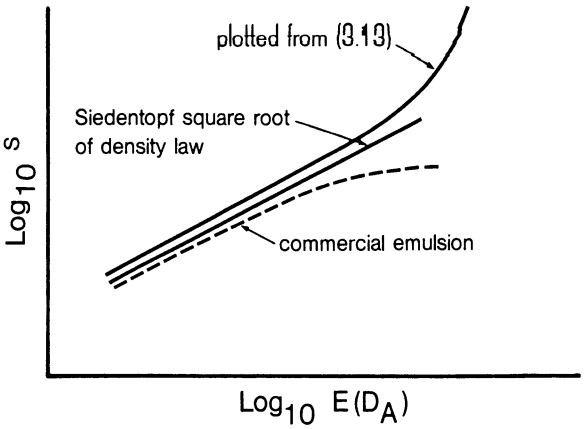

Figure 8. *Noise to signal plots.*

From (3.9) and (3.11), we have *Nutting's formula*

$$E(D_A) = D_b + knga, \qquad (D_b = -\log_{10} t_b, \quad k = \log_{10} e)$$

illustrating the principle of equivalence of optical density $E(D_A)$ and mass density nga. From (3.10) and (3.12) we have

$$S^2 = 4k^2\pi \int_0^\infty h \left(\exp(ng^2 E(\pi r^2 \gamma(h/2r))) - 1\right) \gamma(h/2R) dh \qquad (3.13)$$

for Selwyn's granularity. If in (3.13), we use the fact that $e^x - 1 \geq x$, for $x \geq 0$, we find

$$\begin{aligned} S^2 &\geq 4k^2\pi \int_0^\infty ng^2 E(\pi r^2 \gamma(h/2r)) \gamma(h/2R) h dh \\ &= k'(E(D_A) - D_b) \end{aligned}$$

(where $k' = a^{-1} 4k\pi g \int_0^\infty E(\pi r^2 \gamma(h/2r)) \gamma(h/2R) h dh$ is independent of n) with approximate equality for small n. Thus the model is consistent with *Siedentopf's formula*, an empirically determined principle which states that for small values of density, Selwyn granularity is proportional to the square root of density.

Of great interest to photographic scientists is the noise-to-signal plot of log S versus log $E(D_A)$, shown in Figure 8. The dotted curve is typical of a real emulsion, while the top solid curve results from equation (3.13). The middle solid line of slope 1/2 results from Siedentopf's formula.

Trabka and Doerner (1976), using carefully prepared single grain-size emulsions and a special densitometer for which (3.9) is *exact*, found that (3.13) gave a good fit at low and medium densities to the noise to signal plot of these emulsions, while the Siedentopf formula was only valid at low densities.

Example 2. (Benton, 1977)

Assumptions:

(a) N is stationary Poisson with rate $n > 0$.

(b) $X(\rho) = g(1 - (\rho/r)^2)^b I_{B_r}(\rho)$ where $b \geq 0$ is a constant.

Benton remarks that assumption (b) describes grains with centre opacity g and variable edge sharpness moderated by b. As in example 1, it is easily seen that

$$\mu_t = t_b \exp(-\frac{nag}{b+1}), \qquad C(h) = \mu_t^2 \left(e^{nJ(h)} - 1\right), \tag{3.14}$$

where

$$J(|\, z \,|) = E_2 \int_{B_r \cap (B_r + z)} \left(1 - \left(\frac{|\, s \,|^2}{r}\right)\right)^b \left(1 - \left(\frac{|\, z - s \,|^2}{r}\right)\right)^b ds.$$

Benton evaluates J numerically and examines the noise to signal plot resulting from (3.14). He claims that 'excess granularity' (the difference between the upper solid curve in Figure 8 and the dotted curve for a real emulsion) is reduced in this model, especially with increasing b, but in fact any such reduction is only apparent and results by rescaling the parameters.

Example 3. (Benton, 1977)

In the same paper, Benton uses the same model as in Example 2, but replaces assumption (b) with (b') $X(\rho) = ge^{-(\rho/r)^2}$. Easy computations give

$$\mu_t = t_b e^{-nag}, \quad C(h) = \mu_t^2 (\exp(\frac{1}{2} n g^2 E_2(\pi r^2 \exp(-h^2/(2r)))) - 1).$$

Again, any claimed reduction in excess granularity is due only to scale changes.

Example 4. (Dainty and Shaw, 1982)

Dainty and Shaw attempt to incorporate grain 'clustering' into the random dot model by assuming:

(a) N is a doubly stochastic Poisson point process with probability generating functional given by

$$G(\phi) = E_\mu[\exp \int (\phi(s) - 1) d\mu(s)],$$

where $\mu(\cdot)$ is a random measure on $\mathcal{B}(R^2)$ and E_μ denotes expectation with respect to μ.

(b) $X(\rho) = gI_{B_r}(\rho)$ with r a constant.

From the outset, the authors assume $\mu(\cdot)$ is stationary, so that in effect $G(\phi) = E_\mu[\exp(\mu \int(\phi(s) - 1)ds)]$, where μ is a random variable, and we return to Example 1 with n replaced by μ. μ is then assumed to be gamma distributed with mean n and variance n^2/m, where m is an integer. Expressions for μ_t and $C(h)$ are easily derived. The authors claim that clustering of grains increases as m increases, but on the one hand it is hard to see how clustering can arise from a doubly stochastic model, and on the other hand it is not clear what relevance, if any, m has for the photographic emulsion.

Example 5. (Tanaka and Uchida, 1983)

Tanaka and Uchida observe that "it is known that there are grain aggregations in several types of photographic images. Such grain aggregations are often called mottle." The authors propose to incorporate this clustering into the random dot model by assuming:

(a) N is a cluster point process with probability generating functional

$$G(\phi) = \exp\{w \int \{[\exp \int (\phi(s) - 1)\lambda(|s - x)|)ds] - 1\}dx\}$$

consisting of

(i) a stationary Poisson base process of 'mottle centres', of intensity $w > 0$. The mottle centres are not considered points of N.

(ii) Poisson cluster member processes which are rotation invariant and generated by translation. If x is a mottle centre, the intensity at a point s of the cluster member process initiated from x is $\lambda(|\, s - x\,|)$. The points of the cluster member processes are the locations of grain centres. In their calculations, the authors take $\lambda(\rho) = qI_{B_m}(\rho)$, where m is called the mottle radius.

(b) $X(\rho) = gI_{B_r}(\rho)$, where r is constant with $r << m$.

Using the approximations

$$|\, B_r \cap (B_m + x)\,| \cong \begin{cases} 0 & \text{if } |\, x\,| > m \\ a & \text{if } |\, x\,| \leq m, \end{cases}$$

$$|\, B_r \cap (B_r + s) \cap (B_m + x)\,| \cong \begin{cases} 0 & \text{if } |\, x\,| > m \text{ or } |\, s - x\,| > m \\ a\gamma(|\, s\,|/2r) & \text{otherwise} \end{cases}$$

and equation (3.2), we find after a fair amount of computation that

$$\mu_t \cong t_b \exp(-w\pi m^2(1 - e^{(-gqa)})), \quad C(h) = t_b^2 e^{wJ(h)} - \mu_t^2,$$

where

$$J(h) = \pi m^2(\gamma(h/2m)\left(\exp(g^2qa\gamma(h/2r) - 2gqa)\right) - 1) + 2(1 - \gamma(h/2m)(\exp(-gqa) - 1)).$$

Examples 2 to 5 hope to reduce excess granularity on the noise-to-signal plot and improve fit with experimental results by introducing extra parameters into the random dot model, while keeping the underlying point process basically Poisson. While fit may be improved, it is clear that the drop in the noise to signal plot at high densities for real emulsions is caused by grain overcrowding, and cannot be modeled with a process N of grain centres which is infinitely divisible. What is needed is to view the emulsion as a finite number of two-dimensional layers, in each of which the underlying point process of grain centres is such that grains cannot overlap. The problem, at present, is intractable in two dimensions.

Example 6. (Castro *et al.*, 1972)

To study how crowding of grains affects the noise-to-signal plot, Castro *et al.* (1972) model a one-dimensional version of a monolayer emulsion with a point process of grain centres which prohibits grain overlap. To construct this point process, they use an alternating renewal process (Karlin and Taylor (1975) call this a renewal process involving two components to each interval). Specifically, let $X_1, X_2, \ldots$ and $Y_1, Y_2, \ldots$ be sequences of positive identically distributed random variables with distribution functions $F_X(x)$ and $F_Y(y)$ respectively, means m_X and m_Y respectively, and variances σ_X^2 and σ_Y^2 respectively. In addition, the random vectors $(X_1, Y_1), (X_2, Y_2), \ldots$ are assumed to be i.i.d. We think of the Y_i's as grains and the X_i's as gap-lengths between grains, as in Figure 9, starting with a gap (X_1) from some arbitrary initial point $y = 0$. The mid-points of the Y intervals are the grain reference points and make up the underlying point process N. Rather than work through (3.1) and (3.2) it is easier to proceed directly using renewal theory.

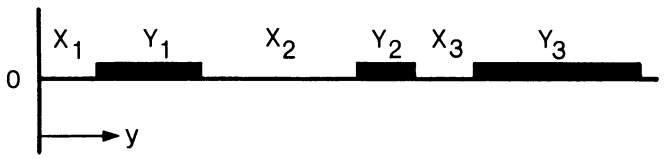

Figure 9. *Alternating renewal process model for one-dimensional monolayer emulsion.*

Given $y > 0$, define

$$I_y = \begin{cases} 1 & \text{if } y \text{ is covered by a } Y\text{-interval (i.e., a grain)} \\ 0 & \text{otherwise.} \end{cases}$$

and let $p(y) = P(I_y = 1)$. Then the point transmittance function for this emulsion is $t(y) = t_b(1-g)^{I_y}$ (where $0^0 = 1$). It is a simple matter to check that $E(t(y)) = t_b(1-gp(y))$ and $\mathrm{Cov}(t(y), t(y+h)) = g^2 t_b^2 (P(I_y = 1,\ I_{y+h} = 1) - p(y)p(y+h))$. We will want to simulate a stationary emulsion, and so we will determine

$$\mu_t = \lim_{y\to\infty} E(t(y)) = t_b(1 - g \lim_{y\to\infty} p(y))$$

and

$$C(h) = \lim_{y\to\infty} \mathrm{Cov}(t(y), t(y+h)) = g^2 t_b^2 (U(h) - (\lim_{y\to\infty} p(y))^2), \tag{3.15}$$

where

$$U(h) = \lim_{y\to\infty} P(I_y = 1,\ I_{y+h} = 1).$$

An application of the renewal argument gives

$$p^*(s) = F_X^*(s)\,(1 - F_Y^*(s) + p^*(s)F_Y^*(s)), \tag{3.16}$$

where $*$ denotes the Laplace-Stieltjes transform. An application of the key renewal theorem shows (as expected) that

$$\lim_{y\to\infty} p(y) = \frac{m_Y}{m_X + m_Y}. \tag{3.17}$$

Arguing for large y, we have

$$\begin{aligned} U(h) &= \lim_{y\to\infty} P(I_{y+h} = 1 \mid I_y = 1) \lim_{y\to\infty} p(y) \\ &= \frac{m_Y}{m_X + m_Y} \lim_{y\to\infty} (P(y+h) \text{ in same } Y\text{-interval as } y \mid I_y = 1) \\ &\qquad + P(y+h \text{ in different } Y\text{-interval} \mid I_y = 1)) \\ &= \frac{m_Y}{m_X + m_Y} \left(1 - K(h) + \int_0^h p(h-y)dK(y)\right), \end{aligned} \tag{3.18}$$

where $K(y) = (1/m_Y)\int_0^y 1 - F_Y(u)du$ is the limiting residual life distribution function of a Y-interval. From (3.16) and (3.17), we obtain

$$U^*(s) = \frac{m_Y}{m_X + m_Y} \left(1 - \frac{1}{m_Y s} \left(\frac{(1 - F_X^*(s))(1 - F_Y^*(s))}{1 - F_X^*(s)F_Y^*(s)}\right)\right). \tag{3.19}$$

In one dimension, an aperture is an interval A of length $|A|$, and (3.5) becomes

$$\mathrm{Var}(T_A) = \frac{1}{|A|}\int_{-\infty}^{+\infty} C(h)\gamma\left(\frac{h}{|A|}\right)dh,$$

where

$$\gamma(h) = \begin{cases} 1-|h| & \text{if } |h| \le 1 \\ 0 & \text{otherwise.} \end{cases}$$

Let $\mathcal{C}(s) = \int_0^\infty e^{-sh}C(h)dh$ denote the ordinary Laplace transform of $C(h)$, as calculated from (3.15), (3.17), and (3.19). Then for a large aperture A, we have

$$\begin{aligned} |A|\,\mathrm{Var}(T_A) &\cong \int_{-\infty}^{\infty} C(h)dh \\ &= \lim_{s\to 0} 2\mathcal{C}(s) \\ &= g^2t_b^2\frac{m_X^2m_Y^2}{(m_X+m_Y)^3}\left(\left(\frac{\sigma_X}{m_X}\right)^2+\left(\frac{\sigma_Y}{m_Y}\right)^2\right). \end{aligned}$$

Then from (1.2) and (3.9), we have for the Selwyn granularity,

$$S^2 \cong \frac{k^2g^2t_b^2}{\mu_t^2}\frac{m_X^2m_Y^2}{(m_X+m_Y)^3}\left(\left(\frac{\sigma_X}{m_X}\right)^2+\left(\frac{\sigma_Y}{m_Y}\right)^2\right). \tag{3.20}$$

For a computational example, the authors take $g = t_b = 1$, and assume X is exponential and Y is lognormal with coefficient of variation v. Using (3.9), (3.20) becomes

$$S^2 \cong k^2(1+v)(1-\mu_t) = k^2(1+v)\left(1-e^{-E(D_A)/k}\right). \tag{3.21}$$

For small $E(D_A)$, this is $S^2 \cong k(1+v)E(D_A)$, namely Siedentopf's formula, while for all density values, we have $S^2 \le k(1+v)E(D_A)$ so that the noise to signal plot for (3.21) will lie below the Siedentopf formula line.

Example 7. (Lawton *et al.*, 1972)

For a better approximation to reality, Lawton *et al.* consider a one-dimensional emulsion made up of m laminated independent layers of the monolayer emulsion considered in Example 6. Then $t(x) = \prod_{i=1}^m t_i(x)$, where $t_i(x)$ is the point transmittance at x of the ith monolayer. By independence, we have from (3.15) and (3.17),

$$\mu_t(m) = E(t(x)) = t_b\left(1-g\frac{m_Y}{m_X+m_Y}\right)^m = t_b\left(1-\frac{d}{m}\right)^m,$$

where $d = gm\, m_Y/(m_X + m_Y)$ is mass density. Note that Nutting's formula $E(D_A) = D_b + kd$, where $D_b = \log_{10} t_b$ (equivalence of optical and mass density), is obtained as $m \to \infty$. Again by independence, the autocovariance function for the m-layer emulsion is $\mathrm{Cov}(t(x), t(x+h)) = (C(h) + \mu_t^2)^m - \mu_t^2(m)$, where $C(h)$ and μ_t are the monolayer autocovariance function and mean respectively determined in Example 6. The authors go on to study the effect of m on the granularity.

3.3 Additional Models of the Emulsion

Colour photographic emulsions are composed of three layers, sensitive to blue, green, and red light respectively. Each of these layers is an emulsion of silver halide grains in gelatin, together with a dye which is activated when a neighbouring grain is developed. Using methods similar to those of Sections 3.1 and 3.2, Trabka (1977) considers overlapping spheres, representing dye clouds in a layer, whose centres are distributed as a Poisson point process in R^3. The region between two parallel planes represents the heterogeneous distribution of dye in the emulsion.

Most studies of multilayer (or 'thick') emulsions are made under the assumption that the statistics of photons incident on a typical grain are the same as for an area the size of a grain on the top surface of an emulsion. Trabka and Kemperman (1978) examine the consequences of grain-exposure fluctuations due to geometrical shielding by partially absorbing grains. The resulting variability in grain exposure spreads the characteristic curve of the emulsion, resulting in greater 'latitude'.

None of the models discussed in this survey have incorporated grain interaction effects due to development. For example, in a weak developer, the development of a given grain may be suppressed because of developer depletion by neighbouring grains, a common method of enhancing definition at the boundaries between light and dark areas of the image. Conversely, in a strong developer, physical proximity of grains can result in infectious development of grains. These 'adjacency' effects are modeled (Anderson, 1977) by viewing the emulsion as a two-dimensional Gibbs random field. Each point of a finite two-dimensional lattice is occupied by a grain which can be in either of two states—developed or not developed. The probability that a grain is in one of these two states depends on the states of the four neighbouring grains, the exposure which the emulsion received, and the developer strength. The model is used to examine the effect of such interaction on edge sharpness and shape of the characteristic curve.

BIBLIOGRAPHY

Anderson, W. J. (1977), "A random field model for grain interaction effects in the photographic emulsion". *Photographic Science and Engineering* **21**, 1–6.

Anderson, W. J. (1978), "A model for reciprocity failure in photographic materials and its asymptotic behaviour at low and high intensities". *Journal of the Optical Society of America* **68**, 972–978.

Anderson, W. J. (1980), "Concerning the asymptotic behaviour of high intensity reciprocity curves". *Photographic Science and Engineering* **24**, 283–289.

Anderson, W. J. (1984), "A multitrap model for high-intensity reciprocity failure in the photographic grain". *Journal of Applied Probability* **21**, 464–478.

Anderson, W. J. (1987), "A result in queueing theory and its application to photographic science". Manuscript in preparation.

Anderson, W. J., and A. M. Mathai (1986), "A queueing model for reciprocity failure in the photographic grain". *Stochastic Processes and Their Applications* **21**, 229–250.

Benton, S. A. (1977), "Approximation for granularity theory". *Photographic Science and Engineering* **21**, 177–182.

Burge, G. (1983), "A model for latent image formation and chemical sensitization". *Photographic Science and Engineering* **27**, 31–35.

Castro, P. E., J. H. B. Kemperman, and E. A. Trabka (1973), "Alternating renewal model of photographic granularity". *Journal of the Optical Society of America* **63**, 820–825.

Cox, D. R., and Y. Isham (1980), *Point Processes*. London: Chapman and Hall.

Dainty, J. C., and R. Shaw (1982), "Density and granularity of clustered distributions of monosized opaque dot". *Journal of the Optical Society of America* **72**, 662–665.

Ehn, D. C., and M. B. Silevitch (1974), "Diffusion model for the adjacency effect in viscous development". *Journal of the Optical Society of America* **64**, 667–676.

Filimonov, R. P. (1977), "Simulation of two-dimensional fields of the impulse type by means of overlapping sets of randomly distributed in the euclidean plane." *Technicheskaya Kibernetika* **14**, 205–211.

Fisher, L. (1972), "A survey of the mathematical theory of multidimensional point processes". In *Stochastic Point Processes: Statistical Analysis, Theory, and Applications*, ed. P. A. W. Lewis, pp. 468–513. New York: Wiley and Sons.

Froehlich, G. K., J. F. Walkup, and T. F. Krile (1982), "Estimation in signal-dependent film-grain noise". *Applied Optics* **20**, 3619–3626.

Hada, H., M. Kawasaki, and H. Fujimoto (1980), "Minimum size of developable latent image specks and energy levels of small silver specks in photographic emulsions". *Photographic Science and Engineering* **24**, 232–241.

Hamilton, J. F. (1966), "Reciprocity law failure". In *Theory of the Photographic Process*, 3rd edition, ed. T. H. James, pp. 132–142. New York: Macmillan.

Hamilton, J. F. (1972), "Concerning the slopes of low-intensity reciprocity curves". *Photographic Science and Engineering* **16**, 287–290.

Hamilton, J. F. (1974), "Mathematical modelling of latent image formation". *Photographic Science and Engineering* **18**, 371–377.

Hamilton, J. F. (1985), Personal communication with the author.

Hamilton, J. F., W. H. Lawton, and E. A. Trabka (1972), "Some spatial and temporal point processes in photographic science". In *Stochastic Point Processes: Statistical Analysis, Theory, and Applications*, ed. P. A. W. Lewis, pp. 818–868. New York: Wiley and Sons.

Hamilton, J. F., and F. Urback (1966), "The mechanism of the formation of the latent image". In *Theory of the Photographic Process*, 3rd edition, ed. T. H. James, pp. 87–119. New York: Macmillan.

Hautot, André (1976), "Sur la structure et la stabilité des centres de la sensibilité photographique". *Bulletin de la Societé des Sciences de Lièges* **45**, 183–200.

James, T. H., Ed. (1977), *The Theory of the Photographic Process*, 4th edition. New York: Macmillan.

James, T. H., and G. C. Higgins (1968), *Fundamentals of Photographic Theory*. Hastings on Hudson, New York: Morgan and Morgan.

Karlin, S., and H. M. Taylor (1975), *A First Course in Stochastic Processes*, 2nd edition. New York: Academic Press.

Kawasaki, M., S. Fujiwari, and H. Hada (1978), "Analysis of characteristic curves for monodisperse mono-grainlayer emulsions and the minimum size of latent image speck". *Photographic Science and Engineering* **22**, 290–295.

Kozakov, O., V. A. Loiko, Yu. S. Andreev, and E. K. Naumenko (1982), "Dependence of the frequency-contrast characteristic of a photographic material on the parameters of its emulsion layer". *Zhurnal Nauchnòi i Prikladnoi Fotographii i Kinematografii* **26**, 241–245.

Lawton, W. H., E. A. Trabka, and D. R. Wilder (1972), "Crowded emulsions: granularity theory for multilayers". *Journal of the Optical Society of America* **62**, 659–657.

Martin, F., and C. Aime (1978), "Some spectral properties of random arrays of grains". *Journal of the Optical Society of America* **68**, 1782–1784.

Martin, F., and C. Aime (1981), "Harmonic analysis of random arrays of grains: application to the jitter model". *Journal of Photographic Science* **29**, 166–170.

Mitchell, J. W. (1978), "The concentration theory of latent image formation". *Photographic Science and Engineering* **22**, 249–255.

Mitchell, J. W. (1983a), "The trapping of electrons in crystal of silver halides". *Photographic Science and Engineering* **27**, 96–102.

Mitchell, J. W. (1983b), "The statistics of electron trapping process in microcrystals of silver halides". *Journal of Photographic Science* **31**, 227–234.

Modestino, J. W., R. W. Fries, and D. G. Daut (1979), "Generalization of the two-dimensional random checkerboard process". *Journal of the Optical Society of America* **31**, 897–906.

Richards, W., and S. B. Purks (1978), "On random dot texture discrimination". *Journal of the Optical Society of America* **68**, 270–271.

Singh, J. P. (1979), "Grain diameter-dependent probability of silver halide grains of photographic emulsions". *Indian Journal of Pure and Applied Physics* **17**,

688–690.

Stark, H. (1977), "Diffraction patterns of non-overlapping circular grains". *Journal of the Optical Society of America* **67**, 700–703.

Stark, H. (1978), "Spectral properties of random arrays of grains: comment". *Journal of the Optical Society of America* **68**, 1785–1786.

Sturge, J. M., Ed. (1977), *Neblette's Handbook of Photography and Reprography: Materials, Processes, and Systems*, 7th edition. New York: Van Nostrand Reinhold.

Tanaka, K., and S. Uchida (1983), "Extended random dot model". *Journal of the Optical Society of America* **73**, 1312–1319.

Trabka, E. A. (1977), "A random-sphere model for die clouds". *Photographic Science and Engineering* **21**, 183–192.

Trabka, E. A., and E. C. Doerner (1976), "Random-dot parameters for monodisperse photographic emulsions". *Journal of Applied Photographic Engineering* **2**, 1–6.

Trabka, E. A., and J. H. B. Kemperman (1978), "Exposure fluctuations in model photographic emulsions 1: Grain shielding effects on the characteristic curve". *Photographic Science and Engineering* **22**, 281–289.

Trabka, E. A., and W. H. Lawton (1974), "Colour granularity: a layered model". *Journal of Photographic Science* **22**, 131–137.

Westcott, M. (1972), "The probability generating functional". *Journal of the Australian Mathematical Society* **14**, 448–466.

David E. Matthews, [1] Christoph E. Minder, [2] and Ian McMillan [3]

A STOCHASTIC MODEL FOR THE EFFECT OF INCIDENT LIGHT INTENSITY ON CO_2 UPTAKE IN LEAVES

ABSTRACT

A continuous-time Markov model is developed to describe the absorption of energy from incident light and the fixation of CO_2 molecules in a single photosynthetic unit (PSU). Equilibrium probabilities and mean sojourn times derived from this Markov process are then used to model the CO_2 uptake in an aggregate of PSU's, for example a leaf, as the superposition of modified renewal processes. From this aggregate process we derive a shifted rectangular hyperbola for expected CO_2 uptake, as a function of the incident light intensity λ , over a fixed observation period of length T. Non-linear regression methods are used to fit this function to experimental data collected in a study of CO_2 uptake in the leaves of various vines. The excellent fit obtained provides empirical support for the proposed stochastic model.

1. INTRODUCTION

In a descriptive article summarizing recent findings in photosynthesis research, Campbell (1984) described photosynthesis as "a classic example of a 'scientific black box' ". Though we know the inputs—carbon dioxide gas and water vapour—and the outputs—glucose sugar and oxygen gas—a complete knowledge of the sequence of events that occurs still eludes plant photochemists and other researchers.

[1] Department of Statistics and Actuarial Science, University of Waterloo, Waterloo, Ontario N2L 3G1

[2] Institut für Sozial-und Präventivmedizin, Universität Bern, CH-3012 Bern, Switzerland

[3] Department of Animal and Poultry Science, University of Guelph, Guelph, Ontario, N1G 2W1

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 41–50.

The techniques of mathematical modelling readily lend themselves to "black box" problems. Indeed, two of the more important functions of such models are prediction and explanation. Although these activities are not necessarily mutually exclusive, prediction models are often empirical in nature with no clear mechanistic relation to the data under study. Nevertheless, the utility of such models is often impressive. For example, the hyperbolic pattern of response of leaf photosynthesis, F, to changing incident light flux density, I, can be expressed as

$$F = \alpha I F^*/(\alpha I + F^*) - R,$$

where α represents leaf photochemical efficiency, F^* is the light-saturated photosynthetic rate and R specifies the rate of dark respiration. From this description of the photosynthetic behaviour of a single leaf, models have been derived for canopy net photosynthesis that agree quite well with experimental data (see, for example, Charles-Edwards, 1982).

In contrast to their prediction counterparts, mechanistic or process-oriented models are usually the result of mathematical descriptions of biochemical processes. These models are generally deterministic, and frequently employ differential equations to describe changes in the essential components of a biological system. The model which is developed here departs from the usual mechanistic approach to photosynthesis by incorporating stochastic elements in its description of a process which is still only partly understood.

2. A STOCHASTIC MODEL OF A PHOTOSYNTHETIC UNIT

To avoid undue complexity and yet incorporate necessary features in our stochastic description of the photosynthetic process, the model which we develop is based on a description of activity at the level of a photosynthetic unit (PSU). A detailed account of the known events which occur in a PSU was given by Nobel (1974). Incident light, in the form of photons, strikes the PSU and quanta of energy are captured. Although the biochemistry of photosynthesis is not completely understood, it is generally believed that at least eight quanta of light energy are required to trigger the chemical reaction which converts carbon dioxide and water into oxygen and glucose sugar. The fundamental aspects of this process appear to be quantum capture and the resulting chemical reaction. The following two subsections outline the assumptions, and the consequences, of a stochastic model for a single PSU.

2.1 Quantum Capture

We shall assume that all PSU's have the same area, and that quantum flux is uniform. Although the description of reality which these assumptions

imply is not strictly correct, neither assumption is critical to the model which we develop. The essential features which characterize the process of photon strike and capture within a single PSU are:

(i) The point process of photon strikes in a particular PSU can be represented by a Poisson process of intensity $\lambda > 0$;
(ii) Given that a photon strike has occurred, effective quantum capture follows with probability p, $0 < p < 1$;
(iii) Distinct quantum captures by the same PSU are independent and identically distributed events.

By effective quantum capture we refer to the transfer of excitation from the periphery of a PSU to the reaction centre. This transfer can depend on many different circumstances; however, the net effect is summarized by (ii) above.

It is well-known (see, for example, Takács, 1960, §2.5) that these three assumptions result in a model for the point process of effective quantum capture in a single PSU which is Poisson with intensity $\alpha = \lambda p$.

2.2 CO_2 Uptake and O_2 Generation

In providing energy to drive the photochemical reaction, the PSU acts like a photovoltaic battery; as soon as a specified energy threshold has been achieved, the reaction is triggered. Clearly, if we know the energy level of a PSU, we can determine whether or not the reaction has begun. Let $\{E_t\}$, $t \geq 0$ be the energy level of a particular PSU at time t, and let N be the threshold level, in quanta, which stimulates the photochemical reaction. The Poisson process of effective quantum capture succinctly describes successive increases in the value of E_t from 0 to N. When the reaction which converts water and carbon dioxide to oxygen and glucose sugar has run its course, the energy level of the PSU is once more 0 and the PSU must begin again the process of accumulating quanta. Therefore, if we could characterize the change of state of E_t from 0 to N, we would have a stochastic model of the photovoltaic activity of a PSU.

One quite general model of this change of state might be to assume that the length of time involved in CO_2 uptake and O_2 generation has an unspecified distribution with mean $1/\beta$, and that these durations are independent of other events. This assumption leads quite naturally to a semi-Markov model for $\{E_t\}$ (see Pyke, 1961a,b), provided we also assume that during CO_2 uptake and O_2 generation, additional effective quantum capture does not occur. According to Nobel (1974, p. 240) this latter assumption is quite realistic since "the rate-limiting step for photosynthesis is not light absorption, excitation transfer or photochemistry (electron donation by trap chl*), but the subsequent steps leading to O_2 evolution and CO_2 fixation".

As an alternative to this semi-Markov model for $\{E_t\}$, we could specify that the length of time involved has an exponential distribution with the same mean, i.e., $1/\beta$. Then $\{E_t\}$ will be a Markov process (see Feller, 1968, §17.6). The correctness of this latter assumption is not crucial to the aggregate model which we develop in §3 , and it simplifies, slightly, the intermediate results. Therefore, we have chosen to model the activity of a PSU as a time-homogeneous Markov process, $\{E_t\}$, with instantaneous transition matrix $Q = (q_{ij})$, where

$$q_{ij} = \begin{cases} \alpha & j = i+1,\ i = 0,\ldots,N-1 \\ -\alpha & j = i,\ i = 0,\ldots,N-1 \\ \beta & i = N,\ j = 0 \\ -\beta & i = j = N \\ 0 & \text{otherwise.} \end{cases}$$

Let π_j, $j = 0,\ldots,N$, be the equilibrium probabilities $\lim_{t\to\infty} Pr(E_t \mid E_o)$. These probabilities can be determined by solving the system of equations $\boldsymbol{\pi}Q = \mathbf{0}$, where $\boldsymbol{\pi} = (\pi_0, \pi_1, \ldots, \pi_N)$, subject to the usual normalizing condition $\Sigma\pi_j = 1$. The values of $\pi_0,\ldots,\pi_N$ determined by the above Q are

$$\pi_j = \beta/(N\beta+\alpha),\quad j = 0,\ldots,N-1 \quad \text{and} \quad \pi_N = \alpha/(N\beta+\alpha). \tag{2.1}$$

Each value corresponds to the stabilized proportion of PSU's in an ensemble which would be observed to occupy state j, $j = 0,\ldots,N$, (see Feller, 1968, §15.7).

A second consequence of the Markov model for $\{E_t\}$ concerns the mean sojourn times in each of the states. These values are $1/\alpha$ for the states $0,1,\ldots,N-1$ and $1/\beta$ for state N (the reaction state). Thus, the total average time that a single PSU at energy level j requires to capture $(N-j)$ quanta and complete the photochemical reaction is

$$\mu_j = \{(N-j)\beta+\alpha\}/(\alpha\beta),\quad j = 0,\ldots,N. \tag{2.2}$$

3. AN AGGREGATE MODEL FOR CO_2 UPTAKE IN A LEAF

The data which prompted the development of the stochastic model described in this paper specify CO_2 uptake over an observation period of fixed length, say $(0,T)$. These data were derived from a single leaf, which is an aggregate of PSU's. To extend the single PSU model which we developed in §2 to the level of a leaf we require two additional assumptions:

(i) A leaf consists of K PSU's which are identical and which act independently;

(ii) The aggregate of PSU's in a leaf has achieved statistical equilibrium when the observation period begins.

Clearly, neither of these assumptions is likely to be strictly correct. However, in the aggregate, our description may be adequate as a model for the combined photosynthetic activity of the constituent PSU's in a single leaf.

Define $U(T)$ to be the expected CO_2 uptake of a single leaf during the observation period. Clearly, the aggregate process of CO_2 uptake in K PSU's is the superposition of K independent, renewal processes (see Cox, 1970). However, these processes are not identical. At the beginning of the observation period not all K PSU's will occupy state 0 and move in lockstep with each other. Rather, a fraction π_j will be in state j, $j = 0, \ldots, N$, and the expected time which elapses until the initial photochemical reaction is completed will be $\mu_j = \{(N-j)\beta + \alpha\}/(\alpha\beta)$. Since $\{E_t\}$ is a Markov process, this is the only adjustment which we must make to account for initial conditions in the observation period. All subsequent intervals during which a single PSU captures N quanta and completes the photochemical reaction are independent and identically distributed with mean value $\mu_0 = (N\beta + \alpha)/(\alpha\beta)$; we call these intervals complete PSU cycles. Let $U_j(T)$ be the expected CO_2 uptake in $(0, T)$ which is due to a PSU having initial state j. The function $U_j(T)$ is well-known as a modified renewal function (see Cox, 1970); its asymptotic form can be shown to equal

$$U_j(T) \approx T/\mu_0 + \{\frac{1}{2}(\sigma^2 + \mu_0^2)/\mu_0^2 - \mu_j/\mu_0\}, \quad j = 0, \ldots, N,$$

where $\sigma^2 = (N\beta^2 + \alpha^2)/(\alpha^2\beta^2)$ is the theoretical variance of the intervals known as complete PSU cycles.

Since the aggregate of PSU's in a leaf is assumed to be in statistical equilibrium when the observation period begins, there will be $K\pi_j$ PSU's, on average, in state j, $j = 0, \ldots, N$. At the conclusion of the observation period, the expected CO_2 uptake for each PSU initially occupying state j is $U_j(T)$; therefore

$$U(T) = K\pi_0 U_0(T) + \ldots + K\pi_N U_N(T).$$

A final algebraic expression for $U(T)$ in terms of the parameters of the model is quite complicated. However, using formulae (2.1) and (2.2) the form of the asymptotic expression can readily be shown to be

$$\begin{aligned} U(T) &\approx K\alpha\beta T/(N\beta + \alpha) + C \\ &= \lambda/(A + B\lambda) + C, \end{aligned}$$

where $A = N/(pKT)$, $B = 1/(K\beta T)$ and C are constants which depend on the parameters of the model. Thus, the equation which summarizes

our aggregate model corresponds to a shifted rectangular hyperbola for the expected CO_2 uptake, expressed as a function of the incident light intensity λ over an observation period of fixed length T.

4. SOME EXPERIMENTAL RESULTS

The data recorded in Table 1 pertain to the uptake of CO_2 in photosynthesis and consist of six sets of measurements obtained from the leaves of various vines, including *Vitis vinifera*, *Vitis labrusca* and several hybrid vines. Each data set contains 14 observation pairs, (λ_i, y_i), of light intensities, λ_i, and CO_2 uptake, y_i, during an observation period of fixed length.

Table 1. *The observed amounts of CO_2 uptake (y) by single leaves of six different varieties of vine. The measurements were recorded during an observation period of constant length at 14 different levels of incident light intensity (λ).*

	Variety					
Intensity (λ)	Seibel 1000	Gamay	Seibel 9110	Marechal Foch	De Chaunac	Seibel 10878
40	0.40	0.34	0.28	0.33	0.28	0.42
200	0.74	0.68	0.60	0.67	0.60	0.81
300	0.86	0.79	0.75	0.73	0.72	0.90
400	1.02	0.93	0.86	0.93	0.85	0.98
600	1.20	1.12	1.03	1.13	1.10	1.13
800	1.31	1.29	1.19	1.39	1.23	1.31
1200	1.53	1.49	1.33	1.65	1.44	1.51
1600	1.67	1.65	1.47	1.79	1.61	1.72
2000	1.81	1.80	1.61	1.90	1.76	1.93
2500	1.90	1.94	1.79	2.00	1.92	2.11
3000	2.01	2.04	1.87	2.05	2.01	2.24
3500	2.06	2.11	1.92	2.08	2.14	2.34
4000	2.11	2.16	1.99	2.12	2.19	2.40
5000	2.13	2.20	2.04	2.14	2.25	2.46

In terms of observation pairs, (λ_i, y_i), for a given data set, the result developed in §3 relating expected CO_2 uptake to incident light intensity may be written as

$$U = E(Y) = \lambda/(A + B\lambda) + C, \tag{4.1}$$

i.e., the regression of CO_2 uptake on incident light intensity is given by a shifted rectangular hyperbola where A, B and C are parameters determined by various aspects of the leaf and the experiment.

Non-linear regression techniques of a standard type were used to fit the model (4.1) to the six different data sets. Figure 1 contains a plot of the *Seibel* 1000 observations and the fitted regression model, while Figure 2 shows the corresponding residual plot. Figure 2 provides no apparent evidence of lack of fit, and is characteristic of the residual plots which were obtained in the other five data sets. The estimated parameter values for the six data sets are presented in Table 2. In every case, the regression model accounted for at least 99.4% of the observed variation in CO_2 uptake.

Charles-Edwards (1981) has observed that mechanistic models of leaf photosynthesis are frequently criticized because they assume the homogeneity of various properties of individual chloroplasts of the leaf. However, he also notes that even if the details of a particular process are obscure, a mathematical model can be expected to exhibit the right sort of qualitative behaviour if the model correctly formalizes the essential features of the process. In fact, the model could also provide a good quantitative description of experimental data, although estimates of the model parameters might not enable researchers to unequivocally resolve the fine detail of the biochemical and physical processes. Models with these characteristics perform the useful service of identifying which are the important aspects of the process under study. In addition, they can sometimes bring order to a welter of otherwise disordered experimental information. In our view, the satisfactory fit of these data sets to the model which we have developed provides empirical support for the adequacy of a stochastic model as a description, in the aggregate, for the effect of incident light intensity on CO_2 uptake in leaves.

ACKNOWLEDGMENT

This work has been supported by the Natural Sciences and Engineering Research Council of Canada.

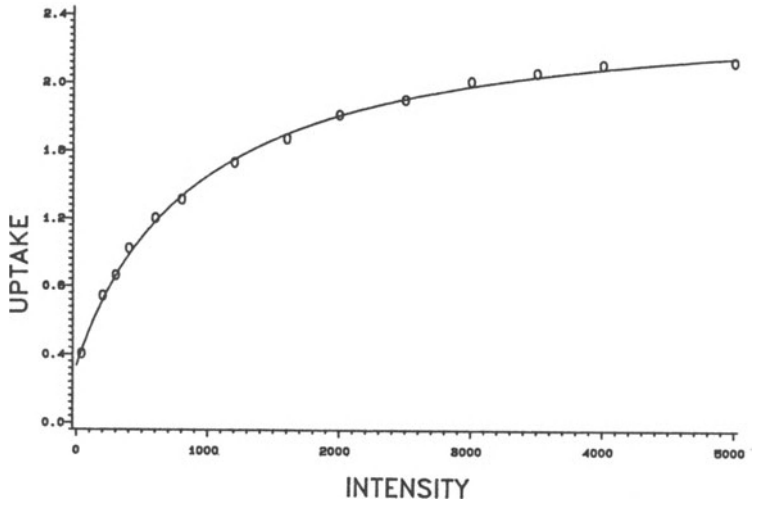

Figure 1. *A scatterplot of the observed CO_2 uptake (y) versus incident light intensity (λ) for the Seibel 1000 leaf; observed values are indicated by the symbol* 0. *The solid line, represents the fitted regression curve.*

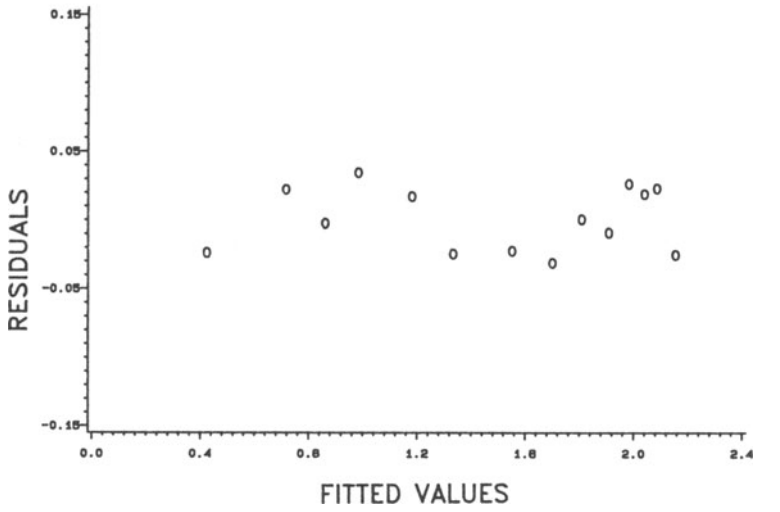

Figure 2. *A scatterplot of the Seibel 1000 residuals $y_i - \hat{y}_i$, versus the values $\hat{y}_i = \hat{C} + \lambda/(\hat{A} + \hat{B}\lambda)$ predicted by the fitted regression model at 14 levels of incident light intensity (λ).*

Table 2. *Estimated parameter values and corresponding asymptotic 95% confidence intervals*[1] *for the six data sets (see Table 1) fitted by the nonlinear regression model* $U = E(Y) = C + \lambda/(A + B\lambda)$.

	Parameter		
Variety	*A*	*B*	*C*
Seibel 1000	429.3	0.463	0.335
	(375.1,483.4)	(0.450,0.476)	(0.279,0.391)
Gamay	467.2	0.421	0.285
	(414.5,519.8)	(0.410,0.433)	(0.233,0.336)
Seibel 9110	517.8	0.456	0.255
	(415.0,620.7)	(0.434,0.478)	(0.172,0.338)
Marechal Foch	334.8	0.424	0.170
	(255.6,414.0)	(0.402,0.445)	(0.050,0.291)
De Chaunac	498.3	0.393	0.233
	(433.2,563.5)	(0.380,0.407)	(0.172,0.294)
Seibel 10878	632.5	0.357	0.443
	(497.0,768.0)	(0.330,0.384)	(0.346,0.540)

[1] The asymptotic confidence intervals were obtained via the method described by Ralston and Jennrick (1978).

REFERENCES

Campbell, W. (1984), "Photons into foodstuffs." *Science Dimension* **16**, 20–29.

Charles-Edwards, D. A. (1981), *The Mathematics of Photosynthesis and Productivity.* London: Academic Press.

Charles-Edwards, D.A. (1982), *Physiological Determinants of Crop Growth.* North Ryde, Australia: Academic Press.

Cox, D. R. (1970), *Renewal Theory.* London: Methuen.

Feller, W. (1968), *An Introduction to Probability Theory and Its Applications,* Volume I. New York: Wiley and Sons.

Nobel, P. S. (1974), *Introduction to Biophysical Plant Physiology.* San Francisco: Freeman.

Pyke, R. (1961a), "Markov renewal processes: definitions and preliminary properties." *Annals of Mathematical Statistics* **32**, 1231–1242.

Pyke, R. (1961b), "Markov renewal processes with finitely many states." *Annals of Mathematical Statistics* **32**, 1243–1259.

Ralston, M. L., and R. I. Jennrich (1978), "Dud, a derivative-free algorithm for nonlinear least squares." *Technometrics* **20**, 7–14.

Takács, L. (1960), *Stochastic Processes: Problems and Solutions.* London: Methuen.

A. F. Desmond [1]

AN APPLICATION OF SOME CURVE-CROSSING RESULTS FOR STATIONARY STOCHASTIC PROCESSES TO STOCHASTIC MODELLING OF METAL FATIGUE

ABSTRACT

The stress history experienced by a metal component or system is modelled as a stationary Gaussian process. Under the influence of repeated stressing, the strength of the component decreases. The time to fatigue failure is modelled as the first crossing time of the stress history to a decreasing curve representing residual strength. Some typical residual strength functions are reviewed. Bounds and approximations to the reliability function are obtained based on curve crossing results for stationary processes.

1. SOME BACKGROUND

A variety of approaches to mathematical modelling of metal fatigue are available in the engineering literature. For a survey of these approaches, see Desmond (1983). Among these, the theory of fracture mechanics (see, for example, Barnby, 1972, Chapter 3) is a relatively recent approach to modelling the fatigue process. According to this theory, fatigue failure is due to the initiation and steady propagation of a dominant crack. Thus the failure time in fatigue consists of two parts:

(i) the formation of a noticeable dominant crack

(ii) the propagation of the dominant crack until a critical size is reached, at which point catastrophic failure ensues.

Crack growth laws obtained via the fracture mechanics approach take the form

$$\frac{da}{dn} = KS^b a^{b/2}, \tag{1}$$

[1] Department of Mathematics and Statistics, University of Guelph, Guelph, Ontario N1G 2W1

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 51–63.

where K and b are constants, $a = a(n)$ is the crack size after n cycles and S is the applied stress in a constant amplitude loading. For random loading S^b is replaced by its mean value (Paris, 1964).

Equation (1) is usually treated as a deterministic equation in the engineering literature. Treated deterministically, (1) can be integrated from an initial crack size a_0 to the crack size $a(t)$ at time t to yield

$$a(t) = [(1 - \frac{b}{2})KS^b t + a_0^{1-\frac{b}{2}}]^{\frac{1}{1-\frac{b}{2}}}.$$

For aluminum, $b = 4$ (Yang and Trapp, 1974) so that

$$a(t) = a_0/[1 - ta_0KS^4]. \tag{2}$$

In general, however, crack length $a(t)$ at time t is best regarded as a stochastic process. An increase in crack length is associated with a corresponding decrease in the strength of the specimen. From fracture mechanics, the relationship between the residual strength R of a structure containing a crack of size a is given by the Griffith-Irwin equation

$$K_c = R(\pi a/2)^{1/2}, \tag{3}$$

where K_c, referred to as the critical stress intensity factor, is a material constant. Relation (3) may be combined with (2) to give residual strength as a function of time. However, (3) only applies to certain structures referred to as non-redundant, which restricts its applicability somewhat.

In this paper the model we suggest for fatigue failure will employ the residual strength function $R(t)$ rather than the crack length $a(t)$ as the description of progressive deterioration under random loading.

In Section 2 we describe some previous studies of residual strength of metals under loading. Section 3 formulates the problem mathematically as a first crossing time for a monotonically decreasing curve representing residual strength. This type of problem represents a very difficult area of stochastic process theory and explicit solutions are not, in general, available. Rather than obtaining an exact solution, we note that the moments of the number of crossings and, in particular, the mean number of crossings may be used to provide bounds on the distribution of fatigue life. Also an approximation to the distribution function of fatigue life is obtained based on an assumption of non-homogeneous Poisson upcrossings.

To summarize, in this paper we shall be concerned with fatigue failure due to a stochastically varying load which promotes the fatigue process of initiation and growth of a dominant crack and consequently a steady decay in strength. The mathematical model we use embodies a description

of the time-varying load and the strength decay. As far as is known, the curve-crossing theory used in the model has not previously been employed in fatigue studies.

2. PREVIOUS STUDIES ON RESIDUAL STRENGTH

Yang and Trapp (1974) described a reliability analysis of aircraft structures under random loading and periodic inspection. They used fracture mechanics theory to estimate crack propagation under random loading. They distinguished two cases depending on whether the structure is redundant or non-redundant. In the non-redundant case the Griffith-Irwin equation (3) may be employed to give residual strength R as a function of crack length a. The relationship (3) holds up to the point where R is equal to the ultimate strength R_0. As a result there is a critical crack size a_c beyond which R starts to decrease following (3). Then integrating (1) with $b = 4$ from a_c to $a(t)$ and using (3) the residual strength function $R(t) = R_0[1 - a_c K S^4 t]^{1/2}$ is obtained.

In order to prevent the crack from propagating to a catastrophic size, it has been a design practice to provide crack stoppers in the structure which will arrest the crack. This practice is called "fail-safe design". If a_s denotes the distance between adjacent fail-safe stoppers, then it is the maximum crack size allowable in the structure, and the minimum residual strength at this crack size can be obtained from (3).

For highly redundant structures, (3) no longer applies to give residual strength as a function of crack length. In this case the residual strength function must be obtained by a combination of analysis and testing. However, in general the residual strength is taken to be monotonically decreasing function of time t or crack size a.

Let $R_0\delta$ be the residual strength at the fail-safe crack size a_s which is determined from analysis and testing. Then a possible form for the residual strength function $R(t)$ at time t after crack initiation is (Yang and Trapp, 1974)

$$R(t) = R_0\{1 - (1 - \gamma)(\frac{a(t) - a_0}{a_s - a_0})^{1/2}\},$$

where $a(t)$, the crack size at time t, is computed from (2).

Eggwertz (1972) employed a residual strength function which decreased linearly with time in an investigation of the fatigue life of wing-panels. No stochastic variation of the residual strength function was taken into account in this investigation.

Hooke (1979) also considered the residual strength function. He pointed out that for some materials strength falls linearly with crack length but that

for a material whose behaviour follows the laws of linear elastic fracture mechanics up to a general yield, there is no decay of strength until a particular crack length and thereafter it decays as the inverse square root of crack length. He used a residual strength decay function of the form

$$R(t) = R_0 k_1 [(\frac{t}{H})^9 - k_2]^{-\frac{1}{2}},$$

where k_1, k_2 are constants and H is a random variable assumed normal with known mean and variance.

Saunders (1976) pointed out that although the residual strength as a function of crack length a is always taken as a known decreasing function of a, the concept of strength degradation will certainly depend on the method of construction and the type of material, as well as the loading spectrum and the environment. He also pointed out that the residual strength function must be obtained from engineering tests of the material and a knowledge of the fracture mechanics particular to the geometry of the component. In general, the residual strength of any component is a concave decreasing function of crack length. However, when composed with crack growth as a function of time, which is convex increasing, the residual strength function can be smoothed out into a variety of shapes.

Whittaker and Saunders (1973), in an investigation of cumulative fatigue damage in an aluminum alloy, had employed a residual strength function (as a function of crack length) of the form

$$R(a) = \delta[V_1 - (V_1 - V_2)(\frac{a}{\sigma})^{\frac{1}{3}}], \quad a > 0. \tag{4}$$

In (4), δ (referred to as a design limit load) and σ, a fail-safe crack length, are determined by ratios V_1, V_2 dictated by design criteria as follows:

$$V_1 = \frac{R(0)}{\delta} > 1, \quad V_2 = \frac{R(\sigma)}{\delta} \leq 1.$$

These are respectively the ratios of ultimate strength $R(0)$ and fail-safe strength $R(\sigma)$ with the limit load. As in the analysis of Yang and Trapp, fracture mechanics could have been applied at this point to obtain crack size $a(t)$ and hence residual strength $R(t)$ as a function of time t. Instead, Saunders (1976) modelled crack growth $a(t)$ as a stochastic process with piecewise linear sample functions, the slopes of the line segments and the times between changes of slope being regarded as random variables.

This brief survey of recent literature indicates that a wide variety of possibilities are available for the residual strength function. In the next section, rather than assume any particular form for $R(t)$ we consider a rather

general model which uses the results of Leadbetter (1966) on crossings of curves by continuous time stochastic processes.

3.1 A Model Based on Curve-Crossings

We assume that the load-process may be modelled as a stationary Gaussian stochastic process $\xi(t)$. The residual strength function $R(t)$ is assumed to be a non-increasing function with initial value $R(0) = R_0$, the initial ultimate static strength of the specimen. It is usual to assume that the material strength remains constant during the crack initiation stage and decreases progressively during the crack propagation stage. A generic form (see Saunders, 1976) of the residual strength function is shown in Figure 1 in which T_i represents time to crack initiation (T_i is in general a random variable).

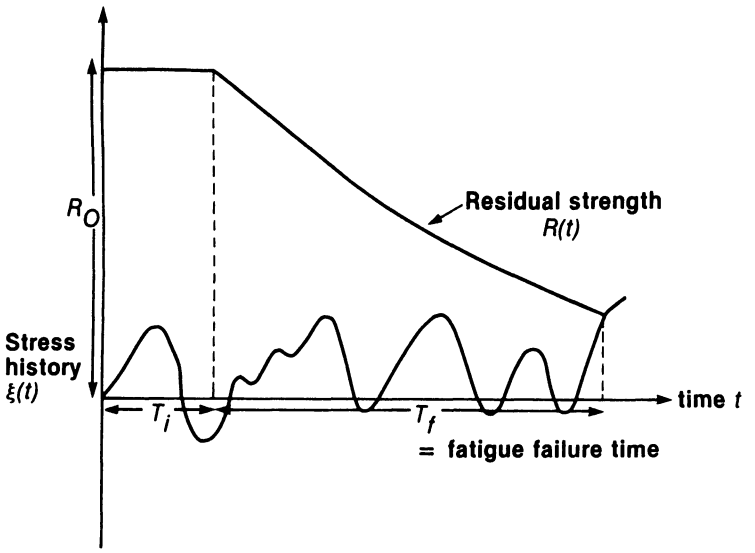

Figure 1. *Generic behaviour of residual strength as a function of time.*

The material strength function $R(t)$ is best regarded as a stochastic process depending on the load history and the material. As such it might be more appropriate to write R as $R(t; \xi(s) : 0 \leq s \leq t)$ to indicate dependence of R on the load history $\xi(t)$. However, since our main purpose in this paper is to illustrate the potential applicability of a hitherto unapplied curve-crossing result we shall for simplicity assume that $R(t) = R_0 h(t - T_i)$, where

$h(t)$ is a known function obtained from engineering testing and fracture mechanics principles. This does not exclude the possibility that $R(t)$ be allowed to depend on various parameters of the loading process, as occurs, for example, in the investigation of Yang and Trapp. This treatment of $R(t)$ as deterministic, while essentially in accord with the approaches adopted in the engineering literature (Section 2), can, however, only be regarded as a first approximation. In the final section we shall discuss one possible stochastic model for $R(t; \xi(s), s \leq t)$, but the mathematical difficulties involved seem formidable.

We also assume $h(\tau)$ is continuously differentiable and monotone with $h(0) = 1$. In addition, we suppose that R_0 is a random variable with p.d.f. $f_{R_0}(r_0)$. The time T_i to crack initiation is a random variable about which little is known. We ignore this phase of the fatigue process and consider only the propagation phase when the residual strength decreases progressively.

The specimen will survive as long as the material strength exceeds the random stress placed on it, i.e., until the condition $\xi(t) \geq R(t)$ is met for the first time. Thus we essentially have a first passage time problem and the probability of survival for service time T (subsequent to crack initiation) is given by the probability of no crossing above the decreasing threshold $R(t) = R_0 h(t - T_i)$ in the interval $(0, T)$.

Thus T_f, the time to fatigue failure (strictly speaking the time spent in the propagation phase), is a random variable with

$$T_f = \min\{\tau \geq 0 : \xi(T_i + \tau) > R_0 h(\tau)\}. \tag{5}$$

The problem of finding the probability of first excursion above a fixed threshold by a stationary Gaussian process has been examined by many authors in the context of random vibrations. It is found that the problem cannot in general be solved without making simplifying assumptions about the nature of the excursions. Based on various assumptions, a variety of approximations to the first passage probability for a fixed threshold have been proposed and compared with numerical results for a single-degree of freedom system excited by white noise (see Yang, 1975). Some of these approximations, particularly those based on an assumption of Poisson upcrossings, have been found useful in the fixed threshold case, which suggests the possibility of applying a non-homogeneous Poisson approximation in the case of a time-dependent threshold. Before applying such an approximation we demonstrate how a useful lower bound for the reliability function may be obtained.

3.2 A Lower Bound for the Reliability Function

The reliability function $F(t)$ is the probability of survival or non-failure due to fatigue in $(0,t)$, i.e., the probability that the fatigue life T_f exceeds t. Thus from (5)

$$\begin{aligned} F(t) &= P(T_f > t) \\ &= P\{\xi^*(\tau) \leq R_0 h(\tau), \quad 0 \leq \tau \leq t\}, \end{aligned}$$

where $\xi*(\tau) = \xi(\tau + T_i)$. Thus $F(t)$ equals the probability that the non-stationary process $\xi^*(t) - R_0 h(t)$ remains negative during the interval $(0,t)$. Since we are assuming R_0 to be a random variable we may use the law of total probability to write

$$F(t) = \int_{R_0} F(t \mid R_0 = r_0) f_{R_0}(r_0) dr_0, \tag{6}$$

where

$$F(t \mid R_0 = r_0) = P\{\max_{0 \leq \tau \leq t} \{\xi^*(\tau) - r_0 h(\tau)\} \leq 0\}.$$

Hence the problem may be regarded either as a zero-crossing problem for the non-stationary process $\xi^*(t) - r_0 h(t)$ or as a curve-crossing problem for the stationary process $\xi^*(t)$. (Assume for simplicity that T_i is independent of the ξ process, so that $\xi^*(t)$ is stationary).

Denote by $U_h(0,t)$ the number of upcrossings of $r_0 h(\tau)$ by $\xi^*(\tau)$ in the interval $(0,t)$. In terms of the corresponding non-stationary point process we may write the reliability function as

$$\begin{aligned} F(t \mid R_0 = r_0) &= P\{\text{no upcrossing of } r_0 h(\tau) \text{ by } \xi(\tau) \text{ in } (0,t)\} \\ &= P\{U_h(0,t) = 0\} \\ &= 1 - \sum_{j=1}^{\infty} P(U_h(0,t) = j), \end{aligned} \tag{7}$$

assuming an upcrossing occurs eventually with probability one.

In general, the probability distribution of $U_h(0,t)$ is very difficult to obtain, but an expression for the mean is more readily derived. Moreover, bounds or estimates of $F(t)$ can be obtained in terms of the factorial moments of $U_h(0,t)$. While we are unaware of any work on higher order factorial moments in the curve-crossing case, Leadbetter (1966) has obtained an expression for the mean number of curve-crossings by a stationary Gaussian process.

Denote by $M_t(r_0, h)$ the mean number of upcrossings in $(0, t)$ i.e. $M_t(r_0, h) = EU_h(0, t)$. Then from (7),

$$F(t \mid R_0 = r_0) \geq 1 - \sum_{j=1}^{\infty} jP(U_h(0, t) = j),$$

while from (6),

$$F(t) \geq 1 - \int_{R_0} M_t(r_0, h) f_{R_0}(r_0) dr_0. \tag{8}$$

In order to make use of this lower bound for design purposes one needs to estimate from data both the density function $f_{R_0}(r_0)$ of the initial strength and the form of the function $h(t)$. A comprehensive discussion of the form of $f_{R_0}(r_0)$ (Freudenthal *et al.*, 1966) has been carried out while various possibilities for $h(t)$ have been described in the previous section. It remains to obtain an expression for $M_t(r_0, h)$, and this we consider in the next section. Before we consider this, however, some remarks on the usefulness of the above lower bound are in order. First, it seems that a considerable amount of data is necessary to estimate the quantities involved. Thus we need extensive data on crack propagation laws and the loading process. Such data are available in the engineering literature for various materials and load processes. Secondly, the question arises as to the sharpness, or otherwise, of the lower bound. Obviously if $E_{R_0} M_t(R_0, h) > 1$ where $E_{R_0} M_t(R_0, h) = \int_{R_0} M_t(r_0, h) f_{R_0}(r_0) dr_0$ then the bound is trivial and of no use whatever. However, in reliability situations one usually designs for a large value of $F(t)$ (i.e., close to 1) or equivalently one hopes for a small value of $E_{R_0} M_t(R_0, h)$. Consequently, in the situations of greatest interest in reliability problems, the case of small $E_{R_0} M_t(R_0, h)$ will be of interest and in such a situation, the lower bound may prove useful.

On the other hand, if one assumes Poisson upcrossings of the residual strength function by $\xi(t)$ one can obtain an expression for the reliability function as

$$\begin{aligned} F(t) &= P\{U_h(0, t) = 0\} \\ &= \exp[-E_{R_0} M_t(R_0, h)]. \end{aligned}$$

In this case $\Lambda(t) = E_{R_0} M_t(R_0, h)$ is the integrated hazard function while the hazard function itself is given as

$$\lambda(t) = \Lambda'(t) = \frac{d}{dt} E_{R_0} M_t(R_0, h).$$

As to the usefulness of the Poisson approximation, Cramer and Leadbetter (1967) and Berman (1970) have given conditions on the covariance

function of $\xi(t)$ which ensure a Poisson limit theorem for high-level crossings of a *fixed* level. While we are unaware of any theoretical work extending these results to the curve-crossing case, a non-homogeneous Poisson limit is intuitively plausible under sufficient smoothness properties of the curve, in view of the fixed level results. A rigorous extension, of the Poisson limit theory to curve-crossings seems worthy of investigation in its own right.

3.3 *Evaluation of* $M_t(r_0, h)$

For crossings of curves by stationary processes one loses the interpretation in terms of stationary streams of events. Also we note that a curve-crossing problem for a stationary process may be regarded as a zero-crossing problem for a non-stationary process. For example, if $\xi(t)$ is a zero-mean stationary process then crossings of the curve $r(t) = r_0 h(t)$ by $\xi^*(t)$ are the same as zero-crossings for the non-stationary process $\xi^{**}(t) = \xi^*(t) - r(t)$. Leadbetter (1966) considered such curve-crossing problems. His argument was essentially an adaptation of Bulinskaya's (1961) argument for the fixed level case.

Leadbetter's results in the Gaussian case is that if $\xi^{**}(t)$ is a non-stationary normal process then the mean number of upcrossings of the zero-level in $0 \leq t \leq 1$ is given by

$$E\{U_0(0,1)\} = \int_0^1 \gamma\sigma^{-1}(1-\mu^2)\phi(\frac{m}{\sigma})[\phi(\eta) + \eta\Phi(\eta)]dt \tag{9}$$

in which (if $\xi^{**}(t)$ has mean $m = m(t)$ and covariance function $r(t,s)$)

$$\sigma^2 = r(t,t), \quad \gamma^2 = \frac{\partial^2 r(t,s)}{\partial t \partial s}\bigg|_{s=t}, \quad \mu = \frac{\partial r(t,s)}{\partial s}\bigg|_{s=t} /(\gamma\sigma)$$

and

$$\eta = (\frac{dm}{dt} - \frac{\gamma\mu m}{\sigma})/\{\gamma(1-\mu^2)^{1/2}\},$$

it being assumed that $\frac{dm}{dt}$ and $\frac{\partial^2 r(t,s)}{\partial t \partial s}$ are continuous functions and that $\sigma > 0$, $|\mu| < 1$ for each t. Here ϕ, Φ are the standard normal p.d.f. and c.d.f. respectively.

In our case, the non-stationary process is of the form $\xi^{**}(t) = \xi^*(t) - r_0 h(t)$ where $\xi^*(t)$ is stationary. In this case, it is easy to see that $\gamma^2 = \lambda_2$, $\mu(t) = 0$, and $\eta(t) = -r_0 h'(t)/\lambda_2^{1/2}$. Hence it follows from (9) (writing $\lambda_2 = \sigma_2^2 = \text{Var } \xi'(t)$) that

$$\begin{aligned} EU_h(0,1) &= M_1(r_0, h) \\ &= \sigma^{-1}\int_0^1 \phi(\frac{r_0 h(t)}{\sigma})[\sigma_2\phi(\frac{r_0 h'(t)}{\sigma_2}) - r_0 h'(t)\Phi(\frac{-r_0 h'(t)}{\sigma_2})]dt. \end{aligned} \tag{10}$$

Moreover, $M_t(r_0, h) = EU_h(0,t)$ is obtained from (10) by simply altering the upper limit of integration in the above to t. Note that in the above it suffices to assume $\lambda_2 < \infty$ where λ_2 is the second spectra moment of the process. This ensures sample function continuity of $\xi(t)$ with probability one and the existence of $\xi'(t)$ in quadratic mean (see Cramer and Leadbetter, 1967).

If one adopts the Poisson upcrossing assumption, the above implies a hazard function of the form

$$\lambda(t) = \sigma^{-1}\phi(\frac{r_0 h(t)}{\sigma})[\sigma_2\phi(\frac{r_0 h'(t)}{\sigma_2}) - r_0 h'(t)\Phi(\frac{-r_0 h'(t)}{\sigma_2})].$$

This hazard function bears no resemblance to those of the distributions commonly employed for analysis of time to failure data. However, in the case where $h'(t) = 0$, corresponding to constant residual strength or no aging with time, one obtains the familiar exponential distribution with parameter

$$\begin{aligned}\lambda &= \sigma^{-1}\phi(\frac{r_0}{\sigma}) \cdot \frac{\sigma_2}{\sqrt{2\pi}} \\ &= \frac{\sigma_2}{2\pi\sigma}\exp[-\frac{1}{2}(r_0/\sigma)^2],\end{aligned}$$

which is the formula of Rice (1945) for the mean upcrossing rate of the level r_0 by $\xi(t)$.

In the foregoing, we have conditioned on the value of r_0. The next step would be to assume some parametric form for $f_{R_0}(r_0)$ and to take expectations as in Subsection 3.2.

Application of (10) and (8) to the specific forms for $h(t)$ discussed in Section 2 will generally involve numerical integration. For example, in the case considered by Eggwertz (1972) a linear reduction of residual strength with time is assumed. This corresponds to letting $h(t) = 1 + kt$ with $k < 0$ whence the following expression for $\lambda(t)$ ensues:

$$\lambda(t) = \sigma^{-1}[\sigma_2\phi(\frac{kr_0}{\sigma_2})] - r_0 k\Phi(\frac{-r_0 k}{\sigma_2})]\phi(\frac{r_0(1+kt)}{\sigma}).$$

4. A STOCHASTIC REPRESENTATION OF THE RESIDUAL STRENGTH FUNCTION

The formulation of $R(t)$ adopted in the previous section was essentially deterministic, although T_i = time to crack initiation and $R_0 = R(0)$, the initial static strength, were assumed to be random variables. Thus, conditional on T_i, $R(t)$ was a random variable for every t with the same distribution as R_0, up to the scaling function $h(t)$. A more accurate model would allow $R(t)$ to be a stochastic process, depending in some way on the stress history $\{\xi(s) : 0 \leq s \leq t\}$. Thus we would write $R(t) = R(t; \xi(s), 0 \leq s \leq t)$ to indicate this dependence. A limited dependence of $R(t)$ on the load history, via mean values of peak stress amplitudes is allowed in the model of Section 3. For example, the residual strength function of Yang and Trapp incorporates load history information via the mean value of the bth power of the peak amplitude distribution. However, this approach does not allow for stochastic variation of this quantity about its mean value. To obtain a stochastic representation for $R(t)$ suppose without loss of generality $b = 2$ in (1) as do Yang and Heer (1971). Then integrating (1) successively with respect to each cycle and summing yields

$$\ln a(n) - \ln a(0) = K \sum_{j=1}^{n} S_j^b, \tag{11}$$

where S_j is the amplitude of the jth stress peak. The stochastic analogue of (11) is

$$\ln a(t) - \ln a(0) = K \sum_{j=1}^{M(t)} [\xi(t_j)]^b, \tag{12}$$

where $M(t)$ is the number of stress peaks in $(0, t)$ and t_j is the time of occurrence of the jth stress peak in $(0, t)$. Using equation (3), we may rewrite (12) as

$$R(t) = R_0 \exp(-\frac{K}{2} \sum_{j=1}^{M(t)} [\xi(t_j)]^b), \tag{13}$$

where (13) is conditional on the event $\{R(t_{j-1}) > \xi(t_j), j = 1, \ldots, M(t)\}$, since otherwise fatigue failure would have occurred before t. The stochastic representation (13) is represented schematically in Figure 2. $R(t)$ is a jump process decreasing by a factor $\exp(-\frac{K}{2}\xi(t_j)^b)$ at the jth stress peak. More

explicitly, (13) can be written

$$R(t) = \begin{cases} R_0, & 0 < t < t_1 \\ R_0 \exp(-\frac{K}{2}\xi(t_1)^b), & t_1 < t < t_2 \\ R_0 \exp(-\frac{K}{2}(\xi(t_1)^b + \xi(t_2)^b), & t_2 < t < t_3 \\ \vdots & \\ R_0 \exp(-\frac{K}{2}\sum_{j=1}^{n}(\xi(t_j)), & t_n < t < t_{n+1}. \end{cases} \tag{14}$$

The fatigue failure time $T_f = \min\{t : R(t) \leq \xi(t)\}$ is the first crossing time of the two stochastic processes $R(t; \xi(s), 0 \leq s \leq t)$, given by (14), and $\xi(t)$. The residual strength representation (14) incorporates the effect of the load history via $\xi(t_j)$, $j = 1, 2 \ldots$, and $M(t)$.

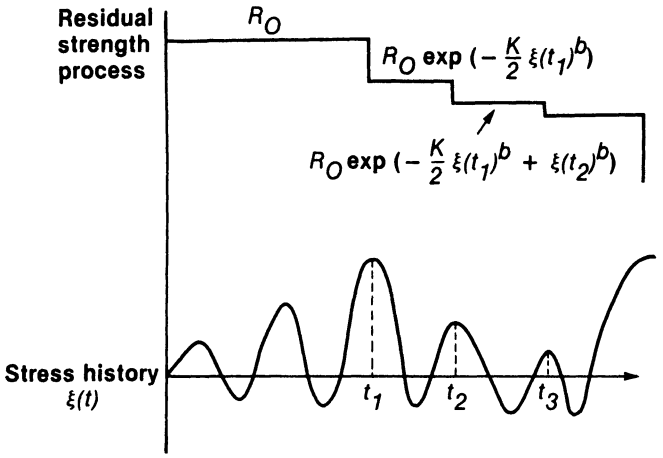

Figure 2. *Stochastic representation of residual strength.*

REFERENCES

Barnby, J. T. (1972), *Fatigue*. London: Mills and Boon.

Berman, S. M. (1971), "Asymptotic independence of the numbers of high and low level crossings of stationary Gaussian processes." *Annals of Mathematical Statistics* **42**, 927–945.

Bulinskaya, E. V. (1961), "On the mean number of crossings of a level by a stationary Gaussian process." *Teoriya Veroyatnostei iee primeneniya* **6**, 474–477.

Cramer, H., and M. R. Leadbetter (1967), *Stationary and Related Stochastic Processes*. New York: Wiley and Sons.

Desmond, A. F. (1983), "Local maxima of stationary stochastic processes and stochastic modelling of fatigue." Ph.D. thesis, University of Waterloo.

Eggwertz, S. (1972), "Investigation of fatigue life and residual strength of wing panel for reliability purposes." In *Probabilistic Aspects of Fatigue* ASTM STP 511, ed. R. A. Heller, pp. 75–105.

Freudenthal, A. M., J. M. Garrelts, and M. Shinozuka (1966), "The analysis of structural safety." *Structural Division Journal, Proceedings of the American Society of Civil Engineers* **92**, 267–325.

Hooke, F. H. (1979), "A new look at structural reliability and risk theory." *American Institute of Aeronautics and Astronautics Journal* **17**, 980–987.

Leadbetter, M. R. (1966), "On crossings of levels and curves by a wide class of stochastic processes." *Annals of Mathematical Statistics* **37**, 260–267.

Paris, P. C. (1964), "The fracture mechanics approach to fatigue". In *Fatigue — an Interdisciplinary Approach, Proceedings of the 10th Sagamore Army Materials Research Conference.* Syracuse, NY: Syracuse University Press.

Rice, S. O. (1976), "Mathematical analysis of random noise." *Bell System Technical Journal* **24**, 46–156.

Saunders, S. C. (1976), "The reliability of structures subject to fatigue under inspection and repair." In *Applications of Statistics*, ed. P. R. Krishnaiah, pp. 481–496.

Whittaker, I. C., and S. C. Saunders (1973), "Exploratory development on application of reliability analysis to aircraft structures considering interaction of cumulative fatigue damage and ultimate strength." Air Force Materials Laboratory Technical Report AFML-TR-72-283.

Yang, J.-N. (1975), "Approximation to first passage probability." *Journal of the Engineering Mechanics Division* **10**. *Proceedings of the American Society of Civil Engineers* **101**, 361–372.

Yang, J.-N., and E. Heer (1971), "Reliability of randomly excited structures." *American Institute of Aeronautics and Astronautics Journal* **9**, 1262–1268.

Yang, J.-N., and W. J. Trapp (1974), "Reliability analysis of aircraft structures under random loading and periodic inspection." *American Institute of Aeronautics and Astronautics Journal* **12**, 1623–1630.

P. Todorovic [1]

LIMIT THEOREMS ARISING IN SOIL EROSION MODELLING

ABSTRACT

It was shown in a recent paper that the effect of soil erosion on crop production can be described by a stochastic process $\{X_n\}_1^\infty$, where $X_n = Y_n \cdot L_n$. Here $\{Y_n\}_1^\infty$ is an independent and identically distributed sequence of non-negative random variables and $\{L_n\}_1^\infty$ is a Markov chain, with stationary transition probabilities, independent of $\{Y_n\}_1^\infty$. In this paper we are concerned with the limiting distributions of the maximum term $\chi_n = \sup_{1 \le k \le n} X_k$ and of the sum $S_n = X_1 + \ldots + X_n$.

1. INTRODUCTION

This paper is concerned with some limit theorems arising in the development of a mathematical model to assess the effect of surface soil erosion on crop production. The erosion process is a result of perpetual activities of various geophysical forces acting upon the surface of earth. The ensuing degradation of farm lands may have a profound impact on the global scale on future food supply. For this reason the Soil and Water Conservation Act requires the United States Department of Agriculture to prepare a report for the U.S. Congress that establishes the current status of soil and water resources in the U.S.A. The impact of surface soil erosion on long-term soil productivity is of particular interest. As was shown in a recent paper (Todorovic and Gani, 1985), under certain conditions this impact can be described by a stochastic process $\{X_n\}_1^\infty$. Asymptotic behavior of certain functionals of this process is the subject of our investigation.

[1] Department of Statistics, University of Kentucky, Lexington, Kentucky 40506

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 65–73.

2. FORMULATION OF THE PROBLEM

The stochastic process $\{X_n\}_1^\infty$ is a sequence of non-negative random variables (r.v.'s) defined as follows: for every $n = 1, 2, \ldots$

$$X_n = Y_n \cdot L_n, \tag{2.1}$$

where

$$L_n = \prod_1^n Z_i. \tag{2.2}$$

Here we assume that the r.v.'s involved satisfy the following conditions:

(i) $\{Y_n\}_1^\infty$ is an i.i.d. sequence of non-negative r.v.'s with common distribution function (d.f.) and probability density (p.d.)

$$Q(y) = P\{Y \leq y\}, \qquad q(y) = \frac{d\,Q(y)}{dy}, \tag{2.3}$$

respectively, with

$$\mu = E\{Y\} < \infty. \tag{2.4}$$

(ii) $\{Z_i\}_1^\infty$ is also an i.i.d. sequence of r.v.'s, independent of $\{Y_n\}_1^\infty$, such that

$$0 \leq Z \leq 1 \quad \text{and} \quad 0 < \alpha = E\{Z\} < 1. \tag{2.5}$$

Note that the r.v.'s $\{X_n\}_1^\infty$ are neither independent nor identically distributed. However, the sequence possesses a monotonicity property (Van Doorn, 1980). In other words, for every $x \geq 0$

$$F_n(x) \geq F_{n+1}(x), \qquad n = 1, 2, \ldots,$$

where $F_n(x) = P\{X_n \leq x\}$.

Denote

$$S_n = \sum_{k=1}^n X_k, \qquad \chi_n = \sup_{1 \leq k \leq n} (X_k), \qquad n = 1, 2, \ldots \tag{2.6}$$

This paper is concerned with distributional convergence of the sequence of partial sums $\{S_n\}_1^\infty$ and of the extreme terms $\{\chi_n\}_1^\infty$. Before we embark on the problem of determining the limiting distributions of S_n and χ_n one should note the following: from (i) and (ii) we have that

$$0 \leq S_1 \leq S_2 \leq \cdots$$

On the other hand, since

$$\sum_{k=1}^{\infty} E\{X_n\} = \alpha\mu(1-\alpha)^{-1},$$

the monotone convergence theorem implies that

$$S_n \uparrow S \text{ almost everywhere (a.e.) as } n \to \infty,$$

where S is an (a.e.) finite-valued r.v. such that

$$E\{S\} = \alpha\mu(1-\alpha)^{-1}.$$

3. LIMITING DISTRIBUTION OF $\{\chi_n\}_1^\infty$.

Many attempts have been made in recent years to extend asymptotic results of classical extreme value theory to include first, discrete parameter and then continuous parameter strictly stationary stochastic processes (Watson, 1954; Berman, 1964; Loynes, 1965; Leadbetter, 1974). A comprehensive account of the existing classical as well as "post classical" results of the theory is given in a recent monograph by Leadbetter *et al.* (1983).

In this section we shall derive the d.f. of χ_n. In addition, we shall specify its limiting form as $n \to \infty$, under the condition that $\{Z_i\}_1^\infty$ is an i.i.d. sequence of r.v.'s with common uniform distribution on $[0,1]$. To this end denote

$$M_n(x) = P\{\chi_n \leq x\}. \tag{3.1}$$

It is clear that $\chi_n \uparrow \chi$ (a.e.), where χ is an (a.e.) finite-valued r.v. Hence,

$$\lim_{n\to\infty} M_n(x) = M(x), \tag{3.2}$$

where $M(x) = P\{\chi \leq x\}$. As we will show, this convergence is uniform. We shall first prove the following result.

Proposition 3.1. Let $\{Z_n\}_1^\infty$ by an i.i.d. sequence of r.v.'s with common uniform distribution on $[0,1]$, then for all $n = 1,2,\ldots$ and $x \geq 0$,

$$M_n(x) = \frac{1}{n!}\int_0^1 \left\{\int_t^1 \frac{1}{s} Q(x/s)ds\right\}^n dt. \tag{3.3}$$

Proof. From a relation (Todorovic and Gani, 1985, p. 6), it follows at once that

$$M_n(x) = E\left\{\prod_1^n Q\left(xL_i^{-1}\right)\right\}$$
$$= \int_{0\le t_n\le} \cdots \int_{\cdots \le t_1\le 1} \phi_{1,\ldots,m}(t_1,\ldots,t_n)\prod_1^n Q(x/t_i)dt_i,$$

where $\phi_{1,\ldots,m}(t_1,\ldots,t_n)$ is the joint probability density of $(L_1,\ldots,L_n)$. Since Z has uniform distribution in $[0,1]$ we have that

$$\phi_{1,\ldots,m}(t_1,\ldots,t_n) = \prod_1^{n-1} 1/t_i. \tag{3.4}$$

Thus,

$$M_n(x) = \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} \left\{\prod_1^{n-1} \frac{1}{t_i} Q(x,t_i)dt_i\right\} Q(x/t_n)dt_n$$
$$= \frac{1}{(n-1)!}\int_0^1 \left\{\int_t^1 \frac{1}{s}Q(x/s)ds\right\}^{n-1} Q(x/t)dt$$

(see Fichtengoltz, 1959, p. 682). On the other hand,

$$\int_0^1 \left\{\int_t^1 \frac{1}{s}Q(x/s)ds\right\}^{n-1} Q(x/t)dt = \frac{1}{n}\int_0^1 t\, d\left\{\int_t^1 \frac{1}{s}Q(x/s)dx\right\}^n$$
$$= \frac{1}{n}\int_0^1 \left\{\int_t^1 \frac{1}{s}Q(x/s)ds\right\}^n dt, \tag{3.5}$$

which proves the proposition.

To find the limiting value of (3.3) when $n \to \infty$ we need the following.

Proposition 3.2. The d.f. $M_n(x)$ satisfies the following difference-differential equation:

$$M_n'(x) = \frac{1}{x}\{M_n(x) - Q(x)M_{n-1}(x)\}. \tag{3.6}$$

Proof. Differentiating both sides of equation (3.3) with respect to x we obtain

$$M_n'(x) = \frac{1}{(n-1)!}\int_0^1 \left\{\int_t^1 \frac{1}{s}Q(x/s)ds\right\}^{n-1}\left(\int_t^1 \frac{1}{s^2}q(x/s)ds\right)dt.$$

By means of the substitution $v = x/s$, after a simple transformation, the last equation can be written as

$$M_n'(x) = \frac{1}{(n-1)!}\int_0^1 \left\{\int_t^1 \frac{1}{s}Q(x/s)ds\right\}^{n-1} \frac{1}{x}\left(\int_x^{x/t} q(v)dv\right) dt$$
$$= \frac{x^{-1}}{(n-1)!}\int_0^1 \left\{\int_t^1 \frac{1}{s}Q(x/s)ds\right\}^{n-1} [Q(x/t) - Q(x)]\, dt.$$

From this and (3.5), after some straightforward calculations, the assertion follows.

The limiting d.f. $M(x)$ is now easy to obtain.

Proposition 3.3. For every $x \geq 0$,

$$M(x) = \exp\left\{-\int_x^\infty \frac{1}{u}[1 - Q(u)]du\right\}. \tag{3.7}$$

Proof. First of all, note that $\{M_n(x)\}_1$ is a sequence of monotonic functions whose limit $M(x)$ exists and represents a d.f. Now, write equation (3.6) as follows:

$$M_n(x) = \int_0^x \frac{1}{z}\{M_n(z) - Q(x)M_{n-1}(z)\}\, dz.$$

From this and the Beppo-Levi theorem we have:

$$M(x) = \int_0^x \frac{1}{z}[1 - Q(z)]\, M(z)dz.$$

Hence,

$$M'(x) = \frac{1}{x}[1 - Q(z)]M(x). \tag{3.8}$$

The general solution of this equation is

$$M(x) = M(a)\exp\left\{\int_a^x \frac{1}{u}[1 - Q(u)]du\right\}. \tag{3.9}$$

Now, since $M(x)$ is a proper d.f. (of the finite valued r.v. χ) $M(x) \to 1$ as $x \to \infty$. From this and (3.9) it follows that

$$M(a) = \exp\left\{-\int_a^\infty \frac{1}{u}[1 - Q(u)]du\right\}.$$

This completes the proof of the proposition.

4. SOME AUXILIARY RESULTS

Denote by

$$G_n(x) = P\{S_n \leq x\}, \qquad G(x) = P\{S \leq x\}, \tag{4.1}$$

the d.f. of S_n and S respectively. Before embarking on the problem of determining the limiting d.f. $G(x)$ some auxiliary results are needed.

Write

$$\Psi(\theta) = E\left\{e^{-\theta Y}\right\}, \qquad L_n^*(\theta) = E\left\{e^{-\theta S_n}\right\}. \tag{4.2}$$

The next lemma gives L_n^* in terms of Ψ.

Lemma 4.1. Suppose that conditions (i) and (ii) hold, then for every $n = 1, 2, \ldots$

$$L_n^*(\theta) = E\left\{\prod_1^n \Psi(\theta L_i)\right\}. \tag{4.3}$$

Proof. From (4.2) it follows that

$$\begin{aligned} L_n^*(\theta) &= \int E\left\{e^{-\theta S_n} \mid L_1, \ldots, L_n\right\} dP \\ &= \int_{0 \leq t_n \leq} \cdots \int_{\cdots \leq t_1 \leq 1} \phi_{1,\ldots,n}(t_1, \ldots, t_n) \prod_1^n \Psi(\theta t_i) dt_i, \end{aligned}$$

where as before $\phi_{1,\ldots,n}(.,\ldots,.)$ stands for the probability density of $(L_1, \ldots, L_n)$. This proves (4.3).

Lemma 4.2. Suppose now that (3.4) holds, then under the same conditions as in the previous lemma we have

$$L_n^*(\theta) = \frac{1}{n!} \int_0^1 \left\{\int_t^1 \frac{1}{s} \Psi(\theta S) ds\right\}^n dt. \tag{4.4}$$

Proof. From (4.3) and the conditions of the lemma it follows at once that

$$\begin{aligned} L_n^*(\theta) &= \int_{0 \leq t_n \leq} \cdots \int_{\cdots \leq t_1 \leq 1} \left\{\prod_1^{n-1} \frac{1}{t_i} \Psi(\theta t_i) dt_i\right\} \Psi(\theta t_n) dt_n \\ &= \frac{1}{(n-1)!} \int_0^1 \left\{\int_t^1 \frac{1}{s} \Psi(\theta s) ds\right\}^{n-1} \Psi(\theta t) dt. \end{aligned} \tag{4.5}$$

Now, since

$$\left\{\int_t^1 \frac{1}{s}\Psi(\theta s)ds\right\}^{n-1} \Psi(\theta t) = -\frac{t}{n}\frac{d}{dt}\left\{\int_t^1 \frac{1}{s}\Psi(s)ds\right\}^n,$$

integration by parts of (4.5) proves the assertion.

5. EVALUATION OF $G(x)$.

We are now in a position to determine the limiting d.f. $G(x)$. To this end note that integral (4.4) is essentially equivalent to that of (3.3). To obtain the limiting value of (4.4) we should apply the same procedure that has been used to prove Proposition 3.1. We obtain

$$\lim_{n\to\infty} L_n^*(\theta) = \exp\left\{-\int_0^\theta \frac{1}{u}[1-\Psi(u)]du\right\}. \tag{5.1}$$

Note that this convergence is uniform.

The right hand side of (5.1) is the Laplace transform of $G'(x) = g(x)$. To obtain $g(x)$, which is our ultimate goal in this section, we must invert the right hand side of (5.1). The standard procedure leads to some cumbersome calculations. To avoid this we shall adopt a different approach. The following proposition is the main result of this section.

Proposition 5.1. The probability density $g(x)$ is a solution of the following non-linear Volterra integro-differential equation:

$$x\,g'(x) + \int_0^x q(x-s)g(s)ds = 0. \tag{5.2}$$

Proof. Differentiating the left and right hand side of equation (4.4), we obtain, after some straightforward calculations, the difference-differential equation

$$\theta L_n^{*'}(\theta) + L_n^*(\theta) = \Psi(\theta)L_{n-1}^*(\theta). \tag{5.3}$$

From the fact that the family of d.f.'s $\{G_n(x)\}_1^\infty$ is sequentially compact and from the Helly-Bray theorem, it follows that the limits

$$L^*(\theta) = \lim_{n\to\infty} L_n^*(\theta) \quad \text{and} \quad L^{*'}(\theta) = \lim_{n\to\infty} L_n^{*'}(\theta) \tag{5.4}$$

exist. Hence, letting $n \to \infty$ in (5.3) we obtain

$$\theta L^{*'}(\theta) + L^*(\theta) = \Psi(\theta)L^*(\theta), \tag{5.5}$$

which can be written as follows:

$$L^{*'}(\theta) + \frac{1}{\theta} L^*(\theta) = \frac{1}{\theta} \Psi(\theta) L^*(\theta).$$

Taking the inverse of the Laplace transform of both sides of the last equation we obtain

$$-xg(x) + G(x) = \int_0^x q(t) \ * \ g(t)dt,$$

where $*$ stands for convolution. Finally, differentiating the left and right hand sides of this equation we obtain (5.2).

Remark 5.1. It is clear from equation (5.2) that the limiting d.f. $G(x)$ depends on $Q(x)$. In addition it follows from the same equation that the p.d. $g(x)$ must be a decreasing function on $[0, \infty)$.

Example 5.1. If $q(x) = \lambda e^{-\lambda x}$ it follows immediately from equation (5.2) that

$$g(x) = \lambda e^{-\lambda x}.$$

Example 5.2. Let $q(x) = \lambda^2 x \ e^{-\lambda x}$; to obtain the limiting d.f. $G(x)$ in this case we will use the Laplace transform

$$L^*(\theta) = \exp\left\{ - \int_0^\infty \frac{1}{u} [1 - \Psi(u)] du \right\} \tag{5.6}$$

rather than the equation (5.2). First of all note that (see equation (4.2))

$$\Psi(\theta) = \left(\frac{\lambda}{\theta + \lambda} \right)^2.$$

Hence,

$$\int_0^\theta \frac{1}{u} [1 - \Psi(u)] du = \ln(\theta + \lambda) - \frac{\lambda}{\theta + \lambda} - \ln \lambda + 1.$$

From this we have:

$$L^*(\theta) = e^{-1} \frac{\lambda}{(\theta + \lambda)} \exp\left\{ \frac{\lambda}{\theta + \lambda} \right\} = e^{-1} \sum_{n=0}^\infty \frac{1}{n!} \left(\frac{\lambda}{\theta + \lambda} \right)^{n+1}.$$

Therefore,

$$\begin{aligned} g(x) &= e^{-(1+\lambda x)} \sum_{n=0}^\infty \frac{(\lambda x)^n}{(n!)^2} \\ &= e^{-(1+\lambda x)} \sum_{n=0}^\infty \left(\frac{2(\lambda x)^{1/2}}{2} \right)^{2n} \frac{1}{(n!)^2} \end{aligned}$$

or

$$g(x) = e^{-(1+\lambda x)} I_o\left(2(\lambda x)^{1/2}\right),$$

where $I_o(u)$ is the modified Bessel's function of the first kind and order zero.

ACKNOWLEDGMENT

The research leading to this work was fully supported by the Office of Naval Research, Grant No. N00014-84-K-0568. It is a pleasure to acknowledge this support.

REFERENCES

Berman, S. M. (1964), "Limit theorems for the maximum term in stationary sequences". *Annals of Mathematical Statistics* **35**, 502–516.

Chung, K. L. (1974), *A Course in Probability Theory*, 2nd edition. New York: Academic Press.

Fichtengoltz, G. M. (1959), *Course on the Differential and Integral Calculus*, Volume 2. Fiz.-Math.-Giz, Moscow (in Russian).

Leadbetter, M. R. (1974), "On extreme values in stationary sequences". *Zeitschrift fur Wahrscheinlichkeitstheorie und Verwandte Gebiete* **28**, 289–303.

Leadbetter, M. R., G. Lindgren, and H. Rootzen (1983), *Extremes and Related Properties of Random Sequences and Processes*. New York: Springer-Verlag.

Loynes, R. M. (1965), "Extreme values in uniformly mixing stationary stochastic processes". *Annals of Mathematical Statistics* **36**, 993–999.

Todorovic, P., and J. Gani (1985), "Modeling the effect of erosion on crop production". University of Kentucky, Department of Statistics Technical Report No. 232, February 1985.

Van Doorn, E. A. (1980), "Stochastic monotonicity of birth-death process". *Advances in Applied Probability* **12**, 59–80.

Watson, G. S. (1954), "Extreme values in samples from m-dependent stationary stochastic processes". *Annals of Mathematical Statistics* **25**, 798–800.

David R. Brillinger [1]

FITTING COSINES: SOME PROCEDURES AND SOME PHYSICAL EXAMPLES

ABSTRACT

The paper is concerned with a variety of time series models that in some sense lead to the fitting of a cosine function of unknown frequency. Both linear and nonlinear models are considered, including both decaying cosines and sustained ones. The discussion is illustrated with examples from seismology (free oscillations of the Earth), geophysics (the Chandler wobble), nuclear magnetic resonance, laser Doppler velocimetry and oceanography (dispersion). The paper ends by surveying a variety of results developed for specific models by various authors. A variety of open problems are indicated.

"The aim of science is to seek the simplest explanation of complex facts ... seek simplicity and distrust it."

A. N. Whitehead

1. INTRODUCTION

There are a broad variety of natural phenomena that are periodic and that have been studied since early times. Some of these, and their researchers, are: the planets (Kepler), pendulums (Galileo), the violin string (Mersenne), light (Huyghens), sound (Newton) and crystals (Kepler, Huyghens). Cosines were fit numerically to orbital data as early as 1754 (see Clairaut, 1754; Heideman *et al.*, 1984). Several arguments may be set down for the genesis of cosines. Linear combinations of cosines provide the general solution of differential equations with constant coefficients—and such equations provide effective descriptions of many phenomena. Cosines and more general periodic functions result from the repeated application of various operators. The input to a system may be periodic, and in consequence

[1] Department of Statistics, University of California, Berkeley, California 94720

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 75–100.

the output is as well. Finally, the experimental setup may be such that periodically varying data is collected.

A key property of cosines is that they persist under linear time invariant operations. This is formalized in Lemma 2.7.1 of Brillinger (1975), but may be illustrated quickly as follows. Suppose

$$Y(t) = \sum_{u=-\infty}^{\infty} a(u)X(t-u). \tag{1}$$

The operation carrying $X(\cdot)$ into $Y(\cdot)$ is linear and time invariant. If $X(t) = \exp\{i\lambda t\}$, then $Y(t) = A(\lambda)\exp\{i\lambda t\}$, with

$$A(\lambda) = \sum_{u} a(u)\exp\{-i\lambda u\}. \tag{2}$$

Here, following de Moivre's formula, $\exp\{i\lambda t\} = \cos\lambda t + i\sin\lambda t$ and because of the linearity of the operation (1), the effect of the operation on the cosine function $\cos\lambda t$ may be seen. In the case that λ is real-valued it is referred to as the *frequency* (in radians per unit time). Because many naturally occurring operations are, to a good approximation, linear and time invariant, the nonentanglement of cosine waves of different frequencies can allow one to look back to the generation process of a phenomenon of interest.

Fourier transforms play essential roles in the study of periodic phenomena and of linear time invariant systems. Definition (2) shows the *transfer function*, $A(\cdot)$, to be the Fourier transform of the *impulse response*, $a(\cdot)$. For the model

$$Y(t) = \rho\cos(\gamma t + \delta) + \varepsilon(t), \tag{3}$$

$t = 0, \pm 1, \pm 2, \ldots$ with $\varepsilon(\cdot)$ a noise process, the least squares estimate of $\rho\exp\{i\delta\}$ is approximately

$$\frac{2}{T}\sum_{t=0}^{T-1} Y(t)\exp\{-i\gamma t\} \tag{4}$$

when γ is known and the data $Y(t)$, $t = 0, \ldots, T-1$ are available. The values

$$\sum_{t=0}^{T-1} Y(t)\exp\{-i2\pi st/T\}, \tag{5}$$

$s = 0, \ldots, T-1$, are referred to as the *discrete Fourier transform* of the data stretch $Y(t)$, $t = 0, \ldots, T-1$. In a variety of circumstances these values may be computed exceedingly rapidly via a fast Fourier transform (FFT)

algorithm (Heideman *et al.*, 1984). Astonishingly, such an algorithm was known to Gauss in 1805, *ibid.*

This paper is a mixture of review of existing results, physical examples, models and methods relating to the fitting of cosines to both linear and nonlinear phenomena. The main sections are: Decaying Cosines, Noise Sustained Oscillations, Dispersion and Modes, a Review of Some Particular Results and Some Open Problems.

2. DECAYING COSINES

2.1 Some Conceptualization

Vibratory motion pervades and unifies the physical sciences. A mathematical conceptualization that is consistent with this observation is that a great variety of natural systems may be described by systems of equations of the form

$$\frac{d\mathbf{Y}(t)}{dt} = \mathbf{A}\mathbf{Y}(t) + \mathbf{X}(t) \tag{6}$$

with $\mathbf{X}(\cdot)$ vector-valued input and with $\mathbf{Y}(\cdot)$ vector-valued output or perhaps a state vector. In the case that the input is $\mathbf{b}\delta(t)$, $\delta(\cdot)$ the Dirac delta, and initial conditions are $\mathbf{Y}(0-) = \mathbf{0}$, then the general solution of (6) may be written

$$\begin{aligned} \mathbf{Y}(t) &= \exp\{\mathbf{A}t\}\mathbf{b} \qquad t > 0 \\ &= \sum_j \alpha_j \exp\{\mu_j t\}\mathbf{u}_j, \end{aligned} \tag{7}$$

where μ_j, $\mathbf{u}_j$ are the (assumed distinct) latents of the matrix $\mathbf{A}$. Focussing on any one of the coordinates of $\mathbf{Y}(\cdot)$ then, its motion has the form

$$\sum_{k=1}^{K} \rho_k \exp\{-\sigma_k t\} \cos(\gamma_k t + \delta_k) \tag{8}$$

for $t > 0$, with $-\sigma_k$ and γ_k the real and imaginary parts of one of the μ_j. This has the empirical implication that one is sometimes led to model time series data as the sum of the term (8) and a noise process.

2.2 Free Oscillations of the Earth

After a great earthquake, the whole Earth may oscillate for many days; see, for example, Bolt (1982, Chapter 6). From these oscillations, or free vibrations, the seismologist infers much about the structure of the Earth.

The equations of motion may be written in the form of (6) for the many particles making up the Earth. A great earthquake may be viewed as providing a delta function type input. In consequence a corresponding seismic record may be viewed as having the form

$$Y(t) = \sum_{k=1}^{K} \rho_k \exp\{-\sigma_k t\} \cos(\gamma_k t + \delta_k) + \varepsilon(t), \tag{9}$$

$\varepsilon(\cdot)$ being a noise process. (It is worth noting that K may be greater than 1500 for some events.) The seismologist is particularly interested in estimating the γ_k and σ_k for he is then able to compare these observed values with corresponding values for an Earth model that he has constructed. A traditional procedure for estimating the γ_k in a model such as (9) is to look for the locations of peaks in the periodogram. Specifically, let

$$d_Y^T(\lambda) = \sum_{t=0}^{T-1} Y(t) \exp\{-i\lambda t\} \tag{10}$$

denote the Fourier transform of a stretch of data, then the periodogram is defined as

$$I_{YY}^T(\lambda) = (2\pi T)^{-1} \mid d_Y^T(\lambda) \mid^2 . \tag{11}$$

It may be expected to show peaks in the neighborhood of the γ_k of (9) with their respective heights depending on the values of the other parameters appearing.

Figure 1 is a record of the Great Chilean earthquake of 22 May 1960 as recorded at Trieste. The tides have been removed from the original displacements measured. Many oscillations are present and it is apparent that these decay. Figure 2 is a graph of the log periodogram, (11), for one frequency interval. It was based on 2548 points with a sampling interval of 2 minutes (hence a longer time period than that shown in Figure 1). Many peaks are apparent. To gain some idea of the reality of these peaks, it may be noted that in the case of stationary noise the distribution of the periodogram is approximately exponential with mean the power spectrum. Using this approximation, one computes that the width of a 95% confidence interval, for the values of Figure 2, is 4.98. The level of fluctuations in Figure 2 is generally greater than this.

2.3 Complex Demodulation

One particularly effective method for assessing the validity of the model (9) and for obtaining initial estimates of the parameters appearing is *complex demodulation*; see, for example, Brillinger (1975, Section 2.7). The basic

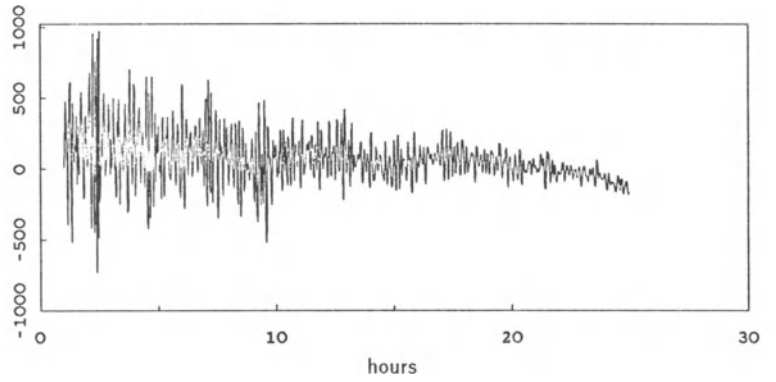

Figure 1. *The Great Chilean Earthquake — Tides Removed*

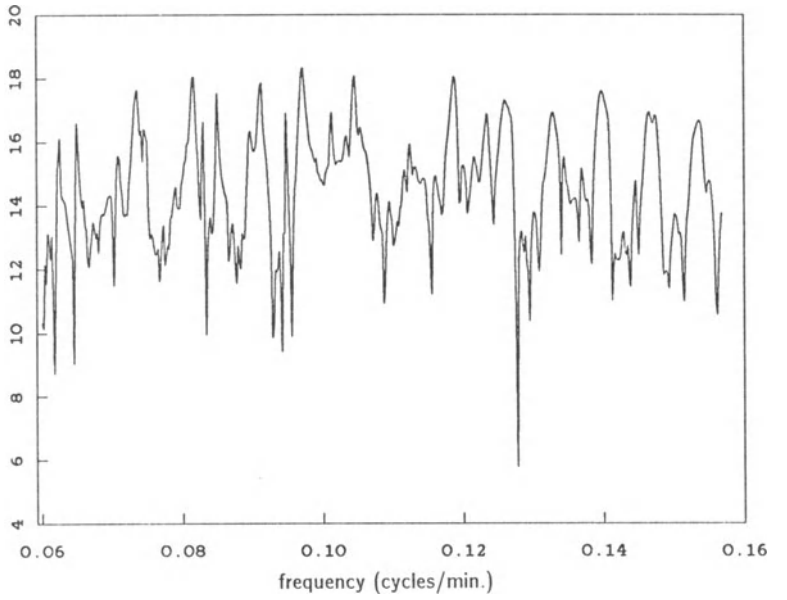

Figure 2. *Log Periodogram — Chilean Earthquake*

ideas are: frequency isolation by narrow band filtering to focus on a single term in (9), followed by frequency translation to slow the oscillations down. The steps are: (i) $Y(t) \rightarrow Y(t)\exp\{i\lambda t\}$, (modulation), then (ii) smooth $Y(t)\exp\{i\lambda t\}$ to obtain $Y(t,\lambda)$, the complex demodulate at frequency λ. In the case that $Y(t) = \rho\ \exp\{-\sigma t\}\cos(\gamma t + \delta)$ one has

$$\begin{aligned} Y(t,\lambda) &\doteq \frac{1}{2}\rho e^{i\delta}e^{-\sigma t}e^{i(\lambda-\gamma)t}, \quad \lambda \text{ near } \gamma \\ &\doteq 0, \qquad\qquad\qquad \text{otherwise.} \end{aligned} \tag{12}$$

Hence $\log \mid Y(t,\lambda) \mid \doteq \log \frac{\rho}{2} - \sigma t$ and $\arg\{Y(t,\lambda)\} \doteq \delta + (\lambda - \gamma)t$. Plots of these quantities versus t provide checks on model adequacy and yield estimates of the parameters appearing. In the case that λ is near γ the phase plot will be approximately horizontal. Figures 3 and 4 provide plots at the frequency .0945 cycles/min. (corresponding to one of the peaks in Figure 2). The results are consistent with an exponentially decaying cosine component. Various other plots for this data set are presented by Bolt and Brillinger (1979).

2.4 Estimation Via Nonlinear Regression

Estimates of parameters are insufficient without accompanying estimates of uncertainty. Fourier inference may be employed to address this problem. Suppose one has a model

$$Y(t) = S(t;\theta) + \varepsilon(t) \tag{13}$$

with $S(\cdot;\theta)$ known up to the finite dimensional parameter θ and with $\varepsilon(\cdot)$ a stationary noise series. Let

$$Y_j = \sum_{t=0}^{T-1} Y(t)\exp\{-i2\pi jt/T\} \tag{14}$$

with similar definitions for $S_j(\theta)$ and ε_j. These are various central limit theorems, (see, for example, Brillinger, 1983), suggesting that the distribution of ε_j may be approximated by a complex normal with mean 0 and variance $2\pi T\ f_{\varepsilon\varepsilon}(2\pi j/T)$ and that ε_j, $\varepsilon_{j'}$, $j \neq j'$ are approximately independent. Here $f_{\varepsilon\varepsilon}(\lambda)$ is the *power spectrum* at frequency λ of the stationary series $\varepsilon(\cdot)$,

$$f_{\varepsilon\varepsilon}(\lambda) = (2\pi)^{-1} \sum_{u=-\infty}^{\infty} \operatorname{cov}\{\varepsilon(t+u), \varepsilon(t)\}\exp\{-i\lambda u\}. \tag{15}$$

Supposing $f_{\varepsilon\varepsilon}(\lambda)$ not to vary too much for λ in a neighborhood I, θ may be estimated by setting down a Gaussian likelihood and maximizing it. This comes down to minimizing

$$\sum_{I} | Y_j - S_j(\theta) |^2, \tag{16}$$

where the summation is over frequencies $2\pi j/T$ in I. For the case of $S(t;\theta) = \rho \exp\{-\sigma t\} \cos(\gamma t + \delta)$, $\theta = (\rho, \sigma, \gamma, \delta)$ one finds for example that the asymptotic variance of the estimate of γ is proportional to $T^{-3}\rho^{-2}4\pi f_{\varepsilon\varepsilon}(\gamma)$. Bolt and Brillinger (1979) and Hasan (1982) give details. For example, for the Chilean data and the frequency of Figures 3 and 4 one finds, converting frequency to period, an estimated period of 10.5681 min. with an estimated standard error of .0014 min. Again, Bolt and Brillinger (1979) give details.

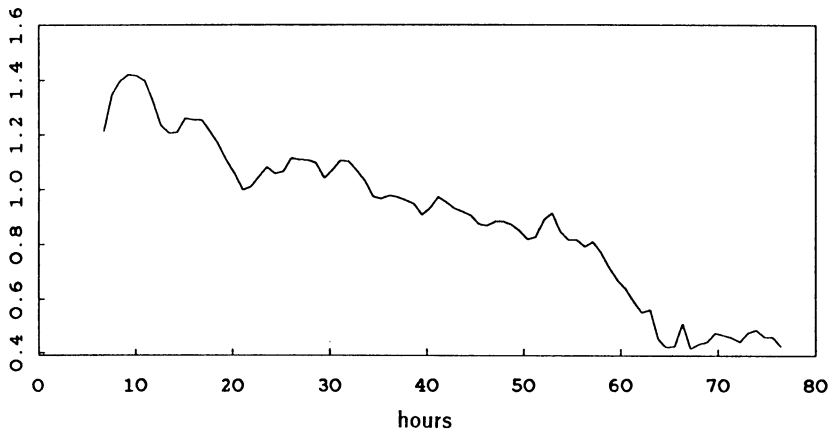

Figure 3. *Log Amplitude at .0945 cycles/min.*

2.5 Estimation of Bifrequency

Suppose that the system of equations (6) is perturbed by replacing the matrix $\mathbf{A}$ by $\mathbf{A} + \varepsilon\langle \mathbf{B}, \mathbf{Y}(t)\rangle$, with ε small and $\langle \mathbf{B}, \mathbf{Y}\rangle$ representing a matrix of the same dimensions as $\mathbf{A}$, linear in $\mathbf{Y}$. The solution of the perturbed, now *nonlinear*, system contains terms in $\exp\{\mu_j t\}$ as at (7), but it also contains interation terms $\exp\{(\mu_k + \mu_\ell)t\}$. A simple form of solution suggested is

$$Y(t) = \sum_{m=1}^{3} \rho_m \cos(\gamma_m t + \delta_m) + \varepsilon(t), \tag{17}$$

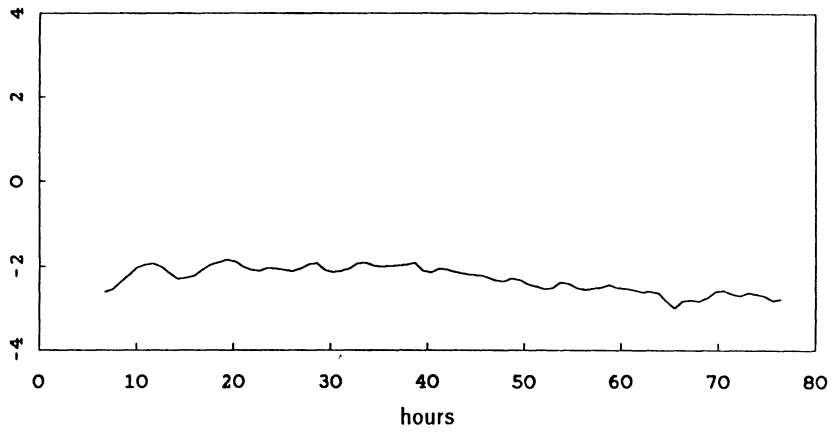

Figure 4. *Phase at .0945 cycles/min.*

where the γ_m are related by $\gamma_1 + \gamma_2 + \gamma_3 = 0$. A triple of frequencies $(\gamma_1, \gamma_2, \gamma_3)$ summing to 0 is referred to as a *bifrequency*; see Brillinger (1980). The *biperiodogram* is a statistic of use in detecting the presence of bifrequencies. It is a direct extension of the (second-order) periodogram (11) and is given by

$$I^T_{YYY}(\lambda_1, \lambda_2) = (2\pi)^{-2} T^{-1} d^T_Y(\lambda_1) d^T_Y(\lambda_2) \overline{d^T_Y(\lambda_1 + \lambda_2)}. \tag{18}$$

Its modulus may be expected to be large when the frequencies $\lambda_1, \lambda_2, \lambda_1 + \lambda_2$ are simultaneously present in the series $Y(\cdot)$.

Zadro and Caputo (1968) develop differential equations for the motion of the Earth in a great earthquake when nonlinearities are present. This work suggests that bifrequencies will be present in that case. Zadro and Caputo (1968) present the results of bispectral computations for the case of the great Alaskan earthquake of 1964. Various suggestive peaks are present in the biperiodogram.

Figure 5 is a contour plot of the modulus of the quantity (18) for the Chilean data and the frequency interval (.08, .12) cycles/min. Peaks are seen to occur both on and off the diagonal $\lambda_1 = \lambda_2$. The largest peak occurs at (.09714, .10459) cycles/min. If one scans Table 1 of Bolt and Currie (1975) one sees that one may have evidence for the interaction of the torsional vibration modes ${}_0T_{10}$, ${}_0T_{11}$ and ${}_0T_{25}$. The results of Brillinger (1980) and further computations may be employed to assess the uncertainties of these values.

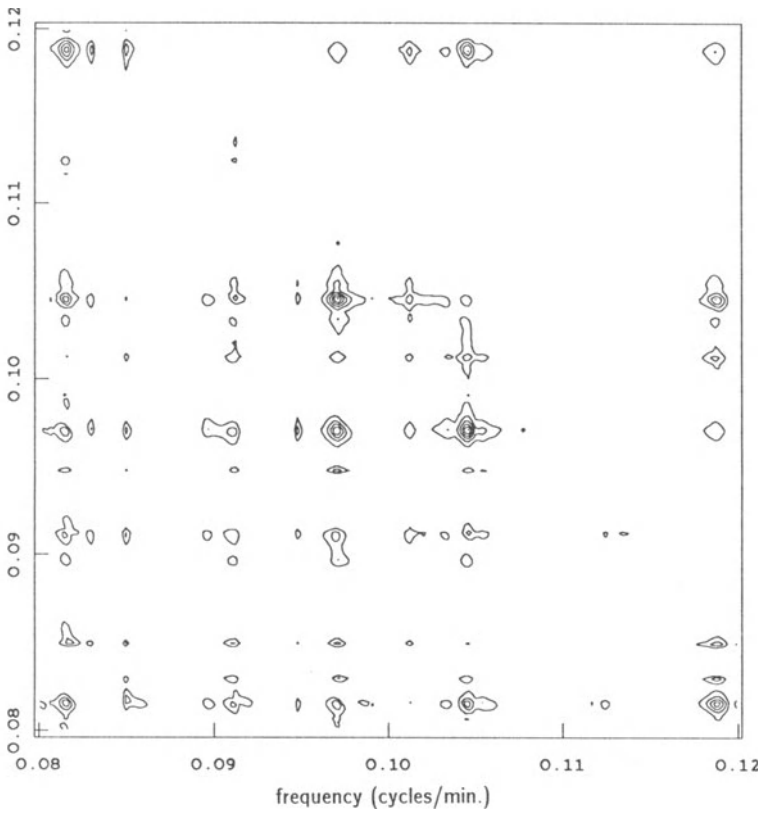

Figure 5. *Modulus Biperiodogram*

3. NOISE SUSTAINED OSCILLATIONS

3.1 Conceptual Background

Consider the case of incoherent light. A model for this situation is the following: electrons of pertinent atoms jump levels. Light of frequency $\gamma = E/h$ is released where E is the change in energy and h is Planck's constant. The time course of the light signal is $a(t) = H(t)e^{-\sigma t}\cos\gamma t$, where $H(t) = 0$ for $t < 0$ and $H(t) = 1$ for $t > 0$. When many atoms are involved the light wave has the form $\sum_j a(t - \tau_j)$, the τ_j being the points of a Poisson process. One is led to consider a process that is a random sum of decaying cosine

waves, all waves having the same frequency γ. The power spectrum of this process has poles at $\lambda = \pm\gamma \pm i\sigma$. It will show peaks for λ near γ.

An analagous result obtains for the system (6) when the input process $\mathbf{X}(\cdot)$ is white noise. Suppose $\mathbf{X}(\cdot)$ is white noise with covariance matrix Σ. Then the spectral density matrix of the process $\mathbf{Y}(\cdot)$ is given by

$$\frac{1}{2\pi}(\mathbf{A} - i\lambda\mathbf{I})^{-1}\,\Sigma\,(\mathbf{A} + i\lambda\mathbf{I})^{-1}. \tag{19}$$

Poles occur for $\lambda = \pm i\mu_j$, the μ_j being the latent values of $\mathbf{A}$. The solution of (6) may be written

$$\begin{aligned}\mathbf{Y}(t) &= \int_0^\infty \exp\{\mathbf{A}u\}\mathbf{X}(t-u)du \\ &= \sum_j \mathbf{v}_j^r \int_0^\infty \exp\{\mu_j u\}\mathbf{X}(t-u)du\ \mathbf{u}_j\end{aligned} \tag{20}$$

(where $\mathbf{u}_j, \mathbf{v}_j$ are the left and right latent vectors of $\mathbf{A}$) and one sees that the process $\mathbf{Y}(\cdot)$ is a random sum of decaying cosine wave frequencies corresponding to the imaginary parts of the latent values of $\mathbf{A}$. Our concern now turns to the estimation of those frequencies. We will proceed via a particular example.

3.2 The Chandler Wobble

The point of intersection of the Earth's axis of rotation with the north polar cap does not remain fixed, rather it wanders about and the Earth is said to "wobble". Figures 6 and 7 give the two coordinates $(X(t), Y(t))$ of the pole for the period 1900–1975. It is convenient to set $Z(t) = X(t) + iY(t)$; then the equations of motion (see Munk and MacDonald, 1960) are

$$\frac{dZ(t)}{dt} = aZ(t) + \frac{d\Phi(t)}{dt} \tag{21}$$

with $\Phi(t)$ corresponding to the excitation process. Supposing the process $\Phi(\cdot)$ to have stationary increments, the power spectrum of the process $Z(\cdot)$ is given by

$$\frac{1}{(\lambda-\gamma)^2 + \sigma^2} f_{\Phi\Phi}(\lambda), \tag{22}$$

writing $a = i\gamma - \sigma$. The periodogram of the data of Figures 6, 7 is given in Figure 8. It shows peaks near frequencies 0, .071 and .083 cycles/year. The first corresponds to trend; see Figure 7. The third corresponds to an annual component present in the excitation process. The second corresponds to the

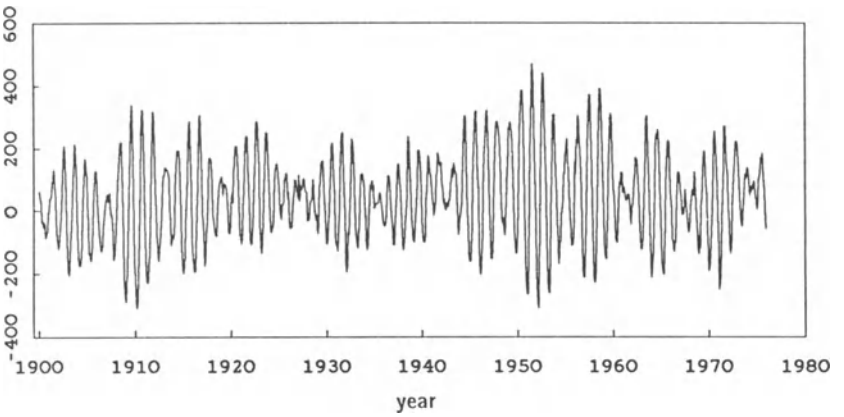

Figure 6. *X-Coordinate Polar Motion*

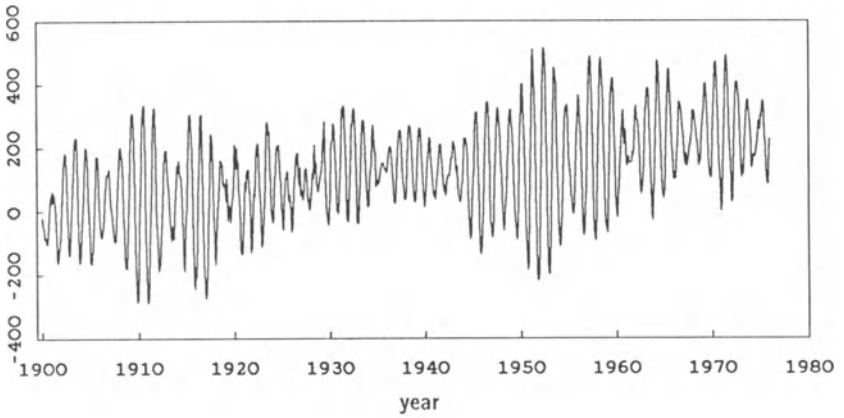

Figure 7. *Y-Coordinate Polar Motion*

Chandler wobble, that is γ of (22). It is of interest to estimate the Chandler period precisely and to provide a measure of uncertainty.

A corresponding finite parameter model is developed by Brillinger (1973). Specifically for seasonally adjusted first differences and measurement error assumed present, the parametric spectrum derived is

$$\frac{\sigma^2}{2\pi}\frac{1-e^{-2\sigma}}{2\sigma}\frac{1}{1-2\exp\{-\sigma\}\cos(\lambda-\gamma)+\exp\{-2\sigma\}}+\frac{\psi^2\mid 1-e^{-i\lambda}\mid^2}{2\pi}. \quad (23)$$

This is then fit (to the data for 1902–1969) by the method of Gaussian

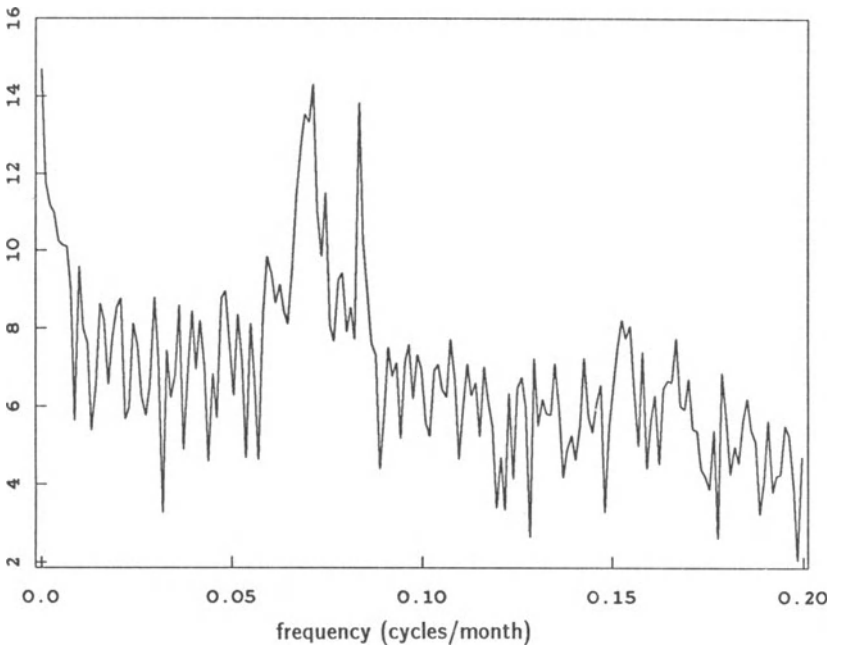

Figure 8. *Log Periodogram—Polar Motion frequency (cycles/month)*

estimation, that is by maximizing the "Gaussian" likelihood

$$\prod_j \frac{1}{f_j} \exp\left\{-I_j^T/f_j\right\}, \tag{24}$$

where I_j^T denotes the periodogram at frequency $2\pi j/T$ and $f_j = f\left(\frac{2\pi j}{T}; \theta\right)$ denotes the theoretical power spectrum as a function of the unknown parameters. This method also leads to estimated standard errors. In particular the value $\hat{\gamma} = .0706$ with an estimated standard error of .0026 was found.

Further examination of the periodogram of Figure 8 shows some power near the frequency .15. It was examined further with a suspicion that it might be due to some nonlinearity. Figures 9, 10 provide the results of complex demodulating the series at a frequency of .153 cycles/year. It was found that the power was predominantly present only for the early part of the series. We have no explanation to present beyond remarking that the individuals responsible for estimating the polar motion changed every so often. The biperiodogram is presented by Brillinger (1973), but it is not strongly suggestive of a nonlinearity.

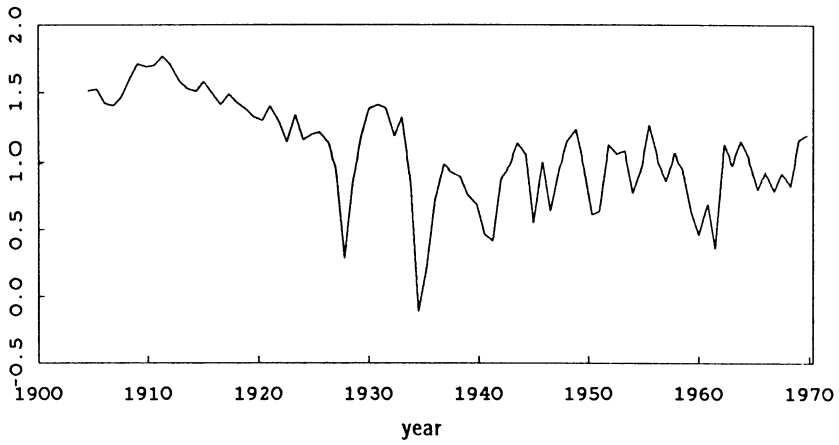

Figure 9. *Log Amplitude at .153 cycles/year*

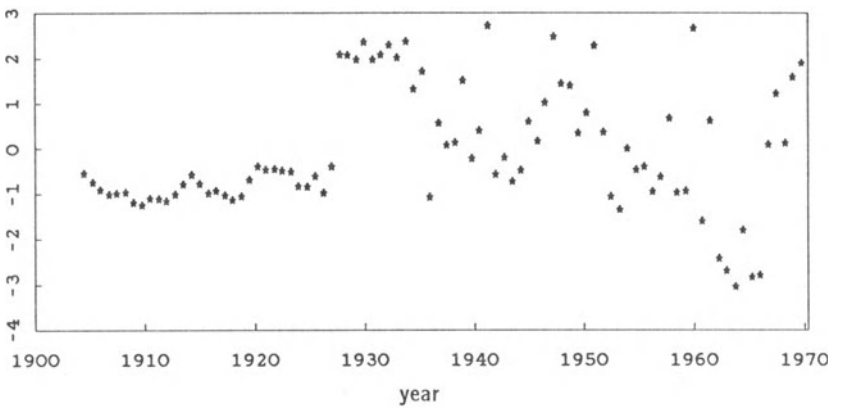

Figure 10. *Phase at .153 cycles/year*

3.3 Nuclear Magnetic Resonance

3.3.1 The Bloch Equations. Nuclear magnetic resonance relies on the interaction between magnetically sensitive nuclei which are exposed to both a strong magnetic field and a radio frequency signal. The nuclei "flip" at characteristic (or resonant) frequencies. The procedures yields information related to molecular structure, interactions and dynamics.

The phenomenon has been described by the Bloch equations. These take

the form

$$\frac{d\mathbf{Y}(t)}{dt} = \mathbf{a} + \mathbf{A}\ \mathbf{Y}(t) + \mathbf{B}\ \mathbf{Y}(t)X(t) \tag{25}$$

with $X(t)$ scalar input, with $\mathbf{Y}(t)$ vector output, with $\mathbf{a}$ a vector and with $\mathbf{A}$, $\mathbf{B}$ matrices. See, for example, Knight and Kaiser (1982).

Various inputs have been employed to identify molecular systems by nuclear magnetic resonance. These include pulses, cosinusoids and noise. The impulse response has been written

$$\sum_k \rho_k \exp\{-\sigma_k t\} \cos \gamma_k t \tag{26}$$

with the γ_k the characteristic frequencies of the substance of concern. One common procedure is to apply a pulse and to look for peaks in the absolute value (periodogram) of the Fourier transform of the output. Peaks are assigned to particular atoms in the molecules present.

3.3.2 Stochastic Nuclear Magnetic Resonance. In stochastic NMR the input, $X(\cdot)$, is taken to be random noise and the particular realization is made use of in the analysis. Blumich (1985) provides a review. In the case that the input is Gaussian white noise, $\mathrm{cov}\{\mathbf{Y}(t+u), X(t)\}$ is found to be given by

$$\sum_k \rho_k \exp\{-\sigma_k u\} \exp\{i\gamma_k u\} \tag{27}$$

for $u > 0$ with the $i\gamma_k - \sigma_k$ the latent values of $\mathbf{A} + \mathbf{B}^2/2$. The Fourier transform of (27) is

$$\sum_k \rho_k \frac{1}{\sigma_k - i(\lambda - \gamma_k)}. \tag{28}$$

The amplitude of this quantity peaks at λ near γ_k, and sample-based quantities may be used to derive estimates. Examples are given by Ernst (1970).

In many important cases second-order spectra are not sufficient to describe structure unequivocally; higher-order spectra are needed. Because of symmetries present, third-order spectra vanish identically. The fourth-order spectrum, which is the Fourier transform of

$$E\{\mathbf{Y}(t)X(t+u_1)X(t+u_2)X(t+u_3)\},$$

has peaks when the frequencies γ_j, γ_k, γ_ℓ, and $\gamma_j+\gamma_k+\gamma_\ell$ are simultaneously present. Examples of sections of such empirical spectra are given by Blumich and Ziessow (1983). The use of such spectra is found to lead to nearly complete assignment of protons to molecules in many substances of concern.

3.4 Particle Processes

Consider a circumstance in which at time t there are $N(t)$ particles situated in space at the locations $\mathbf{r}_j(t), j = 1, \ldots, N(t)$. If $\mathbf{r}$ denotes position in space, then this particle process may be represented by

$$\sum_{j=1}^{N(t)} \delta(\mathbf{r} - \mathbf{r}_j(t)). \tag{29}$$

The motion of the jth particle may be described via $\mathbf{r}_j(t)$. For example if the particle is moving with a constant (directed) velocity then $\mathbf{r}_j(t) - \mathbf{r}_j(0) = \mathbf{v}t$. If the particles motion is Brownian, then $\mathbf{r}_j(t)$ is a spatial Brownian motion with independent Gaussian increments.

With the advent of lasers, the motion of collections of particles may be studied by analysing light scattered when the particles are illuminated by a laser. Briefly through the Doppler effect the frequency of the incident light is shifted slightly by a particle's motion and a study of the frequency distribution of the scattered light gives information on the velocity distribution of the particles.

3.4.1 Laser Doppler Velocimetry. The characteristic property of monochromatic laser light is that it fluctuates very nearly as a cosine wave. Suppose that the incident light comes from a direction $\mathbf{k}_I$ and has a frequency ω. Then the input to the particle system may be represented as

$$X(t) = \exp\{i(\mathbf{k}_I \cdot \mathbf{r} + \omega t)\}. \tag{30}$$

Further the (far-field) scattered output in a direction $\mathbf{k}_S$ may be represented as $Y(t) = S_{\mathbf{k}}(t)X(t)$ where $\mathbf{K} = \mathbf{k}_S - \mathbf{k}_I$, and $s_{\mathbf{K}}(t)$, the complex scattering amplitude, is given by

$$s_{\mathbf{K}}(t) = \sum_j a_j(t) \exp\{-i\mathbf{K} \cdot \mathbf{r}_j(t)\}. \tag{31}$$

Here $X(t), Y(t)$ represent the incident and scattered optical fields and $a_j(t)$ is referred to as the form factor. Supposing that the particles are independent and identical and that the $a_j(\cdot)$ are independent of the $\mathbf{r}_j(\cdot)$, one sees that the autocovariance function of the process $Y(\cdot)$ is given by

$$\begin{aligned} m_{YY}(u) &= E\{s_{\mathbf{K}}(t+u)\overline{s_{\mathbf{K}}(t)}\} \\ &\doteq E\left\{\exp\{-i\mathbf{K} \cdot (\mathbf{r}(t+u) - \mathbf{r}(t))\}\right\}. \end{aligned} \tag{32}$$

This is essentially the characteristic function of the increments of the motion of the particle process. Supposing one has constant (laminar) flow,

then $m_{YY}(u) \doteq \exp\{-i\mathbf{K}\cdot\mathbf{v}u\}$. Supposing Brownian motion, $m_{YY}(u) \doteq \exp\{-DK^2u\}$ with D the diffusion constant and $K = |\mathbf{K}|$. Other models for the motion of the particles, e.g. mixtures of particles with different velocities or different diffusion constants, lead to other functional forms for $m_{YY}(\cdot)$. The problem now is to estimate $m_{YY}(u)$ in practice.

The nature of the situation is that the electric field, $Y(\cdot)$, cannot be observed directly. What can be observed are Poisson processes with rate the modulus-squared of an electric field. In one experimental setup a Poisson process with rate $I(t) = |Y(t)|^2 = |s_K(t)|^2$ is observed. The number of particles, N, is assumed large so that $S_{\mathbf{K}}(t)$ of (31) is approximately Gaussian. From Isserlis's formula then

$$m_{II}(u) = |m_{YY}(0)|^2 + |m_{YY}(u)|^2 \tag{33}$$

and from an estimate of $m_{II}(u)$, an estimate of $|m_{YY}(u)|^2$ may be constructed. This procedure may be employed successfully for particles moving with Brownian motion (see, for example, Nishio *et al.*, 1983); however, in the case of laminar flow $m_{YY}(u) \doteq \exp\{-i\mathbf{K}\cdot\mathbf{v}u\}$, whose modulus contains no information on $\mathbf{K}$. The experimental setup has to be altered.

In Doppler-difference velocimetry, the frequency ω of the input beam is shifted slightly to $\omega+\delta$ giving a second input $X'(t)$ coming from a different direction and the far-field intensity is then

$$I(t) = |s_{\mathbf{K}}(t)X(t) + s_{\mathbf{K}'}(t)X'(t)|^2 . \tag{34}$$

Expanding this shows

$$I(t) \sim \exp\{i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{v}t\}\exp\{-\delta t\} + \ldots \tag{35}$$

in the case of laminar flow and the problem has again become one of estimating the frequency of a cosine. This procedure is used by Pfister *et al.* (1983) and Sato *et al.* (1978), for example. An important advantage of this experimental technique is that rapidly varying velocities may be tracked and even subjected to Fourier analyses themselves (see Pfister *et al.*, 1983).

Cummins (1977) and Shulz-DuBois (1983) are general references to the technique and uses of laser velocimetry.

3.4.2 Discussion. It is worth remarking that the interference procedure used is intimately connected to the technique of complex demodulation described earlier in the paper. By superposing the $X'(t)$ signal one is essentially bringing about multiplication by $\exp\{i(\omega+\delta)t\}$ allowing, as in the case of complex demodulation, attention to be focused on components of frequency near ω.

In the case that the intensity $I(t)$ is low, one will need to take account of sampling fluctuations.

3.4.3 Bispectral Analysis. In an interesting piece of work Sato *et al.* (1978) combine laser Doppler velocimetry with bispectral analysis to obtain information concerning particles in suspension. Their approach has the advantage of "eliminating" Gaussian noise.

The experimental set-up involved vibrating particles (in one case cigar smoke, in another water) by a known sound wave

$$X(t) = A_1 \sin(\omega_0 t + \Phi_1) + A_2 \sin(2\omega_0 t + \Phi_2) \tag{36}$$

and then measuring the particle motion by a laser Doppler velocimeter. The measured signal takes the form

$$Y(t) = a_1 \sin(\omega_0 t + \phi_1) + a_2 \sin(2\omega_0 t + \phi_2) + \varepsilon(t) \tag{37}$$

with the a_i functions of A_1, A_2, particle diameter, relative density of particle material, viscosity of the medium and other things. The series $\varepsilon(\cdot)$ represents noise.

The power spectrum of $Y(\cdot)$ is given by

$$\frac{1}{4\pi}\left(a_1^2\delta(\lambda - \omega_0) + a_2^2\delta(\lambda - 2\omega_0)\right) + f_{\varepsilon\varepsilon}(\lambda) \tag{38}$$

and it should be noted that the noise spectrum appears. Supposing the noise to be Gaussian, in contrast the amplitude of the bispectrum is

$$\frac{1}{32\pi^2} a_1^2 \mid a_2 \mid \delta(\lambda_1 - \omega_0)\delta(\lambda_2 - \omega_0) \tag{39}$$

and the noise component is absent. The value $a_1^2 \mid a_2 \mid$ may be estimated from the bispectral estimate and used in turn to estimate particle parameters. Sato *et al.* (1978) present experimental results demonstrating that this bispectrum based estimate can be much more sensitive than a power spectrum based one.

4. DISPERSION AND MODES

Consider the linear-temporal process

$$Y(x,t) = \rho \cos(\alpha x + \gamma t + \delta). \tag{40}$$

It satisfies the wave equation

$$\frac{\partial^2 Y}{\partial t^2} = c^2 \frac{\partial^2 Y}{\partial x^2} \tag{41}$$

with $c = \gamma/\alpha$, the phase velocity. In the case that there are side conditions, following Sturm-Liouville theory, discreteness occurs. Given frequency γ only a certain number of wavenumbers $\alpha = \alpha_n(\gamma)$, $n = 0, 1, \ldots$ are possible. An implication of this is that for a composite wave different frequency components will travel at different speeds, or disperse. Such a relation between frequency and wavenumber is referred to as a dispersion relation.

From a statistical viewpoint the following problem arises. Given data on $Y(x,t)$ and imagining it to be a superposition of terms of the form (40) satisfying a dispersion relation, how is that relation to be estimated? It is instructive to consider the (two-dimensional) Fourier transform.

One has

$$\int\int \exp\{i(\alpha(\gamma)x + \gamma t)\} \exp\{-i(kx + \lambda t)\}\, dx\, dt$$
$$= \delta(\lambda - \gamma)\delta(k - \alpha(\gamma)). \tag{42}$$

Mass is seen to occur on the curve $k = \alpha(\lambda)$. In the case of a composite process, mass may be expected to occur on a family of curves $k = \alpha_n(\lambda)$.

4.2 Examples

The fields of oceanography, seismology and helioseismology provide empirical examples of the use of Fourier transforms to discern dispersion relations. Gilbert and Dziewonski (1975) provide analyses for the free oscillations of the earth based on seismograms from two deep earthquakes. Munk and MacDonald (1964) analysed sea level fluctuations as measured by a linear array of gauges off the coast of southern California. Estimating a wavenumber-frequency power spectrum, they found most of the energy to be trapped in a few narrow bands in (k, λ) space, corresponding to edge waves. (These are water waves moving sideways to the shore, rather than rolling on to it.)

The most dramatic developments have however been taking place in the field of helioseismology, that is the branch of solar physics concerned with the study of resonant oscillations of the Sun. The motion of the visible portion of the Sun's surface is measured via spectrographs attached to conventional solar telescopes. Velocity of movement is determined through the Doppler effect. The wavenumber-frequency power spectrum is then estimated from the data. The cover of the 6 September 1985 issue of *Science* provides a striking example of such an estimate. References to this work include Deubner and Gough (1984) and Christensen-Dalsgaard *et al.* (1985).

4.3 Discussion

Given a model (e.g., velocity as a function of depth) for the medium of interest, implied dispersion curves may be computed (see, for example, Section

7.2.2 of Aki and Richards, 1980). The empirically determined wavenumber-frequency power spectrum may then be employed to assess the degree of fit of the postulated model. Further one may set up an inverse problem and proceed to improve the model.

The excitement with which researchers view helioseismology is well illustrated by the following remarks of Deubner *et al.* (1975): "... the basic mechanism responsible for the solar 5-minute oscillation is now understood,..." and "... the solutions in Ulrich agree with the observed ridges in all detail to an embarassing extent."

5. A REVIEW OF SOME PARTICULAR RESULTS

In this section the crude details of a variety of results, concerning the fitting of cosine type signals superposed on stationary mixing noise, are presented.

5.1 Whittle (1952)

The model considered is

$$Y(t) = \alpha \cos(\gamma t + \delta) + \varepsilon(t), \tag{43}$$

$t = 0, \ldots, T-1$. The difficult parameter to estimate is γ. It may be estimated either by ordinary least squares or more commonly by maximizing the periodogram

$$|\sum_{t=0}^{T-1} Y(t) e^{-i\lambda t}|^2. \tag{44}$$

The estimate $\hat{\gamma}$ is found to be asymptotically normal with mean γ and variance

$$\frac{48\pi}{T^3\alpha^2} f_{\varepsilon\varepsilon}(\gamma). \tag{45}$$

That the variance falls off as T^{-3} was initially surprising. Hannan (1971, 1973) and Walker (1971, 1973) are related papers.

5.2 Bolt and Brillinger (1979)

This work was referred to earlier in the paper. The model considered is

$$Y(t) = \alpha e^{-\phi t/T} \cos(\gamma t + \delta) + \varepsilon(t), \tag{46}$$

$t = 0, \ldots, T-1$. The parameters are estimated from the (Gaussian) likelihood of the Fourier transform values in the neighborhood of γ. The estimates

$\hat{\gamma}$ and $\hat{\phi}/T$ are found to be asymptotically normal with variance

$$\frac{4\pi}{T^3\alpha^2} f_{\epsilon\epsilon}(\gamma) \int_0^1 e^{-2\phi u} du \Big/ \left[\int_0^1 e^{-2\phi u} du \int_0^1 u^2 e^{-2\phi u} du - \left\{ \int_0^1 u e^{-2\phi u} du \right\}^2 \right]. \quad (47)$$

The parametrization of the decay rate in the form ϕ/T is in order to insure that the signal does not drop out asymptotically. It seems a plausible manner in which to develop asymptotic results.

5.3 Hinich and Shaman (1972)

The work of these researchers is concerned with an areal-temporal process. The model is

$$Y(x,y,t) = \rho \cos(\alpha x + \beta y + \gamma t + \delta) + \varepsilon(x,y,t) \quad (48)$$

for x, y, t taking on values in a latice. Ordinary least squares, maximum likelihood and periodogram maximizing estimates are considered.

5.4 Vere-Jones (1982)

He was concerned with fitting a cyclic model to point process data. A point process $\{\tau_j\}$ is assumed to be Poisson with rate $A \exp\{\alpha \cos(\gamma t + \delta)\}$. The asymptotic distributions of the maximum likelihood estimate and a periodogram maximizing estimate are developed. The asymptotic distribution of $\hat{\gamma}$ is found to be normal with mean γ and variance $12/\left[T^3 A\, \alpha I_1(\alpha)\right]$. Here $I_1(\alpha)$ is a modified Bessel function.

5.5 Isokawa (1983)

This author is concerned with sampled time series data, $Y(\tau_j)$, where the τ_j are the points of a realization of a stationary point process independent of the series $Y(t)$ given by (43). The asymptotic distribution of the estimate of λ maximizing the periodogram

$$\left| \sum_j Y(\tau_j) \exp\{-i\lambda\tau_j\} \right|^2 \quad (49)$$

is determined.

5.6 Hannan (1974)

In this paper Hannan presents results for the model

$$Y(t) = \sum_k \alpha_k \cos(k\gamma t + \delta_k) + \varepsilon(t), \tag{50}$$

$t = 0, \ldots, T-1$. The import of this model is that the expected value has period $2\pi/\gamma$. The asymptotic distribution of the λ maximizing

$$\sum_k \left| d_y^T(k\lambda) \right|^2 / f_{\varepsilon\varepsilon}(k\lambda) \tag{51}$$

is derived. It is found to be normal with mean and variance

$$\left[T^3 \sum_k \frac{\alpha_k^2}{48\pi f_{\varepsilon\varepsilon}(k\gamma)} \right]^{-1} \tag{52}$$

In practice an estimate of $f_{\varepsilon\varepsilon}(\cdot)$ would be inserted in (51).

5.7 Brillinger (1980)

This work was referred to earlier. The model is

$$Y(t) = \sum_{k=1}^{3} \alpha_k \cos(\gamma_k t + \delta_k) + \varepsilon(t) \tag{53}$$

with $\gamma_3 = \gamma_1 + \gamma_2$ or $\gamma_3 = 2\pi - \gamma_1 - \gamma_2$, $0 < \gamma_k < \pi$. This is the model of bifrequencies. The asymptotic distributions of both the ordinary least squares estimate and the estimate (λ_1, λ_2) maximizing the biperiodogram

$$d_Y^T(\lambda_1) d_Y^T(\lambda_2) \overline{d_Y^T(\lambda_1 + \lambda_2)} \tag{54}$$

are determined. Both these asymptotic distributions are found to be normal, but generally different.

5.8 Subba Rao and Yar (1982)

These researchers are concerned with the model of frequency modulation,

$$Y(t) = \alpha \cos(\gamma t + \delta + \varsigma \sin(\psi t + \nu)) + \varepsilon(t). \tag{55}$$

Estimates of γ, ψ are determined by maximizing

$$\sum_k \left| d_Y^T(\gamma + k\psi) \right|^2 / f_{\varepsilon\varepsilon}(\gamma + k\psi). \tag{56}$$

5.9 Brillinger (1985)

This work considers the areal-temporal process (48), but now the sensors are irregularly distributed at locations $(x_j, y_j), j = 1, \ldots, J$. The time period T is thought of as large, and so γ may be treated as known. Let

$$\mathbf{Y}_k = \frac{1}{T} \sum_{t=0}^{T-1} [Y(x_j, y_j, t)] \exp\left\{-i\frac{2\pi kt}{T}\right\}, \tag{57}$$

$$\mathbf{M} = \sum \mathbf{Y}_k \overline{\mathbf{Y}}_k^{\mathrm{T}}, \tag{58}$$

where the summation is over Fourier frequencies $2\pi k/T$ near γ, and

$$\mathbf{S} = \mathbf{M} - \mathbf{Y}_{k'} \overline{\mathbf{Y}}_{k'}^{\mathrm{T}} \tag{59}$$

with $2\pi k'/T = \gamma$. (This last is an estimate of the spectral density matrix of the J noise process $\varepsilon(x_j, y_j, t)$.) Finally define the (steering) vector

$$\mathbf{B} = [\exp\{i(\alpha x_j + \beta y_j)\}]. \tag{60}$$

(In (57) and (60) the $[\cdot]$ notation denotes a J column vector.) The estimate studied is the (α, β) maximizing the "likelihood ratio detection" statistic

$$\frac{\overline{\mathbf{B}}^{\mathrm{T}} \mathbf{S}^{-1} \mathbf{B}}{\overline{\mathbf{B}}^{\mathrm{T}} \mathbf{M}^{-1} \mathbf{B}} - 1. \tag{61}$$

The asymptotic distribution of the estimate is indicated.

5.10 Brillinger (1986)

The previous situation may be viewed as corresponding to a small array of sensors. The work in this reference concerns a large array case, with the measurements irregularly placed with respect to all coordinates. It is convenient to alter the notation somewhat. Suppose

$$Y(t) = a \cos(\omega, t) + b \sin(\omega, t) + \varepsilon(t) \tag{62}$$

for ω, t in R^p and $(\omega, t) = \omega_1 t_1 + \ldots + \omega_p t_p$. Suppose the data available are the values $\{\tau_j, Y(\tau_j)\}$ for τ_j in a region T. The parameter ω is estimated by maximizing, for λ in R^p,

$$\left| \sum_j \exp\{-i(\lambda, \tau_j)\} Y(\tau_j) \right|^2 \tag{63}$$

and given $\hat{\omega}$, (a, b) estimated by ordinary least squares. Asymptotic distributions are obtained assuming $\{\tau_j\}$ is a realization of a stationary mixing point process in R^p with rate c_N and spectrum $f_{NN}(\lambda)$. In particular the estimates are found to be asymptotically normal with covariance matrix

$$c_N^{-2} 2(2\pi)^p f_{VV}(\lambda) \Sigma_T^{-1}, \tag{64}$$

where $f_{VV}(\lambda) = c_N^{-2} f_{\varepsilon\varepsilon}(\lambda) + \int f_{NN}(\lambda - \alpha) f_{\varepsilon\varepsilon}(\alpha) d\alpha$ and

$$\Sigma_T = \begin{bmatrix} |T| & 0 & \beta \int t dt \\ 0 & |T| & -\alpha \int t dt \\ \beta \int t^\tau dt & -\alpha \int t^\tau dt & |\rho| \int t^\tau t dt \end{bmatrix}. \tag{65}$$

The integrals appearing are over the region T. The asymptotics are as $|T| \to \infty$.

6. SOME OPEN PROBLEMS

We end by indicating in cursory form a number of research problems related to the topic of the paper.

1. Diagnostics, influence, robust/resistant procedures.
2. Missing values, quantization, jitter.
3. Estimation of dimension, e.g., by AIC.
4. Inverse problem formulations, ridge regression.
5. Local asymptotic normality, contiguity.
6. Adaptive procedures.
7. The absorbtion model.
8. Signal dependent noise.
9. Law of the iterated logarithm, large deviations, rates of convergence for the estimates.
10. Random effects models.
11. Vector-valued cases.
12. Partially parametric formulations, e.g., the periodic case.
13. Models for the point process and telegraph signal cases.
14. Expansions for distributions.
15. Distributions of test statistics, e.g., of

$$\sup_{\rho,\lambda} \left| \sum \rho^t e^{-i\lambda t} Y(t) \right|^2 \Big/ \sum \rho^{2t} \tag{66}$$

or of

$$\sup_{\lambda_1,\lambda_2} \min \left\{ I_T(\lambda_1), I^T(\lambda_2), I^T(\lambda_1 + \lambda_2) \right\}. \tag{67}$$

16. Properties of the estimates when the model is untrue.
17. The broadband signal case.
18. Parametric analysis of the frequency case.
19. Distribution in the null case of sup over (α, β) of (61).
20. Sampling properties of the NMR estimates.

ACKNOWLEDGMENT

This research was supported by the NSF Grant DMS-8316634.

REFERENCES

Aki, K., and P. G. Richards (1980), *Quantitative Seismology.* San Francisco: Freeman.

Blumich, B. (1985), "Stochastic NMR spectroscopy". *Bulletin of Magnetic Resonance* **7**, 5–26.

Blumich, B., and D. Ziessow (1983), "Nonlinear noise analysis in nuclear magnetic resonance spectroscopy. 1D, 2D, and 3D spectra". *Journal of Chemical Physics* **78**, 1059–1076.

Bolt, B. A. (1982), *Inside the Earth.* San Francisco: Freeman.

Bolt, B. A., and D. R. Brillinger (1979), "Estimation of uncertainties in eigenspectral estimates from decaying geophysical time series". *Geophysical Journal of the Royal Astronomical Society* **58**, 593–603.

Bolt, B. A., and R. G. Currie (1975), "Maximum entropy estimates of Earth torsional eigenperiods from 1960 Trieste data". *Geophysical Journal of the Royal Astronomical Society* **40**, 107–114.

Brillinger, D. R. (1973), "An empirical investigation of the Chandler wobble". *Bulletin of the International Statistical Institute* **45**, 413–433.

Brillinger, D. R. (1975), *Time Series: Data Analysis and Theory.* New York: Holt, Rinehart and Winston.

Brillinger, D. R. (1980), "The comparison of least squares and third-order periodogram procedures in the estimation of bifrequency". *Journal of Time Series Analysis* **1**, 95–102.

Brillinger, D. R. (1983), "The finite Fourier transform of a stationary process". In *Handbook of Statistics* **3**, ed. D. R. Brillinger and P. R. Krishnaiah, pp. 21–37. Amsterdam: Elsevier.

Brillinger, D. R. (1985), "A maximum likelihood approach to frequency-wavenumber analysis". *IEEE Transactions on Acoustics Speech and Signal Processing, ASSP* **33**, 1076–1085.

Brillinger, D. R. (1986), "Regression for randomly sampled spatial series: the trigonometric case". In *Essays in Time Series and Allied Processes*, ed. J. Gani and M. B. Priestley. Sheffield: Applied Probability Trust.

Clairaut, A.-C. (1754), "Mémoire sur l'orbite apparent du soleil autour de la terre, en ayant égard aux perturbations produites par les actions de la lune et des planètes principales". *Mémoires de Mathematique et de Physique de l'Académie Royale des Sciences* **9**, 521–564.

Christensen-Dalsgaard, J., D. Gough, and J. Toomre (1985), "Seismology of the Sun". *Science* **229**, 923–931.

Cummins, H. Z. (1977), "Intensity fluctuation spectroscopy of motile microorganisms". In *Photon Correlation Spectroscopy and Velocimetry*, ed. H. Z. Cummins and R. R. Pike, pp. 200–225. New York: Plenum.

Deubner, F-L., and D. Gough (1984), "Helioseismology". *Annual Review of Astronomy and Astrophysics* **22**, 593–619.

Deubner, F-L., R. K. Ulrich, and E. J. Rhodes (1979), "Solar p-mode oscillations as a tracer of radial differential rotation". *Astronomy and Astrophysics* **72**, 177–185.

Ernst, R. R. (1970), "Magnetic resonance with stochastic excitation". *Journal of Magnetic Resonance* **3**, 10–27.

Gilbert, F., and A. M. Dziewonski (1975), "An application of normal mode theory to retrieval of structural parameters and source mechanisms from seismic spectra". *Philosophical Transactions of the Royal Society of London*, Series A **278**, 187–269.

Hannan, E. J. (1971), "Non-linear time series regression". *Journal of Applied Probability* **8**, 767–780.

Hannan, E. J. (1973), "The estimation of frequency". *Journal of Applied Probability* **10**, 510–519.

Hannan, E. J. (1974), "Time series analysis". *IEEE Transactions on Automatic Control* **AC–19**, 706–715.

Hasan, T. "Non-linear time series regression for a class of amplitude modulated cosinusoids". *Journal of Time Series Analysis* **3**, 109–122.

Heideman, M. T., D. H. Johnson, and C. S. Burrus (1984), "Gauss and the history of the fast Fourier transform". *IEEE ASSP Magazine* **1**, 14–21.

Hinich, M. J., and P. Shaman (1972), "Parameter estimation for an R-dimensional plane wave observed with additive independent Gaussian errors". *Annals of Mathematical Statistics* **43**, 153–169.

Isokawa, Y. (1983), "Estimation of frequency by random sampling". *Annals of the Institute of Statistical Mathematics* **35**, 201–213.

Knight, W. R., and R. Kaiser (1982), "The randomly driven Block equations". *Journal of Magnetic Resonance* **48**, 293–301.

Lawton, J., and D. Williams (1985). *Tiger: A Hockey Story.* Toronto: McClelland and Stewart.

Munk, W. H., and G. J. F. MacDonald (1960), *The Rotation of the Earth.* Cambridge: Cambridge University Press.

Munk, W. H., and G. J. F. MacDonald (1964), "Long waves on the continental shelf: an experiment to separate trapped and leaky modes". *Journal of Fluid Mechanics* **20**, 529–554.

Nishio, I., T. Tanaka, S-T. Sun, Y. Imanishi, and S. T. Ohnishi (1983),

"Hemoglobin aggregation in single red blood cells of sickle cell anemia". *Science* **220**, 1173–1175.

Pfister, G., U. Gerdts, A. Lorenzen, and K. Schatzel (1983), "Hardware and software implementation of on-line velocity correlation measurements in oscillatory and turbulent rotational couette flow". In *Photon Correlation Techniques*, ed. E. O. Schultz-DuBois, pp. 256–262. Berlin: Springer-Verlag.

Sato, T., T. Kishimoto, and K. Sasaki (1978), "Laser Doppler particle measuring system using nonsinusoidal forced vibration and bispectral analysis". *Applied Optics* **17**, 667–670.

Schulz-DuBois, E. O. (ed.) (1983), *Photon Correlation Techniques*. Berlin: Springer-Verlag.

Subba Rao, T., and M. Yar (1982), "Statistical analysis of frequency modulated signals". Technical Report No. 153, Mathematics Department, University of Manchester Institute of Science and Technology.

Vere-Jones, D. (1982), "On the estimation of frequency in point process data". In *Essays in Statistical Science*, ed. J. Gani and E. J. Hannan, pp. 383–394. Sheffield: Applied Probability Trust.

Walker, A. M. (1971), "On the estimation of a harmonic component in a time series with stationary independent residuals". *Biometrika* **58**, 21–36.

Walker, A. M. (1973), "On the estimation of a harmonic component in a time seies with stationary dependent residuals". *Advances in Applied Probability* **5**, 217–241.

Whittle, P. (1952), "The simultaneous estimation of a time series". *Trabajos de Estadistica y de Investigacion Operative* **3**, 43–57.

Zadro, M. B., and M. Caputo (1968), "Spectral, bispectral analysis and Q of the free oscillations of the Earth". *Nuovo Cimento Supplemento* **6**, 67–81.

René Ferland and Gaston Giroux [1]

THE CONVERGENCE OF THE SOLUTION OF A BOLTZMANN TYPE EQUATION RELATED TO QUANTUM MECHANICS

ABSTRACT

McKean (1966), Tanaka (1978), and Sznitman (1984) have obtained existence, uniqueness and asymptotic results for the solution of a Boltzmann type equation, for the cases of Kac's caricature, Maxwell's gas and Boltzmann's gas, respectively. Their methods use Wild's sums. Here we adapt Tanaka's method for his asymptotic result to show, with the help of Wild's sums, the convergence toward the geometric equilibrium of the solution of a Boltzmann type equation related to the Bose-Einstein statistic ($r = 1$) of quantum mechanics.

1. INTRODUCTION

Wild (1951) gave the form of the solution of a Boltzmann type equation when the kernel of the intensity of the collisions belongs to the class of Maxwell gases with cut-off. McKean (1966), Tanaka (1973, 1978), and Sznitman (1984) used this result as a basis for obtaining theorems of existence, uniqueness and convergence in the cases of Kac's caricature, of Maxwell's gas (without cut-off) and of Boltzmann's gas, respectively.

Futcher *et al.* (1980) gave analogous models for closed oscillator systems of quantum mechanics. After having described and situated these models among the numerous models satisfying an equation of Boltzmann type, they obtained another form of the solution by Hilbert space techniques. Their method is thus less general than that of Wild.

The present work shows how Tanaka's method allows one to obtain the convergence of the solution for one of these models.

[1] Département de mathématiques et d'informatique, Université de Sherbrooke, Sherbrooke, Québec J1K 2R1 (both authors)

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 101–112.

2. WILD'S FORM OF THE SOLUTION

We refer to Futcher *et al.* (1980) for the justification of the model which follows. The simplicity of the model comes from the fact that the underlying process takes its values in the natural numbers $\mathcal{N}$. We do not give the explicit description of this process, whose existence and uniqueness have been established by Sznitman (1984). What we want to describe here is the form of the law μ_t, of X_t, in order to show that it converges to a geometric law. The law μ_t satisfies the following Boltzmann equation:

$$\frac{\partial}{\partial t}\mu_t(k) = \sum_{i+j\geq k} \frac{1}{i+j+1}\mu_t(i)\mu_t(j) - \mu_t(k); \quad \mu_0 = \mu. \tag{1}$$

If, for two probability measures μ and ν on $\mathcal{N}$, we put

$$(\mu \circ \nu)(k) = \sum_{i+j\geq k} \frac{1}{i+j+1}\mu(i)\nu(j), \tag{2}$$

we can, like Sznitman (1984), write the Wild's form of the solution as

$$\mu_t = \sum_{n\geq 1} e^{-t}(1-e^{-t})^{n-1}\mu^{(n)}, \tag{3}$$

where

$$\mu^{(1)} = \mu \text{ and } \mu^{(n+1)} = \frac{1}{n}\sum_{k=1}^{n}\left(\mu^{(k)} \circ \mu^{(n-k+1)}\right).$$

Let us point out that $1/(i+j+1)$ is one of the Bose-Einstein statistics; the interested reader may consult Feller (1965).

3. EQUILIBRIUM MEASURE AND CONSERVATION OF MOMENTS

We denote by $\mathcal{M}$ the set of probability measures on $\mathcal{N}$ and by $\mathcal{P}_k$ the subset of those $\lambda \in \mathcal{M}$ whose kth moment $m_k(\lambda)$ is finite. Moreover, we denote by g^p the geometric law with parameter $p \in (0,1)$:

$$g^p(i) = (1-p)^i p, \quad i \in \mathcal{N}.$$

The geometric laws are the equilibrium measures of our system. In fact, they satisfy the following stronger statement.

Lemma 3.1. If $\mu \in \mathcal{M}$ then $\mu \circ \mu = \mu$ if and only if μ is geometric.

Proof. (Necessity) Note that the composition operation introduced in (2) can be written in terms of convolution:

$$(\mu \circ \nu)(i) = \sum_{k \geq i} \frac{1}{k+1} (\mu * \nu)(k),$$

with

$$(\mu * \nu)(i) = \sum_{k=0}^{i} \mu(k)\nu(i-k).$$

The equation $\mu \circ \mu = \mu$ means that

$$\begin{aligned} \mu(i) &= \sum_{k \geq i} \frac{1}{k+1} (\mu * \mu)(k) \\ &= \frac{(\mu * \mu)(i)}{i+1} + (\mu \circ \mu)(i+1) \\ &= \frac{(\mu * \mu)(i)}{i+1} + \mu(i+1). \end{aligned}$$

This recurrence relation implies that μ is geometric.

(Sufficiency) If $g^p \in \mathcal{M}$, then

$$(g^p * g^p)(i) = (i+1)(1-p)^i p^2$$

and

$$\begin{aligned} (g^p \circ g^p)(i) &= \sum_{k \geq i} (1-p)^k p^2 \\ &= (1-p)^i p \\ &= g^p(i). \end{aligned}$$

Proposition 3.2. If in (1) $\mu_0 = g^p$ then $\mu_t = g^p$ for all t.

Proof. With the aid of the lemma it is easy to show by induction that $\mu^{(n)} = g^p$ for every $n \geq 1$ and the result follows from (3).

Lemma 3.3.

(i) If $\mu, \nu \in \mathcal{P}_1$ then $\mu \circ \nu \in \mathcal{P}_1$ and

$$m_1(\mu \circ \nu) = \frac{1}{2}[m_1(\mu) + m_1(\nu)].$$

(ii) If $\mu, \nu \in \mathcal{P}_2$ then $\mu \circ \nu \in \mathcal{P}_2$ and

$$m_2(\mu \circ \nu) = \frac{1}{3}[m_2(\mu) + m_2(\nu)] + \frac{1}{6}[4m_1(\mu)m_1(\nu) + m_1(\mu) + m_1(\nu)].$$

Proof.

(i)

$$\begin{aligned} m_1(\mu \circ \nu) &= \sum_{i \geq 0} i \sum_{k \geq i} \frac{1}{k+1}(\mu * \nu)(k) \\ &= \frac{1}{2}\sum_{i \geq 0} i(\mu * \nu)(i) \\ &= \frac{1}{2}[m_1(\mu) + m_1(\nu)]. \end{aligned}$$

(ii)

$$\begin{aligned} m_2(\mu \circ \nu) &= \sum_{i \geq 0} i^2 \sum_{k \geq i} \frac{1}{k+1}(\mu * \nu)(k) \\ &= \sum_{i \geq 0} \frac{i(2i+1)}{6}(\mu * \nu)(i) \\ &= \frac{1}{3}[m_2(\mu) + m_2(\nu) + 2m_1(\mu)m_1(\nu)] \\ &\quad + \frac{1}{6}[m_1(\mu) + m_1(\nu)]. \end{aligned}$$

The following proposition gives information on the time evolution of the moments of μ_t.

Proposition 3.4. For the solution of equation (1):

(i) if $\mu_0 \in \mathcal{P}_1$, then $\mu_t \in \mathcal{P}_1$ and $m_1(\mu_t) = m_1(\mu_0)$;

(ii) if $\mu_0 \in \mathcal{P}_2$, then $\mu_t \in \mathcal{P}_2$ and $m_2(\mu_t) \leq m_2(\mu_0) + m_1(\mu_0)(1 + 2m_1(\mu_0))$.

Proof.

(i) By induction, using Lemma 3.3 (i), one finds $m_1(\mu^{(n)}) = m_1(\mu_0)$ for every $n \geq 1$ and therefore

$$m_1(\mu_t) = \sum_{n \geq 1} e^{-t}(1 - e^{-t})^{n-1} m_1(\mu^{(n)}) = m_1(\mu_0).$$

(ii) Using Lemma 3.3 (ii) one can show by induction that

$$m_2(\mu^{(n)}) \leq m_2(\mu_0) + m_1(\mu_0)(1 + 2m_1(\mu_0))$$

for every $n \geq 1$. The inequality is obvious for $n = 1$ and by induction

$$\begin{aligned} m_2(\mu^{(m+1)}) &= \frac{1}{m}\sum_{k=1}^{m} m_2(\mu^{(k)} \circ \mu^{(m-k+1)}) \\ &= \frac{1}{m}\sum_{k=1}^{m}\left\{\frac{1}{3}[m_2(\mu^{(k)}) + m_2(\mu^{(m-k+1)})]\right. \\ &\quad \left. + \frac{1}{3}m_1(\mu_0)(1 + 2m_1(\mu_0))\right\} \\ &\leq \frac{1}{m}\sum_{k=1}^{m}\left\{\frac{2}{3}m_2(\mu_0) + m_1(\mu_0)(1 + 2m_1(\mu_0))\right\} \\ &\leq m_2(\mu_0) + m_1(\mu_0)(1 + 2m_1(\mu_0)). \end{aligned}$$

Thus,

$$\begin{aligned} m_2(\mu_t) &= \sum_{n\geq 1} e^{-t}(1 - e^{-t})^{n-1} m_2(\mu^{(n)}) \\ &\leq \sum_{n\geq 1} e^{-t}(1 - e^{-t})^{n-1}[m_2(\mu_0) + m_1(\mu_0)(1 + 2m_1(\mu_0))] \\ &\leq m_2(\mu_0) + m_1(\mu_0)(1 + 2m_1(\mu_0)). \end{aligned}$$

4. A METRIC ON $\mathcal{P}_1$

Definition 4.1. Let $\mu, \nu \in \mathcal{P}_1$. A coupling C of μ and ν is a probability measure on $\mathcal{N}^2$ such that

(i)
$$\sum_{j\geq 0} C(i,j) = \mu(i); \quad \forall i \in \mathcal{N},$$

(ii)
$$\sum_{i\geq 0} C(i,j) = \nu(j); \quad \forall j \in \mathcal{N}.$$

For $\mu, \nu \in \mathcal{P}_1$ we put $\gamma(C) = \sum_{i\geq 0}\sum_{j\geq 0} | i - j | C(i,j)$ and $\rho(\mu,\nu) = \inf\{\gamma(C) \mid C \in \mathcal{C}(\mu,\nu)\}$, where $\mathcal{C}(\mu,\nu)$ denotes the family of couplings of μ and ν.

Proofs of the following results (as well as complimentary information) are given by Dobrushin (1970), Dudley (1976), and Rachev (1984).

Result 1. If $\mu, \nu \in \mathcal{P}_1$ then there exists C in $\mathcal{C}(\mu, \nu)$ such that $\gamma(C) = \rho(\mu, \nu)$. Such a coupling is called optimal.

Result 2. $(\mathcal{P}_1, \rho)$ is a metric space.

Result 3. $\rho(\mu_n, \mu) \to 0$ is equivalent to $\mu_n \Rightarrow \mu$ and $m_1(\mu_n) \to m_1(\mu)$ (where $\mu_n \Rightarrow \mu$ denotes weak convergence).

Tanaka (1978) contains a general result, of which the following is a special case:

Result 4. Let $(\Omega, \mathcal{P}(\Omega), \lambda)$ be a discrete probability space. Suppose $\{\mu^\omega, \omega \in \Omega\}$ and $\{\nu^\omega, \omega \in \Omega\}$ are two subfamilies of $\mathcal{P}_1$ such that

$$\mu = \sum_{\omega \in \Omega} \lambda(\omega)\mu^\omega \text{ and } \nu = \sum_{\omega \in \Omega} \lambda(\omega)\nu^\omega$$

are also in $\mathcal{P}_1$. Then one has

$$\rho(\mu, \nu) \leq \sum_{\omega \in \Omega} \lambda(\omega)\rho(\mu^\omega, \nu^\omega).$$

For the next lemma U_k denotes the uniform law on $0, 1, \ldots, k$.

Lemma 4.2. For $k_1, k_2 \in \mathcal{N}$, $\rho(U_{k_1}, U_{k_2}) = | k_2 - k_1 | /2$.

Proof. We may assume $0 < k_1 < k_2$. It follows from the complimentary slackness theorem (see, for example, Zoutendijk, 1976) that every coupling C for which $C(i, j) = 0$ for $i > j$ is optimal. Using the coupling

$$\begin{cases} C(i,i) = \frac{1}{k_2+1}, & 0 \leq i \leq k_1, \\ C(i,j) = \frac{1}{(k_2+1)(k_1+1)}, & 0 \leq i \leq k_1 < j \leq k_2, \\ C(i,j) = 0, & \text{elsewhere}, \end{cases}$$

we obtain

$$\begin{aligned} \rho(U_{k_1}, U_{k_2}) &= \frac{1}{(k_2+1)(k_1+1)} \left[\frac{(k_1+1)(k_1+2)}{2} \right. \\ &\quad \left. + \cdots + \frac{(k_1+1)(k_1+2)(k_2-k_1)}{2} \right] \\ &= \frac{(k_2-k_1)}{2}. \end{aligned}$$

5. MONOTONICITY OF THE DISTANCE BETWEEN SOLUTIONS

We will obtain the monotonicity as a consequence of a more precise result. First we will establish three lemmas. The first one is a crucial convex inequality.

Lemma 5.1. If μ_1, μ_2, ν_1 and $\nu_2 \in \mathcal{P}_1$ then

$$\rho(\mu_1 \circ \mu_2, \nu_1 \circ \nu_2) \leq \frac{1}{2}\rho(\mu_1, \nu_1) + \frac{1}{2}\rho(\mu_2, \nu_2).$$

Proof. Let C_1 and C_2 be optimal couplings for $\rho(\mu_1, \mu_2)$ and $\rho(\mu_2, \nu_2)$ respectively and denote by λ the product measure of C_1 and C_2 on $(\mathcal{N}^4, \mathcal{P}(\mathcal{N}^4))$. For each $(i,j,k,\ell) \in \mathcal{N}^4$ put

$$\mu^{(i,j,k,\ell)} = U_{i+k},$$
$$\nu^{(i,j,k,\ell)} = U_{j+\ell}.$$

One easily sees that

$$\sum_{(i,j,k,\ell)\in\mathcal{N}^4} \lambda(i,j,k,\ell)\mu^{(i,j,k,\ell)} = \mu_1 \circ \mu_2$$

and that

$$\sum_{(i,j,k,\ell)\in\mathcal{N}^4} \lambda(i,j,k,\ell)\nu^{(i,j,k,\ell)} = \nu_1 \circ \nu_2.$$

Applying successively Result 4, Lemma 4.2 and the triangle inequality, one then has

$$\begin{aligned}
\rho(\mu_1 \circ \mu_2, \nu_1 \circ \nu_2) &\leq \sum_{(i,j,k,\ell)\in\mathcal{N}^4} \lambda(i,j,k,\ell)\rho(\mu^{(i,j,k,\ell)}, \nu^{(i,j,k,\ell)}) \\
&\leq \sum_{(i,j,k,\ell)\in\mathcal{N}^4} \lambda(i,j,k,\ell)\frac{|j+\ell-i-k|}{2} \\
&\leq \sum_{(i,j)\in\mathcal{N}^2} C_1(i,j)\frac{|j-i|}{2} + \sum_{(k,\ell)\in\mathcal{N}^2} C_2(k,\ell)\frac{|\ell-k|}{2} \\
&\leq \frac{1}{2}\rho(\mu_1, \nu_1) + \frac{1}{2}\rho(\mu_2, \nu_2).
\end{aligned}$$

Lemma 5.2. For each $\mu, \nu \in \mathcal{P}_1$,

$$\rho(\mu^{(n)}, \nu^{(n)}) \leq \rho(\mu, \nu), \quad n \geq 1.$$

Proof. Assuming the inequality for $n \leq m$, we have by Result 4 and Lemma 5.1:

$$\begin{aligned}
\rho(\mu^{(m+1)}, \nu^{(m+1)}) &= \rho\left(\frac{1}{m}\sum_{k=1}^{m} \mu^{(k)} \circ \mu^{(m-k-1)}, \frac{1}{m}\sum_{k=1}^{m} \nu^{(k)} \circ \nu^{(m-k+1)}\right) \\
&\leq \frac{1}{m}\sum_{k=1}^{m} \rho\left(\mu^{(k)} \circ \mu^{(m-k+1)}, \nu^{(k)} \circ \nu^{(m-k+1)}\right) \\
&\leq \frac{1}{m}\sum_{k=1}^{m} \left[\frac{1}{2}\rho\left(\mu^{(k)}, \nu^{(k)}\right) + \frac{1}{2}\rho\left(\mu^{(m-k+1)}, \nu^{(m-k+1)}\right)\right] \\
&\leq \frac{1}{m}\sum_{k=1}^{m} \left[\frac{1}{2}\rho(\mu, \nu) + \frac{1}{2}\rho(\mu, \nu)\right] \\
&\leq \rho(\mu, \nu).
\end{aligned}$$

Lemma 5.3. If $\mu, \nu \in \mathcal{P}_1$ then $\rho(\mu_t, \nu_t)$ is continuous.

Proof. First note that for each $i \in \mathcal{N}$

$$f^i(s) = \sum_{n \geq 1} e^{-s}(1 - e^{-s})^{n-1} \mu^{(n)}(i)$$

is continuous in s. Now the continuity of f^i and

$$| \rho(\mu_s, \nu_s) - \rho(\mu_t, \nu_t) | \leq \rho(\mu_s, \mu_t) + \rho(\nu_s, \nu_t)$$

give, recalling Result 3 and Proposition 3.4 (i), the continuity of $\rho(\mu_t, \nu_t)$.

Remark.
Lemmas 5.2 and 5.3 show that

$$\rho(\mu_t \circ \mu_t, \nu_t \circ \nu_t)$$

is continuous and therefore so is

$$\bar{\rho}(\mu_t, \nu_t) = \rho(\mu_t, \nu_t) - \rho(\mu_t \circ \mu_t, \nu_t \circ \nu_t).$$

Theorem 5.4. If $\mu, \nu \in P_1$ then $\rho(\mu_t, \nu_t) \leq \rho(\mu, \nu)$; in fact,

$$\rho(\mu_t, \nu_t) \leq \rho(\mu, \nu) - \int_0^t \bar{\rho}(\mu_s, \nu_s) ds. \tag{4}$$

Proof. Since the solution of (1) is unique, one has

$$\mu_{t+s} = \sum_{n \geq 1} e^{-s}(1 - e^{-s})^{n-1} \mu_t^{(n)}; \quad t, s \geq 0.$$

Applying Result 4 and Lemma 5.2 we obtain

$$\begin{aligned} \rho(\mu_{t+s}, \nu_{t+s}) &\leq \sum_{n \geq 1} e^{-s}(1 - e^{-s})^{n-1} \rho(\mu_t^{(n)}, \nu_t^{(n)}) \\ &\leq \sum_{n \geq 1} e^{-s}(1 - e^{-s})^{n-1} \rho(\mu_t, \nu_t) \\ &\leq \rho(\mu_t, \nu_t). \end{aligned} \tag{4.1}$$

$t \to \rho(\mu_t, \nu_t)$ is therefore a decreasing function and as such has a derivative $\rho'(t)$ almost everywhere which satisfies

$$\rho(\mu_t, \nu_t) - \rho(\mu, \nu) \leq \int_0^t \rho'(s) ds.$$

From (4.1),

$$\begin{aligned} \rho(\mu_{t+s}, \nu_{t+s}) &\leq e^{-s} \rho(\mu_t, \nu_t) + e^{-s}(1 - e^{-s}) \rho(\mu_t^{(2)}, \nu_t^{(2)}) \\ &\quad + \sum_{n \geq 3} e^{-s}(1 - e^{-s})^{n-1} \rho(\mu_t, \nu_t) \\ &\leq e^{-s} \rho(\mu_t, \nu_t) + e^{-s}(1 - e^{-s}) \rho(\mu_t \circ \mu_t, \nu_t \circ \nu_t) \\ &\quad + \rho(\mu_t, \nu_t)(1 - 2e^{-s} + e^{-2s}). \end{aligned}$$

Therefore,

$$\begin{aligned} &\frac{\rho(\mu_{t+s}, \nu_{t+s}) - \rho(\mu_t, \nu_t)}{s} \\ &\leq \rho(\mu_t, \nu_t) \left[\frac{e^{-2s} - e^{-s}}{s} \right] + \rho(\mu_t^{(2)}, \nu_t^{(2)}) \left[\frac{e^{-s} - e^{-2s}}{s} \right], \end{aligned}$$

hence

$$\overline{\lim_{s \downarrow 0}} \frac{\rho(\mu_{t+s}, \nu_{t+s}) - \rho(\mu_t, \nu_t)}{s} \leq -\rho(\mu_t, \nu_t) + \rho(\mu_t \circ \mu_t, \nu_t \circ \nu_t).$$

This latter inequality means that $\rho'(s)$ is dominated by $-\bar{\rho}(\mu_s, \nu_s)$, which gives (4).

6. CONVERGENCE TO EQUILIBRIUM

Theorem 6.1. If $\mu \in \mathcal{P}_1$ and g is the geometric law with mean $m_1(\mu)$ then $\rho(\mu_t, \mathrm{g})$ decreases to zero. In particular $\mu_t \Rightarrow \mathrm{g}$.

The proof is based on the following lemma.

Lemma 6.2. If $\mu \in \mathcal{P}_1$ is such that $m_1(\mu) = m_1(\mathrm{g})$ and $\mu \neq \mathrm{g}$ then

$$\rho(\mu \circ \mu, \mathrm{g}) < \rho(\mu, \mathrm{g}).$$

Proof. By Lemma 3.1 and Lemma 5.1 one has

$$\rho(\mu \circ \mu, \mathrm{g}) \leq \rho(\mu, \mathrm{g}). \tag{5}$$

Therefore, it is sufficient to show that the equality in (5) implies $\mu = \mathrm{g}$. But there is equality in (5) only if

$$\sum_{(i,j,k,\ell) \in \mathcal{N}^4} C(i,j)C(k,\ell) \mid \ell - k + j - i \mid$$
$$= \sum_{(i,j) \in \mathcal{N}^2} C(i,j) \mid j - i \mid + \sum_{(k,\ell) \in \mathcal{N}^2} C(k,\ell) \mid \ell - k \mid,$$

where C is an optimal coupling of μ and g. This last equality in turn implies, by a simple calculation on the first summation, that

$$\sum_{i>j} \sum_{k \leq \ell} C(i,j)C(k,\ell) \min\{\mid i - j \mid, \mid \ell - k \mid\}$$
$$+ \sum_{i \leq j} \sum_{k > \ell} C(i,j)C(k,\ell) \min\{\mid i - j \mid, \mid \ell - k \mid\} = 0.$$

Hence, $C(i,j)C(k,\ell) = 0$ for $i > j$. Finally, equality of the means then implies that $C(i,j) = 0$ for $i \neq j$, therefore $\mu = \mathrm{g}$.

Proof (of the theorem). By Proposition 3.2, $\rho(\mu_t, \mathrm{g}) = \rho(\mu_t, \mathrm{g}_t)$ and therefore $\rho(\mu_t, \mathrm{g})$ is decreasing. To show that it is decreasing to 0 we proceed in two steps.

Step 1. Suppose $m_2(\mu) < \infty$, then by Proposition 3.4, $m_2(\mu_t)$ is bounded in t, say by M. Denoting by $\mathcal{P}_\epsilon$ the family of probability measures $\lambda \in \mathcal{P}_1$ such that

$$m_1(\lambda) = m_1(\mathrm{g}), m_2(\lambda) \leq M \text{ and } \rho(\lambda, \mathrm{g}) \geq \epsilon,$$

we have that $\mathcal{P}_\epsilon$ is compact for ρ. Indeed, let $\{\lambda_n; n \in \mathcal{N}\}$ be a sequence in $\mathcal{P}_\epsilon$, since $\{\lambda_n(i); n \in \mathcal{N}\}$ is included in $[0,1]$ for each $i \in \mathcal{N}$ there exists a subsequence $\{\lambda_{n_k}; k \in \mathcal{N}\}$ and $\lambda : \mathcal{N} \to [0,1]$ such that

$$\lim_{k \to \infty} \lambda_{n_k}(i) = \lambda(i)$$

for all $i \in \mathcal{N}$. But $m_1(\mu) = m_1(\mathrm{g})$ for all k implies $\lambda \in \mathcal{M}$. On the other hand $m_2(\lambda_{n_k}) \leq M$ for all k, therefore $\lambda_{n_k} \Rightarrow \lambda$ and by Result 3 $\rho(\lambda_{n_k}, \lambda) \to 0$. $\mathcal{P}_\epsilon$ being closed, $\lambda \in \mathcal{P}_\epsilon$ and this shows that $\mathcal{P}_\epsilon$ is ρ-compact.

Now notice that, since

$$| \bar{\rho}(\mu, \mathrm{g}) - \bar{\rho}(\nu, \mathrm{g}) | \leq 2\rho(\mu, \nu)$$

$\bar{\rho}(\cdot, \mathrm{g})$ is ρ-continuous on $\mathcal{P}_\epsilon$. Hence, there exists $\mu^* \in \mathcal{P}_\epsilon$ such that

$$\bar{\rho}(\mu, \mathrm{g}) \geq \bar{\rho}(\mu^*, \mathrm{g}) = \delta > 0 \quad \forall \mu \in \mathcal{P}_\epsilon. \tag{6}$$

Finally, if we suppose $\rho(\mu_t, \mathrm{g}) \geq \epsilon > 0$ for all t, then by Theorem 5.1 and (6) we have

$$\begin{aligned} \rho(\mu_t, \mathrm{g}) &\leq \rho(\mu, \mathrm{g}) - \int_0^t \bar{\rho}(\mu_s, \mathrm{g}) ds \\ &\leq \rho(\mu, \mathrm{g}) - \delta t \end{aligned}$$

and this leads to a contradiction for t sufficiently large.

Step 2. In the general case we can choose for each $\epsilon > 0$ a probability measure μ^ϵ such that

$$m_1(\mu^\epsilon) = m_1(\mu), \quad m_2(\mu^\epsilon) < \infty \text{ and } \rho(\mu, \mu^\epsilon) < \epsilon.$$

Therefore, Result 4 and Lemma 5.3 imply $\rho(\mu_t, \mu_t^\epsilon) < \epsilon$, hence

$$\begin{aligned} \rho(\mu_t, \mathrm{g}) &\leq \rho(\mu_t, \mu_t^\epsilon) + \rho(\mu_t^\epsilon, \mathrm{g}) \\ &\leq \epsilon + \rho(\mu_t, \mathrm{g}). \end{aligned}$$

In this way $\overline{\lim}_{t \to \infty} \rho(\mu_t, \bar{g}) \leq \epsilon$ and the theorem is proved.

REFERENCES

Dobrushin, P. L. (1970), "Prescribing a system of random variables by conditional distributions." *Theory of Probability and its Applications* **15**, 458–486.

Dudley, R. M. (1976), "Probability and metrics." *Aarhus University Lecture Notes* **45**, 1–126.

Feller, W. (1965), *An Introduction to Probability Theory and its Applications.* New York: Wiley and Sons.

Futcher, E., M. R. Hoare, E. M. Hendriks, and M. H. Ernst (1980), "Soluble Boltzmann equations for internal state and Maxwell models." *Physica*, Series A **101**, 185–204.

McKean, Jr., H. P. (1966), "Speed of approach to equilibrium for Kac's caricature of a Maxwellian gas." *Archive for Rational Mechanics and Analysis* **21**, 347–367.

Rachev, S. T. (1984), "On a class of minimal functionals on a space of probability measures." *Theory of Probability and its Applications* **29**, 41–49.

Sznitman, S. S. (1984), "Equations de type de Boltzmann, spatialement homogènes." *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete* **66**, 559–592.

Tanaka, H. (1973), "An inequality for functional of probability distributions and its application to Kac's one-dimensional model of a Maxwellian gas." *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete* **27**, 47–52.

Tanaka, H. (1978), "Probabilistic treatment of the Boltzmann equation of Maxwellian molecules." *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete* **46**, 67–105.

Wild, E. (1951), "On the Boltzmann equation in the kinetic theory of gases." *Proceedings of the Cambridge Philosophical Society* **47**, 602–609.

Zoutendijk, G. (1976), *Mathematical Programming Methods.* Amsterdam: North-Holland.

J. Gani [1]

SOME RECENT WORK IN EPIDEMIC MODELS

1. INTRODUCTION

The modern theory of epidemics could be said to have started with Hamer (1906), who noted that new infectives at the discrete time $t+1$ depended on

$$\beta y_t x_t, \qquad t = 0,1,2,\ldots,$$

where x_t is the number of susceptibles, and y_t the number of infectives at time t, with β the infection parameter. Kermack and McKendrick (1927) later considered the deterministic model of a measles epidemic in a population of size N, governed by the differential equations

$$\frac{dx}{dt} = -\beta xy, \qquad \frac{dy}{dt} = \beta xy - \gamma y, \qquad \frac{dz}{dt} = \gamma y, \tag{1.1}$$

where $x(t)$, $y(t)$, $z(t)$ are susceptibles, infectives and immunes at time $t \geq 0$, with $x(t)+y(t)+z(t) = N$, and β, γ are the infection and removal parameters respectively.

Writing $\rho = \gamma/\beta$, they showed from (1.1) that

$$x = x_0 e^{-z/\rho}, \qquad x_0 = x(0) < N,$$

and denoting $u = x + y = N - z$, obtained from the third equation in (1.1) that

$$\frac{du}{dt} = -\gamma\left(u - x_0 e^{-(N-u)/\rho}\right), \qquad \int_N^u \frac{dv}{v - x_0 e^{(v-N)/\rho}} = -\gamma t. \tag{1.2}$$

We see that as $t \to \infty$, $u \to u_\infty$, which is the solution of $v = x_0 e^{(v-N)/\rho}$, and $u_\infty = x_\infty$ represents the number of survivors of the epidemic ($y_\infty = 0$); see

[1] Statistics Program, Department of Mathematics, University of California, Santa Barbara, California 93106, U.S.A.

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 113–122.

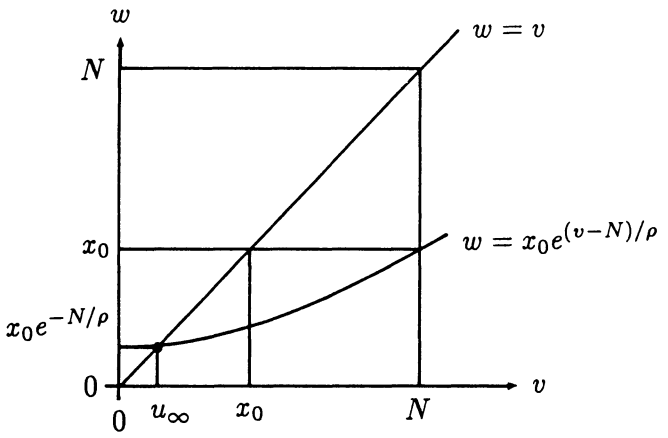

Figure 1. *Survivors u_∞ at the intersection of $w = v$, $w = x_0 e^{(v-N)/\rho}$.*

Figure 1. These results led to the Kermack-McKendrick Threshold Theorem for the deterministic general epidemic.

The Kermack-McKendrick Threshold Theorem:

(a) An epidemic occurs only if

$$\left.\frac{dy}{dt}\right|_{t=0} > 0 \quad \text{or} \quad x_0 > \rho;$$

(b) The survivors u_∞, where u_∞ is the solution of $v = x_0 e^{(v-N)/\rho}$, lie in the range $x_0 e^{-N/\rho} < u_\infty < x_0$.

This deterministic model has a stochastic analogue, which was first considered by Bartlett (1949). He studied the bivariate Markov chain $\{X(t), Y(t); t \geq 0\}$ in continuous time, where $X(t), Y(t)$ are the susceptibles and infectives respectively in a population of size N. The infinitesimal transition probabilities of the chain are now

$$\begin{aligned} &P\{X(t+\delta t) = x-1, Y(t+\delta t) = y+1 \mid X(t) = x, Y(t) = y\} \\ &= \beta xy\delta t + o(\delta t) \end{aligned} \tag{1.3}$$

and

$$\begin{aligned} &P\{X(t+\delta t) = x, Y(t+\delta t) = y-1 \mid X(t) = x, Y(t) = y\} \\ &= \gamma y\delta t + o(\delta t), \end{aligned}$$

with β, γ the infection and removal parameters as before. A realization of the process is illustrated in Figure 2. Note that a downward step in

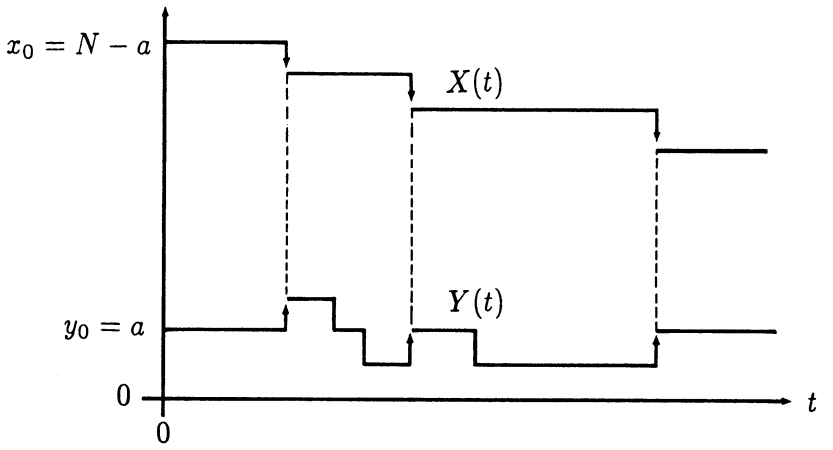

Figure 2. *Realization of* $\{X(t), Y(t);\ t \geq 0\}$.

$X(t)$ corresponds to an upward step in $Y(t)$; $Z(t)$ is given from the relation $X(t) + Y(t) + Z(t) = N$.

The forward Kolmogorov equations for $\{X(t),\ Y(t);\ t \geq 0\}$ with the infinitesimal transition probabilities (1.3) are of the form

$$\frac{d}{dt}p_{xy} = \beta(x+1)(y-1)p_{x+1,y-1} - y(\beta x + \gamma)p_{xy} + \gamma(y+1)p_{x,y+1},$$
$$0 \leq x \leq N - a,\ \ 0 \leq y \leq N,\ \ 0 \leq x + y \leq N, \tag{1.4}$$

where $p_{x,y}(t) = P\{X(t) = x,\ Y(t) = y \mid X(0) = N - a = n, Y(0) = a\}$. Making the time transformation $t' = \beta t$ and writing $\rho = \gamma/\beta$ as before, we obtain that the probability generating function (p.g.f.)

$$\Phi(z, w, t') = \sum_{x=0}^{n} \sum_{y=0}^{n+a-x} z^x w^y p_{xy}(t'),$$

subject to the initial condition $\Phi(z, w, 0) = z^n w^a$, satisfies the partial differential equation

$$\frac{\partial \Phi}{\partial t'} = w(w - z)\frac{\partial^2 \Phi}{\partial z \partial w} + \rho(1 - w)\frac{\partial \Phi}{\partial w} \quad |z|, |w| \leq 1. \tag{1.5}$$

This equation can be derived only because of the forms $\beta x y \delta t$, $\gamma y \delta t$, of the infinitesimal transition probabilities (1.3).

Formal solutions to (1.4) and (1.5) were found by Siskind (1965), Gani (1965) and Sakino (1968), but none was easy to use in practice. Perhaps the simplest was that outlined by Gani (1967).

2. MORE GENERAL INFECTION MECHANISMS

Saunders (1980) studied the spread of myxomatosis among rabbits and found that his data for infectives were better fitted when the infection mechanism was of the form

$$f_{xy} = \frac{\beta xy}{(x+y)^\alpha}, \qquad \alpha = 1/2, \tag{2.1}$$

rather than βxy. It is not difficult to provide a rationalization of this mechanism, which we may refer to as "bunching". We note that $\alpha = 0$ corresponds to the classical "general epidemic", and the values of α which are relevant lie in $0 \leq \alpha \leq 1$.

Kermack and McKendrick (1927) obtained the threshold results for $\alpha = 0$; let us summarize those for $0 < \alpha < 1$ and $\alpha = 1$.

We are now considering the differential equations

$$\frac{dx}{dt} = \frac{-\beta xy}{(x+y)^\alpha}, \qquad \frac{dy}{dt} = \frac{\beta xy}{(x+y)^\alpha} - \gamma y, \qquad \frac{dz}{dt} = \gamma y. \tag{2.2}$$

When $\alpha = 1$, writing $y = x + y$ as before we find

$$x = x_0 \left(\frac{u}{N}\right)^{1/\rho}, \qquad \int_N^u \frac{dv}{v - x_0(v/N)^{1/\rho}} = -\gamma t. \tag{2.3}$$

Thus, for an epidemic to occur

$$\left.\frac{dy}{dt}\right|_{t=0} = \beta y_0 \left(\frac{x_0}{N} - \rho\right) > 0 \quad \text{or} \quad x_0 > \rho N. \tag{2.4}$$

We can see directly that

$$\begin{aligned} u_\infty &= \left(\frac{x_0^\rho}{N}\right)^{1/(\rho-1)} && \text{for } \rho > 1, \\ &= 0 && \text{for } \rho \leq 1; \end{aligned} \tag{2.5}$$

see Figure 3.

Finally, for the case $0 < \alpha < 1$, with $b = 1 - \alpha > 0$, we find that an epidemic occurs only if

$$\left.\frac{dy}{dt}\right|_{t=0} = \beta y_0 \left(\frac{x_0}{(x_0+y_0)^\alpha} - \rho\right) \text{ or } x_0 > \rho N^\alpha. \tag{2.6}$$

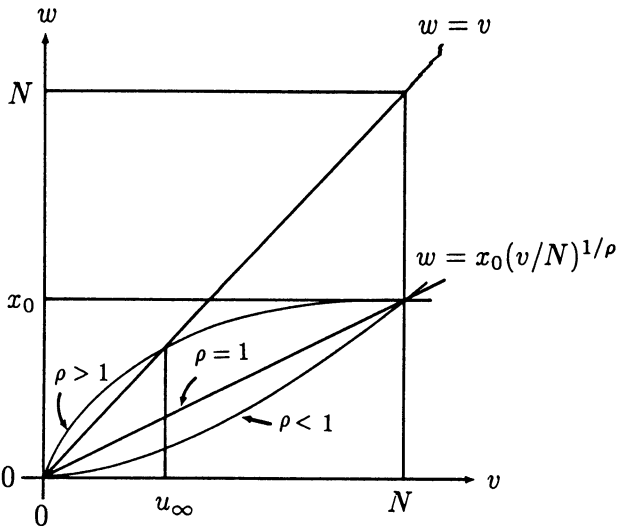

Figure 3. *Survivors* u_∞ *for* $\alpha = 1$.

Also

$$x = x_0 \exp\left\{\frac{1}{\rho b}\left(u^b - N^b\right)\right\},$$

$$\int_N^u \frac{dv}{v - x_0 \exp\left\{\frac{1}{\rho b}\left(v^b - N^b\right)\right\}} = -\gamma t. \tag{2.7}$$

Thus the number of survivors u_∞ will be the solution of

$$v = x_0 \exp\left\{\frac{1}{\rho b}\left(v^b - N^b\right)\right\}; \tag{2.8}$$

see Figure 4.

We note that the methods used to analyze the deterministic epidemic with the more general infection mechanism remain similar to those of Kermack and McKendrick. This proves to be no longer true for the stochastic epidemic $\{X(t), Y(t); t \geq 0\}$, where a solution cannot be obtained using p.g.f. methods.

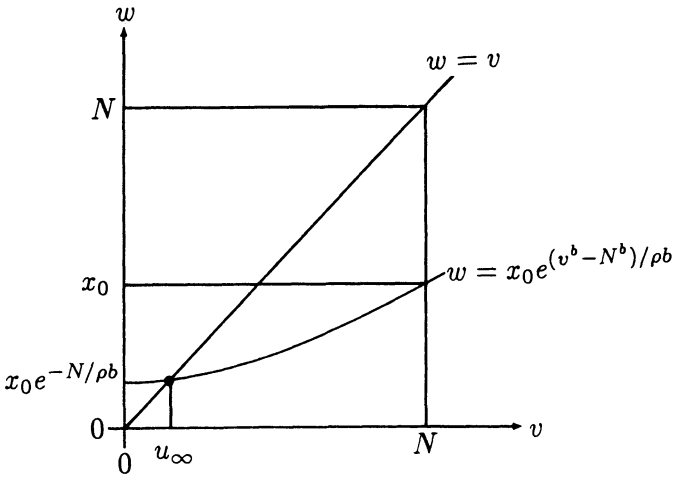

Figure 4. *Survivors* u_∞ *for* $0 < \alpha < 1$.

3. MATRIX GEOMETRIC METHODS FOR THE GENERAL STOCHASTIC EPIDEMIC

Suppose that in order to simplify our formulae, we write, after the usual time transformation ($t' = \beta t$),

$$f_{xy} = \frac{xy}{(x+y)^\alpha}, \quad \rho y = \rho_y. \tag{3.1}$$

The forward Kolmogorov equations now become

$$p'_{xy} = f_{x+1,y-1}p_{x+1,y-1} - (f_{xy} + \rho_y)p_{xy} + \rho_{y+1}p_{x,y+1}, \tag{3.2}$$

$$0 \le x \le n, \quad 0 \le y \le n+a, \quad 0 \le x+y \le n+a,$$

and it is clear that it is no longer possible to use p.g.f. methods in this case. Peter Purdue pointed out that the form of the equations lent itself to the use of matrix-geometric methods and our recent joint paper (Gani and Purdue, 1984) has given details of the procedure.

Briefly, let

$$\underset{(a+1)\times 1}{\mathbf{P}_n(t)} = \begin{bmatrix} p_{n0} \\ \vdots \\ p_{na} \end{bmatrix}, \underset{(a+2)\times 1}{\mathbf{P}_{n-1}(t)} = \begin{bmatrix} p_{n-1,0} \\ \vdots \\ p_{n-1,a+1} \end{bmatrix}, \ldots,$$

$$\underset{(n+a)\times 1}{\mathbf{P}_1} = \begin{bmatrix} p_{10} \\ \vdots \\ p_{1,n+a-1} \end{bmatrix}, \quad \underset{(n+a+1)\times 1}{\mathbf{P}_0} = \begin{bmatrix} p_{00} \\ \vdots \\ p_{0,n+a} \end{bmatrix}$$

be the vectors of probabilities of $\{X(t), Y(t); t \geq 0\}$. Then

$$\mathbf{P}_n' = \{-(B_n + A_n) + \Delta_n A_n\}\mathbf{P}_n, \tag{3.3}$$

where

$$\underset{(a+1)\times(a+1)}{B_n} = \operatorname{diag}(0, f_{n1}, \ldots, f_{n,a-1}, f_{na}),$$

$$A_n = \operatorname{diag}(0, \rho_1, \ldots, \rho_{a-1}, \rho_a),$$

and Δ_n is a matrix with ones on the first upper diagonal and zeros elsewhere.

Similarly

$$\mathbf{P}_x' = \{-(B_x + A_x) + \Delta_x A_x\}\mathbf{P}_x + B_{x+1}^{+}\mathbf{P}_{x+1}^{+}, \quad x = 0, 1, \ldots, n-1, \tag{3.4}$$

where

$$\underset{\substack{(n+a-x+1)\times \\ (n+a-x+1)}}{B_x} = \operatorname{diag}(0, f_{x1}, \ldots, f_{x,n+a-x-1}, f_{x,n+a-x}),$$

$$A_x = \operatorname{diag}(0, \rho_1, \ldots, \rho_{n+a-x-1}, \rho_{n+a-x}),$$

Δ_x is a matrix with ones on the first upper diagonal and zeros elsewhere, and B_{x+1}^{+}, $\mathbf{P}_{x+1}^{+}$ are augmented matrices so that they will have the appropriate number of rows and columns:

$$B_{x+1}^{+} = \begin{bmatrix} 0 & \\ & B_{x+1} \end{bmatrix}, \mathbf{P}_{x+1}^{+} \begin{bmatrix} 0 \\ \mathbf{P}_{x+1} \end{bmatrix}.$$

Using Laplace transform methods, it is possible to obtain the transforms

$$\hat{p}_{xy}(s) = \int_0^\infty e^{-st} p_{xy}(t)\,dt, \quad \operatorname{Re}(s) > 0,$$

in a recursive form, when we write $\rho_y = \rho y$, as

$$\hat{p}_{ny}(s) = \rho^{a-y}\frac{a!}{y!}\prod_{r=y}^{a}(s + f_{nr} + r\rho)^{-1}, \quad y = 0, \ldots, a,$$

$$\hat{p}_{xy}(s) = \sum_{r=y-1}^{n+a-x-1}\frac{(r+1)!}{y!}\rho^{r+1-y}\frac{f_{x+1,r}\hat{p}_{x+1,r}(s)}{\prod_{\ell=y}^{r+1}(s + f_{x\ell} + \ell\rho)},$$

$$x = 1, \ldots, n-1; \qquad y = 1, \ldots, n+a-x. \tag{3.5}$$

Of particular interest are the probabilities of the numbers of survivors as $t \to \infty$, namely

$$\begin{aligned} \pi_{x0} &= \lim_{t\to\infty} p_{x0}(t) \\ &= \lim_{s\to 0} s\hat{p}_{x0}(s) \\ &= \sum_{r=1}^{n+a-x-1} (r+1)!\rho^{r+1} \frac{f_{x+1,r}\hat{p}_{x+1,r}(0)}{\prod_{\ell=1}^{r+1}(f_{x\ell}+\ell\rho)}, \end{aligned} \tag{3.6}$$

which can also be obtained by recursive methods from the $\hat{p}_{xy}(s)$.

It is perhaps worthwhile pointing out that for the general infection mechanism f_{xy}, one can obtain a stochastic threshold theorem by applying Whittle's (1955) method. The value of the matrix-geometric approach is illustrated again in the problem of the epidemic with carriers.

4. EPIDEMICS WITH CARRIERS

This model, in which the carriers $Y(t)$ follow a pure death process, and drive the epidemic, has been studied by Weiss (1965), Dietz (1966), and Downton (1967) when $f_{xy} = xy$. We can once again generalize the infection mechanism to

$$f_{xy} = \frac{xy}{(x+y)^{\alpha}} \tag{4.1}$$

with $\rho_y = \rho y$.

In this case, given $X(0) = n$, $Y(0) = b$, we have

$$\begin{aligned} p'_{xy} = f_{x+1,y}p_{x+1,y} - (f_{xy}+\rho y)\,p_{xy} + \rho(y+1)p_{x,y+1}, \\ 0 \le x \le n, \qquad 0 \le y \le b. \end{aligned} \tag{4.2}$$

Writing

$$\underset{(b+1)\times 1}{\mathbf{P}_x(t)} = \begin{bmatrix} p_{x0}(t) \\ \vdots \\ p_{xb}(t) \end{bmatrix},$$

we find that (4.2) can be written as

$$\mathbf{P}'_n = \{-B_n - A + \Delta A\}\,\mathbf{P}_n, \tag{4.3}$$

where

$$\underset{(b+1)\times(b+1)}{B_n} = \operatorname{diag}(f_{n0}, f_{n1}, \ldots, f_{nb}),$$

$$A = \operatorname{diag}(0, \rho, \ldots, \rho b),$$

and Δ is a matrix with ones on the first upper diagonal and zeros elsewhere. More generally

$$\mathbf{P}'_x = \{-B_x - A - \Delta A\}\mathbf{P}_x + B_{x+1}\mathbf{P}_{x+1}, \quad x = 0, \ldots, n-1, \tag{4.4}$$

where

$$\underset{(b+1)\times(b+1)}{B_x} = \operatorname{diag}(f_{x0}, f_{x1}, \ldots, f_{xb}).$$

Once again, using Laplace transforms, we derive:

$$\hat{p}_{ni}(s) = \frac{b!}{i!}\rho^{b-i}\prod_{k=1}^{b}(s + f_{nk} + k\rho)^{-1}, \quad i = 0, 1, \ldots, n;$$

$$\hat{p}_{xi}(s) = \sum_{j=1}^{b}\frac{j!}{i!}\rho^{j-i}\prod_{k=1}^{j}(s + f_{xk} + k\rho)^{-1} f_{x+1,j}\hat{p}_{x+1,j}(s),$$

$$x = 0, 1, \ldots, n-1. \tag{4.5}$$

Limiting probabilities can be obtained from these. In the particular case where $f_{xy} = xy$, Booth *et al.* (1986) have shown that the earlier results of Weiss, Dietz and Downton can be derived as a special case of the general infection mechanism.

Many problems remain in the area of epidemic modeling, among them the spread of epidemics in groups subdivided by age or genetic constitution. These have yet to be investigated.

REFERENCES

Bartlett, M. S. (1949), "Some evolutionary stochastic processes". *Journal of the Royal Statistical Society*, Series B **11**, 211–229.

Booth, J., J. Gani, M-P. Malice, H. Mansouri, and G. Maravankin (1986), "A general solution for the epidemic with carriers". *Statistics and Probability Letters* **4**, 9–15.

Dietz, K. (1966), "On the model of Weiss for the spread of epidemics by carriers". *Journal of Applied Probability* **3**, 375–382.

Downton, F. (1967), "Epidemics with carriers: a note on a paper of Dietz". *Journal of Applied Probability* **4**, 264–270.

Gani, J. (1965), "On a partial differential equation of epidemic theory, I". *Biometrika* **52**, 617–622.

Gani, J. (1967), "On the general stochastic epidemic". *Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability* **4**, 271–279.

Gani, J., and P. Purdue (1984), "Matrix-geometric methods for the general stochastic epidemic". *IMA Journal of Mathematics Applied to Medicine and Biology* **1**, 333–342.

Hamer, W. H. (1906), "Epidemic disease in England". *Lancet* **1**, 733–739.

Kermack, W. O., and A. G. McKendrick (1927), "Contributions to the mathematical theory of epidemics, I". *Proceedings of the Royal Society,* Series A **115**, 700–721.

Sakino, S. (1968), "On the solution of the epidemic equation". *Annals of the Institute of Statistical Mathematics,* Supplement, **V**, 9–19.

Saunders, I. W. (1980), "A model for myxomatosis". *Mathematical Biosciences* **48**, 1–15.

Siskind, V. (1965), "A solution of the general stochastic epidemic". *Biometrika* **52**, 613–616.

Weiss, G. H. (1965), "On the spread of epidemics by carriers". *Biometrics* **21**, 481–490.

Whittle, P. (1955), "The outcome of a stochastic epidemic—a note on Bailey's paper". *Biometrika* **42**, 116–122.

Michel Blais [1]

TRANSIENCE IN A QUEUEING SYSTEM WITH A FINITE NUMBER OF LOCALLY INTERACTING SERVERS

ABSTRACT

This paper discusses the transience and ergodicity of a queueing system with local interaction. It completes the paper of Malyshev and Tsaregradskii (1982) using the method developed by Malyshev and Menshikov (1981). Then the properties of transience and/or ergodicity can be concluded immediately for other queueing systems.

1. INTRODUCTION

Malyshev and Tsaregradskii (1982) made use of a criterion developed by Malyshev and Menshikov (1981) to determine the ergodicity of their model. This model is one of the simplest possible queueing systems involving a locally interacting finite number of birth-and-death chains with countable states. The difficult but challenging subject of Markov processes with local interaction has been studied mainly for the case where the state space at each point is finite. This simplification of more difficult models in statistical physics has been used in many different areas. See, for instance, Dobrushin *et al.* (1978). Here we only suppose that the state space at each point is countable. This adds new difficulties, but presumably the model is a little more realistic and seems to cover a larger domain of potential applications. Let us first give a description of this model.

Let n servers stand in a line. At each server in each unit time a new call arrives with probability p. Each server in the system services at most one call in its queue in unit time; the service probability equals α if neighbouring servers are occupied and equals α' if at least one neighbouring server is

[1] Département de mathématiques et d'informatique, Université de Sherbrooke, Sherbrooke, Québec J1K 2R1

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 123–129.

free. Suppose furthermore that calls arrive at each server independently and servers serve independently.

This model is a homogeneous Markov chain on Z_+^n with discrete time. The chain is transient if $\alpha < p$ and is ergodic (positive recurrent) if $p < \min\{\alpha, \alpha'\}$. Thus it remains to investigate the non-obvious case $\alpha' \leq p \leq \alpha$; in this case we observe that the chain is irreducible and aperiodic for $0 < p < 1$.

Malyshev and Tsaregradskii (1982) proved that the chain is ergodic if $\alpha' > \alpha p/(\alpha+p)$. They proved transience in particular cases ($\alpha = 1$ or $n = 3$) if $\alpha' < \alpha p/(\alpha + p)$.

The goal of this work is to prove transience in the case

$$\alpha' < \alpha p/(\alpha + p) < p < \alpha$$

and n is odd. The question is to find a suitable function and use it in the method of Malyshev and Menshikov (1981) to show that the chain is transient. Let us first briefly examine this technique.

2. THE METHOD

Let L be a homogeneous irreducible and aperiodic Markov chain on Z_+^n with $\big(P(x,y)\big)_{(x,y)\in Z_+^n \times Z_+^n}$ as its transition matrix. Let $E(x) = \big(E_1(x), \ldots, E_n(x)\big)$ be the vector of the mean jump in one step from the point $x \in Z_+^n$.

Let $\Lambda = (i_1, \ldots, i_k)$ denote an ordered set of natural numbers such that $1 \leq k \leq n$ and $1 \leq i_1 < i_2 < \cdots < i_k \leq n$. For such Λ and $c, t \in R_+$, let

$$B_{c,t}^{\Lambda} = \big\{(r_1, \ldots, r_n) \in R_+^n : r_i > c,\ i \in \Lambda;\ r_i \leq t,\ i \notin \Lambda\big\} \text{ and } B^{\Lambda} = B_{0,0}^{\Lambda}.$$

Condition 1. (Spatial Homogeneity): there exists $c \geq 0$ such that for all Λ,

all $a = (a_1, \ldots, a_n) \in Z_+^n$ with $a_i = 0$ if $i \notin \Lambda$,

all $x \in B_{c,c}^{\Lambda} \cap Z_+^n$ and all $y \in Z_+^n$ we have $P(x,y) = P(x+a, y+a)$.

Condition 2. (Boundedness of Jumps): For all $x \in Z_+^n$ there is a finite number of $y \in Z_+^n$ such that $P(x,y) \neq 0$.

Assuming the first condition, the second is equivalent to: there exists $d > 0$ such that $P(x,y) = 0$ if $\| x - y \| > d$. ($\| \cdot \|$ is any norm in R^n).

The method of Malyshev and Menshikov consists of establishing a generalized Foster's criterion (see Foster, 1953) by considering particular homogeneous Markov chains L^Λ and vectors v^Λ.

For $\Lambda \neq (1,\dots,n)$ we choose an arbitrary point

$$a \in B^\Lambda_{c,0} \cap Z^n_+$$

and define a set

$$C^\Lambda = \left\{x \in Z^n_+ : x_i = a_i,\ i \in \Lambda\right\}.$$

Definition 1.1. L^Λ is the Markov chain on C^Λ with transition matrix

$${}^\Lambda P(x,y) = \sum_{y'} P(x,y'), \qquad x,y \in C^\Lambda,$$

where summation is performed for all $y' \in Z^n_+$ such that $y'_i = y_i$ for $i \notin \Lambda$. It follows from condition 1 that L^Λ does not depend on the choice of $a \in B_{c,0} \cap Z^n_+$.

Condition 3. For any $\Lambda \neq (1,\dots,n)$ the chain L^Λ is irreducible and aperiodic.

Definition 1.2. The vector v^Λ on B^Λ is defined as follows:

(i) if $\Lambda = (1,\dots,n)$ then $v^\Lambda = E[X]$ where $x \in B^\Lambda_{c,c} \cap Z^n_+$;

(ii) if $\Lambda \neq (1,\dots,n)$ and L^Λ is ergodic with $\left(\pi^\Lambda(z)\right)\left(z \in C^\Lambda\right)$ its stationary probabilities, then

$$v^\Lambda_i = \begin{cases} \sum\limits_{z \in C^\Lambda} \pi^\Lambda(z) E_i[z], & i \in \Lambda, \\ 0, & i \in \Lambda; \end{cases}$$

(iii) if $\Lambda \neq (1,\dots,n)$ and L^Λ is nonergodic the vectors v^Λ are not defined.

From Conditions 1 and 2 it follows that

$$\max_\Lambda \| v^\Lambda \| < \infty.$$

Theorem 1.1. Under Conditions 1, 2, and 3, L is transient if for some δ, b, t, $c > 0$ there exists a nonempty set $T \subset R_+^n$ and an unbounded function $f : R_+^n \to R_+$ such that:

1° $| f(x) - f(y) | \leq b \| x - y \|$, for all $x, y \in R_+^n$;

2° $f(x) \geq t$ for all $x \in T$,
$f(x) < t$ for all $x \notin T$;

3° for all Λ such that L^Λ is ergodic, for $\Lambda = (1, \ldots, n)$ and for all $x \in B_{c,0}^\Lambda \cap T$, $f\left(x + v^\Lambda\right) - f(x) \geq \delta$.

3. SOLUTION OF THE PROBLEM

Malyshev and Tsaregradskii (1982) showed that the component v_i^Λ depended only on the number of consecutive servers not in Λ on each side of the ith server, and calculated these components. Denote the component v_i^Λ by $r_{k\ell}$ if $i \in \Lambda$ and there are k consecutive servers not in Λ to the left of the ith server and ℓ consecutive servers not in Λ to the right. Then for $k, \ell \geq 1$ they obtain:

$$
\begin{aligned}
r_{00} &= p - \alpha, \\
r_{0k} = r_{k0} &= \pi_0^{(k)}(p - \alpha') + \left(1 - \pi_0^{(k)}\right)(p - \alpha), \\
r_{k\ell} = r_{\ell k} &= \left[1 - \left(1 - \pi_0^{(k)}\right)\left(1 - \pi_0^{(\ell)}\right)\right](p - \alpha') \\
&\quad + \left(1 - \pi_0^{(k)}\right)\left(1 - \pi_0^{\ell}\right)(p - \alpha),
\end{aligned}
$$

where $\pi_0^{(k)}$ is the stationary probability of the zero state of the first coordinate of the chain L on Z_+^k (by symmetry it could be the last coordinate too, see Malyshev and Tsaregradskii (1982, p. 622). Since the stationary probability is known for $k = 1$ we have

$$
\begin{aligned}
r_{01} &= \alpha'(p - \alpha)/\alpha, \\
r_{11} &= (\alpha - p)\left[\alpha p - \alpha'(\alpha - p)\right]/\alpha^2.
\end{aligned}
$$

Finally we define a function f which verifies the conditions of Theorem 1.1. Let $f = \max\{g, 0\}$, where

$$
g(x_1, \ldots, x_n) = \min_{i \text{ even}} \{x_i\} - 2 \max_{i \text{ odd}} \{x_i\}.
$$

1° $\quad | f(x) - f(y) | \leq 3 \max | x_i - y_i |$.

Actually it suffices to prove this for g,

$$\begin{aligned} |\, g(x) - g(y)\,| &= |\min_{i \text{ even}} \{x_i\} - 2\max_{i \text{ odd}} \{x_i\} - \min_{i \text{ even}} \{y_i\} + 2\max_{i \text{ odd}} \{y_i\}\,| \\ &\le |\min_{i \text{ even}} \{x_i\} - \min_{i \text{ even}} \{y_i\}\,| \\ &\qquad + 2\,|\max_{i \text{ odd}} \{y_i\} - \max_{i \text{ odd}} \{x\}\,| \\ &\le \max_{i \text{ even}} |\, x_i - y_i\,| + 2\max_{i \text{ odd}} |\, x_i - y_i\,| \\ &\le 3\max_{i} |\, x_i - y_i\,|\,. \end{aligned}$$

2° From the definition of f we see that $f(x_1, \ldots, x_n) = 0$ if $x_i = 0$ for an i even. So f may be non-null only on the B^Λ with Λ containing at least all even coordinates.

We set $T = \{x \in Z_+^n : f(x) \ge 1\}$ and then the v_i^Λ may take only the following values when $B^\Lambda \cap T \neq \phi$:

$$\begin{aligned} v_i^\Lambda &\in \{r_{00}, r_{01}, r_{11}\} \qquad \text{for } i \text{ even}, \\ v_i^\Lambda &\in \{0, r_{00}\} \qquad \text{for } i \text{ odd}. \end{aligned}$$

3° There are the following possibilities for $f(x + v^\Lambda) - f(x)$ when $x \in B^\Lambda \cap T$ and n is odd. Set $y = \max_{i \text{ odd}} \{x_i\}$ for simplicity.

(a) If $\min_{i \text{ even}} \{x_i + v_i^\Lambda\} = x_{i_0} + r_{11}$, then $\min_{i \text{ even}} \{x_i\} = x_{i_0}$ since $r_{11} > 0 \ge r_{01} > r_{00}$ in our case; and if Λ contains at least one odd coordinate; then

$$f(x + v^\Lambda) - f(x) = x_{i_0} + r_{11} - 2y - 2r_{00}$$

and

$$-x_{i_0} + 2y = r_{11} - 2r_{00}.$$

(b) If as in (a) but Λ does not contain any odd coordinate, then

$$f(x + v^\Lambda) - f(x) = x_{i_0} + r_{11} - x_{i_0} = r_{11}.$$

(c) If $\min_{i \text{ even}} \{x_i + v_i^\Lambda\} = x_{i_0} + r_{01}$, then $\min_{i \text{ even}} \{x_i\} = x_{i_1} \le x_{i_0}$ and Λ contains at least one odd coordinate, and

$$f(x + v^\Lambda) - f(x) = x_{i_0} + r_{01} - 2y - 2r_{00}$$

and

$$-x_{i_1} + 2y \ge r_{01} - 2r_{00}.$$

(d) If $\min_{i \text{ even}} \{x_i + v_i^\Lambda\} = x_{i_o} + r_{00}$, then $\min_{i \text{ even}} \{x_i\} = x_{i_1} \leq x_{i_o}$, Λ contains at least two odd coordinates, and

$$f(x + v^\Lambda) - f(x) = x_{i_o} + r_{00} - 2y - 2r_{00} - x_{i_1}, +2y \geq -r_{00}.$$

Thus with $\delta = r_{11}$ we have $f(x + v^\Lambda) - f(x) \geq \delta > 0$.

We conclude the chain is transient if $n \geq 3, n$ odd, and

$$0 \leq \alpha' < \alpha p/(\alpha + p) < p < \alpha \leq 1.$$

If n is even we know nothing except of course for $n = 2$ where the chain is ergodic if $0 < \alpha' < \alpha p/(\alpha + p)$.

In order to continue these studies with the method of Malyshev and Menshikov we have to know more about the stationary probability.

4. SERVERS STAND IN A CIRCLE

We suppose now that servers stand in a circle, so that there are two neighbouring servers for each server. This chain is similar to the former one; it is transient if $p > \alpha$ and ergodic if $p < \min\{\alpha, \alpha'\}$. Chains L^Λ are of the previous type since C^Λ represent sets of servers in a line. For the v^Λ there is an alteration if $n \geq 3$ and $\Lambda = (i)$, $1 \leq i \leq n$. In that case L^Λ is a chain on Z_+^{n-1} (servers in a line) with the first and last servers neighbour of the server (i) in Λ. There is not necessarily independence between first and last servers. We have then:

$$\begin{aligned} v_i^\Lambda = r^{n-1} &= (p - \alpha)\left[1 - 2\Pi_0^{(n-1)} + \Pi_{00}^{(n-1)}\right] \\ &\quad + (p - \alpha')\left(2\Pi_0^{(n-1)} - \Pi_{00}^{(n-1)}\right) \\ &= (p - \alpha) + (\alpha - \alpha')\left(2\Pi_0^{(n-1)} - \Pi_{00}^{(n-1)}\right), \end{aligned}$$

where $\Pi_{00}^{(n-1)}$ is the stationary probability of the zero state of the last and first coordinates of the chain L on Z_+^{n-1} (with servers in a line).

We see, since $\Pi_0^{(k)} \leq 1 - p/\alpha$ for $k \geq 1$ (see Malyshev and Tsaregradskii, 1982), that:

$$r^{n-1} < (p - \alpha) + (\alpha - \alpha')\left[2(1 - p/\alpha) - 0\right] \leq 0,$$

if $\alpha' \geq \frac{1}{2}\alpha$. Then Lemma 3 and Theorem 2 of Malyshev and Tsaregradskii (1982) imply that this chain is ergodic if $\frac{1}{2}\alpha \leq \alpha' \leq p < \alpha$.

From the solution of the previous section with exactly the same function we can say that this chain is transient if $\alpha' < \alpha p/(\alpha+p) < p < \alpha$ and $n \geq 4$ even (rather than n odd).

REFERENCES

Dobrushin, R. L., V. I. Kryukov, and A. L. Toom, (1978), *Locally Interacting Systems and their Application in Biology*, Lecture Notes in Mathematics 653. New York: Springer-Verlag.

Foster, F. G. (1953), "On the stochastic matrices associated with certain queueing processes." *Annals of Mathematical Statistics* **24**, 355–360.

Karlin, S., and H. M. Taylor (1975), *A First Course in Stochastic Processes*, 2nd edition. New York: Academic Press.

Malyshev, V. A. (1972), "Classification of two-dimensional positive random walks and almost linear semimartingales." *Soviet Mathematics—Doklady* **13**, 136–139.

Malyshev, V. A., and M. V. Menshikov (1981), "Ergodicity, continuity and analyticity of countable Markov chains." *Transactions of the Moscow Mathematical Society* 1–48.

Malyshev, V. A., and I. P. Tsaregradskii (1982), "A queueing system with local interaction." *Theory of Probability and its Applications* **27**, 619–624.

Menshikov, M. V. (1974), "Ergodicity and transience conditions for random walks in the positive octant of space." *Soviet Mathematics—Doklady* **15**, 1118–1121.

R. J. Kulperger [1]

CENTRAL LIMIT THEOREMS FOR CLUSTER POINT PROCESSES

1. INTRODUCTION

An interesting class of stationary point processes on $\mathbf{R}^d$ is the class of Poisson cluster processes. Consider a parent process $\mathbf{N}$ and a countable sequence of independent and identically distributed (i.i.d.) point processes Y_i on $\mathbf{R}^d$. Each point mass x in $\mathbf{N}$ is replaced by an independent copy of Y centered at x. If $\mathbf{N}$ is a Poisson process, the resulting point process $\mathbf{X}$ is said to be a Poisson cluster point process (Poisson C.P.P.).

Let A be a convex set, centered at 0, and $TA = \{Tx : x \in A\}$, that is TA is the set A scaled up, or expanded, in every direction by a factor $T > 0$. $\mathbf{X}$ is observed on the set TA. Since $TA \uparrow R^d$ as $T \to \infty$, for a fixed A, the asymptotics or limit theorems on $\mathbf{X}$ are obtained as $T \to \infty$, that is when $\mathbf{X}$ is observed on increasingly large sets TA. Central limit theorems (CLT's) have been obtained for $X(TA)$ in the Poisson C.P.P. by Westcott (1972), when $d = 1$ and Y has 2 moments, and by Ivanoff (1980, 1982) when $d \geq 1$ and Y has 3 or 4 moments. Ivanoff (1982) also obtained a functional CLT for $X(T\mathrm{t}A)$, $\mathrm{t} \in [0,1]^d$. Burton and Waymire (1984) also discussed the $d \geq 1$ case and obtained a functional CLT with only a condition of summable covariances by using a notion of positive association. The main tool they used is the probability generating functional (P.G.F.). Ivanoff (1982) also considered other methods on more general point processes. The P.G.F. is not such a useful tool in studying second order statistics of Poisson C.P.P.'s.

Suppose most of the mass of the clusters are contained in a compact set C. When TA is large, $\mathbf{X}$ observed on TA is nearly a random sum of i.i.d. clusters with different centres, ignoring edge effects on TA. CLT's for $X(TA)$ are then, roughly, consequences of random norming CLT's of the type given by Billingsley (1968, Theorem 17.1).

[1] Department of Statistical and Actuarial Sciences, The University of Western Ontario, London, Ontario N6A 5B9

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 131–139.

In this paper, this notion is made more precise. It is not assumed that $\mathbf{N}$ is a Poisson process, but that it satisfies some conditions. The various assumptions are given in Section 2. In Section 3, a CLT and a functional CLT are obtained under a few moment conditions on the clusters Y. In terms of moment conditions on Y, these conditions are weaker than Ivanoff's for the CLT, but are stronger for the version of the functional CLT obtained here. Kulperger (1979) required an infinite number of moments for a similar CLT.

The methods used here should be more useful in the study of higher order intensity estimates for Poisson C.P.P.'s.

2. DEFINITIONS AND ASSUMPTIONS

$\mathbf{N}$ is a simple stationary point process, and Y_i, $i \geq 1$, is an i.i.d. sequence of simple point processes independent of $\mathbf{N}$ (for definitions, see Moyal, 1962).

Definition. $\mathbf{X}$ defined by

$$X(A) = \sum_{x \in \mathbf{N}} Y_x(A - x)$$

is said to be a (simple) C.P.P.

Since $\mathbf{N}$ is a simple point process, all of its point masses are isolated, so the definition is sensible. The notation is $X(A)$ = number of points of the $\mathbf{X}$ process in A and a similar definition for Y_x, the cluster replacing the $\mathbf{N}$-point mass at x. As will be seen later, under some moment conditions on Y, for compact A, $X(A)$ is almost surely finite. The point processes Y are called the cluster mechanisms or simply the clusters.

Some assumptions on $\mathbf{N}$ and Y are now given. If $\mathbf{N}$ is a Poisson process, it satisfies all the assumptions made here. If $\mathbf{N}$ is a strong mixing process or a Poisson C.P.P., with appropriate moment assumptions it will also satisfy the assumptions made here (Ivanoff, 1982).

Some notation used is the following:

(i) $p_{\mathbf{N}}$, $p_{\mathbf{N}}(x)$, $p_{\mathbf{N}}(x_1, x_2)$, $p_{\mathbf{N}}(x_1, x_2, x_3)$, $c_{\mathbf{N}}(x)$ are the first order through fourth order intensities and covariance density, respectively, of $\mathbf{N}$,

(ii) $p_Y(x)$, $p_Y(x, y), \ldots$, are the first and second order intensity (and so on), functions of the cluster mechanism, and

(iii) $\mu_Y = \int_{R^d} p_Y(x)dx = E(Y(R^d))$ = expected cluster size. Notice $p_{\mathbf{N}}(x)$ is a function of only one variable since $\mathbf{N}$ is stationary.

For $\delta > 0$, let $A_\delta = \{x : d(x, A) \leq \delta\}$ and $A^\delta = \{x : d(x, A^c) > \delta\}$, where d is Euclidean distance. $A \setminus B$ means the set difference A minus B.

The following assumptions will be made in various parts of the next section.

A.1 $Y(R^d)$ has two finite moments, $E(Y(R^d)^2) < \infty$, and $\mathbf{N}$ has two locally finite moments and $\int \mid c_{\mathbf{N}}(u) \mid du < \infty$.

A.2 Let $h : \mathbf{R}^d \to \mathbf{R}$ with $\int \mid h(y) \mid dy < \infty$, and for $0 \leq t \leq 1$,

$$U_T'(t) = T^{-d/2} \left\{ \int_{(TtA)^\delta \setminus (TtA)_\delta} \int_{TtA} h(y-x)dy(N(dx) - p_N dx) \right\}$$

Then

$$\sup_{0 \leq t \leq 1} |U_T'(t)| \xrightarrow{Pr} 0 \quad T \to \infty.$$

A.3 Suppose $\mathbf{N}$ satisfies a functional CLT: for A convex and compact, for $0 \leq t \leq 1$,

$$T^{-d/2}(N(TtA) - p_{\mathbf{N}} \mid TtA \mid) \Rightarrow \mid A \mid^{\frac{1}{2}} \sigma_{\mathbf{N}} B_1(t),$$

where B_1 is a standard Brownian motion and $\sigma_{\mathbf{N}}^2 = p_{\mathbf{N}} + \int c_{\mathbf{N}}(u)du$.

A.4 The cluster size $Y(R^d)$ has four finite moments, and $\mathbf{N}$ has four factorial moment intensities which are integrable in the same sense that

$$\int p_{\mathbf{N}}(x)dx < \infty, \quad \int \int p_{\mathbf{N}}(x_1, x_2)dx_1 dx_2 < \infty$$

and

$$\int \int \int p_{\mathbf{N}}(x_1, x_2, x_3)dx_1\, dx_2\, dx_3 < \infty.$$

A.5 There exists a $\delta_0 > 0$ such that for all $\delta \geq \delta_0$,

$$T^{-d/4} \sup_{0 \leq s \leq T} N((sA)^\delta \setminus (sA)_\delta) \xrightarrow{\Pr} 0 \text{ as } T \to \infty.$$

See Leadbetter *et al.* (1983) for various types of mixing conditions for which A.5 could hold.

The following formula will be useful in the next section, and can be obtained in a straightforward way.

Lemma 2.1. For a C.P.P. X, the first moment and covariance function are given as follows:

(*i*) $$E(X(A)) = p_{\mathbf{N}} \mu_Y \mid A \mid .$$

(ii)

$$\operatorname{Cov}(X(A), X(B)) = p_{\mathbf{N}}\mu_Y \mid A \cap B \mid + p_{\mathbf{N}} \int_{R^d} \int_A \int_B p_Y(y_1 - x, y_2 - x) c_N(x) dy_2 dy_1 dx.$$

If $\mathbf{N}$ has independent increments, that is, it is a Poisson process, then $c_{\mathbf{N}}(u) = 0$ for $u \neq 0$.

3. THE CENTRAL LIMIT THEOREMS

Let $C \subseteq \mathbf{R}^d$ be a compact rectangle centred at 0. For a cluster Y_x centered at x, write $Y_x = Y_x^C + Y_x^R$, where Y_x^C and Y_x^R are the parts on $C+x$ and the remainder. In obvious notation, one can decompose $\mathbf{X} = \mathbf{X}^C + \mathbf{X}^R$. The process $\mathbf{X}^C$ is a C.P.P. in which the cluster mechanism has compact support. Let δ = diameter (C). If $\mathbf{X}^C$ has a point mass in A, then its $\mathbf{N}$-parent must lie in A^δ. CLT's for the simpler process $\mathbf{X}^C$ and then it is shown that the remainder process $\mathbf{X}^R$ is not too large.

Let A be a convex set in $\mathbf{R}^d$ with 0 in the interior of A. Let $0 \leq t \leq 1$. Observe $\mathbf{X}$ on TA. $TA \uparrow R^d$ as $T \to \infty$. For each T and A, $\{TtA : 0 \leq t \leq 1\}$ is a nested family of sets indexed by $[0,1]$, and for $s \leq t$, $sA \subseteq tA$. For each T and A, $X(TtA)$ is a stochastic process indexed by $[0,1]$, and for $0 \leq s \leq t \leq 1$, $X(TsA) \leq X(TtA)$.

$$\begin{aligned} X(TtA) - p_{\mathbf{N}}\mu_Y \mid TtA \mid &= \int_{\mathbf{R}}^d Y_x(TtA - x)N(dx) - p_{\mathbf{N}}\mu_Y \mid TtA \mid \\ &= \int_{\mathbf{R}}^d Y_x^C(TtA - x)N(dx) - p_{\mathbf{N}}\mu_Y^C \mid TtA \mid \quad (3.1) \\ &\quad + \int_{\mathbf{R}}^d Y_x^R(TtA - x)N(dx) - p_{\mathbf{N}}\mu_Y^R \mid TtA \mid, \end{aligned}$$

where $\mu_Y = \int_C p_Y(y)dy + \int_{C^c} p_Y(y)dy \stackrel{\text{def}}{\equiv} \mu_Y^C + \mu_Y^R$. The CLT for $\mathbf{X}$ is obtained from the case $t = 1$.

Lemma 3.1. Suppose A.1 holds. Let $\epsilon > 0$, $\gamma > 0$. Take C so large that

$$E(Y^R(\mathbf{R}^d)^2) \leq \{\mid A \mid p_{\mathbf{N}} + \int_{\mathbf{R}^d} C_{\mathbf{N}}(u)du\}^{-1} \epsilon\gamma^2.$$

Then

$$P(T^{-d/2} \mid X^R(TA) - p_{\mathbf{N}}\mu_Y^R \mid TA \mid\mid \geq \gamma) \leq \epsilon$$

for T sufficiently large.

Proof. Apply Lemma 2.1 to the C.P.P. $\mathbf{X}^R$ to calculate $T^{-d}\mathrm{Var}(\mathrm{X^R(TA)})$. Also noting, for example,

$$\begin{aligned} & T^{-d}\int_{\mathrm{R}^d}\int_{TA}\int_{TA} p_Y^R(y_1-x,y_2-x)dy_2dy_1dx \\ & \leq T^{-d}\int_{TA}\int_{R^d}\int_{R^d} p_Y^R(y_1-x,y_2-x)dy_2dxdy_1 \\ & \leq |\,A\,|\,E[Y(\mathbf{R}^d)(Y(\mathbf{R}^d)-1)] \end{aligned}$$

and a similar bound for the last term from Lemma 2.1, this lemma follows from Chebyshev's inequality.

Consider the first term on the right hand side (RHS) of (3.1).

$$\begin{aligned} & \int_{R^d} Y_x^C(TtA-x)N(dx) - p_N\mu_Y^C|TtA| \\ & \quad = \int_{(TtA)^\delta\setminus(TtA)_\delta} X_x^C(TtA-x)N(dx) \\ & \qquad - E\left[\int_{(TtA)^\delta\setminus(TtA)_\delta} Y_x^C(TtA-x)N(dx)\right] \\ & \qquad + \int_{(TtA)_\delta} Y_x^C(R^d)N(dx) - E\left[\int_{(TtA)_\delta} Y_x^C(R^d)N(dx)\right], \quad (3.2) \end{aligned}$$

since if $x \in B_\delta$ then $Y_x^C(B) = Y_x^C(R^d)$. A central limit theorem is now obtained for $X(TA)$.

Theorem 3.2 Suppose A.1 holds. Then

$$T^{-d/2}(X(TA) - p_{\mathrm{N}}\mu_Y\,|\,TA\,|) \Rightarrow N(0,\sigma_{\mathrm{X}}^2\,|\,A\,|),$$

where $\sigma_{\mathrm{X}}^2 = p_{\mathrm{N}}\mathrm{Var}(\mathrm{Y}(\mathrm{R}^{\mathrm{d}})) + \mu_{\mathrm{Y}}^2\sigma_{\mathrm{N}}^2$.

Proof. Consider (3.1) and (3.2) at $t=1$, and multiply by $T^{-d/2}$. In Lemma 3.1 take $\epsilon = \gamma$ and C so large that the remainder term from (3.1) is at most ϵ with probability $\geq 1-\epsilon$ for T sufficiently large. By direct calculation

$$T^{-d}\mathrm{Var}\left(\int_{(TA)^\delta\setminus(TA)_\delta} Y_x^C(TA-x)N(dx)\right) = O(T^{-1}).$$

Therefore $T^{-d/2}$ (first term on RHS of (3.2)) $\xrightarrow{\Pr} 0$. A law of large numbers argument gives $T^{-d}N((TA)_\delta) \xrightarrow{\Pr} p_N \mid A \mid > 0$. Therefore by a minor variation of the simple random norming CLT (Billingsley, 1968, Theorem 17.1),

$$T^{-d}\left\{\int_{(TA)^\delta} Y_x^C(R^d)N(dx) - E\left[\int_{(TA)_\delta} Y_x^C(R^d)N(dx)\right]\right\} \Rightarrow N(0,V(C)),$$

where the limiting variance $V(C) \uparrow \sigma_X^2 \mid A \mid$ as $C \uparrow R^d$. Since $\epsilon > 0$ is arbitrary, the theorem will follow.

Next a functional CLT is obtained. Let

$$W_T(t) = T^{-d/2}(X(TtA) - p_N\mu_Y \mid TtA \mid), \quad 0 \le t \le 1. \tag{3.3}$$

Another interesting version is to replace the index set $[0,1]$ by $[0,1]^d$, as has been done by Ivanoff (1982). Here the index set $[0,1]$ is used so that the truncation method is not obscured. Basically the same methods can be used in the $[0,1]^d$ index case.

Lemma 3.3. Suppose A.4 holds and let $0 \le t_1 < t < t_2 \le 1$. Then for some constant K depending on $\mathbf{N}$, but not t_1, t, t_2 or the cluster mechanism,

$$E\{[W_T(t_2) - W_T(t)]^2[W_T(t) - W_T(t_1)]^2\}$$
$$\le K\ E[Y(\mathbf{R}^d)^4] \mid A \mid^2 (t_2^d - t_1^d)^2.$$

Proof. By first conditioning on $\mathbf{N}$, this is a straightforward but tedious computation, similar to that in Lemma 3.1.

Corollary 3.4. Suppose A.4 holds. For any $\epsilon > 0$, $\gamma > 0$, there exists C sufficiently large so that for all T sufficiently large,

$$P\left\{\sup_{0\le t\le 1} T^{-d/2}\left|X^R(TtA) - p_N\mu_Y^R \mid TtA \right|\right| \ge \gamma\right\} \le \epsilon.$$

Proof. A proof of this can follow the details of the proof given by Billingsley (1968, Theorem 15.6, pp. 128–30), yielding in place of (15.30), upon using Lemma 3.3,

$$P\{w''(W_T,\delta_1) \ge \epsilon\} \le \frac{2K_1}{\epsilon^4} \mid A \mid \sqrt{KE(Y(\mathbf{R}^d)^4}\cdot 2\delta_1 d(1+2\delta_1)^{d-1},$$

where K_1 is some constant and w'' is the modulus of continuity on p. 118 of Billingsley. Combining this with Lemma 3.1 yields the corollary.

A functional CLT for the family of random variables $X(TtA)$, $0 \le t \le 1$, is now obtained. Recall $\{TtA : 0 \le t \le 1\}$ is a nested family of subsets of TA.

Theorem 3.5. Under assumptions A.2 – A.5,

$$W_T(t) \Rightarrow | A |^{1/2} \sigma_{\mathbf{X}} B(t), \quad 0 \le t \le 1,$$

where B is standard Brownian motion and $\sigma_{\mathbf{X}}$ is given in Theorem 3.2, and W_T is given by (3.3).

Proof. Let $\epsilon > 0$. In Corollary 3.4, take $\gamma = \epsilon$ and C sufficiently large. Following (3.1), write $W_T(t) = U_T(t) + T^{-d/2}(X^R(TtA) - p_{\mathbf{N}}\mu_Y^R \mid TtA \mid)$, where $U_T(t) = T^{-d/2}(X^C(TtA) - p_{\mathbf{N}}\mu_Y^C \mid TtA \mid)$. By Corollary 3.4,

$$\sup_{0 \le t \le 1} | W_T(t) - U_T(t) | \xrightarrow{\Pr} 0 \text{ as } T \to \infty, \tag{3.4}$$

where

$$\begin{aligned} U_T(t) = {} & T^{-d/2} \int_{(TtA)_\delta} (Y_x^C(\mathbf{R}^d) - \mu_Y^C) N(dx) \\ & + \mu_Y^C T^{-d/2}(N((TtA)_\delta) - p_{\mathbf{N}} \mid (TtA)_\delta \mid) \\ & + T^{-d/2} \left\{ \int_{(TtA)^\delta \setminus (TtA)_\delta} [Y_x^C(TtA - x) - \int_{(TtA)} p_Y^C(y - x)dy] N(dx) \right\}. \\ & + T^{-d/2} \left\{ \int_{(TtA)^\delta \setminus (TtA)_\delta} \left[\int_{TtA} p_Y^C(y - x)dy \right] N(dx) \right. \\ & \left. - p_{\mathbf{N}}\mu_Y^C(\mid TtA \mid - \mid (TtA)_\delta \mid) \right] \Big\} \end{aligned}$$

Each term on the RHS has mean 0. By A.2, $\sup_t \mid \text{last term} \mid \xrightarrow{\Pr} 0$. For the third term proceed as follows: conditional on $\mathbf{N}$, $Y_x(TtA - x) \le Y_x(\mathbf{R}^d)$, an i.i.d. sequence with finite fourth moments. Then

$$N(TA)^{-1/4} \sup_{x \in TA} Y_x(TtA - x) \to 0,$$

since $T^{-d}N(TA) \to p_N \mid A \mid > 0$. Then using A.5,

$$T^{-d/2} \int_{(Tta)^\delta \setminus (TtA)_\delta} Y_x(TtA - x)N(dx)$$
$$= O_p\left(N(TA)^{-1/4} \sup_x Y(TtA - x)\right)$$
$$\cdot T^{-d/4} \sup_t (N(TtA)\delta \setminus (TtA)_\delta)) \xrightarrow{\Pr} 0.$$

The other part of the third term is handled similarly. By a minor variation on the simple random norming CLT (Billingsley, 1968, Theorem 17.1) and A.3 we then obtain

$$U_T(t) \Rightarrow (|A|p_N\mu_Y^C \mathrm{Var}(Y^C(\mathbf{R}^d)))^{\frac{1}{2}} B_1(t) + (|A|\mu_Y^C\sigma_N^2)^{\frac{1}{2}} B_2(t)$$
$$\stackrel{D}{=} |A|^{\frac{1}{2}}\sigma_X^C B(t), \tag{3.5}$$

since B_1 and B_2 are independent Brownian motions, and $\sigma_{\mathbf{X}}^C$ is given by $\sigma_{\mathbf{X}}$ with $\mathbf{X}^C$ replacing $\mathbf{X}$. Also $\sigma_{\mathbf{X}}^C \to \sigma_{\mathbf{X}}$ as $C \uparrow R^d$. Since $\epsilon > 0$ is arbitrary, the theorem now follows from (3.4) and (3.5).

4. REMARKS

In Theorems 3.2 and 3.5, the constant $\sigma_{\mathbf{X}}^2$ appears. However, $\sigma_{\mathbf{X}}^2 = (2\pi)^d f_{\mathbf{X}}(0)$, where $f_{\mathbf{X}}$ is the spectral density of $\mathbf{X}$. Under A.4, $\mathbf{X}$ has four moments. It can then be shown that a consistent estimate of $f_{\mathbf{X}}(0)$ can be constructed by a weighted sum of periodograms (see Brillinger (1978) for relevant details, or Kulperger (1982) for a similar time series example). In this way Theorem 3.5 or its analogues can be used to construct a graphical test of constancy of the first order intensity of a C.P.P.

The methods used here may be used to obtain results on higher order intensity estimates of Poisson C.P.P.'s, under mild moment conditions. By conditioning on N, the C.P.P. observed on a large set is then viewed as a superposition of randomly centred i.i.d. point processes, except for some edge effects. These types of statistics are currently under investigation.

In the case of the CLT (Theorem 3.2) with compact clusters and $\mathbf{N}$ being Poisson, a direct proof could also be obtained by using Lindeberg-Feller type conditions and a method similar to that used to prove a CLT for sums of an M-dependent process (see, for example, Rao (1984) for the M-dependent CLT).

ACKNOWLEDGMENT

This work has been supported under NSERC grant number A5724.

REFERENCES

Billingsley, P. (1968), *Convergence of Probability Measures.* New York: Wiley and Sons.

Brillinger, D. R. (1978), "Comparative aspects of the study of ordinary time series and point processes." *Developments in Statistics* **1**, 33–133.

Burton, R. M., and E. Waymire (1984), "Scaling limits for point random fields." *Journal of Multivariate Analysis* **15**, 237–251.

Ivanoff, B. G. (1980), "The branching random field." *Advances in Applied Probability* **12**, 825–847.

Ivanoff, B. G. (1982), "Central limit theorems for point processes." *Stochastic Processes and Their Applications* **12**, 171–186.

Kulperger, R. J. (1979), "Parametric estimation for a simple branching diffusion process." *Journal of Multivariate Analysis* **9**, 101–115.

Kulperger, R. J. (1982), "Testing for non-linear shifts in stationary ϕ-mixing processes." In *Time Series Methods in Hydrosciences*, ed. A. El-Sharaawi and S.R. Esterby, pp. 37–44. Amsterdam: Elsevier.

Leadbetter, M. R., G. Lindgren, and H. Rootzen (1983), *Extremes and Related Properties of Random Sequences and Processes.* New York: Springer-Verlag.

Moyal, J. E. (1962), "The general theory of stochastic population processes." *Acta Mathematica* **108**, 1–31.

Rao, M. M. (1984), *Probability Theory with Applications.* New York: Academic Press.

Westcott, M. (1972), "The probability generating functional." *Journal of the Australian Mathematical Society* **14**, 448–466.

B. L. S. Prakasa Rao [1]

ASYMPTOTIC THEORY OF ESTIMATION IN NONLINEAR REGRESSION

1. INTRODUCTION

Nonlinear regression models occur frequently in the modeling of stochastic phenomena. Several examples of such modeling are given by Bard (1974). The study of asymptotic properties of the least squares estimator (LSE) for parameters occurring in nonlinear regression has been the subject of investigation by several authors in view of the fact that it is, in general, difficult to obtain the exact distribution of the LSE for any fixed sample. Malinvaud (1970), Jennrich (1969), Bunke and Schmidt (1980) and Wu (1981) are a few authors among the many who have investigated the asymptotic properties of the LSE in nonlinear regression. Schmidt (1982) has given a survey of testing of hypotheses in nonlinear regression. All the earlier work cited above on asymptotic distribution theory for least squares estimators in nonlinear regression models assume regularity conditions which include, in particular, the condition on the twice differentiability of the regression function with respect to the parameter in a neighbourhood of the true value in addition to other conditions. Schmidt (1982, p. 18) says that "up to my knowledge, there is no idea how to prove the asymptotic normality of the LSE when $g(x, \theta)$ is not differentiable with respect to θ since all the proofs use the normal equations". Recently we have given an alternate approach for the study of asymptotic distribution theory. The least squares is considered as a stochastic process in the parameter and the limiting distribution, if any, is obtained via the study of weak convergence of the least squares process. A similar approach was used for the first time in obtaining the asymptotic distribution of the maximum likelihood estimator for the estimation of the location of the cusp of a continuous density by Prakasa Rao (1968). We present a brief survey of some recent results in the asymptotic theory of least squares estimators. These include the rates of convergence,

[1] Indian Statistical Institute, 7, SJS Sansanwal Marg, New Delhi, India 110 016

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 141–165.

among others.

It has been noticed that, even in linear models, the least modulus estimator (LME) is better in performance than the least squares estimator when errors have a heavy tailed distribution. Even though analytically the LME is not tractable and it is difficult to get a closed form expression for the LME in general, computationally it is no longer a problem to obtain the LME. For instance, in linear models it can be reduced to a linear programming problem which can be solved using standard techniques. An excellent discussion of the LME and its properties in linear models are given by Basser and Koenker (1978) and Taylor (1974). We discuss some recent work of Ivanov (1984b) on the rate of consistency and asymptotic normality of the least modulus estimator for nonlinear regression models. For applications of the least modulus estimators, see Bloomfield and Steiger (1983).

2. PRELIMINARIES

Consider a nonlinear regression model

$$X_j = g_j(\theta) + \varepsilon_j, \ j \geq 1, \tag{2.1}$$

where ε_j, $j \geq 1$ are random variables with $E(\varepsilon_j) = 0$, $j \geq 1$ and $\theta \in \Theta \subset R^k$. Let

$$Q_n(\theta) = \sum_{j=1}^{n} [X_j - g_j(\theta)]^2 , R_n(\theta) = \sum_{j=1}^{n} | X_j - g_j(\theta) | \tag{2.2}$$

and $\mathbf{B}^k$ denote the Borel σ-algebra of subsets of R^k. A $\mathbf{B}^n$-measurable mapping $\hat{\theta}_n : R^n \to \bar{\Theta}$ for which

$$Q_n(\hat{\theta}_n) = \inf_{\theta \in \Theta} Q_n(\theta) \tag{2.3}$$

is called a *least squares estimator* (LSE) for the parameter θ based on the observations $X_1, \ldots, X_n$. Here $\bar{\Theta}$ denotes the closure of the set Θ. A $\mathbf{B}^n$-measurable mapping $\theta_n^* : R^n \to \bar{\Theta}$ for which

$$R_n(\theta_n^*) = \inf_{\theta \in \bar{\Theta}} R_n(\theta) \tag{2.4}$$

is called a *least modulus estimator* (LME) for the parameter θ based on the observations $X_1, \ldots, X_n$.

Lemma 2.1. Suppose $u(x, \theta)$ is continuous in $\theta \in \Theta \subset R^k$ and measurable in x for any fixed $\theta \in \Theta$. Suppose further that Θ is compact. Then there exists a measurable function $\theta(x)$ such that

$$u(x, \theta(x)) = \inf_{\theta \in \Theta} u(x, \theta). \tag{2.5}$$

For a proof of this lemma, see Schmetterer (1974, p. 307). As a consequence of this lemma, it follows that a sufficient condition for the existence of either a LSE or a LME is that the sequence of functions $g_j(\theta)$ are continuous in θ for $j \geq 1$ and Θ is compact in R^k.

In the following discussion, we assume that there exists a measurable LSE $\hat{\theta}_n$ or LME θ_n^*.

The notion of a minimum contrast estimator (MCE) has been introduced by Pfanzagl (1968). This generalizes the concept of a maximum likelihood estimator (MLE) for independent and identically distributed (i.i.d.) observations. He obtained the Berry-Esseen type bound for the distribution function of a MCE (Pfanzagl, 1971). The concept of a contrast function has been generalized by Prakasa Rao (1975) to a sequence of families of contrast functions and a Berry-Esseen type bound for the distribution function of a MCE is obtained by Prakasa Rao (1975) for the case of independent but not necessarily identically distributed (i.n.i.d.) observations. It can be shown that the least squares estimator (LSE) and the least modulus estimator (LME) are special cases of the minimum contrast estimators, discussed by Prakasa Rao (1975), for suitable choices of contrast functions. These results pertain to the case when θ is a scalar. Pfanzagl (1973) extended his results to a vector parameter case. However, the extension of his results in the vector parameter case for i.n.i.d. random vectors has not been done as far as this author is aware of, even though it should be possible to do the same in principle. In view of the fact that the concept of MCE is more general than a LSE or a LME, the regularity conditions imposed to obtain the rates of convergence and the Berry-Esseen type bound for the MCE are much stronger than are needed to obtain the same for the LSE or the LME directly. In the following discussion, we will not pursue this approach. For a discussion of the results via this approach, see Prakasa Rao (1985) and Ivanov and Kozlov (1981).

3. CONSISTENCY AND RATE OF CONVERGENCE FOR LSE

3.1 Scalar Parameter Case

Consider a nonlinear regression model

$$X_i = g_i(\theta) + \varepsilon_i, \quad i \geq 1, \tag{3.1}$$

where $\theta \in \Theta \subset R$ and $\{\varepsilon_i, i \geq 1\}$ is a sequence of random variables with $E(\varepsilon_i) = 0$, $i \geq 1$.

Theorem 3.1. (Ivanov, 1976). Suppose that ε_i, $i \geq 1$ are i.i.d. random variables with $E \mid \varepsilon_1 \mid^s < \infty$ for some integer $s \geq 2$. Further suppose that there exists $0 < K_1 \leq K_2 < \infty$ such that

$$nK_1(\theta_1 - \theta_2)^2 \leq \sum_{j=1}^{n} [g_j(\theta_1) - g_j(\theta_2)]^2 \leq n K_2(\theta_1 - \theta_2)^2 \tag{3.2}$$

for all θ_1, θ_2 in Θ. Then there exists a constant $c > 0$ independent of n and ρ such that

$$P_{\theta_0}\left\{n^{\frac{1}{2}} \mid \hat{\theta}_n - \theta_0 \mid > \rho\right\} \leq c\rho^{-s} \tag{3.3}$$

for every $\rho > 0$.

Let θ_0 denote the true parameter. Note that

$$\begin{aligned} Q_n(\theta_0) &= \sum_{i=1}^{n} \varepsilon_i^2 = \sum_{i=1}^{n} [X_i - g_i(\theta_0)]^2 \\ &\geq \sum_{i=1}^{n} [X_i - g_i(\hat{\theta}_n)]^2 \\ &= \sum_{i=1}^{n} \varepsilon_i^2 + n\,\Psi_n(\hat{\theta}_n, \theta_0) - 2n\,U_n(\hat{\theta}_n)\Psi_n(\hat{\theta}_n, \theta_0), \end{aligned} \tag{3.4}$$

where

$$U_n(\theta) = \begin{cases} \frac{1}{n}\sum_{j=1}^{n} \varepsilon_j \left\{\frac{g_j(\theta) - g_j(\theta_0)}{\Psi_n(\theta, \theta_0)}\right\}, & \theta \neq \theta_0 \\ 0, & \theta = \theta_0 \end{cases}$$

and

$$n\Psi_n(\theta_1, \theta_2) = \sum_{i=1}^{n} [g_i(\theta_1) - g_i(\theta_2)]^2. \tag{3.6}$$

Relation (3.4) implies that, for any $\varepsilon > 0$,

$$P_{\theta_0}\left(\mid \hat{\theta}_n - \theta_0 \mid > \varepsilon\right) \leq P_{\theta_0}\left\{\sup_{\mid \theta - \theta_0 \mid > \varepsilon} \mid U_n(\theta) \mid \geq \frac{1}{2}\right\}.$$

In particular, for any $\rho > 0$,

$$\begin{aligned} P_{\theta_0}\left\{n^{\frac{1}{2}} \mid \hat{\theta}_n - \theta_0 \mid > \rho\right\} &\leq P_{\theta_0}\left\{\sup_{\mid \theta - \theta_0 \mid > \rho} \mid U_n(\theta) \mid \geq \frac{1}{2}\right\} \\ &\quad + P_{\theta_0}\left\{\sup_{\rho n^{-\frac{1}{2}} < \mid \theta - \theta_0 \mid \leq \rho} \mid U_n(\theta) \mid \geq \frac{1}{2}\right\}. \end{aligned}$$

It can be checked that there exists $c_1 > 0$ and $c_2 > 0$ such that

$$P_{\theta_0}\left\{\sup_{|\theta-\theta_0|>\rho} |\, U_n(\theta)\,| \geq \frac{1}{2}\right\} \leq c_1\rho^{-e}$$

and

$$P_{\theta_0}\left\{\sup_{\rho n^{-\frac{1}{2}}<|\theta-\theta_0|\leq\rho} |\, U_n(\theta)\,| \geq \frac{1}{2}\right\} \leq c_2\rho^{-e}$$

(for details, see Ivanov, 1976, or Prakasa Rao, 1984a). The last inequality follows from studying the oscillations of the stochastic processes

$$\{V_n(\theta), \theta \in [m^\theta, (m+1)^\theta]\}, \qquad n \geq 1,$$

where

$$V_n(\theta) = \frac{1}{n^{\frac{1}{2}}}\sum_{j=1}^{n}\varepsilon_j\{g_j(\theta) - g_j(\theta_0)\},$$

$$m^\theta = \theta_0 + \rho n^{-\frac{1}{2}} + m\rho\left[n^{\frac{1}{2}}\right]^{-1}.$$

This result has been generalized by Prakasa Rao (1984a) to the case when $\{\varepsilon_i,\ i \geq 1\}$ form a dependent sequence not necessarily identically distributed.

Theorem 3.2. (Prakasa Rao, 1984a). Let $\{\varepsilon_j, j \geq 1\}$ be a ϕ-mixing process satisfying the following conditions:

(i)

$$E(\varepsilon_i) = 0, \qquad i \geq 1 \quad \text{and} \quad \sup_i E\,|\,\varepsilon_i\,|^4 < \infty,$$

(ii)

$$\sum_{i=1}^{\infty}(i+1)\{\phi(i)\}^{\frac{1}{2}} < \infty, \tag{3.7}$$

where $\phi(\cdot)$ is the mixing coefficient. Further suppose that the condition (3.2) holds. Then there exists a constant $c > 0$ independent of n and $\rho > 0$ such that, for every $\rho > 0$,

$$P_{\theta_0}\left\{n^{\frac{1}{2}}\,|\,\hat{\theta}_n - \theta_0\,| > \rho\right\} \leq c\rho^{-4}. \tag{3.8}$$

Remark 3.1. This result continues to hold if $\{\varepsilon_i\}$ is a strong-mixing process provided there exists $\delta > 0$ such that

(i)

$$E(\varepsilon_i) = 0, \quad i \geq 1 \text{ and } \sup_i E \mid \varepsilon_i \mid^{4+2\delta} < \infty,$$

(ii)

$$\sum_{i=1}^{\infty} (i+1) \{\alpha(i)\}^{\delta/(4+\delta)} < \infty, \tag{3.7}'$$

where $\alpha(\cdot)$ is the strong mixing coefficient (see Prakasa Rao, 1984a). One can prove an analogous result under some conditions for an absolutely regular sequence $\{\varepsilon_i, i \geq 1\}$ by using some inequalities due to Yoshihara (1978). Note that the condition of absolute regularity is weaker than ϕ-mixing or strong mixing. For results on the strong consistency of least squares estimator in nonlinear regression model, see Ivanov and Kozlov (1981) or Wu (1981) when the errors are i.i.d. and Nelson (1980) when the errors form a martingale difference sequence. Observe that, as a consequence of (3.8), it follows that eventually

$$n^{\frac{1}{2}} \mid \hat{\theta}_n - \theta_0 \mid \leq n^{\gamma} \text{ a.s.} [P_{\theta_0}] \tag{3.9}$$

whenever $1/4 < \gamma < 1/2$ by the Borel-Cantelli lemma. In particular, it follows that

$$\hat{\theta}_n \to \theta_0 \text{ a.s.} [P_{\theta_0}] \text{ as } n \to \infty. \tag{3.10}$$

Theorem 3.2 stated above can also be generalized to the case of a weighted least squares estimator provided the sequence of weights is bounded (see Prakasa Rao, 1984a). The rate obtained in Theorem 3.1 or Theorem 3.2 can be improved when the errors $\{\varepsilon_i\}$ form an i.i.d. Gaussian sequence.

Theorem 3.3. (Prakasa Rao, 1984b). Let $\{\varepsilon_j, j \geq 1\}$ be i.i.d. Gaussian random variables with mean 0 and known variance σ^2. Further suppose that the condition (3.2) holds. Then there exists constants $B > 0$ and $b > 0$ such that

$$P_{\theta_0} \left\{ n^{\frac{1}{2}} \mid \hat{\theta}_n - \theta_0 \mid > \rho \right\} \leq B \, e^{-b\rho^2} \tag{3.11}$$

for every $\rho > 0$ and $n \geq 1$.

The bounds obtained in the inequalities (3.3), (3.8) and (3.11) can be shown to be uniform on compact sets $K \subset \Theta$.

The proof of the last theorem can be given by considering

$$Z_n(\phi) = \exp \left\{ \frac{1}{2} (Q_n(\theta) - Q_n(\theta + \phi n^{-\frac{1}{2}})) \right\}$$

as a stochastic process with ϕ as the index for any fixed $\theta \in \Theta$ and studying the oscillation of the process. Note that for any $\rho > 0$,

$$P_\theta \left(n^{\frac{1}{2}} \mid \hat{\theta}_n - \theta \mid > \rho \right) \leq P_\theta \left\{ \sup_{|\phi| \geq \rho} Z_n(\phi) \geq 1 \right\}.$$

For details, see Prakasa Rao (1984b).

3.2 Vector Parameter Case

Let us now consider the nonlinear regression model

$$X_i = g_i(\theta) + \varepsilon_i, \ i \geq 1, \tag{3.12}$$

where $\theta \in \Theta \subset R^k$ and $\{\varepsilon_i\}$ is a sequence of random variables with $E(\varepsilon_i) = 0$ for all $i \geq 1$.

The following result gives the rate of convergence of the LSE in this case.

Theorem 3.4. (Prakasa Rao, 1984c). Suppose $\{\varepsilon_i\}$ is a sequence of independent random variables such that

$$E(\varepsilon_i) = 0, \ i \geq 1, \ \sup_i E \mid \varepsilon_i \mid^m < \infty \text{ for some } m > k \text{ and } m \geq 4. \tag{3.13}$$

Let $K \subset \Theta$ be compact. Assume that there exists positive constants $0 < K_1 \leq K_2 < \infty$ such that

$$K_1 \parallel \theta_1 - \theta_2 \parallel^2 \leq \Psi_n(\theta_1, \theta_2) \leq K_2 \parallel \theta_1 - \theta_2 \parallel^2, \tag{3.14}$$

where

$$\Psi_n(\theta_1, \theta_2) = n^{-1} \sum_{i=1}^{n} [g_1(\theta_1) - g_i(\theta_2)]^2.$$

Then there exists a constant $c_K > 0$ depending only on the compact set K and m such that

$$\sup_{\theta \in K} P_\theta \left(n^{\frac{1}{2}} \parallel \hat{\theta}_n - \theta \parallel > \rho \right) \leq c_K \rho^{-m} \tag{3.15}$$

for every $\rho > 0$ and $n \geq 1$.

Remark 3.2. The proof of this result is based on the technique of fluctuation inequalities as in the scalar parameter case. It was assumed that $m > k$ and $m \geq 4$ where k is the dimension of the parameter. This condition is too

strong for theoretical purposes and it is connected with the method of proof. We conjecture that the result holds for $m \geq 4$. The condition that $m > k$ is analogous to the condition (3.4), p. 185 of Ibragimov and Hasminskii (1981) in their study of the properties of the maximum likelihood estimator in the vector parameter case via the weak convergence of the normalized log-likelihood ratio process.

The following result is due to Ivanov (1984a) when the errors $\{\varepsilon_i\}$ are i.i.d. random variables with $E(\varepsilon_i) = 0, i \geq 1$.

Let $d_n = d_n(\theta), \theta \in \Theta$ be a diagonal matrix of order $k \times k$ with diagonal elements d_{in}, $1 \leq i \leq k$. Suppose that, for any compact $K \subset \Theta$,

$$\lim_{n \to \infty} \inf_{\theta \in K} n^{-\frac{1}{2}} d_{in}(\theta) > 0, \qquad 1 \leq i \leq k. \tag{3.16}$$

Define

$$n\Psi_n(\theta_1, \theta_2) = \sum_{j=1}^{n} [g_j(\theta_1) - g_j(\theta_2)]^2, \quad \theta_1, \theta_2 \in \Theta$$

and

$$\phi_n(\mathbf{u}_1, \mathbf{u}_2) = n\Psi_n(\theta + n^{\frac{1}{2}} d_n^{-1} \mathbf{u}_1, \theta + n^{\frac{1}{2}} d_n^{-1} \mathbf{u}_2)$$

for all $\mathbf{u}_1, \mathbf{u}_2 \in U_n(\theta)$ where

$$U_n(\theta) = \{\theta^* : \theta + n^{\frac{1}{2}} d_n^{-1} \theta^* \in \Theta\}.$$

For any $r > 0$, let $B(r) = \{\mathbf{u} \in R^k : \| \mathbf{u} \| \leq r\}$. Let $K \subset \Theta$ be compact. Suppose the following regularity conditions hold:

For any $\varepsilon > 0$ and $\rho > 0$, there exists $\delta > 0$ such that for $n > n_0$ (depending on K),

$$\sup_{\theta \in K} \left(\sup_{\substack{\mathbf{u}_1, \mathbf{u}_2 \in B(\rho) \cap \overline{U_n(\theta)} \\ \| \mathbf{u}_1 - \mathbf{u}_2 \| \leq \delta}} n^{-1} \phi_n(\mathbf{u}_1, \mathbf{u}_2) \right) \leq \varepsilon. \tag{3.17}$$

For some $\rho_0 > 0$ and for any $0 < r \leq \rho_0$, there exists $\Delta > 0$ and $\rho > 0$ such that, for $n > n_0$,

(i)

$$\inf_{\theta \in K} \left(\inf_{\mathbf{u} \in B(\rho_0) \setminus B^0(r) \cap \overline{U_n(\theta)}} \{ n^{-1} \phi_n(0, \mathbf{u}) \} \right) \geq \rho$$

(ii)

$$\inf_{\theta \in K} \left(\inf_{\mathbf{u} \in \overline{U_n(\theta)} \setminus B^0(\rho_0)} n^{-1} \phi_n(0, \mathbf{u}) \right) \geq 4\sigma^2 + \Delta. \tag{3.18}$$

$\{\varepsilon_i, i \geq 1\}$ are i.i.d. random variables with $E(\varepsilon_1) = 0$,

$\sigma^2 = E(\varepsilon_1^2)$ and $E \mid \varepsilon_1 \mid^s < \infty$ for some integer $s \geq 3$. (3.19)

Theorem 3.5. (Ivanov, 1984a). Under the conditions (3.17) to (3.19), for any $\rho > 0$,

$$\sup_{\theta \in K} P_\theta \left\{ \| n^{\frac{1}{2}} d_n(\theta)(\hat{\theta}_n - \theta) \| \geq \rho \right\} = o(n^{-(s-2)/2}). \tag{3.20}$$

Remark 3.3. Ivanov (1984a) has also obtained a moderate deviation result for the vector parameter case. Under some additional conditions, he has shown that if $E \mid \varepsilon_1 \mid^s < \infty$ for some s such that $s^2 > s + k$, then there exists $c > 0$ such that

$$\sup_{\theta \in K} P_\theta \left\{ \| d_n(\theta)(\hat{\theta}_n - \theta) \| \geq c(\log n)^{\frac{1}{2}} \right\} = o(n^{-(s-2)/2}). \tag{3.21}$$

We will not discuss the details here.

Unaware of the results of Prakasa Rao (1975), Ivanov and Kozlov (1981) extended the concept of minimum contrast estimators to i.n.i.d. observations and obtained the following results on the n^α-strong consistency of the least squares and least modulus estimators. Their definition of a sequence of contrast functions differs from that given by Prakasa Rao (1975).

Definition 3.1. A sequence of estimators θ_0 is said to be *n^α-strongly consistent* for θ_0 if

$$n^\alpha \| \theta_n - \theta_0 \| \to 0 \quad \text{a.s. } [P_{\theta_0}] \text{ as } n \to \infty.$$

Theorem 3.6. (Ivanov and Kozlov, 1981). Assume that $\{\varepsilon_i\}$ are i.i.d. random variables with $E(\varepsilon_1) = 0$, $\text{var}(\varepsilon_1) < \infty$. Further suppose that the following conditions hold. Let K be compact contained in θ. For every $\theta_0 \in \Theta$, there exists $\alpha > 0$ such that for every $\varepsilon > 0$

$$\lim_{n \to \infty} \left(\inf_{\theta \in K \setminus v(\theta_0, \varepsilon n^{-\alpha})} \Psi_n(\theta, \theta_0) \right) > 0, \tag{3.22}$$

where $v(\theta_0, \varepsilon n^{-\alpha}) = \{\theta : \| \theta - \theta_0 \| \leq \varepsilon n^{-\alpha}\}$, and

$$\overline{\lim_{n \to \infty}} \left(\sup_{\theta_1, \theta_2 \in K} \{\Psi_n(\theta_1, \theta_2) - \Psi(\theta_1, \theta_2)\} \right) \leq 0, \tag{3.23}$$

where $\Psi(\theta_1, \theta_2)$ is uniformly continuous on the diagonal $[\theta_1 = \theta_2]$, in the sense that for every $\varepsilon > 0$ there is a $\delta > 0$ such that $\Psi(\theta_1, \theta_2) < \varepsilon$ whenever $\| \theta_1 - \theta_2 \| < \delta$. Then the LSE $\hat{\theta}_n$ defined by

$$Q_n(\hat{\theta}_n) = \inf_{\theta \in K} Q_n(\theta)$$

is n^{α}-strongly consistent.

Remark 3.4. The condition (3.23) is not necessary for strong consistency. For example, consider the nonlinear regression model

$$x_i = \cos i\theta + \varepsilon_i, \qquad i \geq 1, \tag{3.24}$$

where $\theta \in \Theta = (0, \pi)$ and $\{\varepsilon_i, i \geq 1\}$ are i.i.d. random variables with $E(\varepsilon_i) = 0$. If $K = [\beta, \gamma], 0 < \beta < \gamma < \pi$, then $\hat{\theta}_n$ is n-strongly consistent but the condition (3.23) fails.

4. CONSISTENCY AND RATE OF CONVERGENCE FOR LME

Let $f_i(x_i, \theta) = | x_i - g_i(\theta) |$, $i \geq 1$. Suppose that sequence $\{f_i\}$ satisfies the following conditions:

(i)

$$E_{\theta_0} f_i(X_i, \theta) < \infty \text{ for } i \geq 1, \ \theta_0, \theta \in \Theta, \text{ and}$$

(ii)

for every $\theta_0 \in \Theta$, there is an $\alpha \geq 0$ such that for every $\varepsilon > 0$

$$\lim_{n \to \infty} \inf_{\theta \in K \setminus v(\theta_0, \varepsilon n^{-\alpha})} \left\{ n^{-1} \sum_{i=1}^{n} E_{\theta_0} f_i(X_i, \theta) - n^{-1} \sum_{i=1}^{n} E_{\theta_0} f_i(X_i, \theta_0) \right\} > 0, \tag{4.1}$$

where K is a compact set contained in Θ. Let θ_n^* be defined by

$$R_n(\theta_n^*) = \inf_{\theta \in K} R_n(\theta). \tag{4.2}$$

Theorem 4.1 (Ivanov and Kozlov, 1981). Suppose that ε_i, $i \geq 1$ are i.i.d. symmetric random variables with $E(\varepsilon_1^2) < \infty$ for every $\theta \in K$. Further suppose that

$$\overline{\lim_{n \to \infty}} \sup_{\theta_1, \theta_2 \in K} \left(n^{-1} \sum_{i=1}^{n} | g_i(\theta_1) - g_i(\theta_2) | - \eta(\theta_1, \theta_2) \right) \leq 0, \tag{4.3}$$

where $\eta(\theta_1, \theta_2)$ is uniformly continuous on the diagonal $\theta_1 = \theta_2$, and

$$\overline{\lim_{n\to\infty}} \Psi_n(\theta, \theta_0) < \infty \text{ for any } \theta, \theta_0 \in K, \tag{4.4}$$

where $\Psi_n(\theta_1, \theta_2) = n^{-1} \sum_{i=1}^{n} (g_i(\theta_1) - g_i(\theta_2))^2$. Then

$$n^{\alpha} \| \theta_n^* - \theta_0 \| \to 0 \text{ a.s. } [P_{\theta_0}] \text{ as } n \to \infty. \tag{4.5}$$

Under some conditions similar to those given in (3.17) to (3.19), Ivanov (1984b) stated an analogue of Theorem 3.5. We now discuss this result.

Let $d_n = d_n(\theta), \theta \in \Theta$ be a diagonal matrix of order $k \times k$ with $d_{in}, 1 \leq i \leq k$ as the diagonal elements satisfying (3.16). Define

$$f(j, \mathbf{u}) = g_j(\theta + n^{\frac{1}{2}} d_n^{-1} \mathbf{u}),$$

$$\Psi_{pn}(\mathbf{u}_1, \mathbf{u}_2) = \sum_{j=1}^{n} | f(j, \mathbf{u}_1) - f(j, \mathbf{u}_2) |^p, \ p \geq 1.$$

Fix $\theta \in \Theta$. Let

$$U_n(\theta) = n^{\frac{1}{2}} d_n(\theta) (\Theta - \theta)$$

and

$$B(r) = \{\mathbf{u} \in R^k : \| \mathbf{u} \| \leq r\}$$

as defined earlier. Let $K \subset \Theta$ be compact. Suppose the following conditions hold.

For any $\varepsilon > 0$ and $\rho > 0$, there exists $\delta > 0$ such that, for $n > n_0$ (depending on K),

$$\sup_{\theta \in K} \sup_{\substack{\mathbf{u}_1, \mathbf{u}_2 \in B(\rho) \cap \overline{U_n(\theta)} \\ \| \mathbf{u}_1 - \mathbf{u}_2 \| \leq \delta}} n^{-1} \Psi_{1n}(\mathbf{u}_1, \mathbf{u}_2) \leq \varepsilon. \tag{4.6}$$

For any $\rho > 0$ and for $n > n_0$,

$$\sup_{\theta \in K} \sup_{\mathbf{u} \in \overline{U_n(\theta)} \cap B(\rho)} \max_{1 \leq j \leq n} | f(j, \mathbf{u}_1) - f(j, \mathbf{0}) | \leq \chi_1(\rho), \text{ if } s = 1$$

and

$$\sup_{\theta \in K} \sup_{\mathbf{u} \in \overline{U_n(\theta)} \cap B(\rho)} n^{-1} \Psi_{sn}(\mathbf{u}, 0) \leq \chi_s(\rho), \quad \text{if } s \geq 2. \tag{4.7}$$

For any $r > 0$, there exists $\Delta(r) > 0$ such that, for $n > n_0$,

$$\inf_{\theta \in k} \inf_{\mathbf{u} \in \overline{U_u(\theta)} \setminus B^0(r)} n^{-1} E_\theta R_n(\theta + n^{\frac{1}{2}} d_n^{-1} \mathbf{u}) \geq \mu_1 + \Delta(r)$$

given that there exists $R_0 > 0$ such that $\Delta(R_0) = \rho_0\mu_1 + \Delta_0$ where $\rho_0 > 0$ and $\Delta_0 > 0$ are some numbers and $\mu_1 = E \mid \varepsilon_1 \mid$. Here

$$R_n(\theta) = \sum_{j=1}^{n} \mid X_j - g_j(\theta) \mid . \tag{4.8}$$

$\{\varepsilon_i\}$ are i.i.d. random variables with $E(\varepsilon_1) = 0$ and

$$E \mid \varepsilon_1 \mid^s = \mu_s < \infty \text{ for some } s \geq 1. \tag{4.9}$$

Theorem 4.2. (Ivanov, 1984b). Under the conditions (4.6) to (4.9), there exists a constant $c > 0$ not depending on ρ and n such that, for any $\rho > 0$,

$$\sup_{\theta \in K} P_\theta \left\{ \| n^{-\frac{1}{2}} d_n(\theta) (\theta_n^* - \theta) \| \geq \rho \right\} \leq c q_n(s), \tag{4.10}$$

where $q_n(s) = n^{-(s-1)}$ for $s \geq 2$ and $q_n(1) \to 0$ as $n \to \infty$.

A proof of this proposition is not given by Ivanov (1984b) and the reader is referred to Ivanov and Kozlov (1981).

5. ASYMPTOTIC DISTRIBUTION OF LSE

We will now study the asymptotic distribution of LSE via the weak convergence of the least squares process in the scalar parameter case and the least squares random field in the vector parameter case. For an alternative classical approach via normal equations, see Wu (1981).

5.1 Scalar Parameter Case

Consider the nonlinear regression model

$$X_i = g_i(\theta) + \varepsilon_i, \qquad i \geq 1, \tag{5.1}$$

where ε_i, $i \geq 1$ are i.i.d. random variables with mean 0 and finite positive variance σ^2 and $\theta \in \Theta \subset R$. Without loss of generality, assume that $\sigma^2 = 1$. Let $\hat{\theta}_n$ be a LSE as defined in section 3. Define

$$\Psi_n(\theta_1, \theta_2) = \frac{1}{n} \sum_{i=1}^{n} [g_i(\theta_1) - g_i(\theta_2)]^2 .$$

Suppose that the following regularity conditions hold.

There exists $0 < k_1 < k_2 < \infty$ such that

$$k_1 (\theta_1 - \theta_2)^2 \leq \Psi_n (\theta_1, \theta_2) \leq k_2 (\theta_1 - \theta_2)^2 \tag{5.2}$$

for all $n \geq 1$ and θ_1, θ_2 in θ.

$g_i(\theta)$ is differentiable with respect to θ for every $i \geq 1$ and for any $\theta_0 \in \Theta$, there exists a neighbourhood V_{θ_0} of θ_0 in Θ such that, for all $i \geq 1$,

(i)

$$| g_i(\theta) - g_i (\theta_0) - (\theta - \theta_0) g_1^{(1)} (\theta_0) | \leq d_i (\theta_0) | \theta - \theta_0 |^2$$

for all $\theta \in V_{\theta_0}$ where $g_i^{(1)}(\theta_0)$ denotes the derivative of $g_i(\theta)$ at θ_0 and

(ii)

$$\overline{\lim_{n \to \infty}} \frac{1}{n} \sum_{i=1}^{n} d_i^2 (\theta_0) < \infty. \tag{5.3}$$

(iii)

$$0 < K = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \left[g_i^{(1)} (\theta_0) \right]^2 < \infty. \tag{5.4}$$

Note that $\hat{\theta}_n$ minimizes $Q_n(\theta) - Q_n(\theta_0)$ over $\theta \in \Theta$ for any fixed $\theta_0 \in \Theta$. Let

$$J_n(\phi) = Q_n(\theta_0 + n^{-\frac{1}{2}} \phi) - Q_n (\theta_0) \tag{5.5}$$

for all ϕ such that $\theta_0 + n^{-\frac{1}{2}} \phi \in V_{\theta_0}$.

Theorem 5.1. (Prakasa Rao, 1984d). Suppose the conditions (5.2) to (5.4) hold. Then, for any $\tau > 0$, the sequence of processes $\{J_n(\phi), -\tau \leq \phi \leq \tau\}$ converge in distribution on $C[-\tau, \tau]$ to the process $\{J(\phi), -\tau \leq \phi \leq \tau\}$, where

$$J(\phi) = 2K^{\frac{1}{2}} \phi \xi + K\phi^2. \tag{5.6}$$

Here K is as given by (5.4) and ξ is $N(0,1)$.

In view of Theorems 3.1 and 5.1, applying the results and methods in the theory of weak convergence of probability measures on complete separable metric spaces (see, for example, Prakasa Rao, 1968), it follows that

$$n^{\frac{1}{2}} (\hat{\theta}_n - \theta_0) \xrightarrow{L} \hat{\phi}, \tag{5.7}$$

where $\hat{\phi}$ is defined by the relation

$$J(\hat{\phi}) = \min_{\phi} J(\phi) \tag{5.8}$$

and $J(\phi)$ is as defined by (5.6). Note that

$$\hat{\phi} = -K^{-\frac{1}{2}}\xi \tag{5.9}$$

and hence

$$n^{\frac{1}{2}}(\hat{\theta}_n - \theta_0) \xrightarrow{L} N\left(0, K^{-1}\right).$$

Theorem 5.2. (Ivanov, 1976; Prakasa Rao, 1984d). Under the conditions (5.2) to (5.4),

$$P_{\theta_0}\left(n^{\frac{1}{2}} \mid \hat{\theta}_n - \theta_0 \mid > \rho\right) = O\left(\rho^{-2}\right) \tag{5.10}$$

and

$$n^{\frac{1}{2}}(\hat{\theta}_n - \theta_0) \xrightarrow{L} N(0, K^{-1}) \text{ as } \to \infty, \tag{5.11}$$

where $0 < K = \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} [g_i^{(1)}(\theta_0)]^2 < \infty$ as given in (5.4).

Remark 5.1. For variations of the above result and an application to the study of asymptotic properties of the LSE in the nonlinear regression model

$$X_i = \mid a_i - \theta \mid + \varepsilon_i, \qquad i \geq 1, \tag{5.12}$$

where ε_i are i.i.d. random variables with mean 0 and finite positive variance and $\{a_i\}$ is a real sequence satisfying some conditions; see Prakasa Rao (1984d). Note that this model is not amenable to study via the classical methods since $g_i(\theta) = \mid a_i - \theta \mid$ is not differentiable with respect to θ at $\theta = a_i$.

5.2 Vector Parameter Case

Consider the nonlinear regression model

$$X_i = g_i(\theta) + \varepsilon_i, \qquad i \geq 1, \tag{5.13}$$

where $\{g_i(\theta), 1 \geq 1\}$ is a sequence of functions possibly nonlinear in $\theta \in \Theta \subset R^k$ and ε_i, $i \geq 1$ are independent random variables with mean 0 and finite variances. Let $\sigma_i^2 = E\left(\varepsilon_i^2\right)$ and $\hat{\theta}_n$ be a LSE as defined in Section 3. Define

$$\Psi_n(\theta_1, \theta_2) = n^{-1} \sum_{i=1}^{n} \left[g_i(\theta_1) - g_i(\theta_2)\right]^2. \tag{5.14}$$

Suppose the following regularity conditions hold. There exists $0 < k_1 < k_2 < \infty$ such that

$$k_1 \parallel \theta_1 - \theta_2 \parallel^2 \leq \Psi_n(\theta_1, \theta_2) \leq k_2 \parallel \theta_1 - \theta_2 \parallel^2 \tag{5.15}$$

for all $n \geq 1$ and θ_1, θ_2 in Θ.

$g_i(\theta)$ has partial derivatives with respect to the components of θ and, for any $\theta_0 \in \Theta$, there exists a neighbourhood V_{θ_0} of θ_0 in Θ such that, for all $i \geq 1$,

$$| g_i(\theta) - g_i(\theta_0) - (\theta - \theta_0)' \nabla g_i(\theta_0) | \leq d_i(\theta_0) \| \theta - \theta_0 \|^2$$

for all $\theta \in V_{\theta_0}$, where $\nabla g_i(\theta_0)$ is $\left(\frac{\partial g_i}{\partial \theta_1}, \ldots, \frac{\partial g_i}{\partial \theta_k}\right)$ evaluated at θ_0. Further,

$$\overline{\lim_n} \frac{1}{n} \sum_{i=1}^{n} d_i^2(\theta_0) < \infty. \tag{5.16}$$

$\{\varepsilon_i\}$ are independent random variables with $E(\varepsilon_i) = 0$, $E(\varepsilon_i^2) = \sigma_i^2$ and

$$\sup_i E | \varepsilon_i |^m < \infty \text{ for some } m > k \text{ and } m \geq 4 \text{ and}$$

$$\inf_i E(\varepsilon_i^2) \geq \sigma^2 > 0. \tag{5.17}$$

The matrices
(i)

$$K = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \left[\nabla g_i(\theta_0) \nabla g_i(\theta_0)'\right] \sigma_i^2$$

and
(ii)

$$K^* = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \left[\nabla g_i(\theta_0) \nabla g_i(\theta_0)'\right] \tag{5.18}$$

exist and are positive definite.

Fix $\theta_0 \in \Theta$. Define

$$J_n(\phi) = Q_n(\theta_0 + n^{-\frac{1}{2}}\phi) - Q_n(\theta_0) \tag{5.19}$$

for all ϕ such that $\theta_0 + n^{-\frac{1}{2}}\phi \in V_{\theta_0}$.

Theorem 5.3. (Prakasa Rao, 1984e). Under the conditions (5.15) to (5.17), the sequence of random fields $\{J_n(\phi), \| \phi \| \leq \tau\}$ converge in distribution to the random field $\{J(\phi), \| \phi \| \leq \tau\}$ on the space C of continuous functions on $\{\phi : \| \phi \| \leq \tau\}$ for any fixed $\tau > 0$, where

$$J(\phi) = \phi' K^* \phi + 2\phi' \xi \tag{5.20}$$

and ξ is k-variate normal with mean vector zero and covariance matrix K. Here K and K^* are as defined by (5.18).

In view of Theorem 3.4 and Theorem 5.3, and applying again the theory of weak convergence, it follows that

$$n^{\frac{1}{2}}(\theta_n - \theta_0) \xrightarrow{L} \hat{\phi}, \tag{5.21}$$

where $\hat{\phi}$ is defined through the relation

$$J(\hat{\phi}) = \inf_{\phi \in R^k} J(\phi) \tag{5.22}$$

and $J(\phi)$ is as defined by (5.20). Observe that

$$\hat{\phi} = K^{*-1}\xi. \tag{5.23}$$

Hence

$$n^{\frac{1}{2}}(\hat{\theta}_n - \theta_0) \xrightarrow{L} N_k\left(0, K^{*-1}KK^{*-1}\right) \text{ as } n \to \infty, \tag{5.24}$$

where $N_k(0, \Sigma)$ denotes the k-variate normal distribution with mean vector 0 and covariance matrix Σ.

Theorem 5.4. (Prakasa Rao 1984c, 1984e). Suppose the conditions (5.15) to (5.18) hold. Then, for any $\rho > 0$,

$$P_{\theta_0}\left(n^{\frac{1}{2}} \| \hat{\theta}_n - \theta_0 \| > \rho\right) = O\left(\rho^{-m}\right) \tag{5.25}$$

and

$$n^{\frac{1}{2}}(\hat{\theta}_n - \theta_0) \xrightarrow{L} N_k\left(0, K^{*-1}KK^{*-1}\right) \text{ as } n \to \infty. \tag{5.26}$$

Since $m \geq 4$, it follows that

$$\hat{\theta}_n \xrightarrow{a.s.} \theta_0 \text{ as } n \to \infty \tag{5.27}$$

from (5.25) by the Borel-Cantelli lemma. For an example of an application of Theorem 5.4, see Prakasa Rao (1984e).

Remarks 5.2. The condition (5.17) that $\sup_i E \mid \varepsilon_i \mid^m < \infty$ for some $m > k$ and $m \geq 4$ is purely a technical condition. It is imposed due to the method used in the proof based on fluctuation inequalities for random fields. We conjecture that the result continues to hold if for some $\delta > 0$,

$$E(\varepsilon_i) = 0, \quad \sup_i E \mid \varepsilon_i \mid^{2+\delta} < \infty, \quad \inf_i E \mid \varepsilon_i \mid^2 \geq \sigma^2 > 0. \tag{5.17}'$$

We further remark that it should be possible to relax the condition (5.17) to (5.17)′, at least in case $g_i(\cdot)$ are sufficiently differentiable as in Deshayes and Picard (1984). Asymptotic theory of LSE, under the weaker condition (5.17)′ but stronger additional conditions, has been discussed by Prakasa Rao (1986). Methods used there are similar to those of Inagaki and Ogata (1975), Prakasa Rao (1972) and Huber (1967).

We now discuss briefly the results of Prakasa Rao (1986).

Suppose the following regularity conditions hold in addition to (5.16) and (5.17)′.

$$\sum_{i=1}^{\infty} [g_i(\theta_1) - g_i(\theta_2)]^2 > 0 \text{ if } \theta_1 \neq \theta_2 \text{ in } \Theta. \tag{5.28}$$

Observe that

$$\begin{aligned} \frac{1}{2}\nabla Q_n(\theta) &= \sum_{i=1}^{n} [X_i - g_i(\theta)] \nabla g_i(\theta) \\ &= \sum_{i=1}^{n} \eta_i(Y_i, \theta) \qquad \text{(say)} . \end{aligned} \tag{5.29}$$

Suppose that $E\eta_i(Y_i, \theta) = \lambda_i(\theta)$ exists where E denotes the expectation under the true model. Suppose there exists $\theta_0 \in \Theta$ such that $\lambda_i(\theta_0) = 0$, $i \geq 1$.

There exists a neighbourhood U_{θ_0} of θ_0 such that the following conditions hold:

(i)

$$\bar{\lambda}_n(\theta) = \frac{1}{n}\sum_{i=1}^{n} \lambda_i(\theta) \to \lambda(\theta) \qquad \text{as } n \to \infty,$$

where

$$\lambda(\theta) \neq \lambda(\theta_0) \text{ if } \theta \neq \theta_0, \qquad \theta \in U_{\theta_0}.$$

(ii) $\lambda_i(\theta)$ are continuously differentiable for $i \geq 1$ such that

$$\bar{\Lambda}_n(\theta) = \frac{1}{n}\sum_{i=1}^{n} \Lambda_i(\theta) \to \Lambda(\theta) \tag{5.30}$$

uniformly for $\theta \in U_{\theta_0}$, where $\Lambda_i(\theta) = \frac{\partial \lambda_i(\theta)}{\partial \theta}$.

Let

$$u_i(y, \theta, d) = \sup_{\|\tau - \theta\| \leq d} |\, \eta_i(y, \tau) - \eta_i(y, d) \,| . \tag{5.31}$$

Suppose that for every compact $K \subset \Theta$, there exists $d_0 > 0, H_1 > 0$ and $H_2 > 0$ such that

$$\sup_{\theta \in K} E\left(u_i(X_i, \theta, d)\right) < H_1 d, \qquad i \geq 1,$$

and

$$\sup_{\theta \in K} E\left(u_i^2(X_i, \theta, d)\right) < H_2 d, \qquad i \geq 1.$$

For any fixed ϕ_1 and ϕ_2,

(i)

$$\sum_{i=1}^{n} \sigma_i^2 [g_i(\theta_0) - g_i(\theta_0 + \phi_1 n^{-\frac{1}{2}})][g_i(\theta_0) - g_i(\theta_0 + \phi_2 n^{-\frac{1}{2}})]$$

$$= \phi_1' K(\theta_0) \phi_2 + o(1), \tag{5.32}$$

(ii)

$$\sum_{i=1}^{n} [g_i(\theta_0) - g_i(\theta_0 + \phi_1 n^{-\frac{1}{2}})]^2 = \phi_1' K^*(\theta_0) \phi_1 + o(1), \tag{5.33}$$

where $K(\theta_0)$ and $K^*(\theta_0)$ are positive definite matrices.

$$\sup_{i \geq 1} | g_i(\theta_0) - g_i(\theta_0 + \phi n^{-\frac{1}{2}}) | \leq M \| \phi \| n^{-\frac{1}{2}} \tag{5.34}$$

for some $M < \infty$, uniformly in ϕ and n.

Let

$$J_n(\phi) = Q_n(\theta_0 + \phi n^{-\frac{1}{2}}) - Q_n(\theta_0). \tag{5.35}$$

Suppose there exists $\eta > 0$ such that

$$\lim_{M \to \infty} \overline{\lim_{n \to \infty}} P\left[\inf_{\|\phi\| \geq M} J_n(\phi) \geq \eta\right] = 1.$$

Under the regularity conditions (5.16), (5.17)′ and (5.28) to (5.35), it can be shown that

$$n^{\frac{1}{2}}(\hat{\theta}_n - \theta_0) \xrightarrow{L} N_k\left(0, K^{*-1} K K^{*-1}\right) \text{ as } n \to \infty.$$

For details, see Prakasa Rao (1986).

5.3 Nonregular Case

The cases considered for the study of the asymptotic distribution of the least squares estimator discussed above may be termed smooth cases or regular cases. We have earlier indicated a regression model where the standard classical approach via normal equations is not applicable. We now present another example where the classical approach is not applicable. The result here is due to Prakasa Rao (1984f).

Consider the nonlinear regression model

$$X_i = |\, a_i - \theta \,|^{\lambda} + \varepsilon_i, \qquad i \geq 1, \tag{5.36}$$

where $0 < \lambda < \frac{1}{2}$, λ known, $\{\varepsilon_i\}$ are i.i.d. random variables with mean zero and variance 1. Suppose that $\{a_i, i \geq 1\}$ is a real sequence with the property

$$\sum_{i=1}^{n} \left\{ |\, a_i - \theta \,|^{\lambda} - |\, a_i - \theta_0 \,|^{\lambda} \right\}^2 = 2nC(\lambda) \,|\, \theta - \theta_0 \,|^{2\lambda+1} \left(1 + o(1)\right), \tag{5.37}$$

where $C(\lambda) \neq 0$ and there exists $0 < k_1 < k_2 < \infty$ such that

$$nk_1 \,|\, \theta_1 - \theta_2 \,|^{2\lambda+1} \leq \sum_{i=1}^{n} \left\{ |\, a_i - \theta_1 \,|^{\lambda} - |\, a_i - \theta_2 \,|^{\lambda} \right\}^2 \leq nk_2 \,|\, \theta_1 - \theta_2 \,|^{2\lambda+1} \tag{5.38}$$

for all θ_1 and θ_2 in Θ, Θ compact contained in R.

Theorem 5.5. (Prakasa Rao, 1984f). Suppose the conditions (5.37) and (5.38) hold. Let $\hat{\theta}_n$ be a LSE of θ based on $X_1, \ldots, X_n$. Then there exists $c > \theta$ such that, for any $r > 0$ and for any $n \geq 1$,

$$P_{\theta_0}\left(n^{\rho} \,|\, \hat{\theta}_n - \theta_0 \,| > r \right) \leq cr^{-(2\lambda+1)} \tag{5.39}$$

and

$$n^{\rho}(\hat{\theta}_n - \theta_0) \xrightarrow{L} \hat{\phi} \text{ as } n \to \infty, \tag{5.40}$$

where $\rho = (2\lambda + 1)^{-1}$ and $\hat{\phi}$ is the location of the minimum of the non-stationary Gaussian process $\{R(\phi), -\infty < \phi < \infty\}$ with

(i)

$$E[R(\phi)] = 2C(\lambda) \,|\, \phi \,|^{2\lambda+1},$$

(ii)

$$\begin{aligned} &\text{Cov } [R(\phi_1), R(\phi_2)] \\ &\quad = 4C(\lambda) \left[|\, \phi_1 \,|^{2\lambda+1} + |\, \phi_2 \,|^{2\lambda+1} - |\, \phi_1 - \phi_2 \,|^{2\lambda+1} \right]. \end{aligned} \tag{5.41}$$

Remark 5.3. Note that $\rho > \frac{1}{2}$ if $0 < \lambda < \frac{1}{2}$ and the asymptotic variance of the LSE is $O\left(n^{-2\rho}\right)$ which is small as compared to that in the smooth case when it is $O\left(n^{-1}\right)$.

As was mentioned in the introduction, one can obtain the Berry-Esseen bound for the distribution of the least squares estimator as a special case of the results of Prakasa Rao (1975). Ivanov (1976a) obtained the Berry-Esseen bound for the distribution of the least squares estimator by methods analogous to those in Pfanzagl (1971). He has also obtained an asymptotic expansion for the same (Ivanov, 1976b), again by methods similar to those of Pfanzagl (1973). In all these papers, the case of the scalar parameter is treated. Recently Ivanov and Zwanzig (1983) obtained Berry-Esseen bounds and asymptotic expansions for the distribution of the least squares estimator in the vector parameter case under some strong assumptions on the characteristic functions of ε_i. Second order asymptotics in nonlinear regression were discussed by Schmidt and Zwanzig (1983), extending the work of Pfanzagl (1973) for MCE in the i.i.d. case.

6. ASYMPTOTIC DISTRIBUTION OF LME

Consider the nonlinear regression model

$$X_i = g_i(\theta) + \varepsilon_i, \qquad i \geq 1, \tag{6.1}$$

where $\Theta \subset R^k$ and $g_i(\theta), i \geq 1$ is a sequence of continuous functions, possibly nonlinear in $\theta \in \Theta$, and ε_i, $i \geq 1$ is a sequence of independent and identically distributed random variables. Let K be compact contained in Θ.

Suppose $g_j(\theta)$ is differentiable with respect to θ and let

$$d_{in}(\theta) = \left(\sum_{j=1}^{n} g_{ij}^2(\theta)\right)^{\frac{1}{2}},$$

where

$$g_{ij}(\theta) = \frac{\partial}{\partial \theta_i} g_j(\theta), \qquad 1 \leq i \leq k.$$

Denote

$$g_{ij}(\theta + n^{\frac{1}{2}} d_n^{-1} \mathbf{u}) = f_{ij}(\mathbf{u}), \qquad 1 \leq i \leq k.$$

In addition to the conditions (4.8) and (4.9), suppose the following regularity conditions hold.

Θ is convex. The functions $g_j(\theta), j \geq 1$ are continuous on $\bar{\Theta}$ and continuously differentiable on Θ. Further, for any $R > 0$, there exists n_0 depending on the compact K such that for $n > n_0$,

$$\sup_{\theta \in K} \left\{ \sup_{u \in B^0(R) \cap U_n(\theta)} n^{\frac{1}{2}} d_{in}^{-1}(\theta) \left(\max_{1 \leq j \leq n} | f_{ij}(\mathbf{u}) | \right) \right\} \leq \chi_i(R), \ 1 \leq i \leq k. \tag{6.2}$$

Suppose $g_{ij}(\theta), 1 \leq i \leq k, j \geq 1$ are differentiable with respect to θ. Let

$$d_{i\ell n}(\theta) = \left(\sum_{j=1}^{n} g_{i\ell j}^2(\theta) \right)^{\frac{1}{2}},$$

$$g_{i\ell j}(\theta) = \frac{\partial g_j(\theta)}{\partial \theta_i \partial \theta_\ell},$$

and

$$\Psi_{2n}^{(i)}(\mathbf{u}_1, \mathbf{u}_2) = \sum_{j=1}^{n} \left(f_{ij}(\mathbf{u}_1) - f_{ij}(\mathbf{u}_2) \right)^2.$$

Θ is convex. The functions $g_{ij}(\theta), 1 \leq i \leq k, j \geq 1$ are continuous on $\bar{\Theta}$ and continuously differentiable in θ. In addition, for every $R > 0$ and $n > n_0$,

$$\sup_{\theta \in K} \left\{ \sup_{u \in B^0(R) \cap U_n(\theta)} n^{\frac{1}{2}} d_{in}^{-1}(\theta) d_{i\ell n} \left(\theta + n^{\frac{1}{2}} d_n^{-1}(\theta) \mathbf{u} \right) \right\}$$

$$\leq \chi_{i\ell}(R), \quad 1 \leq i, \ell \leq k. \tag{6.3}$$

Let

$$I_n(\theta) = \left(\left(\left(d_n^{-1}(\theta) \right) \left(\sum_{j=1}^{n} g_{ij}(\theta) g_{kj}(\theta) \right) d_n^{-1}(\theta) \right) \right)_{k \times k}$$

and $\lambda_{\min}(I_n(\theta))$ be the smallest eigenvalue of the matrix $I_n(\theta)$.

$$\overline{\lim_n} \inf_{\theta \in K} \lambda_{\min}(I_n(\theta)) > 0. \tag{6.4}$$

The random variable ε_1 possesses bounded density $\phi(x) = F^{(1)}(x)$ such that

$$| \phi(x) - \phi(0) | \leq H | x |, \qquad x \in R \tag{6.5}$$

for some $H > 0$.

Theorem 6.1. (Ivanov, 1984b). Under the conditions (4.8), (4.9) and (6.2) to (6.5),

$$\sup_{\theta \in K} \sup_{C \in \mathcal{C}^k} \mid P_\theta \left\{ 2\phi(0) I_n^{\frac{1}{2}}(\theta) d_n(\theta) (\theta_n - \theta) \in C \right\} - \phi_{I_k}(C) \mid \to 0$$

as $n \to \infty$, where $\mathcal{C}^k$ denotes the class of Borel convex subsets of R^k and ϕ_A denotes the k-variate normal distribution with mean 0 and covariance matrix A.

7. OPEN PROBLEMS

(i) Find the rates of convergence when the errors $\{\varepsilon_i\}$ form an absolutely regular sequence (Yoshihara, 1978), which is weaker than either the ϕ-mixing or the strong mixing property.

(ii) Extend the results on the rate of consistency in the multiparameter case as well as the scalar case to a general growth rate condition on $\Psi_n(\theta_1, \theta_2)$ as defined in (3.14) or (3.6).

(iii) Extend the approach to the study of asymptotic theory of LSE, via the least squares process or the least squares random field to the case when $\{\varepsilon_i\}$ is a stochastic process which satisfies some type of mixing condition, or is absolutely regular.

(iv) The conditions of Ivanov (1984b) for deriving asymptotic normality of LME are not satisfactory. Is it possible to derive a Berry-Esseen type bound for the distribution of LME under the conditions stated by Ivanov (1984b)?

(v) Extend the stochastic process approach as discussed in Section 5 of this paper to a weighted least squares estimator, where the weights may be random or the weight corresponding to the ith observation X_i depends on the earlier observations X_j, $1 \leq j \leq i$, for instance.

(vi) Study asymptotic theory for least squares estimators in the presence of nuisance parameters.

(vii) Consider the nonlinear regression model

$$X_i = g_i(\theta) + \varepsilon_i, \qquad i \geq 1.$$

Suppose $\theta \in \Theta$ and λ is a prior density on Θ. Let

$$Q_n(\theta) = \sum_{i=1}^{n} (X_i - g_i(\theta))^2 .$$

Since there is a prior information about θ, it might be useful to minimize $\lambda(\theta)Q_n(\theta)$ instead of $Q_n(\theta)$ and obtain a Bayesian type LSE. If the prior is uniform and Θ is compact, then it reduces to the ordinary LSE. It would be interesting to study the asymptotic properties of this Bayesian type LSE by the methods described in Sections 3 and 5. See Prakasa Rao (1987).

(viii) Consider the nonlinear regression model

$$X_i = g_i(\theta) + \varepsilon_i, \qquad i \geq 1.$$

Suppose the process $\{X_i, i \geq 1\}$ is such that there is a change in the value of θ, say from θ_1 to θ_2, at some instant τ and the problem is the estimation of θ_1, θ_2 and τ. It is likely that this problem can be tackled by the methods discussed in Section 4 by studying the weak convergence of the process

$$Q_n^{(t)}(\theta) = \sum_{j=1}^{[nt]} (X_i - g_i(\theta))^2,$$

for $0 \leq t \leq 1$ and applying methods similar to those of Deshayes and Picard (1984).

REFERENCES

Bard, Y. (1974), *Nonlinear Parameter Estimation.* New York: Academic Press.

Basser, G., and R. Koenker (1978), "Asymptotic theory of least absolute error regression." *Journal of the American Statistical Association* **73**, 618–622.

Bloomfield, P., and W. L. Steiger (1983), *Applications of Least Absolute Deviations.* Basel, Switzerland: Birkhauser Verlag.

Bunke, H., and W. H. Schmidt (1980), "Asymptotic results on nonlinear approximation of regression functions and weighted least squares." *Mathematische Operationsforschung und Series Statistics* **11**, 3–32.

Deshayes, J., and D. Picard (1984), "Principe de invariance sur le processus de vraisemblance." *Annales de l'Institut Henri Poincaré* **20**, 1–20.

Huber, P. (1967), "The behaviour of maximum likelihood estimates under nonstandard conditions." *Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability* **1**, 221–233.

Ibragimov, I. A., and R. Z. Hasminskii (1981), *Statistical Estimation: Asymptotic Theory.* New York: Springer-Verlag.

Inagaki, N., and Y. Ogata (1975), "The weak convergence of likelihood of ratio random fields and its applications". *Annals of the Institute of Statistical Mathematics* **27**, 391–419.

Ivanov, A. V. (1976a), "The Berry-Esseen inequality for the distribution of the least squares estimate." *Mathematical Notes* **20**, 721–727.

Ivanov, A. V. (1976b), "An asymptotic expansion for the distribution of the least squares estimator of the nonlinear regression parameter." *Theory of Probability and its Applications* **21**, 557–570.

Ivanov, A. V. (1984a), "Two theorems on consistency of a least squares estimator." *Theory of Probability and Mathematical Statistics* **28**, 25–34.

Ivanov, A. V. (1984b), "On consistency and asymptotic normality of least modulus estimator." *Ukrainian Mathematical Journal* **36**, 297–303 (In Russian).

Ivanov, A. V., and O. M. Kozlov (1981), "On consistency of minimum contrast estimators in the case of nonidentically distributed observations." *Theory of Probability and Mathematical Statistics* **23**, 63–72.

Ivanov, A. V., and S. Zwanzig (1983), "An asymptotic expansion for the distribution of the least squares estimator in nonlinear regression model." *Mathematische Operationsforschung und Series Statistics* **14**, 7–27.

Jennrich, R. I. (1969), "Asymptotic properties of nonlinear least squares estimators." *Annals of Mathematical Statistics* **40**, 633–643.

Malinvaud, E. (1970), "The consistency of nonlinear regression." *Annals of Mathematical Statistics* **41**, 956–969.

Nelson, P. I. (1980), "A note on strong consistency of least squares estimators in regression model with martingale difference errors." *Annals of Statistics* **8**, 1057–1064.

Pfanzagl, J. (1968), "On the measurability and consistency of minimum contrast estimates." *Metrika* **14**, 249–272.

Pfanzagl, J. (1971), "The Berry-Esseen bound for minimum contrast estimates." *Metrika* **17**, 82–91.

Pfanzagl, J. (1973), "Asymptotic expansions related to minimum contrast estimators." *Annals of Statistics* **1**, 993–1026.

Prakasa Rao, B. L. S. (1968), "Estimation of the location of the cusp of a continuous density." *Annals of Mathematical Statistics* **39**, 76–87.

Prakasa Rao, B. L. S. (1972), "Maximum likelihood estimation for Markov processes." *Annals of the Institute of Statistical Mathematics* **24**, 333–345.

Prakasa Rao, B. L. S. (1975), "The Berry-Esseen bound for minimum contrast estimators in the independent not identically distributed case." *Metrika* **22**, 225–239.

Prakasa Rao, B. L. S. (1984a), "The rate of convergence of the least squares estimator in a nonlinear regression model with dependent errors." *Journal of Multivariate Analysis* **14**, 315–322.

Prakasa Rao, B. L. S. (1984b), "On the exponential rate of convergence of the least squares estimator in the nonlinear regression model with Gaussian errors." *Statistics and Probability Letters* **2**, 139–142.

Prakasa Rao, B. L. S. (1984c), "On the rate of convergence of the least squares estimator in nonlinear regression model for multiparameter." (Preprint) New Delhi: Indian Statistical Institute.

Prakasa Rao, B. L. S. (1984d), "Weak convergence of least squares process in the smooth case." (Preprint) New Delhi: Indian Statistical Institute.

Prakasa Rao, B. L. S. (1984e), "Weak convergence of the least squares random

field in the smooth case." (Preprint) New Delhi: Indian Statistical Institute. (to appear in *Statistics and Decisions* **4**.)

Prakasa Rao, B. L. S. (1984f), "Asymptotic theory of least squares estimator in a nonregular nonlinear regression model." *Statistics and Probability Letters* **3**, 15–18.

Prakasa Rao, B. L. S. (1985), "Remarks on the asymptotic properties of least squares estimator and least modulus estimator." (Preprint) New Delhi: Indian Statistical Institute.

Prakasa Rao, B. L. S. (1986), "The weak convergence of least squares random field and its application." *Annals of the Institute of Statistical Mathematics* (to appear).

Schmetterer, L. (1974), *Introduction to Mathematical Statistics*. Berlin: Springer-Verlag.

Schmidt, W. H. (1982), "Testing hypothesis in nonlinear regressions." *Mathematische Operationsforschung und Series Statistics* **13**, 3–19.

Schmidt, W. H., and S. Zwanzig (1983), "Second order asymptotics in nonlinear regression." (Preprint) Akadamie Der Wissenschafleñ Der DDR Institut für Mathematik.

Taylor, L. D. (1974), "Estimation by minimizing the sum of absolute errors." In *Frontiers in Econometrics*, ed. Paul Zarembka, pp. 169–190. New York: Academic Press.

Wu, C. F. (1981), "Asymptotic theory of nonlinear least squares estimation." *Annals of Statistics* **9**, 501–513.

Yoshihara, K. (1978), "Probability inequalities for sums of absolutely regular processes and their applications." *Zeitschrift für Wahrscheinlichkeitstheorie und Verwandte Gebiete* **43**, 319–329.

D. L. McLeish and Christopher G. Small [1]

LIKELIHOOD ASYMPTOTICS FOR THE DISCRIMINATION PROBLEM

ABSTRACT

Suppose $\mathbf{X}_i, i = 1, 2, \ldots, n$ are independent random vectors such that k are drawn from a known density $g(\mathbf{x})$ and $n - k$ from a known density $f(\mathbf{x})$. We consider the discrimination problem of allocating observations to their parent densities in such a way as to minimize a linear combination of the expected number of the two types of misclassification. The rule minimizing this risk function is written as a function of k.

1. INTRODUCTION

Suppose $\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_n$ are n independent p-dimensional random column vectors, each of which has one of two known distributions $F(\mathbf{x})$ or $G(\mathbf{x})$ with densities $f(\mathbf{x})$, $g(\mathbf{x})$ respectively. We assume that $f(\mathbf{x})$ and $g(\mathbf{x})$ are distinct but have common support. Let $(d_1, d_2, \ldots, d_n)$ be a vector of binary values $(d_i = 0, 1)$ such that $\mathbf{X}_i$ has density $(1 - d_i)f(\mathbf{x}) + d_i g(\mathbf{x})$. The vector $(d_1, \ldots, d_n) \in \{0, 1\}^n$ is presumed to be unknown. Let $\mathbf{X} = (\mathbf{X}_1, \ldots, \mathbf{X}_n)$. For convenience of terminology, we label those observations with $d_i = 1$ "contaminants".

One of the tasks of discriminant analysis is to construct a vector $\boldsymbol{\delta}(\mathbf{X}) = (\delta_1, \ldots, \delta_n)$ of binary values $(\delta_i = 0, 1)$ so as to minimize a risk function. See, for example, Anderson (1958, p. 197).

Suppose the costs of the two types of classification errors are in some

[1] Department of Statistics and Actuarial Science, University of Waterloo, Waterloo, Ontario N2L 3G1 (both authors)

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 167–177.

ratio $\alpha : 1$. In particular, suppose the risk function is defined by

$$\mathbf{E}[L(\mathbf{d}, \delta)] = \mathbf{E}\left[\sum_{i=1}^{n} \{(\delta_i - d_i)^+ + \alpha(d_i - \delta_i)^+\}\right]$$
$$= \mathbf{E}\left\{\alpha \sum_{\{i,\delta_i=0\}} d_i + \sum_{\{i,\delta_i=1\},} (1 - d_i)\right\},$$

where $x^+ = 1$ if $x > 0$, 0 if $x \leq 0$. The task is usually solved by the construction of a real-valued discriminant function $D(\mathbf{x})$ together with a real constant c_D so that δ is defined by

$$\delta_i = \begin{cases} 0 & D(\mathbf{X}_i) \geq c_D \\ 1 & D(\mathbf{X}_i) < c_D. \end{cases} \tag{1}$$

Rules of this form are discussed, for example, by Kendall *et al.* (1966, pp. 370–380). If there is no constraint on the function D, e.g., that it be linear, then the Neyman-Pearson lemma can be used to find an optimal choice of D. We set

$$D(\mathbf{x}) = f(\mathbf{x})/g(\mathbf{x}). \tag{2}$$

This is optimal in the Neyman-Pearson sense, namely that for all discriminant functions with fixed misclassification error $P_F[D(\mathbf{x}) < c_D]$, the choice $D = f/g$ minimizes the error $P_G[D(\mathbf{x}) \geq c_D]$.

If (2) is used, then

$$\mathbf{E}[L(\mathbf{d}, \delta)] = (n - k_0)P_F[f(\mathbf{x})/g(\mathbf{x}) < c] + \alpha k_0 P_G[f(\mathbf{x})/g(\mathbf{x}) \geq c], \tag{3}$$

where $k_0 = \sum_{i=1}^{n} d_i$. So the choice of c minimizing the expected number of misallocations is $c = \alpha k_0/(n - k_0)$.

It should be noted that allocating by (2) is only optimal when δ_i is restricted to be a function of $\mathbf{x}_i$ alone. For example, k_0 must be known for the best choice of c to be obtained. Paradoxically, it will be shown in Section 2 that if k_0 is known, there exists a discrimination rule superior to rules of the form (1).

2. PERMUTATION EQUIVARIANT ALLOCATION RULES: k_0-KNOWN

Consider the class of allocation rules δ which are equivariant under permutations of the vectors $\mathbf{X}_1, \ldots, \mathbf{X}_n$. More specifically, let τ be any $(n \times n)$-dimensional permutation matrix. We restrict attention to rules $\delta(\mathbf{X})$, such that

$$[\delta(\mathbf{X})]\tau = \delta(\mathbf{X}\tau). \tag{4}$$

Note that this restriction still includes rules of the form (1) as a special case. The requirement (4) that δ be permutation equivariant can be justified by the natural requirement that the allocation of observations $\mathbf{X}_i$ should not depend upon their labels $i = 1, 2, \ldots, n$.

We shall now generalize the concept of order statistics to p dimensions. Let $\mathbf{A}$ be a subset of the space $\mathbf{M}_{p\times n}$ of all $(p \times n)$ matrices such that $\mathbf{X}$ lies in $\mathbf{A}$ with probability one. Let $\sigma : \mathbf{X} \to \sigma_X$ be a function from $\mathbf{A}$ into the class of $(n \times n)$ permutation matrices. We require that

(2.A) for each $(n \times n)$ permutation matrix ν, $A_\nu = \{\mathbf{X} : \sigma_X = \nu\}$ is measurable in $\mathbf{M}_{p\times n}$;

(2.B) for each $(n\times n)$ permutation τ, and for every $\mathbf{X} \in \mathbf{A}$, $\mathbf{X}\sigma_X = \mathbf{X}\tau\sigma_{X\tau}$.

Under these conditions, we shall call σ a *canonical ordering operator*. Let $\mathbf{Y} = (\mathbf{Y}_1, \ldots, \mathbf{Y}_n) = \mathbf{X}\sigma_X$. We call $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$ the corresponding *generalized order statistics* of $\mathbf{X}$. For convenience we can arbitrarily set $\mathbf{Y}_1 = \mathbf{Y}_2 = \cdots = \mathbf{Y}_n = \mathbf{0}$ on the null set $\mathbf{X} \notin \mathbf{A}$. The matrix $\mathbf{Y}$ can be recognized as an almost sure maximal invariant under the column permutation group. The joint density of $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$ is given by

$$L^n(k_0) = L_n(k_0; \mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n)$$
$$= \begin{cases} \sum_{\tau} \prod_{i=1}^{n-k_0} f[\mathbf{y}_{\tau(i)}] \prod_{i=n-k_0+1}^{n} g[\mathbf{y}_{\tau(i)}], & (\mathbf{y}_1, \ldots, \mathbf{y}_n) \in \bigcup_{X\in\mathbf{A}} X\sigma_X \\ 0 & (\mathbf{y}_1, \ldots, \mathbf{y}_n) \notin \bigcup_{X\in\mathbf{A}} X\sigma_X. \end{cases} \tag{5}$$

The summation above is understood to be over all permutations τ of the integers $i = 1, \ldots, n$. Expression (5) also defines a marginal likelihood $L^n(k)$ over $k = 0, 1, 2, \ldots, n$, for the case where k_0 is unknown. We shall consider its properties in the next section.

For k_0 known, we construct the optimal equivariant δ by formally identifying the minimum risk equivariant estimator (using risk function given in (3)) with the Bayes estimator to the same decision problem assuming the prior on the parameter space $\{(d_1, \ldots, d_n) : \sum_{i=1}^n d_i = k_0\}$ induced by the right invariant Haar measure on the group of column permutations. See, for example, Hora and Buehler (1966). As the permutation group is finite, the left and right Haar measures are identical and induce the uniform distribution on the parameter space $\{(d_1, \ldots, d_n) : \sum_{i=1}^n d_i = k_0\}$.

For equivariant δ,

$$\mathbf{E}[L(\mathbf{d}, \delta) \mid \mathbf{Y}] = \mathbf{E}^B[L(\mathbf{d}, \delta) \mid \mathbf{X}], \tag{6}$$

where $\mathbf{E}^B[. \mid \mathbf{X}]$ is the Bayes posterior expectation with respect to the uni-

form prior, given $\mathbf{X}$. Now,

$$\mathbf{E}^B[L(\mathrm{d},\delta)\ \mathbf{X}] = \mathbf{E}^B\left[\alpha \sum_{\{i:\delta_i=0\}} d_i \,\middle|\, \mathbf{X}\right] + \mathbf{E}^B\left[\sum_{\{i:\delta_i=1\}} (1-d_i) \,\middle|\, \mathbf{X}\right]. \quad (7)$$

So setting $\mathbf{E}^B[d_i \mid \mathbf{X}] = W_i(k_0)$, we see that

$$\mathbf{E}[L(\mathrm{d},\delta) \mid \mathbf{Y}] = \sum_{\{i:\delta_i=0\}} \alpha W_i(k_0) + \sum_{\{i:\delta_i=1\}} [1 - W_i(k_0)]. \quad (8)$$

The conditional expectation on the left-hand side of (8) is minimized by

$$\delta_i = \begin{cases} 0 & W_i(k_0) < \frac{1}{1+\alpha} \\ 1 & W_i(k_0) \geq \frac{1}{1+\alpha}. \end{cases} \quad (9)$$

It is interesting to compare the optimal allocation given in (9) with the rule based upon (1), (2) with $c = \alpha k_0/(n-k_0)$. If the conditional expectation $\mathbf{E}^B[d_i \mid \mathbf{X}]$ in (9) is replaced by $\mathbf{E}^B[d_i \mid \mathbf{X}_i]$, the resulting rule is precisely the optimal allocation based upon marginal distributions given by (1), (2). The reason for the suboptimality is then in evidence: $\mathbf{E}^B[d_i \mid \mathbf{X}_i]$ is based upon partial information from the complete data set.

The relationship between these rules is further clarified by the following representation of $W_i(k_0)$. Some algebra will provide from (5) the representation for each $1 \leq i \leq n$,

$$\begin{aligned} &L^n(k_0; \mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_n) \\ &= k_0 g(\mathbf{y}_i) L^{n-1}(k_0 - 1; \mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_{i-1}, \mathbf{y}_{i+1}, \cdots, \mathbf{y}_n) \\ &\quad + (n - k_0) f(\mathbf{y}_i) L^{n-1}(k_0; \mathbf{y}_1, \cdots, \mathbf{y}_{i-1}, \mathbf{y}_{i+1}, \cdots, \mathbf{y}_n) \end{aligned} \quad (10)$$

and from (10), if X_j corresponds to the ith order statistic $\mathbf{Y}_i$,

$$W_j(k_0) = \frac{k_0 g(\mathbf{y}_i) L^{n-1}(k_0 - 1; \mathbf{y}_1, \cdots, \mathbf{y}_{i-1}, \mathbf{y}_{i+1}, \cdots, \mathbf{y}_n)}{L^n(k_0; \mathbf{y}_1, \cdots, \mathbf{y}_n)}. \quad (11)$$

In view of (11), the criterion $W_j(k_0) > \frac{1}{1+\alpha}$ becomes

$$\frac{f(\mathbf{y}_i)}{g(\mathbf{y}_i)} < \frac{\alpha k_0}{n - k_0} \frac{L^{n-1}(k_0 - 1; \mathbf{y}_1, \cdots, \mathbf{y}_{i-1}, \mathbf{y}_{i+1}, \cdots, \mathbf{y}_n)}{L^{n-1}(k_0; \mathbf{y}_1, \cdots, \mathbf{y}_{i-1}, \mathbf{y}_{i+1}, \cdots, \mathbf{y}_n)}, \quad (12)$$

and this can be compared with the optimal Neyman-Pearson rule based on the marginal distribution of $\mathbf{X}_j$,

$$\frac{f(\mathbf{X}_j)}{g(\mathbf{X}_j)} \leq \frac{\alpha k_0}{n - k_0}. \quad (13)$$

In fact (12) is also a Neyman-Pearson rule but based on the joint distribution of the order statistics $\mathbf{Y}$. It clearly adjusts the right-hand side of (13) to account for the relative likelihood that there are either k_0 or $k_0 - 1$ contaminants in the data set with y_i removed. To show the effects of this adjustment, we compare the risk for rules (12) and (13) in the univariate case $n = 8$, $k_0 = 1$, $\alpha = 1$ and $f(x)$, $g(x)$ are normal (0,1) normal $(\mu, 1)$ respectively, in Table 1.

Table 1

Risk: $\alpha = 1$, $n = 8$, $k_0 = 1$, known

Rule	$\mu = .5$	$\mu = 1.0$	$\mu = 2.0$	$\mu = 2.5$
(12)	1.00	.96	.57	.32
(13)	1.00	.98	.67	.50

3. THE EFFECT OF UNKNOWN k_0

In general, of course, we do not know the value of k_0, and cannot put (12) into practice directly. Under these circumstances, it seems a reasonable modification of (12) to replace k_0 by an estimator obtained from the data.

In this section, we examine properties of the maximum (marginal) likelihood estimator of the parameter k_0 and note that the essential difference between rules of the form (12) and (13) disappears. Since one might expect the difference to depend on the efficiency of our estimator $\hat{k}$ maximizing $L^n(k)$, we first investigate the asymptotic properties of this estimator.

An alternative to maximum likelihood estimation of k_0 is an empirical Bayes approach to the problem. Suppose we assume k_0 is an observation from a binomial (n, π) distribution. The unknown parameter π appearing in the prior distribution for k_0 is replaced by a maximum likelihood estimator $\hat{\pi}$ obtained from the data X and the posterior probabilities that $d_i = 1$ given $\mathbf{X}$ are now computed assuming this value $\hat{\pi}$ for the parameter. It is not hard to show, in this case, that these probabilities are given by $w_i(\hat{\pi})$, where $w_i(p)$ is the function on $0 \leq p \leq 1$

$$w_i(p) = pg(\mathbf{X}_i)/[(1-p)f(\mathbf{X}_i) + pg(\mathbf{X}_i)], \qquad i = 1, 2, \ldots, n. \tag{14}$$

The rule $w_i(\hat{\pi}) \geq \frac{1}{1+\alpha}$ therefore reduces to a rule with form similar to (13), viz;

$$\frac{f(\mathbf{X}_i)}{g(\mathbf{X}_i)} \leq \frac{\alpha\hat{\pi}}{1-\hat{\pi}}. \tag{15}$$

This analysis leads to the same rule as a "mixture model" likelihood based rule where we assume the observations $\mathbf{X}_i$ are independent, each with mixture probability density function of the form $\pi g(\mathbf{x}) + (1-\pi)f(\mathbf{x})$ and the parameter π is estimated by maximum likelihood from the observed order statistics $\mathbf{Y}$. The following properties of the mixture likelihood are well-known:

(a) The mixture marginal likelihood function of $\mathbf{Y}$ is

$$\lambda^n(\pi) = \begin{cases} n! \prod_{i=1}^{n} [(1-\pi)f(\mathbf{Y}_i) + \pi g(\mathbf{Y}_i)] & \text{if } \mathbf{Y} = \mathbf{X}\sigma_X \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

(b) Provided $f(x_i) \neq g(x_i)$ for some $i = 1, 2, \ldots, n$, there is a unique value $\hat{\pi}$ maximizing $\lambda^n(\pi)$ and satisfying the likelihood equation

$$\mu_n(\hat{\pi}) = n\hat{\pi}, \tag{17}$$

where

$$\mu_n(\pi) = \sum_{i=1}^{n} w_i(\pi). \tag{18}$$

(c) *If the mixture model holds* with π_0 the true value of the parameter, $\sqrt{n}(\hat{\pi} - \pi_0)$ is asymptotically normal $(0, J^{-1}(\pi_0))$ where

$$J(\pi_0) = \frac{\mathbf{E}_G[w(\pi_0)] - \pi_0}{\pi_0(1-\pi_0)^2}$$

and $\mathbf{E}_G w(\pi_0)$ denotes the expected value of a weight $w_i(\pi_0)$ of an observation $\mathbf{X}_i$ drawn from density $g(\cdot)$.

We begin by comparing the estimator defined by (17) with the estimator $\hat{k}$ maximizing $L^n(k)$ for data obtained from a contamination model. The main result is the following:

Theorem. Let $n \to \infty$ and k_0, the number of contaminants, be the integer part of np_0 for some $0 < p_0 < 1$. Then:

(a) $| n\hat{\pi} - \hat{k} | < 1$.

(b) $n^{\frac{1}{2}}(\hat{\pi} - p_0)$ and $n^{-\frac{1}{2}}(\hat{k} - k_0)$ are asymptotically $N(0, I^{-1}(p_0))$ where $I^{-1}(p) = J^{-1}(p) - p(1-p)$.

(c) Provided $k - k_0 = o(\sqrt{n \log n})$,

$$L^n(k) \sim \frac{\sqrt{n\hat{\pi}(1-\hat{\pi})}}{\sigma_n(\hat{\pi})} \exp\left\{ \frac{-(k-n\hat{\pi})^2}{2} \left[\frac{1}{\sigma_n^2(\hat{\pi})} - \frac{1}{n\hat{\pi}(1-\hat{\pi})} \right] \right\} \lambda^n(\hat{\pi}) \tag{19}$$

almost surely, where

$$\sigma_n^2(p) = \sum_{i=1}^{n} w_i(p)[1 - w_i(p)].$$

Before proving this theorem, we comment on some of the results. (a) indicates that, whatever the origin of the data, the estimators $\hat{k}$ and $n\hat{\pi}$ (motivated by completely different models) of the number of contaminants in the sample are essentially equivalent when large. (b) is a standard result, required if we wish to test hypotheses or construct a confidence interval for the number of contaminants *actually appearing* in a sample, rather than some parameter (e.g., π in the mixture model) which generates this number. $I(p)$, although it takes the place usually occupied by the Fisher information in comparable results, is not strictly speaking the Fisher information. Indeed, since the parameter in a contamination model k_0 is necessarily discrete, there is no obvious analogue of Fisher information. Since $I(\pi) > J(\pi)$, there is generally more "information" in a sample on the number of contaminants than there is on the parameter π describing, in the mixture model, the probability a given observation will be a contaminant. (c) is a result comparable to that of Heyde and Johnstone (1979) describing the asymptotic form of the likelihood function. It indicates that the likelihood takes the form of a normal likelihood asymptotically, and is useful in the construction of fiducial or Bayes intervals for k_0.

Proof. We begin by proving (1). Conditionally on $\mathbf{Y}$ choose $Z_1, Z_2, \ldots, Z_n$ to be independent binary variates such that $P(Z_i = 1 \mid \mathbf{Y}) = w_i(p) = 1 - P(Z_i = 0 \mid \mathbf{Y})$. Then the (marginal) likelihood of k, $L^n(k)$, can be written as

$$L^n(k) = \frac{P\left[\sum_{i=1}^{n} Z_i = k \middle| \mathbf{Y}\right]}{Bin(k; n, p)} \lambda^n(p) \tag{20}$$

for arbitrary $0 < p < 1$, where

$$Bin(k; n, p) = \binom{n}{k} p^k (1-p)^{n-k}.$$

In equation (20), $P[\sum_{i=1}^n Z_i = k \mid \mathbf{Y}]$ is calculated conditionally on the order statistics and, hence, conditionally on $w_1(p), \ldots, w_n(p)$. We can interpret (20) as a mixture likelihood $\lambda^n(p)$ in p that has been corrected by the ratio of two probabilities. Note that p appears superficially only on the right-hand side of (20), where it cancels out and does not affect $L^n(k)$. Note also that the distribution of the order statistics is dependent on k only through the ratio $P[\sum_{i=1}^n Z_i = k \mid \mathbf{Y}]/Bin(k; n, p)$. As $0 < p < 1$ is arbitrary in equation (20), we set $p = \hat{\pi}$. We begin by showing that $L^n(k)$ decreases for $k \geq n\hat{\pi}$. For arbitrary $k \geq n\hat{\pi}$, let

$$h(s) = \begin{cases} \frac{1}{Bin(k+1;n,\hat{\pi})} & \text{if } s = k+1 \\ \frac{-1}{Bin(k;n,\hat{\pi})} & \text{if } s = k \\ 0 & \text{otherwise.} \end{cases} \tag{21}$$

Then $L^n(k+1) - L^n(k) = \lambda(\hat{\pi})\mathbf{E}\{h[\sum_{i=1}^n Z_i]\}$ where $Z_1, \ldots, Z_n$ are binary variates with $P[Z_i = 1 \mid \mathbf{Y}] = w_i(\hat{\pi}) = w_i$. By Corollary 2.1 of Hoeffding (1956), the maximum value of $\mathbf{E}\{h[\sum_{i=1}^n Z_i]\}$ over all $w_1, w_2, \ldots, w_n$ subject to the constraint $\sum_{i=1}^n w_i = n\hat{\pi}$ occurs when $w_1, \ldots, w_n$ take on at most three distinct values, at most one of which lies strictly between 0 and 1. Suppose the maximizing w_i are such that n_0 values are $0, n_1$ are 1 and n_2 values are $(n\hat{\pi} - n_1)/n_2$ where $n_2 = n - n_0 - n_1$. Then it is easy to see that in this case $L^n(k+1) - L^n(k) \leq 0$ if and only if

$$\frac{Bin\left(k+1-n_1; n_2, \frac{n\hat{\pi}-n_1}{n_2}\right)}{Bin\left(k-n_1; n_2, \frac{n\hat{\pi}-n_1}{n_2}\right)} \leq \frac{Bin(k+1; n, \hat{\pi})}{Bin(k; n, \hat{\pi})}$$

or equivalent, if

$$\frac{n-n_0-k}{n-n_0-n\hat{\pi}} \frac{n\hat{\pi}-n_1}{k+1-n_1} \leq \frac{n-k}{1-\hat{\pi}} \frac{\hat{\pi}}{k+1}. \tag{22}$$

Since $k \geq n\hat{\pi}$, this occurs for any $n_0, n_1 \geq 0$ with equality if and only if $n_0 = n_1 = 0$. Thus, we have shown that the maximized value of $L^n(k+1) - L^n(k)$ is less than or equal to zero for all $k \geq n\hat{\pi}$. Similarly, $L^n(k)$ is nondecreasing for $k \leq n\hat{\pi}$. Hence, $L^n(k)$ is unimodal and maximized by an integer $\hat{k}$ such that $| \hat{k} - n\hat{\pi} | < 1$.

We now prove (b). In view of (a) it is sufficient to prove that $n^{\frac{1}{2}}(\hat{\pi} - p_0)$ is asymptotically $N(0, I^{-1}(p_0))$. Define

$$u(\mathbf{x}_i; p) = \frac{w_i(p) - p}{p(1-p)} = \frac{[g(\mathbf{x}_i) - f(\mathbf{x}_i)]}{f(\mathbf{x}_i) + p[g(\mathbf{x}_i) - f(\mathbf{x}_i)]}. \tag{23}$$

It is easy to see that $u(\mathbf{x}_i; p)$ is a non-increasing function of p for each $\mathbf{x}_i$ and $\partial u/\partial p = -u^2$. Provided $f(\mathbf{x}_i) \neq g(\mathbf{x}_i)$ for some i, the m.l.e. $\hat{\pi}$ will be the unique solution to

$$\sum_{i=1}^{n} u(\mathbf{x}_i; \hat{\pi}) = 0. \tag{24}$$

Since F and G are distinct, the probability that $f(\mathbf{x}_i) = g(\mathbf{x}_i)$ for all $i = 1, 2, \ldots$, is zero. We suppose the data $\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_n$ obtain from a contamination model with k_0 equal to the integer part of np_0. Let $q_n = k_0/n$. Then for any $\epsilon > 0$,

$$\hat{\pi} \geq q_n + \epsilon \text{ iff } 0 \leq \sum_{i=1}^{n} u(\mathbf{X}_i; q_n + \epsilon). \tag{25}$$

Now $q_n \to p_0$ and for n sufficiently large,

$$q_n \mathbf{E}_G[u(\mathbf{X}; q_n + \epsilon)] + [1 - q_n]\mathbf{E}_F[u(\mathbf{X}; q_n + \epsilon)] < \delta < 0, \tag{26}$$

where δ does not depend on n. Here and in the remainder of the proof, $\mathbf{E}_G u(\mathbf{X}_i; p)$ denotes the expectation of $u(\mathbf{X}_i; p)$ for any X_i drawn from the distribution G. So applying the strong law of large numbers to the two components of the sample in (25) and using (26) we see that the probability is zero that (25) holds infinitely often as $n \to \infty$. We treat the case $\hat{\pi} \leq q_n - \epsilon$ similarly. Thus, $\hat{\pi} \to p_0$ almost surely.

Similarly, for $c > 0$,

$$\begin{aligned} P\left[\hat{\pi} > p + \frac{c}{\sqrt{n}}\right] &= P\left[0 < \sum_{i=1}^{n} u(\mathbf{X}_i; p_0 + cn^{-\frac{1}{2}})\right] \\ &\sim P\left[0 < \sum_{i=1}^{n} \left\{u(\mathbf{X}_i; p_0) - cn^{-\frac{1}{2}} u^2(\mathbf{X}_i; p_0)\right\}\right] \\ &\sim P\left[c\mathbf{E}(u^2) < n^{-\frac{1}{2}} \sum_{i=1}^{n} (\mathbf{X}_i; p_0)\right]. \end{aligned} \tag{27}$$

Now it is easy to see that $\mathbf{E}(u^2) = \mathbf{E}_G(u)/(1 - p_0)$. It can also be shown that $n^{-\frac{1}{2}} \sum_{i=1}^{n} u(\mathbf{X}_i; p_0)$ is asymptotically normal with mean zero and variance

$$\frac{\mathbf{E}_G[u(\mathbf{x}; p_0)]}{1 - p_0} \{1 - p_0 \mathbf{E}_G[u(\mathbf{x}; p_0)]\}. \tag{28}$$

Substituting this in (27), we obtain that $\sqrt{n}(\hat{\pi} - p_0)$ is asymptotically normal with mean zero and variance

$$\frac{\{1 - p_0 \mathbf{E}_G[u(\mathbf{x}; p_0)]\}(1 - p_0)}{\mathbf{E}_G[u(\mathbf{x}; p_0)]}. \tag{29}$$

Substituting the form $u(\mathbf{x};p_0) = [w(\mathbf{x};p_0) - p_0]/[p_0(1-p_0)]$ the variance (29) takes the form $I^{-1}(p_0)$.

To prove (c), we verify the conditions of the local central limit theorem (see Petrov, 1975, p. 195, Theorem 4) to approximate $P[\sum_{i=1}^n Z_i = k \mid \mathbf{Y}]$ using $p = \hat{\pi}$ in (20). First observe that as a consequence of (a) above, $\sigma_n^2(\hat{\pi}) \sim \sigma_n^2(p_0)$ a.s. as $n \to \infty$. We begin by showing

$$\left|\frac{k - \mu_n(\hat{\pi})}{\sigma_n(\hat{\pi})}\right| = o(\sqrt{\log n}) \text{ a.s.} \tag{30}$$

Note that since $\sigma_n^2(\hat{\pi}) \sim \sigma_n^2(p_0) \sim n\ \mathbf{E}\{w(\mathbf{X};p_0)[1 - w(\mathbf{X};p_0)]\}$, we only need to show

$$| k - \mu_n(\hat{\pi}) | = o(\sqrt{n \log n}) \text{ a.s.} \tag{31}$$

Now the left side of (31) is less than or equal to

$$\begin{aligned} &| k - k_0 | + | k_0 - \mu_n(k_0/n) | + | \mu_n(k_0/n) - \mu_n(\hat{\pi}) | \\ &= o(\sqrt{n \log n}) + O(\sqrt{n \log \log n}) + \left(\frac{k_0 - n\hat{\pi}}{n}\right) O(\sigma_n^2(p_0)) \text{ a.s.} \end{aligned}$$

The order of the middle term follows from the law of the iterated logarithm applied to the two components of the sample. The order in the last term follows from the fact that $\partial \mu_n(p)/\partial p = \sigma_n^2(p)/[p(1-p)]$. The entire expression is $o(\sqrt{n \log n})$.

Having established (30), we now apply the local central limit theorem to obtain

$$\begin{aligned} P\left[\sum_{i=1}^n Z_i = k \,\middle|\, \mathbf{Y}\right] &\sim N\left[k; \mu_n(\hat{\pi}), \sigma_n^2(\hat{\pi})\right] \\ &= N[k; n\hat{\pi}, \sigma_n^2(\hat{\pi})] \text{ a.s.}, \end{aligned} \tag{32}$$

where $N(x;\mu,\sigma^2) = (\sqrt{2\pi}\sigma)^{-1} \exp[-(x-\mu)^2/(2\sigma^2)]$. Similarly in the denominator of (20)

$$Bin(k;n,\hat{\pi}) \sim N[k; n\hat{\pi}, n\hat{\pi}(1-\hat{\pi})]. \tag{33}$$

The expression (19) now follows from (32), (33).

We are now in a position to compare the discrimination rules for unknown number of contaminants. The rule (15) is obtained from the mixture model in the empirical Bayes analysis, and this is to be compared with a rule of the form (9) or (12) with k_0 replaced by its maximum likelihood estimator $\hat{k}$. We have seen that $\alpha\hat{k}/(n-\hat{k})$ and $\alpha\hat{\pi}/(1-\hat{\pi})$ are nearly identical for large

$\hat{k}$ not too close to n since $| \hat{k} - n\hat{\pi} | < 1$. Furthermore, the second term on the right-hand side of (12), while providing a correction when k_0 is unknown, is almost exactly equal to 1 when k_0 is replaced by $\hat{k}$, since this is the ratio of the likelihood function L^{n-1} at its maximum and a value adjacent to its maximum. This observation can be verified asymptotically fairly easily using the expression (c) of the Theorem; we can show that for each i, the two weights are asymptotically equivalent in the sense that $W_i(\hat{k})/w_i(\hat{\pi}) \to 1$ almost surely.

We verify this result for small samples with a simulation in the case discussed earlier: $n = 8$, $k_0 = 1$, $\alpha = 1$. The results, tabulated in Table 2, can now be compared with those of Table 1 and we see that a large penalty is paid for lack of knowledge of the value of k_0. This table was generated from 4,000 simulations of each case.

Table 2

Risk: $n = 8, \alpha = 1, k_0 = 1$ unknown

Rule	$\mu = .5$	$\mu = 1.0$	$\mu = 2.0$	$\mu = 2.5$
$W_i(\hat{k}) > \frac{1}{1+\alpha}$	2.77	1.81	.92	.62
(15)	2.77	1.80	.92	.62

REFERENCES

Anderson, T. W. (1958), *An Introduction to Multivariate Statistical Analysis.* New York: Wiley and Sons.

Heyde, C. C., and I. M. Johnstone (1979), "On asymptotic posterior normality for stochastic processes." *Journal of the Royal Statistical Society,* Series B **41,** 184–189.

Hoeffding, W. (1956), "On the distribution of the number of successes in independent trials." *Annals of Mathematical Statistics* **27,** 713–721.

Hora, R. B., and R. J. Buehler (1966), "Fiducial theory and invariant estimation." *Annals of Mathematical Statistics* **37,** 643–656.

Kendall, M. G., A. Stuart, and J. K. Ord (1966), *The Advanced Theory of Statistics,* Volume 3. London: Griffin.

Petrov, V. V. (1975), *Sum of Independent Random Variables.* Berlin: Springer.

Truc T. Nguyen [1]

ON FRÉCHET BOUNDS OF BIVARIATE DISTRIBUTIONS

ABSTRACT

The Fréchet bounds of a set of bivariate distributions with fixed marginals are characterized by the monotonicity of their supports. Also they are characterized by their totally positive dependence of order 2 (TP2) and reverse regular of order 2 (RR2) properties. A corollary of these results is the existence of a measurable transformation which transforms two different random variables of a location-scale parameter family defined by a symmetric probability density function into the same continuous random variable.

1. INTRODUCTION

Let X and Y be jointly distributed random variables with the joint cumulative distribution function (c.d.f.) $H(x, y)$ and with fixed marginals c.d.f.'s $F(x)$ and $G(y)$. The convex set of all such bivariate c.d.f.'s is denoted by $\mathcal{F}(F, G)$. The characterizations of extreme distributions of this set are given in a number of papers, under different forms and cases. Douglas (1964) and Lindenstrauss (1965) considered the case of continuous F and G. Letac (1966), Denny (1980) and Nguyen and Sampson (1982) give characterizations in the discrete case. In this note, we study two special extreme distributions of $\mathcal{F}(F, G)$, namely, the upper Fréchet bound and the lower Fréchet bound of the set $\mathcal{F}(F, G)$. In Section 2, the Fréchet bounds are characterized by the monotonicity of their supports. A corollary of this result in the case of continuous F and G is a result of Kimeldorf and Sampson (1978), a monotone dependence characterization of the Fréchet bounds. The transformations between two continuous random variables are also studied in this section. In Section 3, inside the set of extreme distributions of $\mathcal{F}(F, G)$, the Fréchet

[1] Department of Mathematics and Statistics, Bowling Green State University, Bowling Green, Ohio 43403

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 179–188.

bounds will be characterized by their TP2 and RR2 properties. In Section 4, using the transformations defined by the Fréchet bounds, we construct transformations which map two different random variables of a location-scale parameter family into the same random variable of the family.

2. FRÉCHET BOUNDS AND FRÉCHET BOUND TRANSFORMATIONS

The following theorem defines the greatest lower bound and the least upper bound of the set $\mathcal{F}(F,G)$.

Theorem 2.1. (Hoeffding, 1940; Fréchet, 1951)

Let $H^-(x,y) = \max(0, F(x) + G(y) - 1)$ and $H^+(x,y) = \min(F(x), G(y))$. Then for any c.d.f. H of $\mathcal{F}(F,G)$ and for all $(x,y) \in R^2$,

$$H^-(x,y) \leq H(x,y) \leq H^+(x,y).$$

Note that H^- and H^+ both are c.d.f.'s in $\mathcal{F}(F,G)$. H^- and H^+ are called the lower Fréchet bound and the upper Fréchet bound of $\mathcal{F}(F,G)$, respectively. They both are extreme c.d.f.'s in $\mathcal{F}(F,G)$.

In this section, the Fréchet bounds are characterized by the monotonicity of their supports.

Definition 2.1. A set C of R^2 is said to be a monotone non-decreasing (non-increasing) curve if $\forall$ (x_1,y_1), (x_2,y_2) of C, $x_1 < x_2$, implies $y_1 \leq y_2$ $(y_1 \geq y_2)$.

Between the set of probability measures μ in R^2 (R^1) and the set of bivariate c.d.f.'s (univariate c.d.f.'s) $H(F)$, there exists a one to one correspondence determined by

$$\mu(I_1 \times I_2) = H(x_2,y_2) + H(x_1,y_1) - H(x_1,y_2) - H(x_2,y_1),$$

where $I_1 = (x_1,x_2]$, $I_2 = (y_1,y_2]$ are two arbitrary intervals of R^1 such that $\mu(I_1) = F(x_2) - F(x_1)$. The support of a c.d.f. is the support of the corresponding probability measure. The support of a c.d.f. H is denoted by $\text{Supp}(H)$.

Theorem 2.2. Let X and Y be r.v.'s with respective c.d.f.'s F and G. A necessary and sufficient condition that their joint c.d.f. is H^+, the upper Fréchet bound (H^-, the lower Fréchet bound) of $\mathcal{F}(F,G)$ is that the support of their joint c.d.f. is a non-decreasing (non-increasing) curve.

Proof. *Necessity.* Suppose that the joint c.d.f. of X and Y is H^+ and (x_1, y_1), (x_2, y_2) are two arbitrary points of $\text{Supp}(H^+)$ with $x_1 < x_2$. It must be shown that $y_1 \leq y_2$. The proof follows by contradiction. Suppose that $y_1 > y_2$. Let $0 < \delta < \min((x_2 - x_1)/2, (y_1 - y_2)/2)$. Then $x_1 + \delta < x_2$ and $y_2 + \delta < y_1$. Since (x_1, y_1) and (x_2, y_2) are points of $\text{Supp}(H^+)$ and both do not belong to $(-\infty, x_1 + \delta] \times (-\infty, y_2 + \delta]$, the following inequalities hold:

$$H^+(x_1 + \delta, y_2 + \delta) < F(x_1 + \delta)$$

and

$$H^+(x_1 + \delta, y_2 + \delta) < G(y_2 + \delta).$$

These two inequalities imply that $H^+(x_1 + \delta, y_2 + \delta) < \min(F(x_1 + \delta), G(y_2 + \delta))$ and this is a contradiction with H^+.

Sufficiency. Suppose that the joint c.d.f. of X and Y is H with $\text{Supp}(H)$ being a non-decreasing curve. Let (x_0, y_0) be an arbitrary point of R^2. It must be shown that $H(x_0, y_0) = \min(F(x_0), G(y_0))$. The proof also follows by contradiction. Suppose that $H(x_0, y_0) < \min(F(x_0), G(y_0))$. Hence, each of the sets $\text{Supp}(H) \cap (x_0, \infty) \times (-\infty, y_0]$, and $\text{Supp}(H) \cap (-\infty, x_0] \times (y_0, \infty)$ are not empty. Suppose (x_1, y_1) and (x_2, y_2) are points in these two sets, respectively. Then $x_1 > x_0 \geq x_2$, $y_1 \leq y_0 < y_2$. This implies that $\text{Supp}(H)$ is not a non-decreasing curve, a contradiction.

The proof of the lower Fréchet bound is similar.

In the case where X and Y are both continuous r.v.'s, that is F and G are absolutely continuous c.d.f.'s, the Fréchet bounds are characterized by their monotone dependency.

Corollary 2.1. (Kimeldorf and Sampson, 1978) Let X and Y be continuous random variables with respective c.d.f.'s F and G. A necessary and sufficient condition that X and Y have their joint c.d.f. as their upper (lower) Fréchet bound of $\mathcal{F}(F, G)$ is that there exists a monotone increasing (decreasing) function g^+ (g^-) for which $P(Y = g^+(X)) = 1$ ($P(Y = g^-(X)) = 1$), i.e., Y and $g^+(X)$ (Y and $g^-(X)$) are almost surely identical.

The function g^+ (g^-) is called by us the upper (lower) Fréchet bound transformation of X into Y. The functions g^+ and g^- are defined by Theorem 2.1 by the following implicit forms:

$$F(x) = G(g^+(x))$$

and

$$F(x) + G(g^-(x)) = 1,$$

for every $x \in$ Range (X). Without loss of generality, suppose that both Range (X) and Range (Y) are open. The domain of g^+ and g^- is Range (X) and their range is Range (Y). g^+ and g^- are both differentiable (and hence continuous and measurable) on Range (X). For given F and G, g^+ and g^- are uniquely defined (up to a set of measure 0, with respect to the Lebesgue measure on Range (X)).

Definition 2.2. (Barlow and Proschan, 1975) Let X and Y have joint density (or in the discrete case, joint probability mass function) $f(x, y)$. Then $f(x, y)$ is totally positive of order 2, TP2 (reverse regular of order 2, RR2; see Karlin, 1968) if

$$\begin{vmatrix} f(x_1, y_1), & f(x_1, y_2) \\ f(x_2, y_1), & f(x_2, y_2) \end{vmatrix} \geq (\leq)\ 0$$

for all $x_1 < x_2$, $y_1 < y_2$ in the ranges of X and Y, respectively.

This definition has been extended to handle the case when p.d.f.'s do not exist. For disjoint intervals I and J in R^1, with end points a, b, and c, d, respectively, we say $I < J$ if $b < c$.

Definition 2.3. (Block *et al.*, 1982) Let μ be a probability measure on R^2. The measure μ is TP2 (RR2) if

$$\mu(I_1 \times J_1) \times \mu(I_1' \times J_1') \geq (\leq)\ \mu(I_1 \times J_1') \times \mu(I_1' \times J_1) \qquad (2.1)$$

where $I_1 < I_1'$, $J_1 < J_1'$ are disjoint intervals of R^1.

For the case where (X, Y) has a p.d.f. or a p.m.f., it is easily shown that Definitions 2.2 and 2.3 are equivalent.

The c.d.f. H is said to be TP2 (RR2) if its corresponding probability measure μ is TP2 (RR2).

Suppose μ^+ and μ^- are the measures corresponding to H^+ and H^-, respectively. We show in Lemma 2.1 that the upper Fréchet bound is TP2 and the lower Fréchet bound is RR2.

Lemma 2.1. μ^+ is TP2 and μ^- is RR2.

Proof. Suppose $I_1 = (x_1, x_2]$, $I_1' = (x_1', x_2']$, $J_1 = (y_1, y_2]$, $J_1' = (y_1', y_2']$, where $I_1 < I_1'$, $J_1 < J_1'$. Without loss of generality, we can suppose that $F(x_1) \leq G(y_1)$. The proof then follows by Definition 2.3 and by considering the two cases separately, namely $F(x_2) \leq G(y_2)$ and $F(x_2) > G(y_2)$.

3. A TP2 AND RR2 CHARACTERIZATION OF FRÉCHET BOUNDS

The marginal c.d.f.'s of $\mathcal{F}(F,G)$ can be written under the following forms:

$$F = a_1F_d + a_2F_s + (1-a_1-a_2)F_{ac},\ 0 \le a_1,\ a_2 \le 1,\ a_1+a_2 \le 1,$$

and

$$G = b_1G_d + b_2G_s + (1-b_1-b_2)G_{ac},\ 0 \le b_1,\ b_2 \le 1,\ b_1+b_2 \le 1,$$

where F_d, G_d are discrete parts, F_{ac}, G_{ac} are absolutely continuous parts and F_s, G_s are singular parts of F and G, respectively. In this note, we suppose that both F and G do not have singular parts (that is, they are non-singular c.d.f.'s). Then $F = a_1F_d + (1-a_1)F_{ac}$, $G = b_1G_d + (1-b_1)G_{ac}$.

Theorem 3.1. Let X and Y be random variables with respective c.d.f.'s F and G (both without singular parts). A necessary and sufficient condition for the joint c.d.f. of X and Y to be the upper (lower) Fréchet bound of $\mathcal{F}(F,G)$ is that H is an extreme c.d.f. of $\mathcal{F}(F,G)$ and H is TP2 (RR2).

Proof. The necessity follows immediately from Lemma 2.1. To show sufficiency, we need to show that Supp(H) is a non-decreasing curve in the case of upper Fréchet bound and is a non-increasing curve in the case of lower Fréchet bound. The proof follows by Theorem 2.2.

To prove sufficiency, we need the following results, proofs of which are omitted.

Lemma 3.1. Let H be a c.d.f. If H is TP2 (RR2) and if (x_1,y_1), (x_2,y_2) are two points of Supp(H) with $x_1 < x_2$, $y_1 > y_2$ ($y_1 < y_2$), then (x_1,y_2) and (x_2,y_1) are also points of Supp(H).

Theorem 3.2. (Nguyen and Sampson, 1982) Let X and Y be discrete r.v.'s with respective c.d.f.'s F and G. Their joint c.d.f. H is an extreme point of $\mathcal{F}(F,G)$ if and only if for every finite rectangle $S_I \times S_J$ in Supp(F)$\times$ Supp(G), there exists a row or a column containing at most one point of Supp(H).

Theorem 3.3. (Lindenstraus, 1965) Let X and Y be continuous r.v.'s with respective c.d.f.'s F and G. Suppose their joint c.d.f. H is an extreme element of $\mathcal{F}(F,G)$. Then the corresponding probability measure μ of H is singular with respect to Lebesgue measure on R^2.

Let H be a c.d.f. of $\mathcal{F}(F,G)$, where F and G are two non-singular part univariate c.d.f.'s. In general H can be written under the form $H =$

$aH_d + bH_s + (1-a-b)H_{ac}$, where H_d, H_s and H_{ac} are discrete, singular and absolutely continuous parts of H, respectively, $0 \le a,\ b \le 1$, $a+b \le 1$. If H has a singular part, i.e., $b \neq 0$, H_s itself can be decomposed into two parts, one with continuous marginals, denoted by H_{sc}, the other is denoted by H_{sd}. Set $C_{sc} = \{(x,y) : (x,y) \in \text{Supp } (H_s),\ x \in \text{Supp } (F_c)$ and $y \in \text{Supp } (G_c)\}$, $C_{sd} = \{(x,y);\ (x,y) \in \text{Supp } (H_s),\ x \in \text{Supp } (F_d)$ or $y \in \text{Supp } (G_d)\}$.

Let μ_{sc} and μ_{sd} be two measures on R^2, defined by $\mu_{sc} = 0$ if $\mu_s(C_{sc}) = 0$, $\mu_{sd} = 0$ if $\mu_s(C_{sd}) = 0$ and $\mu_{sc}(E) = \mu_s(E \cap C_{sc})/\mu_s(C_{sc})$ if $\mu_s(C_{sc}) \neq 0$, $\mu_{sd}(E) = \mu_s(E \cap C_{sd})/\mu_s(C_{sd})$ if $\mu_s(C_{sd}) \neq 0$, where E is a measurable subset of R^2 and μ_s is the probability measure corresponding to H_s. In the case $\mu_{sc} \neq 0$ and $\mu_{sd} \neq 0$, H_{sc} and H_{sd} are the c.d.f.'s corresponding to μ_{sc} and μ_{sd}, respectively. In the general case, H_s can be written as $H_s = cH_{sc} + (1-c)H_{sd}$, $0 \le c \le 1$. Note that $c = 0$ if $\mu_s(C_{sc}) = 0$ and $c = 1$ if $\mu_s(C_{sd}) = 0$. This decomposition of H_s is unique by the uniqueness of C_{sc} and C_{sd}. Substituting this form of H_s in H, one obtains $H = aH_d + b_1H_{sc} + b_2H_{sd} + (1-a-b_1-b_2)H_{ac}$, $0 \le a,\ b_1,\ b_2 \le 1$, $a+b_1+b_2 \le 1$.

If F and G are both discrete, then $a = 1$, and $H = H_d$. If F and G both are absolutely continuous, then $a = b_2 = 0$, and $H = b_1H_{sc} + (1-b_1)H_{ac}$.

By Theorem 3.3, if H is an extreme c.d.f. of $\mathcal{F}(F,G)$ then $1-a-b_1-b_2 = 0$, and $H = aH_d + b_1H_{sc} + (1-a-b_1)H_{sd}$. Thus, H_d, H_{sc} and H_{sd} are extreme c.d.f.'s of $\mathcal{F}(H_d)$, $\mathcal{F}(H_{sc})$, and $\mathcal{F}(H_{sd})$, respectively, where $\mathcal{F}(H_d)$, $\mathcal{F}(H_{sc})$, and $\mathcal{F}(H_{sd})$ are the sets of c.d.f.'s with fixed marginals defined by H_d, H_{sc}, and H_{sd}, respectively.

Proof of the Sufficiency Part of Theorem 3.1.

Let H be a TP2 extreme c.d.f. of $\mathcal{F}(F,G)$. To show that H is the upper Fréchet bound of $\mathcal{F}(F,G)$, we are going to show that Supp(H) is a non-decreasing curve, then the proof follows by Theorem 2.2.

Let (x_1,y_1) and (x_2,y_2) be two arbitrary points of Supp(H) with $x_1 < x_2$. We need to show that $y_1 \le y_2$. The proof follows by contradiction.

Suppose $y_1 > y_2$. By Lemma 3.1 (x_1,y_2) and (x_2,y_1) are also points of Supp(H). Now, there are different cases to be considered.

(a) *F and G both are discrete c.d.f.'s.* The contradiction follows by considering the rectangle $\{x_1,x_2\} \times \{y_1,y_2\}$, and from Theorem 3.2.

(b) *F and G are both absolutely continuous c.d.f.'s.* It is known that if F is an absolutely continuous c.d.f., $F(X)$ is a r.v. with uniform distribution on $(0,1)$. For every measurable set E of R^1, let $\mu_F(E) = m(F(E))$, where m is the Lebesgue measure on R^1. Then, $\forall 0 < \delta < \min((x_2-x_1)/2, (y_1-y_2)/2)$, it follows that $\mu_H((x_1-\delta, x_1+\delta) \times$

$(y_1 - 0, y_1 + \delta)) > 0$, and $\mu_H((x_2 - \delta, x_2 + \delta) \times (y_2 - \delta, y_2 + \delta)) > 0$. Set $C_1 = \{x : (x, y) \in (x_2 - \delta, x_2 + \delta) \times (y_2 - \delta, y_2 + \delta) \cap \text{ Supp } (H)\}$, $C_2 = \{y : (x, y) \in (x_1 - \delta, x_1 + \delta) \times (y_1 - \delta, y_1 + \delta) \cap \text{ Supp } (H)\}$. Then $\mu_F(C_1) > 0$ and $\mu_G(C_2) > 0$. F and G are both absolutely continuous, hence $m(C_1) > 0$ and $m(C_2) > 0$. By Lemma 3.1, $C_1 \times C_2$ is a subset of Supp(H), $\mu_H(C_1 \times C_2) > 0$, and $m \times m(C_1 \times C_2) = m(C_1) \times m(C_2) > 0$. The contradiction then follows by Theorem 3.3.

(c) *F and G are two c.d.f.'s with no singular parts.* The proof follows upon considering the following different subcases.

(x_1, y_1) and (x_2, y_2) are:

(1) both in Supp (H_d) or both in Supp (H_{sc}),

(2) one in Supp (H_{sd}) and one in Supp (H_{sc}),

(3) both in Supp (H_{sd}),

(4) one in Supp (H_d) and one in Supp (H_{sd}), and

(5) one is in Supp (H_d) and one in Supp (H_{sc}).

The proof for the lower Fréchet bound and RR2 is similar.

Corollary 3.1. Let H be a TP2 (RR2) c.d.f. in $\mathcal{F}(F, G)$. If H is not the upper (lower) Fréchet bound of $\mathcal{F}(F, G)$, then H is not an extreme c.d.f. of $\mathcal{F}(F, G)$.

Fréchet (1958) investigated the case of two parameter c.d.f.'s with fixed marginals under the form

$$aH^+ + bH^- + (1 - a - b)H_I : 0 \leq a,\ b \leq 1,\ a + b \leq 1, \text{ where } H_I = FG.$$

Konijn (1959) used mixtures of H_I, H^+, and H^- to investigate the power of certain tests of independence. Ahmed *et al.* (1979) used the set $\{aH_I + (1 - a)H^+ : 0 \leq a \leq 1\}$ as a model for a test of independence versus strictly positive quadrant dependence. We now study these sets with respect to TP2 and RR2.

Corollary 3.2. Let H_I and H^+ (H^-) be the independent c.d.f. and the upper (lower) Fréchet bound of $\mathcal{F}(F, G)$ where F and G are two absolutely continuous c.d.f.'s. Then $H = aH_I + (1 - a)H^+$ $(aH_I + (1 - a)H^-)$ is not TP2 (RR2) for every $0 < a < 1$.

Corollary 3.3. Let H_I, H^+ and H^- be the independent c.d.f., the upper Fréchet bound and the lower Fréchet bound of $\mathcal{F}(F, G)$, respectively, where F and G are two absolutely continuous c.d.f.'s. Then $H = aH^+ + bH^- +$

$(1-a-b)H_I$, $0 \le a, b \le 1$, $a+b \le 1$, is neither TP2 nor RR2 if $0 < a < 1$ or $0 < b < 1$.

4. A PROBLEM RELATED TO FRÉCHET BOUND TRANSFORMATIONS

Let X_0 be a continuous random variable with range R^1, with c.d.f. F, and symmetric p.d.f. f. The location-scale parameter family of distributions defined by X_0 is denoted by

$$\mathcal{F}_{L,S} = \{F_{a,b} : F_{a,b}(x) = F((x-a)/b),\ -\infty < a < +\infty,\ b > 0\}.$$

Lemma 4.1. Let X_1, X_2 and X_3 be r.v.'s with respective c.d.f.'s $F_1 = F_{a_1,b_1}$, $F_2 = F_{a_2,b_2}$ and $F_3 = F_{a_3,b_3}$, where F_1, F_2 and F_3 are in $\mathcal{F}_{L,S}$ and at least $a_1 \neq a_2$ or $b_1 \neq b_2$. Then there does not exist any linear transformation which transforms both of X_1 and X_2 into X_3.

Proof. The proof follows by contradiction. Suppose there exists a linear transformation $T(x) = ax+b$ which transforms both of X_1 and X_2 into X_3. If $a > 0$, then T is increasing by Corollary 2.1 and by the upper Fréchet bound transformation from X_1 into X_3 and from X_2 into X_3. The transformation T is then defined by $F_1(x) = F((x-a_1)/b_1) = F_3(T) = F((T-a_3)/b_3)$, such that $T(x) = (b_3/b_1)x + a_3 - (b_3/b_1)a_1$, or $F_2(x) = F((x-a_2)/b_2) = F_3(T) = F((T-a_3)/b_3)$, such that $T(x) = (b_3/b_2)x + a_3 - (b_3/b_1)a_2$. If $a < 0$, then T is decreasing by Corollary 2.1. and by the lower Fréchet bound transformation from X_1 into X_3 and from X_2 into X_3. The transformation T is then defined by $F_3(T) = 1-F_1(x) = 1-F((x-a_1)/b_1) = F(-(x-a_1)/b_1)$, then $T(x) = -(b_3/b_1)x + a_3 + (b_3/b_1)a_1$, or $F_3(T) = 1-F_2(x) = 1-F((x-a_2)/b_3) = F(-(x-a_2)/b_2)$, then $T(x) = -(b_3/b_2)x + a_3 + (b_3/b_2)a_2$.

In both cases, it implies that $a_1 = a_2$ and $b_1 = b_2$ and the contradiction follows.

Theorem 4.1. If X_1 and X_2 are two r.v.'s with respective c.d.f.'s $F_1 = F_{a_1,1}$ and $F_2 = F_{a_2,1}$, with $a_1 \neq a_2$ then there exists a nonlinear (measurable) transformation T which transforms both X_1 and X_2 into X_0.

Proof. Let $t(x) = (x-(a_1+a_2)/2)^2$. Then $W = t(X_1) = t(X_2)$ (i.e., $t(X_1)$ and $t(X_2)$ are identically distributed).

$P(t(X_1) \le w) = P(t(X_2) \le w) = 0$ if $w \le 0$.

$$
\begin{aligned}
&P\{t(X_1) = (X_1 - (a_1 + a_2)/2)^2 \le w\} \\
&= P\{-(w)^{\frac{1}{2}}) \le X_1 - (a_1 + a_2)/2 \le (w)^{\frac{1}{2}}\} \\
&= P\{-(w)^{\frac{1}{2}} + (a_1 + a_2)/2) \le X_1 \le (w)^{\frac{1}{2}} + (a_1 + a_2)/2\} \\
&= P\{-(w)^{\frac{1}{2}} + (a_1 + a_2)/2 - a_1 \le X_1 - a_1 \le (w)^{\frac{1}{2}} + (a_1 + a_2)/2 - a_1\} \\
&= P\{-(w)^{\frac{1}{2}} + (a_2 - a_1)/2 \le X_0 \le (w)^{\frac{1}{2}} + (a_2 - a_1)/2\} \\
&= P\{-(w)^{\frac{1}{2}} - (a_2 - a_1)/2 \le X_0 \le (w)^{\frac{1}{2}} - (a_2 - a_1)/2\} \\
&\text{(by symmetry of the distribution of } X_0\text{)} \\
&= P\{-(w)^{\frac{1}{2}} - (a_2 - a_1)/2 + a_2 \le X_0 + a_2 \le (w)^{\frac{1}{2}} - (a_2 - a_1)/2 + a_2\} \\
&= P\{-(w)^{\frac{1}{2}} + (a_1 + a_2)/2 \le X_2 \le (w)^{\frac{1}{2}} + (a_1 + a_2)/2\} \\
&= P\{-(w)^{\frac{1}{2}} \le X_2 - (a_1 + a_2)/2 \le (w)^{\frac{1}{2}}\} \\
&= P(t(X_2) = (X_2 - (a_1 + a_2)/2)^2 \le w) \ \forall\ w > 0.
\end{aligned}
$$

$W = t(X_1) = t(X_2)$ is a continuous random variable with range$(0, +\infty)$.

Let g^+_{W,X_0} and g^-_{W,X_0} be the upper and lower Fréchet bound transformations from W into X_0, respectively. Then $T_1 = (g^+_{W,X_0}) \circ t$ and $T_2 = (g^-_{W,X_0}) \circ t$ are, by Lemma 4.1, two nonlinear (measurable) transformations which transform X_1 and X_2 into X_0.

When $X_0 \sim N(0, 1)$, the result of Theorem 4.1 is an answer to a question of D. Basu given by Kagan *et al.* (1973): Does there exist a nonlinear (measurable) transformation $T : R^1 \to R^1$ which transforms two normal distributions with different means into the same normal distribution? For a complete solution of this problem, see Nguyen (1985).

REFERENCES

Ahmed, A. H. N., N. A. Lanberg, R. V. Leon, and F. Proschan (1978), "Partial ordering of positive quadrant dependence, with applications." Technical Report, The Florida State University, Tallahassee, Florida.

Barlow, R. E., and F. Proschan (1975), *Statistical Theory of Reliability and Life Testing.* New York: Holt, Rinehart and Winston.

Block, H. W., T. H. Savits, and M. Shaked (1982), "Some concepts of negative dependence." *Annals of Probability* **10**, 765–772.

Denny, J. L. (1980), "The support of discrete extreme measures with given marginals." *Michigan Mathematics Journal* **27**, 59–64.

Douglas, R. G. (1964), "On extreme measures and subspace density." *Michigan Mathematics Journal* **11**, 243–246.

Fréchet, M. (1951), "Sur les tableaux de corrélation dont les marges sont données." *Annales de l'Université de Lyon*, Section A, Series 3, **14**, 53–77.

Fréchet, M. (1958), "Remarques au sujet de la note précédente." *Comptes Rendus des Séances Academie des Sciences* **246**, 2719–2720.

Hoeffding, S. (1940), "Masstabinvariante Korrelations-Theorie." *Schriften Mathematische Institut Universität Berlin* **5**, 181–233.

Kagan, A. M., Y. V. Linnik, and C. R. Rao (1973), *Characterization Problems in Mathematical Statistics*. New York: Wiley and Sons.

Karlin, S. (1968), *Total Positivity*, Volume 1. Stanford, California: Stanford University Press.

Kimeldorf, G., and A. R. Sampson (1978), "Monotone dependence." *Annals of Statistics* **6**, 895–903.

Konijn, H. S. (1959), "Positive and negative dependence of two random variables." *Sankhyā* **21**, 269–280.

Letac, G. (1966), "Représentation des mesures de probabilités sur le produit de deux espaces dénombrables de marges données." *Illinois Journal of Mathematics* **10**, 497–507.

Lindenstrauss, J. (1965), "A remark on extreme doubly stochastic measures." *American Mathematical Monthly* **72**, 379–382.

Nguyen, T. T. (1985), "A note on Fréchet bounds and transformations between normal random variables." Technical Report, Bowling Green State University, Bowling Green, Ohio.

Nguyen, T. T., and A. R. Sampson (1982), "Extreme points of bivariate discrete distributions with fixed marginals." Technical Report. No. 82–21. University of Pittsburgh, Pittsburgh, Pennsylvania.

Colin M. Ramsay [1]

STRONG LIMIT THEOREMS FOR SUMS OF RANDOM VARIABLES DEFINED ON A FINITE MARKOV CHAIN

ABSTRACT

Let $\{X_k, J_k\}$ be a bivariate sequence of random variables, where J_k is a finite ergodic Markov chain. Assume the random variables X_k are conditionally independent given $\{J_k\}$. By decomposing $S_n = \sum_{k=1}^{n} X_k$ into the sum of i.i.d. random variables plus two 'remainder' terms, it is proved that S_n satisfies both the Strong Law of Large Numbers and the Law of the Iterated Logarithm under the conditions of finite first and second moments, respectively, of $[X_k \mid J_{k-1}, J_k]$.

1. INTRODUCTION

Let $\{X_k, J_k\}$ be a bivariate Markov process such that $\{J_k\}$ is an ergodic finite Markov chain with state space $\Omega = \{1, 2, \ldots, N\}$. A real-valued random sequence $\{X_k\}$ is defined on the Markov chain $\{J_k\}$ if it satisfies:

$$\begin{aligned} &X_0 = 0 \quad \text{and} \quad |X_n| < \infty \quad \text{a.s.}, \\ &\Pr[X_k \le x,\ J_k = j \mid X_0, J_0, X_1, J_1, \ldots, X_{n-1}, J_{n-1} = i] \\ &\quad = \Pr[X_k \le x,\ J_k = j \mid J_{k-1} = i] \\ &\quad = p_{ij} F_{ij}(x) \quad \text{for} \quad i, j \in \Omega \quad \text{and} \quad -\infty < x < \infty. \end{aligned} \tag{1.1}$$

The matrix $\mathbf{P} = (p_{ij})$, called the transition matrix for the Markov chain $\{J_n\}$, is ergodic with stationary distribution $\boldsymbol{\pi} = (\pi_1, \pi_2, \ldots, \pi_N)$ satisfying

$$\boldsymbol{\pi}\mathbf{P} = \boldsymbol{\pi}. \tag{1.2}$$

[1] Actuarial Science, 310 Burnett Hall, University of Nebraska, Lincoln, Nebraska 68588-0307

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 189–196.

Miller, (1961, 1962a,b) investigated the random walk S_n, where X_k is given in (1.1) and

$$S_n = \sum_{k=0}^{n} X_k, \tag{1.3}$$

from the point of view of first passage probabilities. Miller used Wiener-Hopf factorization techniques to analyse these probabilities. This so-called Wiener-Hopf factorization is a technique that employs Fourier transformations in the complex plane. This has been the most popular method used for studying the behaviour of X_n; see, for example, Keilson and Wishart (1964, 1965, 1967), Presman (1969), Mogul'skii (1976), Takács (1978), Borovkov (1980) or Arndt (1980).

The literature on the limits of functions of the random sequence S_n is not very extensive. Keilson and Wishart (1964) established the Central Limit Theorem for S_n. Wolfson (1977) proved that under certain conditions on the sequence of constants $\{a_n, b_n\}$, that $(S_n/b_n - a_n)$ converges in distribution to a stable law $F(x)$. Fabens and Neuts (1970), and Resnick and Neuts (1970) investigated the distribution of the maximum term of the sequence $\{X_n\}$ and proved that its distribution, if non-trivial, is of the extreme value form. Resnick (1971) investigated the asymptotic location and recurrence properties of this maximum. Arndt (1980) developed expressions for the asymptotic distribution of $\max\{S_0, S_1, \ldots, S_n\}$. Strong limit theorems for S_n were developed by Janssen and by O'Brien. Janssen (1969) established the Strong Law of Large Numbers (SLLN) for S_n using complicated renewal theory methods, while O'Brien (1974) used the theory of stationary processes to prove that the chain dependent process S_n obeys both the SLLN and the Law of the Iterated Logarithm (LIL).

In the sequel the SLLN and the LIL for S_n, defined in (1.3), are established using methods simpler than those used by either Janssen or O'Brien. The method used is to decompose S_n into sums of independent and identically distributed (i.i.d.) random variables plus two random remainder terms. By using certain theorems due to Richter (1965) and Chow *et al.* (1981), these limit laws are proved. The LIL is established under more general conditions than those used by O'Brien.

2. MAIN RESULTS

For the Markov chain J, let $\{T_k^{(j)}\}$ be the sequence of random times of successive entries into state $j \in \Omega$, $k = 1, 2, \ldots$. Assume, for convenience, that $T_0^{(j)} = 0$ for all $j \in \Omega$ and that $J_0 = i$. The length of time between successive entries into state j (i.e., $T_{k+1}^{(j)} - T_k^{(j)}$, $k = 1, 2, \ldots$) are i.i.d. with

all moments finite, since $\{J_k\}$ is a finite ergodic Markov chain. S_n can be decomposed, after at least one transition into state j (i.e., after sufficiently large n), as follows:

$$S_n = W_{ij} + \sum_{m=1}^{N(n,j)} Z_m^{(j)} + R_n^{(j)}, \tag{2.1}$$

where

$$W_{ij} = X_0 + X_1 + \ldots + X_{T_1^{(j)}}, \tag{2.2}$$

$$Z_m^{(j)} = X_{T_m^{(j)}+1} + \ldots + X_{T_{m+1}^{(j)}}, \tag{2.3}$$

$$N(n,j) = \sup_{k \geq 1} \left\{ k : T_k^{(j)} \leq n \right\}, \tag{2.4}$$

and

$$R_n^{(j)} = X_{T_{N(n,j)}^{(j)}+1} + \ldots + X_n \tag{2.5}$$

with $R_n^{(j)} = 0$ if $T_{N(n,j)}^{(j)} = n$. It is clear that $Z_m^{(j)}$, $m = 1, 2, \ldots$, are i.i.d. for each $j \in \Omega$. W_{ij} and $R_n^{(j)}$ are the random remainder terms, while $N(n,j)$ is the number of entries into state j after n transitions.

Clearly for any real-valued positive sequence of constants b_n with $b_n \uparrow \infty$,

$$\lim_{n \to \infty} \frac{W_{ij}}{b_n} = 0 \text{ a.s.} \qquad \text{for all } i, j \in \Omega. \tag{2.6}$$

Can a similar result be established for $R_n^{(j)}$? Note that

$$| R_n^{(j)} | \leq \sum_{k=T_{N(n,j)}^{(j)}+1}^{n} | X_k | \leq \sum_{k=T_{N(n,j)}^{(j)}+1}^{T_{N(n,j)+1}^{(j)}} | X_k | = Y_n^{(j)}, \text{ say, } j \in \Omega.$$

The sequence $Y_1^{(j)}, Y_2^{(j)}, \ldots, Y_n^{(j)}, \ldots$ is a sequence of i.i.d. almostly surely finite non-negative random variables.

Now,

$$\lim_{n \to \infty} \frac{Y_n^{(j)}}{b_n} = 0 \text{ a.s. } \Rightarrow \frac{R_n^{(j)}}{b_n} = 0 \text{ a.s.}$$

Of interest are $b_n = n$ and $b_n = (2n\sigma^2 \log \log n)^{1/2}$, where σ^2 is a positive constant. It is easily seen from Laha and Rohatgi (1979, Proposition 2.2.1, Corollary 2, page 73) that, for all $j \in \Omega$,

(i) $\lim_{n\to\infty} Y_n^{(j)}/n = 0$ a.s. if $E[Y_n^{(j)}] < \infty$,
and (2.7)
(ii) $\lim_{n\to\infty} Y_n^{(j)}/(n \log\log n)^{1/2} = 0$ a.s. if $E[(Y_n^{(j)})^2] < \infty$.

Under the conditions of Theorem 1 below, $E[Y_n^{(j)}] < \infty$. Under the assumption (2.11) below, $E[(Y_n^{(j)})^2] < \infty$.

The main results, as expressed in Theorems 1 and 2, can now be established.

Theorem 1. (Strong Law of Large Numbers) If X_n and S_n are defined in (1.1) and (1.2) respectively, with

$$\int_{-\infty}^{\infty} | x | \, dF_{ij}(x) < \infty \text{ for all } i, j \in \Omega,$$

then

$$\lim_{n\to\infty} \frac{S_n}{n} = \mu \text{ a.s.}, \tag{2.8}$$

where μ is a constant.

Proof. From the ergodic theorem for Markov chains (see, for example, Cox and Miller, 1965, Section 3.4), it follows that $\lim_{n\to\infty} N(n,j)/n = \pi_j$. Also Theorem 1 of Richter (1965) gives

$$\lim_{n\to\infty} \frac{1}{N(n,j)} \sum_{r=1}^{N(n,j)} Z_r^{(j)} = E[Z_r^{(j)}] \qquad \text{a.s.},$$

where $\{Z_r^{(j)}\}$ is the sequence of i.i.d. random variables with finite mean defined in (2.3) and the random increasing sequence $N(n,j) \to \infty$ a.s. as $n \to \infty$. Therefore,

$$\begin{aligned}
\lim_{n\to\infty} \frac{S_n}{n} &= \lim_{n\to\infty} \frac{1}{n} \left\{ W_{ij} + \sum_{r=1}^{N(n,j)} Z_r^{(j)} + R_n^{(j)} \right\} \\
&= \lim_{n\to\infty} \frac{1}{n} \left\{ \sum_{r=1}^{N(n,j)} Z_r^{(j)} \right\} \text{ a.s.} \\
&= \lim_{n\to\infty} \left\{ \frac{N(n,j)}{n} \right\} \left\{ \frac{1}{N(n,j)} \sum_{r=1}^{N(n,j)} Z_r^{(j)} \right\} \\
&= \pi_j \beta^{(j)} \text{ a.s.} \quad \text{for} \quad j \in \Omega,
\end{aligned} \tag{2.9}$$

where $\beta^{(j)} = E[Z_r^{(j)}]$ and π_j is given by (1.2). Since S_n/n converges to the same limit regardless of j, then $\pi_j\beta^{(j)} = \mu$ (independent of $j \in \Omega$).

A corollary of Theorem 1 is that $E[Z_t^{(j)}] = \mu/\pi_j$, where μ is a constant independent of $j \in \Omega$. The case where $X_n \geq 0$ a.s. is called a Markov renewal process. Pyke and Schaufele (1964, Lemma 4.1), using Markov renewal theory, proved for

$$Z_k^{(j)}(f) = \sum_{n=T_k^{(j)}+1}^{T_{k+1}^{(j)}} f(X_n)$$

with $f : R \to R$ being a Lebesgue measurable function satisfying

$$\int_{-\infty}^{\infty} | f(x) | dF_{ij}(x) < \infty \quad \text{and} \quad \int_{-\infty}^{\infty} f^2(x) dF_{ij}(x) < \infty,$$

that

$$E[Z_k^{(j)}(f)] = \frac{1}{\pi_j} A_f, \tag{2.10}$$

where A_f is a constant independent of $j \in \Omega$. The result (2.10), without the restriction that $X_n \geq 0$ a.s., is a corollary of Theorem 1 obtained simply by replacing X_n by $f(X_n)$.

Next consider the LIL. Assume that for each $i, j \in \Omega$,

$$\int_{-\infty}^{\infty} x dF_{ij}(x) = 0 \qquad \text{and} \qquad \int_{-\infty}^{\infty} x^2 dF_{ij}(x) < \infty. \tag{2.11}$$

For some positive constant σ^2, define b_n as

$$b_n = \left(2n\sigma^2 \log \log n\right)^{1/2}. \tag{2.12}$$

This leads from (2.6) and (2.7) to

$$\lim_{n\to\infty} \frac{W_{ij}}{b_n} = \lim_{n\to\infty} \frac{R_n^{(j)}}{b_n} = 0 \qquad \text{a.s.}$$

Since for any positive constant a

$$\lim_{n\to\infty} \frac{\log(a + \log n)}{\log \log n} = 1,$$

then

$$\lim_{n\to\infty}\left[\frac{2\ N(n,j)\sigma_j^2 \log\ \log\ N(n,j)}{2n\ \log\ \log\ n}\right]^{1/2} = \left(\pi_j\sigma_j^2\right)^{1/2} \quad \text{a.s.} \tag{2.13}$$

for a positive constant σ_j^2. Choose σ_j^2 so that

$$\sigma_j^2 = \mathrm{Var}[Z_k^{(j)}]. \tag{2.14}$$

In order to establish the LIL for S_n one has to establish for the sequences $\{Z_k^{(j)}\}_{k=1}^{\infty}$ given in (2.3). Since the $Z_k^{(j)}$'s are i.i.d., it is necessary to assume the following hold for $Z_k^{(j)}$:

$$\text{(i)}\ \ E[Z_k^{(j)}] = 0 \quad \text{and} \quad \text{(ii)}\ \ \mathrm{Var}[Z_k^{(j)}] = \sigma_j^2 < \infty,$$

in order for the LIL to be applicable, that is, for

$$\overline{\lim_{n\to\infty}} \frac{\sum_{k=1}^{n} Z_k^{(j)}}{(2n\sigma_j^2\ \log\ \log\ n)^{1/2}} = 1.$$

From the assumptions in (2.11), it is clear that both (i) and (ii) hold.

Since $\lim_{n\to\infty} N(n,j)/k_n = 1$ a.s., where $k_n = n\pi_j$, then from Chow *et al.* (1981, Corollary 1.1),

$$\overline{\lim_{n\to\infty}} \frac{\sum_{k=1}^{N(n,j)} Z_k^{(j)}}{\left(2N(n,j)\sigma_j^2\ \log\ \log\ N(n,j)\right)^{1/2}} = 1 \ \text{ a.s.} \tag{2.15}$$

Thus using b_n given by (2.12), the result in (2.15), and a method similar to (2.9), leads to

$$\overline{\lim_{n\to\infty}} \frac{S_n}{b_n} = \left(\frac{\pi_j\sigma_j^2}{\sigma^2}\right)^{1/2} \quad \text{a.s.} \tag{2.16}$$

for $j \in \Omega$. Since S_n/b_n converges to the same limit, independently of $j \in \Omega$, then $\pi_j\sigma_j^2$ is independent of j. Therefore the positive constant σ^2 in (2.12) can be taken as $\sigma^2 = \pi_j\sigma_j^2$, independent of $j \in \Omega$. The following theorem is now clear.

Theorem 2. (Law of the Iterated Logarithm) If $\{X_k, J_k\}$, as defined in (1.1), satisfies

$$\int_{-\infty}^{\infty} x^2 dF_{ij}(x) < \infty, \qquad i,j \in \Omega,$$

and

$$\int_{-\infty}^{\infty} x dF_{ij}(x) = 0 \qquad i, j \in \Omega,$$

and $\sigma^2 = \pi_j \sigma_j^2$, then

$$\overline{\lim_{n\to\infty}} \frac{S_n}{(2n\sigma^2 \log \log n)^{1/2}} = 1 \quad \text{a.s.}$$

3. CONCLUSIONS

Equation (2.1) says that, in essence, S_n behaves as a random sum of independent random variables. This observation is basic to the proofs of the theorems in Section 2. This can be used to prove that $\overline{S} = \sup_{n\geq 1} S_n$ is finite almost surely if and only if $\lim_{n\to\infty} E[X_n] < 0$; see Arndt (1980).

It is hoped that this method of decomposing S_n, as in (2.1) can be used to demonstrate other limit theorems for S_n.

ACKNOWLEDGMENTS

The author is grateful for the referee's comments and suggestions, and for Dr. Reg Kulperger's assistance in the editing of the final revision of this paper.

REFERENCES

Arndt, K. (1980), "Asymptotic properties of the distribution of the supremum of a random walk on a Markov chain". *Theory of Probability and its Applications* **25**, 309–324.

Borovkov, K. A. (1980), "Stability, theorems and estimates of the rate of convergence of the components of factorizations for walks defined on Markov chains". *Theory of Probability and its Applications* **25**, 325–334.

Chow, Y. S., H. Teicher, C. Z. Wei, and K. F. Yu (1981), "Iterated logarithm laws with random subsequences". *Zeitschrift fur Wahrscheinlichkeitstheorie und Verwandte Gebiete* **57**, 215–251.

Cox, D. R., and H. D. Miller (1965). *The Theory of Stochastic Processes.* London: Chapman and Hall.

Fabens, A. J., and M. F. Neuts (1970), "The limiting distribution of the maximum term in a sequence of random variables defined on a Markov chain". *Journal of Applied Probability* **7**, 754–760.

Janssen, J. (1969), "Les Processus $(J-X)$". *Cahiers. Centre d'Etudes de Recheche Opérationnelle* **11**, 181–214.

Keilson, J., and D. M. G. Wishart (1964), "A central limit theorem for processes defined on a finite Markov chain". *Proceedings of the Cambridge Philosophical Society* **60**, 547–567.

Keilson, J., and D. M. G. Wishart (1965), "Boundary problems for additive processes defined on a finite Markov chain". *Proceedings of the Cambridge Philosophical Society* **61**, 173–190.

Keilson, J., and D. M. G. Wishart (1967), "Addenda to processes defined on a Markov chain". *Proceedings of the Cambridge Philosophical Society* **63**, 187–193.

Laha, R. G., and V. K. Rohatgi (1979), *Probability Theory.* New York: Wiley and Sons.

Miller, H. D. (1961), "A convexity property in the theory of random variables defined on a finite Markov chain". *Annals of Mathematical Statistics* **32**, 1260–1270.

Miller, H. D. (1962a), "A matrix factorization problem in the theory of random variables defined on a finite Markov chain". *Proceedings of the Cambridge Philosophical Society* **58**, 268–285.

Miller, H. D. (1962b), "Absorption probabilities for sums of random variables defined on a finite Markov chain". *Proceedings of the Cambridge Philosophical Society* **58**, 286–298.

Mogul'skii, A. A. (1976), "Factorization identities for processes with independent increments given on a finite Markov chain". *Theory of Probability and Mathematical Statistics* **11**, 87–96.

O'Brien, G. L. (1974), "Limit theorems for sums of chain-dependent processes". *Journal of Applied Probability* **11**, 582–587.

Presman, E. L. (1969), "Methods of factorization and a boundary problems for sums of random variables defined on a Markov chain". (In Russian.) *Izvestija Akademii Nauk SSSR, Serija Matematiceskaja* **33**, 861–990.

Pyke, R., and R. Schaufele (1964), "Limit theorems for Markov renewal processes". *Annals of Mathematical Statistics* **35**, 1746–1764.

Resnick, S. I. (1971), "Asymptotic location and recurrence properties of maxima of a sequence of random variables defined on a Markov chain". *Zeitschrift fur Wahrscheinlichkeitstheorie und Verwandte Gebiete* **18**, 197–217.

Resnick, S. I., and M. F. Neuts (1970), "Limit laws for maximum of a sequence of random variables defined on a Markov chain". *Advances in Applied Probability* **2**, 323–343.

Richter, W. (1965), "Limit theorems for sequences of random variables with sequences of random indices". *Theory of Probability and its Applications* **10**, 74–84.

Takács, L. (1978), "On fluctuations of sums of random variables". *Studies in Ergodic Theory: Advances in Mathematics Supplementary Studies* **2**, 45–93. New York: Academic Press.

Wolfson, D. B. (1977), "Limit theorems for sums of a sequence of random variables defined on a Markov chain". *Journal of Applied Probability* **14**, 614–620.

Malay Ghosh [1]

ON ADMISSIBILITY AND UNIFORM ADMISSIBILITY IN FINITE POPULATION SAMPLING

ABSTRACT

The paper surveys admissibility and uniform admissibility results in finite population sampling starting with the pioneering work of Professor Joshi, Professor Godambe and others. The recently introduced "stepwise Bayes" technique of Meeden and Ghosh has been explored in the proof of admissibility of well-known estimators as well as in the construction of new admissible estimators of the finite population mean and the finite population variance.

1. INTRODUCTION

It is a great honor to speak on the occasion of the seventieth birthday of Professor V. M. Joshi. The topic of admissibility and uniform admissibility in finite population sampling owes much to Professor Joshi's pioneering research, and I can say with great enthusiasm that this area of research remains as fertile as it was nearly twenty years ago.

The current paper is largely a review article with no attempt of being complete. The selection of topics reflects my personal bias, and the exclusion of an article within the domain of my selection is more a reflection on my unawareness than on the relevance of the paper.

The outline of my paper is as follows. In Section 2, I will review the admissibility results of Professor Joshi, Professor Godambe and others who have followed their line of approach. In Section 3, I will present the recently introduced "stepwise Bayes" technique of Meeden and myself in proving admissibility in finite population sampling. Several new estimators of the population mean and variance will be generated by suitable use of this tech-

[1] Department of Statistics, University of Florida, Gainesville, Florida 32611

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 197–213.

nique. In Section 4, I will introduce the notion of "uniform admissibility" and review the research in this area starting with the pioneering papers of Professor Joshi (1966) and Professor Godambe (1969).

2. ADMISSIBILITY IN FINITE POPULATION SAMPLING

Consider a finite population $\mathcal{U}$ with units labelled $1, \ldots, N$. Let y_i denote the value of a single characteristic attached to the unit i. The vector $y = (y_1, \ldots, y_N)$ is the unknown state of nature, and is assumed to belong to Θ. A subset s of $\{1, \ldots, N\}$ is called a sample. Let $n(s)$ denote the number of elements belonging to s. The set of all possible samples is denoted by S. A design is a function p defined on S such that $p(s) \in [0,1]$ for all $s \in S$ and $\sum_{s \in S} p(s) = 1$. Given $y \in \Theta$ and $s = \{i_1, \ldots, i_{n(s)}\}$ with $1 \leq i_1 < \cdots < i_{n(s)} \leq N$, let $y(s) = \{y_{i_1}, \ldots, y_{i_{n(s)}}\}$. The problem is to estimate different parameters $\gamma(y)$ of interest based on s, $y(s)$. An estimator $e(s,y)$ of $\gamma(y)$ is a function on $S \times \Theta$ which depends on y only through $y(s)$; $e(s,y)$ is said to be *linear* if

$$e(s,y) = \sum_{u \in s} \beta(s,u) y(s), \tag{2.1}$$

where β is a function on $S \times \mathcal{U}$ such that $\beta(s,u) = 0$ if $u \notin s$; $e(s,y)$ is said to be a p-unbiased estimator of $\gamma(y)$ if

$$\sum_{s \in S} e(s,y) p(s) = \gamma(y), \tag{2.2}$$

for all $y \in \Theta$. Also, if $L\big(a, \gamma(y)\big)$ denotes the loss in estimating $\gamma(y)$ by a, then e is said to be a p-admissible estimator of $\gamma(y)$ if there does not exist any estimator $e'(s,y)$, of $\gamma(y)$ such that

$$\sum_{s \in S} L\big(e'(s,y), \gamma(y)\big) p(s) \leq \sum_{s \in S} L\big(e(s,y), \gamma(y)\big) p(s), \tag{2.3}$$

for all $y \in \Theta$ with strict inequality for some $y \in \Theta$.

First consider the situation $\gamma(y) = \sum_{i=1}^{N} y_i$, the population total, and $\Theta = R^N$. The classic result of Godambe (1955) is the non-existence of a uniformly minimum variance unbiased (UMVU) estimator in the class of all linear unbiased estimators of $\gamma(y)$.

One time-honored estimator of $\gamma(y)$ is the celebrated Horvitz-Thompson (HT) estimator. In order to describe this estimator, let $\Pi_i = \sum_{s \ni i} p(s)$ denote the inclusion probability of the ith unit in the sample, when the sampling design is p. We assume that $\Pi_i > 0$ for all $i = 1, \ldots, N$ and

$\sum_1^N \Pi_1 = n$. Then, the HT estimator of $\gamma(y)$ is $e_{HT}(s,y) = \sum_{i\in s} y_i/\Pi_i$. It is easy to check that e_{HT} is a p-unbiased estimator of $\gamma(y)$. It is proved by Godambe (1960) and Roy and Chakravarti (1960) that under squared error loss (i.e. , $L(a,\gamma(y)) = (a-\gamma(y))^2$) the HT estimator is admissible within the class of linear unbiased estimators irrespective of the sampling design. It was proved by Godambe and Joshi (1965) that the linearity restriction could be removed and the HT estimator was admissible within the class of all unbiased estimators under squared error loss. Joshi (1965b) has shown that for fixed sample size designs (i.e., $n(s) \neq n \Rightarrow p(s) = 0$ for some positive integer n), the HT estimator was admissible within the class of all estimators of $\gamma(y)$. However, if the fixed sample size design restriction was removed, then it was shown by an example of Godambe and Joshi (1965) that the HT estimator could be inadmissible.

The special case when $\Pi_i = n/N$ $(i = 1,\ldots,N)$ leads to the classical estimator $e_0(s,y) = (N/n)\sum_{i\in S} y_i$ of $\gamma(y)$. In this case, it was shown by Joshi (1965a) that the estimator e_0 was always an admissible estimator of $\gamma(y)$.

The above results were all established under squared error loss. Joshi (1968, 1969) used a more general bowl-shaped loss of the form $L(a,\gamma(y)) = W(|\gamma(y)-a|)$, where $W(u) \nearrow$ in u, $W(0) = 0$, and for every $k > 0$, $\int_0^\infty W(u)\exp(-ku^2/2)\,du < \infty$. Under this loss, e_0 was shown to be an admissible estimator of $\gamma(y)$ in the class of all estimators.

Suppose now for *every* unit i in the population, information is available on an auxiliary characteristic x_i $(> 0)(i = 1,\ldots,N)$. The classical estimator of the population total in the presence of auxiliary information is given by the ratio estimator

$$e_R(s,y) = \left\{\left(\sum_{i\in s} y_i\right) / \left(\sum_{i\in s} x_i\right)\right\} \sum_{i=1}^N x_i. \tag{2.5}$$

The admissibility of e_R under squared error loss was proved by Joshi (1966), while its admissibility under the more general loss W as given in (2.4) was proved by Joshi (1968, 1969).

Most of Joshi's admissibility proofs are done in two stages. For proving the admissibility of an estimator $e(s,y)$ of $\gamma(y)$, he first shows that e is a "weakly admissible" estimator of γ.

Definition 1. An estimator $e(s,y)$ is said to be *weakly admissible* for estimating $\gamma(y)$ if there does not exist any estimator $e'(s,y)$ such that the inequality (2.3) holds for almost all (Lebesgue) $y \in R^N$ with strict inequality holding for a subset of R^N with positive measure. The second (and

usually the more difficult) step is to show that weak admissibility implies admissibility.

Recenty, Tsui (1983) has extended Joshi's ideas to obtain a general class of p-admissible estimators for estimating $\gamma(y)$. He considers the class of estimators of the form

$$e_W(s,y) = \sum_{i\in s} y_i + \left(\sum_{i\in s} W_i y_i / \sum_{i\in s} W_i x_i\right) \sum_{i\notin s} x_i, \tag{2.6}$$

where W_i 's (> 0) are known constants. Putting $W_i = W$ (a constant) for all $i = 1,\ldots,N$ leads to the classical ratio estimator, while putting $W_i = \Pi_i^{-1} - 1$ where Π_i (> 0) is the inclusion probability of the ith unit leads to an estimator proposed by Brewer (1979). Further, putting $W_i = x_i^{-1}$, one gets an estimator proposed by Basu (1971), while $W_i = x_i\sigma_i^{-2} (i = 1,\ldots,N)$ leads to an estimator proposed by Royall (1970). Many of these estimators can also be motivated from a model-based approach as follows. Suppose we consider the model $y_i = \beta x_i + \epsilon_i$ $(i = 1,\ldots,N)$, where the ϵ_i's are independently distributed with $E(\epsilon_i) = 0$ and $V(\epsilon_i) = \sigma_i^2 \equiv \sigma_i^2(x_i)$. Under the assumed model, the BLUE of β is $\hat{\beta} = \sum_{i\in s} y_i x_i \sigma_i^{-2} / \sum_{i\in s} x_i^2 \sigma_i^{-2}$. Now, based on the prediction theory approach, the estimator of $\gamma(y)$ is $\sum_{i\in s} y_i + \hat{\beta}\sum_{i\notin s} x_i$ which is precisely (2.6) with $W_i = x_i\sigma_i^{-2}$. Putting $\sigma_i^2 = x_i^2$, one gets the estimator considered by Basu.

Other extensions of these ideas involve estimation of parameters of interest other than the population mean. Liu and Thompson (1983) have considered estimation of parameters of the form $g_1(y) = \sum_{i=1}^N \sum_{j=1}^N c_{ij} y_i y_j$, $g_2(y) = \sum_{i=1}^N \sum_{j=1}^N b_{ij}(y_i - y_j)^2$ and $g_3(y) = \sum_{i=1}^N \sum_{j=1}^N b_{ij}(x_i - x_j)$ $(y_i - y_j)$, where the c_{ij}'s and b_{ij}'s are known constants. An important special case is when $b_{ij} = N^{-1}(N-1)^{-1}$, i.e., when g_2 and g_3 are respectively the population variance and the population covariance.

One well-known estimator of the variance of the HT estimator is due to Sen (1953) and Yates and Grundy (1952). This estimator is given by

$$e_V(s,y) = \sum_{i\in s}\sum_{j\in s} \left(\frac{\Pi_i\Pi_j}{\Pi_{ij}} - 1\right)\left(\frac{y_i}{\Pi_i} - \frac{y_j}{\Pi_j}\right)^2. \tag{2.7}$$

In the above, $\Pi_{ij} = \sum_{s\ni(i,j)} p(s)$ is assumed to be > 0 for all $1 \le i,j \le N$. Joshi (1970) showed that if the sampling design was of fixed sample size 2, then, under squared error loss, e_V is an admissible estimator of

$$V(e_{HT}) = \sum_{j=1}^N\sum_{j=1}^N (\Pi_i\Pi_j - \Pi_{ij})\left(\frac{y_i}{\Pi_i} - \frac{y_j}{\Pi_j}\right)^2$$

within the class of all unbiased estimators. Biyani (1982) provided examples to show that for sample sizes ≥ 3, e_V is an inadmissible estimator of e_{HT} in the narrower class of nonnegative unbiased quadratic estimators, while for $n = 2$, e_V is inadmissible in the class of nonnegative quadratic estimators (not necessarily unbiased).

The admissibility results proved by Joshi are typically independent of the choice of designs. Indeed, if an estimator is p-admissible, then it is also p_0-admissible for every $p_0 << p$ (i.e., $p(s) = 0 \Rightarrow p_0(s) = 0$ for every $s \in S$). This important result is due to Scott (1975).

3. STEPWISE BAYES TECHNIQUE

We examine in this section how stepwise Bayes techniques could be useful in deriving admissible estimators of the population mean or other parameters of interest. First we recall the following from Meeden and Ghosh (1981).

With $\Theta = \{\theta_1, \ldots, \theta_k\}$, let $\{f_\theta, \theta \in \Theta\}$ be a family of possible probability functions for X taking on values in some finite sample space $\mathcal{X}$. Assume that for each $x \in \mathcal{X}$, $f_{\theta_i}(x) > 0$ for at least one $\theta_i \in \Theta$. Consider estimation of $\gamma(\theta)$, some real valued function of θ, with squared error loss. Let $\lambda = (\lambda_1, \ldots, \lambda_k)$ denote a prior distribution on Θ. The marginal probability function of X under λ is $g(x; \lambda) = \sum_{i=1}^k f_{\theta_i}(x)\lambda_i$. Let $\theta(\lambda) = \{\theta_i : \lambda_i > 0\}$. Two prior distributions λ and λ' are said to be "mutually singular" if $\theta(\lambda) \cap \theta(\lambda') = \emptyset$. Theorem 1 below characterizes the class of admissible estimators for this problem. This theorem is a slight variation of Theorem 1 by Meeden and Ghosh (1981).

Theorem 1. *If δ is admissible, then there exists a nonempty finite set of mutually singular prior distributions $\lambda^1 = (\lambda_1^1, \ldots, \lambda_k^1), \ldots, \lambda^n = (\lambda_1^n, \ldots, \lambda_k^n)$ such that*

(i) if

$$\Lambda^1 = \{x : g(x; \lambda^1) > 0\}$$

and for $i = 2, \ldots, n$,

$$\Lambda^i = \left\{ x : g(x; \lambda^i) > 0 \text{ and } x \notin \bigcup_{j=1}^{i-1} \Lambda^j \right\},$$

then each Λ^i is nonempty and $\cup_{i=1}^n \Lambda^i = \mathcal{X}$;

(ii) *if $\delta_i^*(x)$ denotes the Bayes estimate of $\gamma(\theta)$ against λ^i, then, for $x \in \Lambda^i$,*

$$\delta(x) = \delta_i^*(x) \text{ for all } x \in \Lambda^i,\ i = 1, \ldots, n.$$

Conversely, if there exists a set of mutually singular prior distributions $\lambda^1, \ldots, \lambda^n$ *which satisfies* (i), *then* δ *given in* (ii) *is admissible. This* δ *defined as in* (ii) *is called a stepwise Bayes estimate with respect to the sequence of priors* $\lambda^1, \ldots, \lambda^n$.

Theorem 1 shows how admissible estimators can be constructed in finite problems. First a prior distribution, say λ^1, is specified. For all $x \in \Lambda^1$, the Bayes estimate is computed; if $\Lambda^1 = \mathcal{X}$, we are done. Otherwise, a second prior distribution, say λ^2, singular to λ^1, is chosen and then the Bayes estimate against λ^2 is computed for those $x \in \Lambda^2$. If $\Lambda^1 \cup \Lambda^2 = \mathcal{X}$, we are done. If not, choose another prior, say λ^3 singular to both λ^1 and λ^2, and continue until we have an estimator defined at all points of the sample space.

In finite population sampling, the above technique is useful for proving admissibility when the parameter space contains a finite number of elements, the so-called *scale-load* situation (see Hartley and Rao, 1968, or Royall, 1968). More important, this technique is useful for proving "finite admissibility" of an estimator.

Definition 2. An estimator $e(s, y)$ is said to be *finitely p-admissible* for estimating $\gamma(y)$ if for every $y^0 \in \Theta$, there exists a subset $\Theta(y^0)$ of Θ containing a *finite* number of points including y^0 such that if $y \in \Theta(y^0)$, then e is p-admissible.

Theorem 2. Every finitely p-admissible estimator e is p-admissible.

Proof. Suppose not. Then there exists an estimator e' such that $R_p(e', y) \leq R_p(e, y)$ for all $y \in \Theta$ with strict inequality for at least one point, say y^0. Then e' dominates e when y is restricted to $\Theta(y^0)$ containing a finite number of points including y^0, a contradiction to the finite admissibility of e.

As an illustration of this technique, we prove admissibility of Basu's estimator for estimating the population total. Recall from Section 2 that this estimator is given by

$$e_B(s, y) = \sum_{i \in s} y_i + n^{-1}(s) \sum_{i \in s} (y_i / x_i) \sum_{i \notin s} x_i. \tag{3.1}$$

Consider first the situation when the parameter space is $\overline{\mathcal{Y}}_x(\alpha_1, \ldots, \alpha_r) = \{y : y_i / x_i = \alpha_j \text{ for some } j = 1, \ldots, r \text{ and for all } i = 1, \ldots, N\}$. Also, let $\overline{\overline{\mathcal{Y}}}_x(\alpha_1, \ldots, \alpha_r) = \{y : y_i / x_i = \alpha_j \text{ for some } j = 1, \ldots, r \text{ and for all } i = 1, \ldots, N \text{ and each } \alpha_j \text{ appears for at least one } j,\ j = 1, \ldots, r\}$. If $y \in \overline{\overline{\mathcal{Y}}}_x(\alpha_1, \ldots, \alpha_r)$, we say that y is of order r for $\alpha_1, \ldots, \alpha_r$. Similarly, if $y(s)$ is a sample point with $r \leq n(s)$, we say that $y(s)$ is of order r

for $\alpha_1, \ldots, \alpha_r$ if each y_i/x_i equals one of the i values $\alpha_1, \ldots, \alpha_r$, and if for each value α_j, there exists at least one i_ℓ such that $y_{i_\ell}/x_{i_\ell} = \alpha_j$. If $y \in \overline{\overline{y}}_x(\alpha_1, \ldots, \alpha_r)$, let $W_y(j)$ be the number of (y_i/x_i) 's which are equal to α_j. Note that for each j, $W_j(j) \geq 1$ and $\sum_{j=1}^{r} W_y(j) = N$. If $y(s)$ is a sample point of order r for $\alpha_1, \ldots, \alpha_r$, let $W_y(j; s)$ be the number of observed (y_i/x_i) 's $(i \in s)$ which are equal to α_j.

We now exhibit a family of mutually orthogonal prior distributions on $\overline{y}_x(\alpha_1, \ldots, \alpha_r)$ against which Basu's estimator is the unique stepwise Bayes estimator for any design p.

The first prior λ^1 puts mass r^{-1} on the r points $y = (x_1\alpha_j, \ldots, x_N\alpha_j)$ for $j = 1, \ldots r$. For such a prior all the observed ratios y_i/x_i in a sample s are the same and the Bayes estimator is just Basu's estimator in this case.

The second prior λ^2 is defined over the set $\cup_{\{i<i'\}} \overline{\overline{y}}_x(\alpha_i, \alpha_{i'})$. The set contains all parameter vectors of order two for some α_i and $\alpha_{i'}$. If y is of order two for α_i and $\alpha_{i'}$ with $i < i'$, then

$$\lambda^2(y) \propto \int_0^1 p^{W_y(i)-1}(1-p)^{W_y(i')-1}dp = \frac{\Gamma\big(W_y(i)\big)\Gamma\big(W_y(i')\big)}{\Gamma(N)}.$$

For a sample $y(s)$ of order 2 for α_i and $\alpha_{i'}$, the marginal probability of $y(s)$ is given by $\lambda^2\big(y(s)\big) \propto \Gamma\big(W_y(i; s)\big)\,\Gamma\big(W_y(i'; s)\big) \,/\, \Gamma\big(n(s)\big)$. The sample points having positive marginal probability under λ^2, but not under λ^1 are just those of order two for some α_i and $\alpha_{i'}$ with $i < i'$. Let $y(s)$ be such a point, and suppose $i^* \notin s$. Then

$$E\left[(y_{i^*}/x_{i^*}) \mid s, y(s)\right] = \left[\alpha_i W_y(i; s) + \alpha_{i'} W_y(i'; s)\right]/n(s).$$

For such a sample s, the Bayes estimator of the population total for λ^2 at $y(s)$ is

$$\alpha_i \sum_{j \in s(i)} x_j + \alpha_{i'} \sum_{j \in s(i')} x_j + \left\{\left[\alpha_i W_y(i; s) + \alpha_{i'} W_y(i'; s)\right]/n(s)\right\} \sum_{i^* \notin s} x_{i^*},$$

where $s(i) = \{k \in s : y_k/x_k = \alpha_i\}$. This agrees again with Basu's estimator.

The third prior is defined over $\cup_{\{i<i'<i''\}} \overline{\overline{y}}_x(\alpha_i, \alpha_{i'}, \alpha_{i''})$, and is given by

$$\lambda^3(y) \propto \int_0^1 \int_0^1 p_1^{\,W_y(i)-1} p_2^{\,W_y(i')-1}(1-p_1-p_2)^{W_y(i'')-1}dp_1dp_2.$$

The sample points which have positive marginal probability under λ^3 but not under λ^1 and λ^2 are those which are of order 3 for some $\alpha_i, \alpha_{i'}$ and $\alpha_{i''}$.

Again for such points, the Bayes estimator against λ^3 can be shown to be equal to Basu's estimator. Continuing in this way, it follows from Theorem 1 that e_B is admissible when the parameter space is $\overline{y}_x(\alpha_1, \ldots, \alpha_r)$ for every choice of $(\alpha_1, \ldots, \alpha_r), r = 1, 2, \ldots, N$. This proves the finite admissibility of e_B. Hence, by Theorem 2, e_B is an admissible estimator of $\lambda(y) = \sum_1^N y_i$ when the parameter space is R_N as well.

The special case when $x_i = 1$ for all $i = 1, \ldots, N$ leads to the classical estimator $e_c(s, y(s)) = \sum_{i \in s} y_i + \left[(N - n(s))/n(s)\right] \sum_{i \in s} y_i = (N/n(s)) \sum_{i \in s} y_i$ of the population total. Thus, this estimator is also a stepwise Bayes estimator against the same sequence of priors λ^1, λ^2 defined over the parameter space $\overline{y}(\alpha_1, \ldots, \alpha_r) = \{y : y_i = \alpha_j$ for some $j = 1, \ldots, r$ and for all $i = 1, \ldots, N\}$. Suppose now for each unit i in the population k characteristics $y_i^{(1)}, y_i^{(2)}, \ldots, y_i^{(k)}$ are measured. Let $\mathbf{y}_i = (y_i^{(1)}, \ldots, y_i^{(k)}), i = 1, \ldots, N$. Consider now the parameter space $\Gamma(\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_r) = \{\mathbf{y} = (\mathbf{y}_1, \ldots, \mathbf{y}_N) : \mathbf{y}_i = \boldsymbol{\alpha}_j$ for some $j = 1, \ldots, r$, and for all $i = 1, \ldots, N\}$. Writing $W_j(\mathbf{y}(s))$ as the number of $\mathbf{y}_i$'s $(i \in s)$ equal to $\boldsymbol{\alpha}_j$, and using the same sequence of priors $\lambda^1, \lambda^2, \lambda^3, \ldots$ as above defined on $\Gamma(\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_r)$, it follows that $\left((N/n)\sum_{i \in s} y_i^{(1)}, \ldots, (N/n)\sum_{i \in s} y_i^{(k)}\right)$ is an admissible estimator of $\sum_{i=1}^N y_i = \left(\sum_{i=1}^N y_i^{(1)}, \ldots, \sum_{i=1}^N y_i^{(k)}\right)$ the vector of population totals under squared error loss when the parameter space is $\Gamma(\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_r)$ and eventually when the parameter space is R^{Nk} for any arbitrary k. This shows the lack of *Stein effect* in finite population sampling. This particular approach is taken by Meeden *el al.* (1985). This was demonstrated earlier by Joshi (1977) using a different line of approach.

Meeden *et al.* (1985) have established a duality between admissibility in nonparametric problems and admissibility in finite population sampling problems. For example, if we can construct an admissible estimator of a certain functional of interest in the nonparametric set up, it is possible to obtain an admissible estimator of the corresponding parameter in finite population sampling. Examples include estimation of the distribution function, say $F(t)$, and also functionals of the form $\int \ldots \int \phi(t_1, \ldots, t_m) F(dt_1) \ldots F(dt_m)$ which include as special cases the population mean $\left(m = 1, \phi(t_1) = t_1\right)$ and the population variance $\left(m = 2, \phi(t_1, t_2) = \frac{1}{2}(t_1 - t_2)^2\right)$ under squared error loss. Estimation of the distribution function is also considered by Cohen and Kuo (1985).

Although the estimator e_B (given in (3.1)), and in particular e_c does not have a Bayesian derivation, such an estimator can be given a Bayes-like interpretation. If one acts as if "a posteriori" any *unobserved ratio* $r_i = y_i/x_i$ has the empirical distribution of the r_i for $i \in s$, then Basu's estimator can be written as $E\left(\sum_1^N y_i \mid s, y(s)\right) = \sum_{i \in s} y_i + \sum_{i \notin s} E(y_i \mid s, y(s))$. This is when the prior information is essentially nil. On the other hand,

suppose a pseudo-Bayesian statistician has slightly more prior feeling about $r = (r_1, \ldots, r_N)$. In particular, suppose he has a guess for $\mu = N^{-1}\sum_{i=1}^{N} r_i$, say μ_* in mind. One possibility open to such a person is, of course, to adopt a prior according to which r_i's are independent with a common marginal mean μ_*. One then obtains the estimator

$$e_G(s,y) = \sum_{i\in s} y_i + \mu_* \sum_{i\notin s} x_i \tag{3.2}$$

of the population total. Among others, Godambe (1969) has studied properties of such estimators.

An examination of (3.1) and (3.2) suggests yet another possibility to the pseudo-Bayesian, i.e., some average of $\bar{r}(s) = n^{-1}(s)\sum_{i\in s} r_i$ and μ_* might be appropriate for an unobserved r_i. A convenient representation of the resulting estimator will be

$$e_M(s,y) = \sum_{i\in s} y_i + \left(\frac{M}{M+n}\mu_* + \frac{n}{M+n}\bar{r}(s)\right)\sum_{i\notin s} x_i. \tag{3.3}$$

The choice of M reflects the degree of prior belief about $u*$ as compared to the sample evidence. With this notation e_B and e_G are easily identified as e_0 and e_∞ respectively. This estimator is suggested by Vardeman and Meeden (1983a). It can be derived using a two stage normal prior as by Ericson (1969). The estimator can also be arrived at using Dirichlet process priors as by Binder (1982). Binder considered the special case when $x_i = 1$ for all $i = 1, \ldots, N$, but his arguments can be generalized.

A useful way to think about the estimators e_0, e_M and e_∞ is that prior belief is not symmetric in $y_1, \ldots, y_N$, but it is symmetric in $r_1, \ldots, r_N$. This line of thinking suggests yet more possibilities. For example, one might be willing to say that though the prior belief is not symmetric in the ratios y_i/x_i it is symmetric in the *differences* $d_i = y_i - x_i$ $(i = 1, \ldots, N)$. This leads to the difference estimators

$$e_0'(s,y) = \sum_{i\in s} y_i + \sum_{i\notin s} x_i + (N-n)\bar{d}(s), \tag{3.4}$$

$$e_M'(s,y) = \sum_{i\in s} y_i + \sum_{i\notin s} x_i + (N-n)\left(\frac{M}{M+n}\mu_* + \frac{n}{M+n}\bar{d}(s)\right), \tag{3.5}$$

$$e_\infty'(s,y) = \sum_{i\in s} y_i + \sum_{i\notin s} x_i + (N-n)\mu_*, \tag{3.6}$$

where $\bar{d}(s) = n^{-1}(s)\sum_{i\in s} d_i$.

Again there could be situations in which before declaring prior beliefs to be symmetric, the pseudo-Bayesian might rescale the differences between the y_i and x_i according to some (known) constants $c_1, \ldots, c_N$. Then one can assume the exchangability of $z_i = (y_i - x_i)/c_i$ $(i = 1, \ldots, N)$ leading to estimators of the form

$$e_0''(s, y) = \sum_{i \in s} y_i + \sum_{i \notin s} x_i + \bar{z}(s) \sum_{i \notin s} c_i; \tag{3.7}$$

$$e_M''(s, y) = \sum_{i \in s} y_i + \sum_{i \notin s} x_i + \left(\frac{M}{M+n} \mu_* + \frac{n}{M+n} \bar{z}(s) \right) \sum_{i \notin s} c_i; \tag{3.8}$$

$$e_\infty''(s, y) = \sum_{i \in s} y_i + \sum_{i \notin s} x_i + \mu_* \sum_{i \notin s} c_i. \tag{3.9}$$

Of course one does not have to motivate estimators arising necessarily out of exchangability of the ratios (y_i/x_i), the differences $(y_i - x_i)$, or the $(y_i - x_i)/c_i$'s. For example, instead of assuming that the posterior distribution of any unobserved r_j is the empirical distribution of the observed r_i's, it is possible to assume that *a posteriori* any unobserved r_j assumes the value r_i $(i \in s)$ with probability proportional to x_i $(i \in s)$. This leads to the pseudo-Bayes estimator

$$\begin{aligned} e_R(s, y) &= \sum_{i \in s} y_i + \left\{ \sum_{i \in s} (y_i/x_i) \frac{x_i}{\sum_{i \in s} x_i} \right\} \sum_{i \notin s} x_i \\ &= \sum_{i \in s} y_i + \frac{\sum_{i \in s} y_i}{\sum_{i \in s} x_i} \sum_{i \notin s} x_i = \frac{\sum_{i \in s} y_i}{\sum_{i \in s} x_i} \sum_{i=1}^{N} x_i, \end{aligned}$$

which is the classical ratio estimator. The HT estimator can be generated as

$$e_{HT}(s, y) = \sum_{i \in s} y_i + \left\{ \sum_{i \in s} \frac{y_i}{\Pi_i} \frac{1 - \Pi_i}{\sum_{i \in s} (1 - \Pi_i)} \right\} \sum_{i \notin s} \Pi_i. \tag{3.10}$$

This is shown by Meeden and Ghosh (1984). In deriving (3.10) we have used the restriction $\sum_{i=1}^{N} \Pi_i = n$ so that

$$\sum_{i \in s} (1 - \Pi_i) = n - \sum_{i \in s} \Pi_i = \sum_{i=1}^{N} \Pi_i - \sum_{i \in s} \Pi_i = \sum_{i \notin s} \Pi_i.$$

Other applications exist of the stepwise Bayes technique. Vardeman and Meeden (1983b) have shown that the trimmed and the Winsorized means given respectively by

$$e_T(s,y) = (n-p-q)^{-1} \sum_{i=p+1}^{n-q} y_{(i)}, \tag{3.11}$$

where $y_{(1)} \leq \cdots \leq y_{(n)}$ denote the ordered y_i's ($i \in s$) for fixed sample designs with size n, and

$$e_W(s,y) = n^{-1}\left[py_{(p+1)} + \sum_{i=p+1}^{n-q} y_{(i)} + qy_{(n-q)}\right] \tag{3.12}$$

are stepwise Bayes (and hence admissible) estimators of the finite population total employing a suitable sequence of priors. Again Vardeman and Meeden (1984) have applied the stepwise Bayes technique in estimating the finite population total under various forms of stratification including the usual stratified sampling (where attached to every unit i is a stratum membership j_i and $\mathbf{j} = (j_1, \ldots, j_N)$ is completely known) and poststratification where the j_i are known only for those units sampled.

So far, the discussion has been confined to the estimation of the population total. We may as well be interested in estimating the population variance. The population variance is defined by

$$\sigma^2(y) = (N-1)^{-1} \sum_{i=1}^{N} (y_i - \bar{y})^2 \, (N \geq 2). \tag{3.13}$$

The usual estimator of $\sigma^2(y)$ is given by

$$T = T(s,y) = \big(n(s)-1\big)^{-1} \sum_{i \in s} \big(y_i - \bar{y}(s)\big)^2,$$

which is unbiased under simple random sampling. However, it is shown by Ghosh and Meeden (1983) that T is in general an inadmissible estimator of $\sigma^2(y)$. Specifically, the following theorem is proved.

Theorem 3. *Let $n \geq 2$ be a fixed positive integer, and let p be a design such that $p(s) > 0 \Rightarrow n(s) = n$. If either $N \geq \max(4, n+2)$, or $N = n+1$ (≥ 3) is odd, then T is an inadmissible estimator of σ^2. Moreover, in the special case $n = 2, N = 3$, any estimator of the form cT with $c \neq 2/3$ is inadmissible.*

The sequence of priors $\lambda^1, \lambda^2, \lambda^3, \ldots$ used in proving that $(N/n(s))\sum_{i\in s} y_i$ is an inadmissible estimator of the population total $\sum_1^N y_i$ can also be used in generating a stepwise Bayes (and hence admissible) estimator of σ^2. The estimator generated this way is given by (see Ghosh and Meeden, 1983)

$$T' = \frac{(n(s)-1)(N+1)}{(n(s)+1)(N-1)}T. \tag{3.14}$$

This result was generalized by Mazlom (1984) to estimation of functionals of the form $\int\cdots\int \phi\,(x_1,\ldots,x_m)\,F(dx_1)\ldots F(dx_m)$ and such estimators turned out to be the corresponding U-statistics multiplied by some appropriate shrinking factors.

A very general class of stepwise Bayes estimators of the population variance is proposed by Vardeman and Meeden (1983a). This was motivated from the use of Dirichlet process priors. This estimator is given by

$$\begin{aligned} V_M = {} & \frac{n(s)(N+M)\big(NM+Nn(s)+n(s)\big)}{N^2\big(M+n(s)\big)\big(M+n(s)+1\big)}T \\ & + \frac{\big(N-n(s)\big)M\big(NM+Nn(s)-M\big)}{N^2\big(M+n(s)\big)\big(M+n(s)+1\big)}\sigma_*^2 \\ & + \frac{\big(N-n(s)\big)n(s)M(N+M)}{N^2\big(M+n(s)\big)\big(M+n(s)+1\big)}\big(\bar{y}(s)-\mu_*\big)^2, \end{aligned} \tag{3.15}$$

where μ_* (real) or σ_*^2 (>0) are the mean and the variance of the Dirichlet process prior. With this notation $V_0 \equiv T'$. Also,

$$V_\infty = \frac{n(s)}{N}T + \frac{n(s)\big(N-n(s)\big)}{N^2}\big(\bar{y}(s)-\mu_*\big)^2 + \frac{\big(N-n(s)\big)(N-1)}{N^2}\sigma_*^2. \tag{3.16}$$

The estimator V_∞ arises when the y_i's are assumed to be *independent* with common mean μ_* and common variance σ_*^2. This estimator was proposed by Liu (1974), Chaudhuri (1978) and Zacks and Solomon (1981). Vardeman and Meeden (1983a) employed a sequence of priors generating V_M, V_0 or V_∞ as stepwise Bayes estimators.

4. UNIFORM ADMISSIBILITY

In this section, we introduce the notion of "uniform admissibility" which is stronger than the notion of p-admissibility as given in (2.3). The question is that for a given strategy (p, e), (where p denotes the design and e the estimator) can there be another strategy (p', e') which is uniformly better than (p, e)? More precisely, we have the following definition.

Definition 3. A strategy (p, e) belonging to some class e is said to be *uniformly admissible* if there does not exist any strategy $(p', e') \in e$ such that

$$\sum_{s \in \mathcal{s}} L[e'(s, y), \gamma(y)] p'(s) \leq \sum_{s \in \mathcal{s}} L[e(s, y), \gamma(y)] p(s), \tag{4.1}$$

for all $y \in \Theta$ with strict inequality for some $y \in \Theta$.

The name "uniform admissibility" comes from Joshi (1966). (Godambe (1966) calls it global admissibility). Joshi (1966) showed that in the class of all designs with fixed sample size, the sample mean was a uniformly admissible estimator of the population mean under squared error loss. The results of Joshi were extended by Sekkappan and Thompson (1975). They considered the class of all designs C_n' with average sample size $\left(\text{i.e.}, \sum_{s \in \mathcal{s}} n(s) p(s)\right)$ equal to n and inclusion probability of the ith unit $\left(\text{i.e.}, \sum_{s \ni i} p(s)\right)$ equal to Π_i. Also, let C_n be a subclass of C_n' consisting of fixed size designs of size n and inclusion probabilities Π_i. Consider an estimator $e(s, y)$ of the population total such that

$$e(s, y) = \sum_{i \in s} b_i y_i \tag{4.2}$$

where the coefficients b_i satisfy

$$b_i > 1 \ (i = 1, \ldots, N) \quad \text{and} \quad \sum_{i=1}^{N} b_i^{-1} = n. \tag{4.3}$$

The following theorem is then proved by Sekkappan and Thompson (1975).

Theorem 4. *The pair (e, p) where $p \in C_n$ is uniformly admissible among pairs (e', p') when $p' \in C_n'$.*

Putting $b_i = \Pi_i^{-1}$, it follows as a corollary to this theorem that the strategy (p, e_{HT}) with $p \in C_n$ is a uniformly admissible estimator of the population total in the class of all pairs (e', p') with $p' \in C_n'$. Ramakrishnan (1975) proved the result where p could be in C_n' rather than C_n, but attention was restricted only to design unbiased estimators. A generalization

of Ramakrishnan's result is given by Cassel *et al.* (1977) where the class of strategies (p, e_{GD}) is the generalized difference strategy $p \in C_n'$ and e_{GD} is of the form

$$e_{GD}(s, y) = \sum_{i \in s} (y_i - x_i)/c_i + \sum_{i=1}^{N} x_i. \tag{4.4}$$

In another direction, Godambe (1969) proved uniform admissibility of the strategies (p, e_{B_λ}) where $p \in C_n$ and $e_{B_\lambda}(s, y) = \sum_{i \in s} y_i + \sum_{i \notin s} \lambda_i$ for some specified $\lambda_1, \ldots, \lambda_N$ within the class of all strategies (p', e') with $p' \in C_n'$. We have noted earlier that e_{B_λ} is a Bayes estimator of the population total under squared error loss. Later, Ericson (1970) proved uniform admissibility of strategies (p, e_{B_*}) with $e_{B_*}(s, y) = \alpha_n \sum_{i \in s} y_i + \beta_n$, where $\alpha_n \in (1, N/n)$ and β_n is arbitrary within the class of strategies (p', e') with $p' \in C_n'$. It was shown by Scott (1975) that if (p, e) was uniformly admissible with respect to $C_n (C_n')$, then (p_0, e) was uniformly admissible with respect to $C_n (C_n')$ if $p_0 << /p$ (i.e., $p(s) = 0 \Rightarrow p_0(s) = 0$).

For estimating the variance of a finite population, Chaudhuri (1978) proved uniform admissibility of strategies of the form (p, V_∞) within the class of all strategies of the form (p', e') where $p' \in C_n'$. More recently Mazlom and Meeden (1986) have used the stepwise Bayes technique to prove uniform admissibility of strategies of the form (p, e_B), where e_B is defined in (3.1) within the class of all strategies of the form (p', e') with $p' \in C_n$. Certain other results are given by Vardeman and Meeden (1983a).

ACKNOWLEDGMENT

This research was partially supported by the NSF Grant Number DMS-8218091 and partially by the Research Development Award of the Division of Sponsored Research, University of Florida.

REFERENCES

Basu, D. (1971), "An essay on the logical foundations of survey sampling, part one." In *Foundations of Statistical Inference*, ed. V. P. Godambe and D. A. Sprott, pp. 203–242. Toronto: Holt, Rinehart and Winston.

Binder, D. A. (1982), "Non-parametric Bayesian models for samples from finite populations." *Journal of the Royal Statistical Society*, Series B **44**, 388–393.

Biyani, S. H. (1980), "On inadmissibility of the Yates-Grundy variance estimator in unequal probability sampling. *Journal of the American Statistical Association* **75**, 709–712.

Brewer, K. R. W. (1979), "A class of robust sampling designs for large-scale surveys." *Journal of the American Statistical Association* **74**, 911–915.

Cassel, C. M., C. E. Sarndal, and J. H. Wretman (1977), *Foundations of Inference in Survey Sampling*. New York: Wiley and Sons.

Chaudhuri, A. (1978), "On estimating the variance of a finite population." *Metrika* **25**, 65–76.

Cohen, M. P., and L. Kuo (1985), "The admissibility of the empirical distribution function." *Annals of Statistics* **13**, 262–271.

Ericson, W. A. (1969), "Subjective Bayesian models in sampling finite populations" (with discussion). *Journal of the Royal Statistical Society*, Series B **31**, 195–233.

Ericson, W. A. (1970), "On a class of uniformly admissible estimators of a finite population total." *Annals of Mathematical Statistics* **41**, 1369–1372.

Ghosh, M., and G. Meeden (1983), "Estimation of the variance in finite population sampling." *Sankhya*, Series B **45**, 362–375.

Ghosh, M., and G. Meeden (1986), "Empirical Bayes estimation in finite population sampling." *Journal of the American Statistical Association*. To appear.

Godambe, V. P. (1955), "A unified theory of sampling from finite populations." *Journal of the Royal Statistical Society*, Series B **17**, 269–278.

Godambe, V. P. (1960), "An admissible estimate for any sampling design." *Sankhya* **22**, 285–288.

Godambe, V. P. (1966), "Bayes and empirical Bayes estimation in sampling finite populations." (Abstract). *Annals of Mathematical Statistics* **37**, 552.

Godambe, V. P. (1969), "Admissibility and Bayes estimation in sampling finite populations—V." *Annals of Mathematical Statistics* **40**, 672–676.

Godambe, V. P., and V. M. Joshi (1965), "Admissibility and Bayes estimation in sampling finite populations. I." *Annals of Mathematical Statistics* **36**, 1707–1722.

Hartley, H. O., and J. N. K. Rao (1968), "A new estimation theory for sample surveys." *Biometrika* **55**, 547–557.

Joshi, V. M. (1965a), "Admissibility and Bayes estimation in sampling finite populations II." *Annals of Mathematical Statistics* **36**, 1723–1729.

Joshi, V. M. (1965b), "Admissibility and Bayes estimation in sampling finite populations III." *Annals of Mathematical Statistics* **36**, 1730–1742.

Joshi, V. M. (1966), "Admissibility and Bayes estimation in sampling finite populations IV." *Annals of Mathematical Statistics* **37**, 1658–1670.

Joshi, V. M. (1968), "Admissibility of the sample mean as estimate of the mean of a finite population." *Annals of Mathematical Statistics* **39**, 606–620.

Joshi, V. M. (1969), "Admissibility of estimates of the mean of a finite population." In *New Developments in Survey Sampling*, ed. N. L. Johnson and H. Smith, pp. 188–212. New York: Wiley-Interscience.

Joshi, V. M. (1970), "Note on the admissibility of the Sen-Yates-Grundy estimator and Murthy's estimator and its variance estimator for samples of size two." *Sankhya*, Series A **32**, 431–438.

Joshi, V. M. (1977), "A note on estimators in finite populations." *Annals of Statistics* **5**, 1051–1053.

Joshi, V. M. (1979), "Joint admissibility of the sample means as estimators of the means of finite populations." *Annals of Statistics* **7**, 995–1002.

Liu, T. P. (1974), "Bayes estimation for the variance of a finite population." *Metrika* **21**, 127–132.

Liu, T. P., and M. E. Thompson (1983), "Properties of estimators of quadratic finite population functions: the batch approach." *Annals of Statistics* **11**, 275–285.

Mazlom, R. I. (1984), "Admissibility in choosing between experiments with applications." Ph.D. Thesis, Iowa State University.

Mazlom, R. I., and G. Meeden (1986), "Using the stepwise Bayes technique to choose between experiments." *Annals of Statistics*. To appear.

Meeden, G., and M. Ghosh (1981), "Admissibility in finite problems." *Annals of Statistics* **9**, 846–852.

Meeden, G., and M. Ghosh (1983), "Choosing between experiments: applications to finite population sampling." *Annals of Statistics* **11**, 296–305.

Meeden, G., and M. Ghosh (1984), "On the admissibility and uniform admissibility of ratio type estimators." In *Statistics: Applications and New Directions*, ed. J. K. Ghosh and J. Roy, pp. 378–390. Calcutta: Indian Statistical Institute.

Meeden, G., M. Ghosh, and S. Vardeman (1985), "Some admissible nonparametric and related finite population sampling estimators." *Annals of Statistics* **13**, 811–817.

Ramakrishnan, M. K. (1975), "Choice of an optimum sampling strategy—I." *Annals of Statistics* **3**, 669–679.

Roy, J., and I. M. Chakravarti (1960), "Estimating the mean of a finite population." *Annals of Mathematical Statistics* **31**, 392–398.

Royall, R. M. (1968), "An old approach to finite population sampling theory." *Journal of the American Statistical Association* **63**, 1269–1279.

Royall, R. M. (1970), "On finite population sampling theory under certain linear regression models." *Biometrika* **57**, 377–387.

Scott, A. J. (1975), "On admissibility and uniform admissibility in finite population sampling." *Annals of Statistics* **3**, 489–491.

Sekkappan, Rm., and M. E. Thompson (1975), "On a class of uniformly admissible estimators for finite populations." *Annals of Statistics* **3**, 492–499.

Sen, A. R. (1953), "On the estimate of the variance in sampling with varying probabilities." *Journal of the Indian Society of Agricultural Statistics* **5**, 119–127.

Tsui, K. W. (1983), "A class of admissible estimators of a finite population total." *Annals of the Institute of Statistical Mathematics*, Part A **35**, 25–30.

Vardeman, S., and G. Meeden (1983a), "Admissible estimators in finite population sampling employing various types of prior information." *Journal of Statistical Planning and Inference* **7**, 329–341.

Vardeman, S., and G. Meeden (1983b), "Admissible estimators of the population total using trimming and Winsorization." *Statistics and Probability Letters*

1, 317–321.

Vardeman, S., and G. Meeden (1984), "Admissible estimators for the total of a stratified population that employ prior information." *Annals of Statistics* **12**, 675–684.

Yates, F., and P. M. Grundy (1953), "Selection without replacement from within strata with probability proportional to size." *Journal of the Royal Statistical Society*, Series B **15**, 253–261.

Zacks, S., and H. Solomon (1981), "Bayes and equivariant estimators of the variance of a finite population: Part I, simple random sampling." *Communications in Statistics A, Theory and Methods* **10**, 407–426.

Richard M. Royall [1]

OVERLOOKED CORRELATION IN FINITE POPULATION INFERENCE

ABSTRACT

In the prediction approach to finite population inference, probability models play a central role. Here we consider linear regression models and study how errors in specifying a model's covariance structure affect variance estimators and the corresponding large sample confidence intervals for the population mean or total. We focus on local correlation in the form of either serial correlation or clustering. We find that overlooked serial correlation introduces little bias in variance estimators which consist of linear combinations of squared residuals when (i) the sampling fraction is small and (ii) the sample units are well dispersed in the population. Samples that are not well dispersed can produce badly biased variance estimators and misleading confidence intervals. When the sampling fraction is not negligible it is in general impossible to state verifiable sample conditions ensuring that serial correlation effects are unimportant. Clustering which is overlooked in the model can introduce severe biases in variance estimators when more than one unit is selected from each sample cluster, even when the sample is large and the sampling fraction small.

1. INTRODUCTION

In this paper the prediction approach to finite population inference is used to study some effects of overlooked correlation on linear estimators of finite population totals (or means) and on the corresponding variance estimators. This approach treats the population values $y_1, y_2, \ldots, y_N$ as realizations of random variables $Y_1, Y_2, \ldots, Y_N$. Thus after a sample s has been chosen and the sample y-values, $\{y_i; i \in s\}$, have been observed, esti-

[1] Department of Biostatistics, The Johns Hopkins University, Baltimore, Maryland 21205

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 215–226.

mating the population total, $T = \sum_1^N y_i = \sum_s y_i + \sum_r y_i$, is equivalent to predicting the value $\sum_r y_i$ of the unobserved random variable $\sum_r Y_i$, where r is the set of all non-sample units in the population.

The joint probability model for $Y_1, Y_2, \ldots, Y_N$ is the essential link between the sample and the non-sample units. The model provides the formal basis for predicting the non-sample values. It is with respect to this model that basic statistical properties such bias, i.e. $E(\hat{T} - T)$, and variance, $\text{var}(\hat{T} - T)$, are defined for an estimator $\hat{T}$. See Royall and Cumberland (1981) and the discussion following that paper for some general arguments and empirical evidence supporting the prediction approach.

When the values of auxiliary variables $x_1, x_2, \ldots, x_N$ associated with the population units are known, predictive inference about T might be based on a regression model expressing $E(Y_i)$ as a function of x_i. For example, if x_i is a measure of the size of unit i and if y_i is roughly proportional to the size x_i, then a model stating that $E(Y_i) = \beta x_i$ might be entertained. If the variability of the y's also increases with increasing size then the model might be elaborated as

$$\text{Model } M: \quad Y_1 \ldots, Y_N \text{ are independent with}$$
$$E(Y_i) = \beta x_i \quad \text{and} \quad \text{var}(Y_i) = \sigma^2 x_i.$$

Under model M, for a given sample s of n units, the best linear unbiased (BLU) estimator of T is the ratio estimator, $\hat{T} = (\bar{y}_s/\bar{x}_s) \sum_1^N x_i$, and the error variance of $\hat{T}$ is $\text{var}(\hat{T} - T) = (N/f)(1 - f)\ (\bar{x}\bar{x}_r/\bar{x}_s)\sigma^2$, where f is the sampling fraction n/N. An unbiased estimator v_L of the error-variance is obtained when $\hat{\sigma}^2 = \sum_s [y_i - (\bar{y}_s/\bar{x}_s)x_i]^2 / (n-1)x_i$ is substituted for σ^2. If both population and sample grow (subject to some mild constraints) then the standardized error $(\hat{T} - T)/v_L^{1/2}$ converges in law to the standard normal distribution, and this fact validates approximate confidence intervals of the usual form: $\hat{T} \pm z v_L^{1/2}$ (Royall and Cumberland, 1978).

In a potential application to a real population, model M cannot be known, and should not be assumed, to be correct. Such a model is properly thought of as a *working model*, an approximation to guide in planning and inference. Thus robustness, or insensitivity to changes in the model, is a key practical concern. Previous work has studied what happens when the regression and variance functions depart from the forms specified by the working model ($E(Y) = \beta x$ and $\text{var}(Y) = \sigma^2 x$, in the case of model M). Alternatives to the estimator v_L and conditions on the sample s have been identified which preserve the validity of the large-sample CI (confidence interval) under much more general models.

This paper follows Holt and Scott (1981) and Scott and Holt (1982) in addressing the effects of non-zero covariances on statistical properties derived

under a working model which specifies, incorrectly, that those covariances are zero. For a given $\hat{T}$ and variance estimator v, (for which $\hat{T} \pm zv^{1/2}$ is an asymptotically valid CI under a specified working model) we examine key properties under alternative models which allow more general correlation structure. We seek to learn about the effects of departure from the working model and about how we might protect against harmful effects through our choice of the sample and the estimators.

If the data show clearly the flaws in the working model and point to an alternative model, then we might simply adopt the alternative as a new working model. However, we are concerned here with situations which are not so clear-cut, where the working model and various alternatives are all more or less consistent with the available evidence. Such cases are important, not only at the design stage, but also in analysis, because errors which are not sufficiently extreme to show up clearly in typical samples can, under unfavorable circumstances, generate badly misleading inferences.

2. THE SIMPLE I.I.D. WORKING MODEL

The simplest case is adequate for illustrating some basic relations and effects. Consider the working model which states that $Y_1, Y_2, \ldots, Y_N$ are independently and identically distributed (i.i.d.) as Y where $E(Y) = \theta$ and $\text{var}(Y) = \sigma^2$. Consider first the problem of using a sample mean $\overline{Y}_s$ to estimate, not the finite population average, $\overline{Y}$, but the mean θ of the underlying probability law. Under the working model, $\overline{Y}_s$ is unbiased, the statistic $\hat{\sigma}^2/n = \sum_s (Y_i - Y_s)^2/(n(n-1))$ is an unbiased and consistent estimator of $\text{var}(\overline{Y}_s)$, and $\overline{Y}_s \pm z\hat{\sigma}/n^{1/2}$ is an asymptotically valid CI for θ (assuming, as we will throughout, the existence of the necessary moments). But if the Y's are actually correlated, the variance estimator can be biased and the large-sample CI invalidated.

2.1 Global Correlation

If the i.i.d. working model fails, and the Y's are, in fact, exchangeable, with $\text{cov}(Y_i, Y_j) = \rho\sigma^2$ for all $i \neq j$, then $\text{var}(\overline{Y}_s) = \sigma^2\{(1-\rho)/n + \rho\}$, while $E(\hat{\sigma}^2/n) = \sigma^2(1-\rho)/n$, so that the coverage probability of the CI $\overline{Y}_s \pm z\hat{\sigma}/n^{1/2}$ approaches zero as n grows. Thus this type of "global" correlation, corresponding to a common variance component shared by all the observations, can be disastrous to the CI for θ.

If the target of estimation is the finite population mean $\overline{Y}$, global correlation is less troublesome. Under the i.i.d. working model, the sample mean is unbiased with error variance $\text{var}(\overline{Y}_s - \overline{Y}) = (1-f)\sigma^2/n$. The variance estimator $v = (1-f)\hat{\sigma}^2/n$ is unbiased and consistent, providing

an asymptotically valid CI for $\overline{Y}$, namely $\overline{Y}_s \pm zv^{1/2}$. What if the working model fails and global correlation is present? The effect on the CI for $\overline{Y}$ is entirely different from the effect on the CI for θ. This is because the variance estimated, $\text{var}(\overline{Y}_s, \overline{Y}_r)$, is determined not simply by $\text{var}(\overline{Y}_s)$ but also by $\text{var}(\overline{Y}_r)$ and $\text{cov}(\overline{Y}_s, \overline{Y}_r)$. All three of these quantities are influenced by the correlation, and they fit together so that the variance estimate remains unbiased and the CI asymptotically valid; under the global correlation model $E(v) = (1-f)\sigma^2(1-\rho)/n = \text{var}(\overline{Y}_s - \overline{Y})$.

2.2 Local Correlation

For many applications our concern with potential model failure is more realistically directed to *local* correlation alternatives, which express the possibility that a unit's Y-value might be correlated with those of nearby units, and the remainder of this paper is devoted to models of this type. We will consider two varieties of local correlation, namely serial correlation and clustering.

2.2.1 Serial correlation. As a simple starting point we suppose the units are arranged and labelled so that

$$E(Y_i) = \theta \quad \text{and} \quad \text{cov}(Y_i, Y_j) = \begin{cases} \sigma^2 & i = j \\ \rho\sigma^2 & i = j \pm 1 \\ 0 & \text{elsewhere.} \end{cases} \tag{1}$$

Here only the Y-values of adjacent units are correlated, and it is easy to show that if (1) is to apply for general N then the possible values of ρ are $-\frac{1}{2} \leq \rho < \frac{1}{2}$.

Again we start with the problem of estimating θ rather than Y. If in fact model (1) applies then the actual variance will not be simply σ^2/n, as the i.i.d. working model implies, but will depend on the pattern of units in the sample. The key feature of this pattern is the number g of groups of (one or more) adjacent units in the sample. Thus $g = 1$ indicates that the sample consists of one continuous segment of adjacent units such as j, $j+1, \ldots, j+n-1$. At the other extreme, $g = n$ indicates that there are no pairs of adjacent units in the sample, as in the case of the systematic sample $j, j+r, j+2r, \ldots, j+(n-1)r$ obtained by choosing unit j and every rth one thereafter ($r > 1$) until n are selected.

Of course if model (1) applies, $\overline{Y}_s$ is still unbiased and consistent. But the correlation which the i.i.d. working model overlooks does affect the variance and the variance estimator. The actual variance is now

$$\text{var}(\overline{Y}_s) = (\sigma^2/n)\{1 + 2\rho(1 - g/n)\}, \tag{2}$$

while the expected value of the estimator is

$$E\left(\hat{\sigma}^2/n\right) = \left(\sigma^2/n\right)\left\{1 + 2\rho(1 - g/n)/(n-1)\right\}. \tag{3}$$

The variance estimator pays too little attention to the correlation – the coefficient of ρ in (3) equals the coefficient in (2) *divided by* $n-1$. The relative bias, $\{[(3)-(2)]/(2)\}$, is approximately $-2\rho(1-g/n)/\{1+2\rho(1-g/n)\}$, so that the large sample CI for θ, $\overline{Y}_s \pm \hat{\sigma}/n^{1/2}$, is invalidated unless $g/n \to 1$. The problem can obviously be avoided by choosing a sample whose units are dispersed so that $g = n$.

For estimating the finite population mean $\overline{Y}$, $\overline{Y}_s$ remains unbiased under (1) and its error variance is

$$\text{var}(\overline{Y}_s - \overline{Y}) = (\sigma^2/n)\{(1-f) + 2\rho[(1-f-g/n) + (\gamma - f)/N]\}, \quad (4)$$

where $\gamma = 2, 1$, or 0 depending on whether both, one or neither of the extreme units (units 1 and N) is in s. This expression (4) must be compared with the expected value of the variance estimator $v = (1-f)\hat{\sigma}^2/n$ under the same model, (1):

$$E(v) = (\sigma^2/n)\{(1-f) - 2\rho(1-g/n)(1-f)/(n-1)\}. \quad (5)$$

From (4) and (5) we see that as n and N grow,

$$\text{var}(\overline{Y}_s - \overline{Y}) = (\sigma^2/n)\{1-f+2\rho(1-f-g/n) + O(1/N)\}$$

while

$$E(v) = (\sigma^2/n)\{1-f+O(1/n)\}.$$

Thus for n large, the correlation again has a negligible effect on the expectation of the variance estimator, so that the bias in v is determined solely by the effect of ρ on the variance itself. The relative bias is approximately

$$\frac{E(v) - \text{var}}{\text{var}} \doteq \frac{-2\rho(1-f-g/n)}{1-f+2\rho(1-f-g/n)}. \quad (6)$$

When the sample units are dispersed so that $g = n$, (6) equals $2\rho f/\{1-f(1+2\rho)\}$. In such samples the variance estimator has a bias, but this bias is small whenever the sampling fraction f is small. At the other extreme, in compact samples (small g), the situation is much worse. When the sample consists of a single strip of adjacent units ($g = 1$) the relative bias is approximately $-2\rho/(1+2\rho)$; the sign is opposite that of ρ and the magnitude is unbounded on $-\frac{1}{2} < \rho < \frac{1}{2}$.

The approximate relative bias (6) vanishes when $g/n = 1 - f$, that is, when g/n is close to its expected value under simple random sampling without replacement (SRS), $1 - f + 1/N$. In fact, under SRS the expected bias is precisely zero: $E_{SRS}[(5)-(4)] = 0$. If n and N grow so that $f \to f_o$

for some $0 \leq f_o < 1$, then the relative bias under SRS is $O_p\left(1/n^{1/2}\right)$, where this last expression denotes a generic term which, when multiplied by $n^{1/2}$, is bounded in probability. This shows that the problem created by this type of local correlation will rarely be serious in large randomly-selected samples. Of course for the purpose of making inferences based on a specific observed sample, it is the actual value of g/n in that sample which is important, not the value which was expected before the sample was chosen. If misfortune strikes and g/n is not close to $1 - f$ then a substantial bias is present unless ρ is small. This bias is not diminished by the fact that such a sample was improbable. Even if the sample is chosen at random, inferences should be properly conditioned on the characteristics of that sample, and not be distracted by considerations of "what might have been". A simple precaution is to restrict the random sampling plan so that only samples where $g/n \doteq 1 - f$ can be selected.

2.2.2 Clustering. As another alternative to the i.i.d. working model, we consider a model stating that the units are in fact grouped in independent clusters within which the Y's are exchangeable. Thus $E(Y_i) = \theta$ and $\text{var}(Y_i) = \sigma^2$ for all i, but all units belonging to the same cluster have a common covariance, $\rho\sigma^2$. We denote the number of units in cluster k by M_k, and let m_k be the number (possibly zero) of these units in the sample, so that $\sum M_k = N$ and $\sum m_k = n$. Now the true error variance is

$$\text{var}(\overline{Y}_s - \overline{Y}) = \left(\sigma^2/n\right)(1-f)(1-\rho) + \rho(\sigma^2/n^2)\sum\left(m_k - fM_k\right)^2, \quad (7)$$

while

$$E(v) = \left(\sigma^2/n\right)(1-f)\left[1 - \{\rho/(n-1)\}\left\{\left(\sum m_k^2/n\right) - 1\right\}\right]. \quad (8)$$

We will consider only the case of constant $M_k = M$. The results easily generalize to models where the M_k show modest variability. If the non-zero m_k are all equal ($= m$), as in two-stage sampling with equal workloads, the two expressions (7) and (8) simplify:

$$\text{var}(\overline{Y}_s - \overline{Y}) = \left(\sigma^2/n\right)(1-f) + \left(\rho\sigma^2/n\right)\{m(1-f_1) - (1-f)\}, \quad (9)$$

where f_1 is the fraction of clusters selected in the first stage of sampling, and

$$E(v) = \left(\sigma^2/n\right)(1-f)\{1 - \rho(m-1)/(n-1)\}. \quad (10)$$

If $m = 1$ the coefficient of ρ in $E(v)$ vanishes; as in the case of serial correlation, a dispersed sample prevents the correlation from affecting the variance

estimator. More generally, whenever n/m, the number of clusters represented in the sample, is large, the coefficient of ρ is small. In this case the relative bias is approximately

$$\frac{E(v) - \text{var}}{\text{var}} \doteq \frac{-\rho\{m(1-f_1) - (1-f)\}}{1 - f + \rho\{m(1-f_1) - (1-f)\}}.$$

When the first-stage sampling fraction f_1 is small as well (which implies that the overall sampling fraction $f = f_1 m/M$ is also small) the relative bias is approximately $-\rho(m-1)/\{1+\rho(m-1)\}$, which vanishes when $m = 1$ but can be substantial otherwise. Within cluster correlation cannot be safely ignored when estimates are based on a cluster sample with more than one sample unit per cluster ($m > 1$), even when the sample is large and both sampling fractions, f_1 and m/M, are small.

If SRS, not cluster sampling, is used, then there is reason for optimism that the relative bias will be small. Again this is because the SRS expectation of $E(v)$ equals that of $\text{var}(\hat{T} - T)$, i.e., the expected (SRS) bias in v equals zero. But again the key question for inference is whether the expressions (7) and (8) are approximately equal for the sample at hand, not whether equality was expected.

3. SERIAL CORRELATION AND LINEAR REGRESSION MODELS

The general consequences of serial correlation in the simple i.i.d. case carry over to working models having a less simple mean and variance structure, but still specifying zero covariances. For linear statistics, such as ratio, regression, and mean-of-ratios estimators of $\overline{Y}$ or the population total, $T = N\overline{Y}$, and variance estimators which are linear combinations of squared residuals, we find that when n is large:

(i) expected values of the variance estimators are relatively insensitive to serial correlation,

(ii) the error variances themselves ($\text{var}(\hat{T} - T)$) can be strongly affected by serial correlation when g/n is small,

(iii) if both f and $1 - g/n$ are small, the relative bias introduced in variance estimators by serial correlation is small.

3.1 Working Model M

We will sketch these results for the case of the ratio estimator and the working model M. Analogous results for other linear estimators are easily obtained.

The first result, (i), is simple. If the residual $r_i = Y_i - \hat{Y}_i$ has expected value zero, then its square has expected value

$$E(r_i^2) = \text{var}(Y_i) - 2\,\text{cov}(Y_i, \hat{Y}_i) + \text{var}(\hat{Y}_i).$$

The effect of serial correlation appears only in the two final terms, which are both $O(1/n)$. Specifically, in the case of the ratio estimator, the working model M states that the Y's are uncorrelated and that both the mean and the variance of Y_i are proportional to x_i. Under M, $r_i = Y_i - (\overline{Y}_s/\overline{x}_s)\,x_i$, and $E_M(r_i^2) = \sigma^2 x_i(1 - x_i/n\overline{x}_s) = \text{var}_M(Y_i)(1 + O(1/n))$. Now under the more general model

$$\text{Model } M1: \quad E(Y_i) = \beta x_i,\ \text{cov}(Y_i, Y_j) = \begin{cases} \sigma^2 x_i & i = j \\ c_i & j = i+1 \\ c_{i-1} & j = i-1 \\ 0 & \text{elsewhere,} \end{cases}$$

we find that for every i in s

$$E_{M1}(r_i^2) = \sigma^2 x_i - 2x_i\left\{\sigma^2 x_i + c_{i-1}\delta_{i-1}(s) + c_i\delta_{i+1}(s)\right\}/(n\overline{x}_s) + (x_i/\overline{x}_s)^2\left\{\sigma^2 x_s + \psi_s\right\}/n,$$

where $\delta_j(s)$ is a zero-one indicator of whether j is in s and $\psi_s = 2\sum_s c_i\delta_{i+1}(s)/n$. Since $E_{M1}(r_i^2) = \sigma^2 x_i\{1 + O(1/n)\}$, it follows that serial correlation has little effect on the expectation of a variance estimator of the form $\sum_s \ell_i r_i^2$ (such as v_L). If bias is introduced, it is via the correlation's effect on the target of estimation, $\text{var}(\hat{T} - T)$, rather than on the estimator itself.

The estimator v_L, for example, has

$$\begin{aligned} E_{M1}(v_L) &= \{N(1-f)/f\}\,(\overline{x}\overline{x}_r/\overline{x}_s)\,\sigma^2\,\{1 - \psi_s/(\overline{x}_s(n-1))\} \\ &= E_M(v_L)\,\{1 + O(1/n)\}. \end{aligned}$$

The effect of non-zero c's on the expectation of v_L is asymptotically negligible, provided only that the sequences $\{x_i\}$ and $\{c_i\}$ are reasonably stable.

Since the variance estimator from conventional sampling theory (not based on prediction models), $v_C = \{N(1-f)/f\}\sum_s r_i^2/(n-1)$, and the bias-robust estimator, $v_D = \{N(1-f)/f\}\,(\overline{x}_r\overline{x}/\overline{x}_s^2)\sum_s r_i^2/n(1 - x_i/(n\overline{x}_s))$, are also linear functions of the squared residuals, the same general result applies: $E_{M1}(v) = E_M(v)\{1 + O(1/n)\}$.

On the other hand, the actual error-variance under $M1$ is

$$\begin{aligned} \text{var}_{M1}(\hat{T} - T) = &\left\{N(1-f)^2/f\right\}(\overline{x}_r/\overline{x}_s)^2\,(\overline{x}_s\sigma^2 + \psi_s) \\ &- N(1-f)\left\{(\overline{x}_r/\overline{x}_s)\,\phi - \overline{x}_r\sigma^2 - \psi_r\right\}, \end{aligned} \tag{11}$$

where

$$\psi_r = 2\sum_r c_i \delta_{i+1}(r)/(N-n)$$

and

$$\phi = 2\sum_1^N c_i \{\delta_i(s) - \delta_{i+1}(s)\}^2/n.$$

Since the sum in ϕ has only $2g - \gamma$ non-zero terms, the second term in (11) is $O(N)$ as $N \to \infty$ and $f \to 0$, while the first term is $O(N/f)$. This observation, together with the fact that when all the c_i vanish model $M1$ becomes model M, implies that

$$\mathrm{var}_{M1}(\hat{T} - T) = \mathrm{var}_M(\hat{T} - T)\{1 + (\psi_s/(\bar{x}_s\sigma^2)) + O(f)\}.$$

Thus when $M1$ applies and both n and N/n are large, the variance is altered by the factor $1 + \psi_s/(\bar{x}_s\sigma^2))$. This results in a relative bias in the variance estimator v, $RB_{M1}(v) = \{E_{M1}(v) - \mathrm{var}_{M1}(\hat{T} - T)\}/\mathrm{var}_{M1}(\hat{T} - T)$, of approximately

$$RB_{M1}(v) \doteq \{RM_M(v) - \psi_s/(\bar{x}_s\sigma^2)\}/(1 + \psi_s/(\bar{x}_s\sigma^2)). \tag{12}$$

For estimators like v_L and v_D which are unbiased under model M, $RB_{M1}(v) \doteq -\psi/(\bar{x}\sigma^2 + \psi)$. For v_C the relative bias under M is approximately $(\bar{x}_s/\bar{x})^2 - 1$ (Royall and Eberhardt, 1975), so that under $M1$ it becomes

$$RB_{M1}(v_C) \doteq \{(\bar{x}_s/\bar{x})^2 - 1 - \psi_s/(\bar{x}_s\sigma^2)\}/(1 + \psi_s/(\bar{x}_s\sigma^2)).$$

The contribution of the covariance terms to the relative bias (12) is represented by ψ_s, which is an average of n terms, g of which equal zero. Its effect vanishes when the sample units are dispersed so that $g/n \to 1$. In such samples, the presence of serial correlation (as expressed in model $M1$) introduces essentially no bias in v_L and v_D and adds none to the bias in v_C which was already present under the working model, M. Since v_C is inappropriate even under M unless the sample is well-balanced, $\bar{x}_s \doteq \bar{x}$, and since this estimator appears to have no redeeming advantages under the local correlation alternative, we will consider it no further.

Expression (12) shows that samples made up of only a few large groups of units (small g) can produce in v_L and v_D a substantial negative bias when the c_i are positive, and a positive bias when they are negative.

When the sampling fraction f is not small, the possibilities are more varied, with both terms in the variance (11) contributing to the large sample bias in v_D and v_L:

$$E_{M1}(v) - \mathrm{var}_{M1}(\hat{T} - T) = -N(1-f)\{(\bar{x}_r/\bar{x}_s)^2\psi_s(1-f)/f - (\bar{x}_r/\bar{x}_s)\phi + \psi_r + O(1/n)\}. \tag{13}$$

In this case the coefficients of ψ_s, ψ_r, and ϕ all have the same order of magnitude, so that choosing a dispersed sample ($g = n$) to eliminate ψ_s no longer ensures that the relative bias is small.

If the relative bias is to become negligible when f converges to a non-zero limit as N grows, then the term within the braces in (13) must approach zero. This occurs in probability under SRS because, with respect to the SRS probability distribution, the four ratios $\bar{x}_r/\bar{x}_s$, $\psi_s/f\bar{c}$, $\psi_r/(1-f)\bar{c}$, and $\phi/2(1-f)\bar{c}$, where $\bar{c} = \sum_1^N c_i/N$, all converge to unity. In fact, all have the representation $1 + O_p(n^{-1/2})$. On the other hand, for inference from a given sample we want to know whether the four ratios are in fact all approximately unity in that sample. Although the first one, $\bar{x}_r/\bar{x}_s$, can be examined directly, the other three cannot. However an indirect check can be made by noting whether g/n is approximately $1-f$; if not, then the actual numbers of non-vanishing terms in ψ_s, ψ_r, and ϕ ($n-g$, $N-n-g-1+\gamma$, and $2g-\gamma$ respectively) are not close to their SRS-expected values ($(n-1)f$, etc.), suggesting that the desired conditions ($\psi_s \doteq f\bar{c}$, etc.) are not satisfied by this sample.

3.2 Serial Correlation Effects in a More General Context

Robustness of variance estimators to departure of the variance function from the form specified in model M, $\text{var}(y) = \sigma^2 x$, has been studied (Royall and Cumberland, 1978) by considering the alternative

$$\text{Model } G: \; Y_1, \ldots, Y_N \text{ are independent with } E(Y_i) = \beta x_i \text{ and } \text{var}(Y_i)) = v_i,$$

where the v_i are subject only to some mild constraints such as that $\bar{v} = \sum_1^N v_i/N$ converge to a finite limite as N grows. It has been shown that if $f \to 0$ then v_D is robust in the sense of consistency under G, $v_D/\text{var}_g(\hat{T} - T) \to 1$ in probability, and that v_L is not robust.

We can study the effects of serial correlation in this more general framework by considering the alternative

$$\text{Model } G1: \quad E(Y_i) = \beta x, \quad \text{cov}(Y_i, Y_j) = \begin{cases} v_i & i = j \\ c_i & j = i+1 \\ c_{i-1} & j = i-1 \\ 0 & \text{elsewhere.} \end{cases}$$

The results are just as before. There is little effect on the variance estimator, but a potentially large effect on the variance itself:

(i) $E_{G1}(v) = E_G(v)\{1 + O(1/n)\}$

(ii) $\text{var}_{G1}(\hat{T} - T) = \text{var}_G(\hat{T} - T)\{1 + \psi_s/\bar{v}_s + O(f)\}$.

This means that the expression (12) for the relative bias generalizes: when n is large and f is small

$$RB_{G1}(v) \doteq \{RB_G(v) - \psi_s/\bar{v}_s\} \,/\, (1 + \psi_s/\bar{v}_s)\,.$$

Since ψ_s is a sum of $n-g$ non-zero covariances divided by n, this last result implies that

(iii) if both f and $1-g/n$ are small then the relative bias in v is little affected by serial correlation.

Finally, expression (13) for the bias in a variance estimator generalizes to show that the contribution of serial correlation is just as before:

$$\begin{aligned} &E_{G1}(v) - \mathrm{var}_{G1}(\hat{T} - T) \\ &\quad = E_G(v) - \mathrm{var}_G(\hat{T} - T) \\ &\qquad - N(1-f)\left\{(\bar{x}_r/\bar{x}_s)^2\psi_s(1-f)/f - (\bar{x}_r/\bar{x}_s)\phi + \psi_r + O(1/n)\right\}. \end{aligned}$$

Thus the estimator v_D, which remained consistent when model M was replaced by G (so long as $f \to 0$), retains its consistency in the face of serial correlation (G replaced by $G1$) so long as the sequence of samples is one in which $g/n \to 1$.

4. FURTHER WORK AND EXTENSIONS

Generalizations of the serial correlation results in two directions are straightforward. Most of the results for the ratio estimator under model M carry over to other linear estimators and zero-correlation working models. The presence of serial correlation causes no bias in the estimator $\hat{T}$ and has little effect on the expectation of any variance estimator which is a linear function of square residuals. But the target of variance estimation, $\mathrm{var}(\hat{T}-T)$, can be sharply altered by serial correlation. Protection is ensured when f is small if the sample units are dispersed ($g/n \doteq 1$). These results also extend to m-dependent serial correlations models, in which units i and j are correlated if and only if $|\, i-j \,| < m$, where m is a fixed integer which is small relative to n. Protection from the correlation effects is obtained, when n is large and f is small, if the sample units are well-dispersed — separated by at least m units.

The clustering phenomenon is harder to model in the general regression context. One immediate difficulty is that when the working model specifies unequal variances, as M does, the most natural ways to model clustering effects not only introduce correlations but also alter the variance structure as

well. Thus it becomes harder to examine correlation *per se* without simultaneously keeping track of effects of departure from the working model's variance structure. Some preliminary calculations, as well as the results of Scott and Holt (1982) for the related problem of estimating regression coefficients (with a constant variance working model), suggest that the present conclusion applies quite generally—working models which overlook within cluster correlation can lead to serious problems when the correlation is present and the sample contains more than one unit from each cluster sampled.

REFERENCES

Holt, D., and A. J. Scott (1981), "Regression analysis using survey data". *The Statistician* **30**, 169–178.

Royall, R. M., and W. G. Cumberland (1978), "Variance estimation in finite population sampling". *Journal of the American Statistical Association* **73**, 351–358.

Royall, R. M., and W. G. Cumberland (1981), "An empirical study of the ratio estimator and estimators of its variance". *Journal of the American Statistical Association* **76**, 66–77.

Royall, R. M., and K. R. Eberhardt (1975), "Variance estimates for the ratio estimator". *Sankhya*, Series C **37**, 43–52.

Scott, A. J., and D. Holt (1982), "The effect of two-stage sampling on ordinary least square methods". *Journal of the American Statistical Association* **77**, 848–854.

M. E. Thompson [1]

IDEAS FROM THE FOUNDATIONS OF SAMPLING APPLIED TO THE ONE-WAY LAYOUT

ABSTRACT

This paper is an attempt to apply ideas from the foundations of sampling theory to a situation in the design of experiments, namely the one-way layout with two treatments and no technical error. Basic considerations concerning the role and choice of randomization are shown to correspond. There is no obvious value in the design context for analogues of πps sampling. An optimality result for estimation of the difference in treatment effect is given.

1. INTRODUCTION

In the light of the recent reemergence of interest in the analogues between sampling and experimental design, the present paper applies the elements of foundations of sampling, as found, for example, in the paper of Godambe and Joshi (1965), to a simple situation in the design of experiments, namely the one-way layout with two treatments and negligible technical or measurement error.

Applying the principles of sampling to the design of experiments may have a precedent in the work of Neyman, whose pioneering paper on sampling (Neyman, 1934) appeared the year before the paper on design (Neyman, 1935) which set off his controversy with Fisher. His 1935 approach to the comparison of treatment effects can be described as follows.

Let $y_{ij}(k)$ denote the "true yield" for block i, plot j and treatment k. This would be the mean yield if the experiment were repeated indefinitely under no change of vegetative conditions. Let $\eta_{ij}(k)$ be the actual yield on a particular occasion. Then $\varepsilon_{ij}(k) = \eta_{ij}(k) - y_{ij}(k)$ is "technical error", analogous to response error in sampling.

[1] Department of Statistics and Actuarial Science, University of Waterloo, Waterloo, Ontario N2L 3G1

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 227–242.

Let $\bar{\bar{y}}(k)$ denote the mean of the true yields over all plots for treatment k. As Neyman expressed the purpose of the experiment, it was to compare the means $\bar{\bar{y}}(k)$, or more specifically to estimate the differences $\Delta = \Delta(k, k') = \bar{\bar{y}}(k) - \bar{\bar{y}}(k')$. Thus, the problem was reduced to the comparison of means for the *finite population* of experimental units.

In the analysis of a randomized block design, $B_i(k)$ and the "soil error" $z_{ij}(k)$ were defined by the following relations:

$$y_{ij}(k) = \bar{\bar{y}}(k) + B_i(k) + z_{ij}(k),$$
$$\sum_i B_i(k) = 0, \qquad \sum_j z_{ij}(k) = 0.$$

Similarly, for the Latin square design, the decomposition

$$y_{ij}(k) = \bar{\bar{y}}(k) + R_i(k) + C_j(k) + z_{ij}(k),$$

$$\sum_i R_i(k) = 0, \qquad \sum_j C_j(k) = 0$$

was defined.

Assuming n plots with each treatment, the estimate proposed for $\Delta(k, k')$ was

$$d = \bar{\bar{\eta}}(k) - \bar{\bar{\eta}}(k') = \frac{1}{n}\left\{\sum_{i,j} \delta_{ij}(k)\eta_{ij}(k) - \sum_{i,j} \delta_{ij}(k')\eta_{ij}(k')\right\},$$

where

$$\delta_{ij}(k) = 1 \text{ if treatment } k \text{ is applied to } i, j,$$
$$= 0 \text{ otherwise .}$$

On assuming that the $\varepsilon_{ij}(k)$ are all independent $N(0, \sigma_\varepsilon^2)$, then

$$\varepsilon_r(d) = \Delta + \frac{1}{n}\left\{\sum_{i,j} \delta_{ij}(k)z_{ij}(k) - \sum_{i,j} \delta_{ij}(k')z_{ij}(k')\right\},$$

where ε_r denotes the corresponding expectation operator.

If further E denotes expectation with respect to the randomization of the design (randomized block or Latin square) then

$$E[\varepsilon_r(d)] = \Delta.$$

Neyman (1935) computed a "variance" $E[\varepsilon_\tau(d-\Delta)^2]$ for each scheme and showed that there are configurations of the $z_{ij}(k)$ which can make the Latin square less efficient than the randomized block design. The non-superiority of the Latin square could occur because the $z_{ij}(k)$ were allowed to depend on k. Neyman (1935) also developed confidence intervals for Δ, based on the randomization in case $\sigma_\varepsilon^2 = 0$. Note that if $\sigma_\varepsilon^2 = 0$, so that there is no technical error, this variance reduces to $E[(d-\Delta)^2]$, the randomization variance.

Fisher's approach, as described by Joan Fisher Box (1978), was apparently to consider that (for the randomized block design)

$$y_{ij}(k) = \mu + \alpha(k) + B_i + z_{ij},$$

where $\sum_k \alpha(k) = 0$, $\sum_i B_i = 0$, and the z_{ij} have mean 0 in some sense. He considered the purpose of the experiment to be to test the null hypothesis that the treatments had no relative effect, which in the above context would mean

$$H_0 : \alpha(k) = 0 \quad \text{for all } k.$$

The z-tests he derived were justifiable in terms of the randomization distribution, as in Neyman's approach, assuming the constraint $\sum_{ij} z_{ij} = 0$. Fisher, in fact, expressed this kind of justification explicitly elsewhere (Fisher, 1936).

An alternative "modern" randomized block analysis sets

$$\eta_{ij}(k) = \mu(k) + \beta_i(k) + e_{ij}(k),$$

where $\sum_i \beta_i(k) = 0$ and the $e_{ij}(k)$ are independent $N(0, \sigma^2)$. The term $e_{ij}(k)$ includes both soil and technical error. The purpose of the experiment is to compare the means $\mu(k)$, which are analogous to super-population means in sampling theory. Fisher's z tests can be justified in terms of this model. In most texts the randomization plays no role in such a justification. However, as should become clear in the simpler situation discussed in succeeding sections, the interplay of model and randomization scheme which can exist in sampling (Thompson, 1980, 1984) can equally well exist in the design of experiments.

2. THE ONE-WAY LAYOUT

Consider the use of n experimental units, and two treatments A and B. In the absence of technical error the response is

$$y_i(k) = \theta_k + \gamma_i, \quad i = 1, \ldots, m; \; k = A \text{ or } B,$$

where (as assumed by Fisher) the γ_i are noise values (Neyman's "soil error") which are independent of the treatment applied. The object is to find a set of designs (i.e., treatment assignments)

$$D_1, \ldots, D_S,$$

and associated probabilities

$$p_s = P(D_s), \quad s = 1, \ldots, S$$

which would make possible a powerful test of the hypothesis

$$H_0 : \theta_A - \theta_B = 0.$$

This is, of course, closely related to the problem of finding an efficient strategy (randomization scheme and estimator) for estimating $\theta_A - \theta_B$.

In the following sections, a pure randomization approach is described in the same generality as is commonly used in sampling theory. It is then argued that the choice of randomization and estimators or test statistics to be used should involve a stochastic model for the responses. In fact, the author believes that tests and estimates for which the justification is based on the randomization distribution alone have useful interpretations but should not be regarded as inference; the randomization is relevant for inference only when it gives results consistent with those based on an appropriate model (see Thompson, 1980).

Although the role of randomization may be similar in *both* sampling and design contexts, the criteria for choosing randomization strategies may be analogous, some of sampling theory appears to have no counterpart in the design of experiments: Section 5 suggests that there is little reason for analogues of πps sampling to be introduced. Finally, Section 6 gives conditions under which optimal unbiased estimators exist.

3. PURE RANDOMIZATION APPROACH

If we were interested only in the long run frequency properties of the strategies and tests used, it might be quite reasonable to evaluate them first in terms of the distribution induced by the randomization scheme, without introducing any other stochastic element. This would be analogous to the approach to sampling estimation found in the textbooks of Cochran (1977), Murthy (1967), Sukhatme and Sukhatme (1970), etc., and dominating foundational discussions before the 1970's.

Consider a general scheme

$$D_1, \ldots, D_S$$
$$p_1, \ldots, p_S$$

and suppose without loss of generality that $\sum_{i=1}^{m} \gamma_i = 0$. A general homogeneous linear estimator of $\theta_A - \theta_B$ could be written

$$e = \sum_{i,k} \delta_{is}(k) a_{is}(k) y_i(k),$$

where D_s is the design selected, and

$$\delta_{is}(k) = 1 \text{ if } k \text{ is assigned to } i \text{ under } D_s,$$
$$= 0 \text{ otherwise .}$$

The randomization expectation of e is

$$E_R(e) = \sum_s p(s) \sum_{i,k} \delta_{is}(k) a_{is}(k) y_i(k).$$

If we impose the condition that e should be an unbiased estimator of $\theta_A - \theta_B$ then for every θ_A, θ_B and $\gamma = (\gamma_1, \ldots, \gamma_m)$ we would have

$$E_R(e) = \theta_A - \theta_B.$$

Equivalently, if

$$\xi_i = \sum_s p(s) \delta_{is}(A) a_{is}(A)$$

and

$$\eta_i = \sum_s p(s) \delta_{is}(B) a_{is}(B),$$

the conditions for unbiased estimation of $\theta_A - \theta_B$ are that

$$\sum_i \xi_i = 1, \quad \sum_i \eta_i = -1,$$

and

$$\sum_i \gamma_i (\xi_i + \eta_i) = 0$$

for *all* γ such that $\sum_i \gamma_i = 0$. The latter condition implies that $\xi_i + \eta_i =$ a constant ξ, and the former two that $\xi = 0$. Thus, the two conditions which will guarantee unbiasedness are

$$(U1) \quad \xi_i = -\eta_i$$

(average coefficient for each unit response is 0) and

$$(U2) \quad \sum_i \xi_i = 1.$$

The randomization variance would be

$$\mathrm{Var}_R(e_s) = \sum_s p(s) \left(\sum_{k,i} \delta_{is}(k) a_{is}(k) y_i(k) - \theta_A + \theta_B \right)^2 .$$

Since $\theta_A - \theta_B = y_i(A) - y_i(B) = \frac{1}{m} \sum_i (y_i(A) - y_i(B))$, $\mathrm{Var}_R(e)$ may be expressed as a quadratic function of co-ordinates of the vectors $\mathbf{z} = (z_1, \ldots, z_m)$ and $\mathbf{z}' = (z_1', \ldots, z_m')$, where $z_i = y_i(A)$ and $z_i' = y_i(B)$. Let a general quadratic function of $\mathbf{z}, \mathbf{z}'$ be denoted by

$$Q(\mathbf{z}, \mathbf{z}') = \sum_{i \le i'} \sum_{i'} \left(Q_{ii'}^{AA} z_i z_{i'} + Q_{ii'}^{AB} z_i z_{i'}' + Q_{ii'}^{BA} z_i' z_{i'} + Q_{ii'}^{BB} z_i' z_{i'}' \right),$$

and let

$$\pi_{ii'AA} = \sum_s p(s) \delta_{is}(A) \delta_{i's}(A), \quad \pi_{ii'BA} = \sum_s p(s) \delta_{is}(B) \delta_{i's}(A),$$

$$\pi_{ii'AB} = \sum_s p(s) \delta_{is}(A) \delta_{i's}(B), \quad \pi_{ii'BB} = \sum_s p(s) \delta_{is}(B) \delta_{i's}(B);$$

thus $\pi_{ii'rr'}$ is the probability that i receives treatment r and i' receives treatment r', where r, r' take values in the set $\{A, B\}$. A randomization-unbiased estimator of $Q(\mathbf{z}, \mathbf{z}')$ when D_j is selected is

$$\sum_{i \le i'} \sum_i \left\{ \frac{\delta_{is}(A)\delta_{i's}(A)}{\pi_{ii'AA}} Q_{ii'}^{AA} z_i z_{i'} + \frac{\delta_{is}(A)\delta_{i's}(B)}{\pi_{ii'AB}} Q_{ii'}^{AB} z_i z_{i'}' \right.$$
$$\left. + \frac{\delta_{is}(A)\delta_{i's}(B)}{\pi_{ii'BA}} Q_{ii'}^{BA} z_i' z_{i'} + \frac{\delta_{is}(B)\delta_{i's}(B)}{\pi_{ii'BB}} Q_{ii'}^{BB} z_i' z_{i'}' \right\}$$

provided that

$$\pi_{ii'rr'} = 0 \Rightarrow Q_{ii'}^{rr'} = 0.$$

(Note $\pi_{ii'AB} = \pi_{ii'BA} = 0$ if $i = i'$.) Thus, $\mathrm{Var}_R(e)$ possesses a randomization unbiased estimate if

(i) $\pi_{ii'rr'} > 0$ when $i \neq i'$, or $i = i'$ and $r = r'$

and

(ii) $\mathrm{Var}_R(e)$ can be written in the form of $Q(\mathbf{z}, \mathbf{z}')$ with $Q_{ii}^{AB} = 0, Q_{ii}^{BA} = 0$.

A sufficient condition for (ii) to be satisfied is that $\mathrm{Var}_R(e)$ can be written as a function of $\mathbf{z}$ only, which will be true if for each s

$$\sum_i \delta(B)a_{is}(B) = -1. \tag{3.1}$$

Clearly, the analogous condition

$$\sum_i \delta_{is}(A)a_{is}(A) = 1 \tag{3.2}$$

would also suffice to ensure "estimability" of $\mathrm{Var}_R(e)$.

Let $v(e)$ be an estimator of $\mathrm{Var}_R(e)$ such that

$$E_R[v(e)] = \mathrm{Var}_R(e).$$

Under favourable conditions, it may be possible to assume that

$$\frac{e-(\theta_A-\theta_B)}{\sqrt{v(e)}}$$

has a standard normal or even a t-distribution. This may be expected to happen if the "distribution" of the γ_i, $i=1,\ldots,m$ is not very skew and m is large and S, the number of design choices, is also large. It follows that, subject to such conditions, the problem of estimating $\theta_A-\theta_B$ and testing H_0 (not necessarily efficiently) can be solved under a wide variety of strategies.

For example, if the scheme is complete randomization, $m/2$ units being selected at random for A, the most intuitively appealing estimator for $\theta_A-\theta_B$ is

$$e = \frac{2}{m}\sum_{i=1}^{m}(\delta_{is}(A)y_i(A) - \delta_{is}(B)y_i(B)) = \bar{y}_s(A) - \bar{y}_s(B).$$

Clearly,

$$E_R(e) = \theta_A - \theta_B,$$

and (3.1) and (3.2) are both satisfied. Thus, $\mathrm{Var}_R(e)$ is estimable, and in fact

$$E_R[v(e)] = \mathrm{Var}_R(e),$$

where

$$\begin{aligned} v(e) &= \frac{2}{n}(v_A + v_B), \\ v_A &= \frac{1}{\left(\frac{m}{2}-1\right)}\sum_i \delta_{is}(A)\left(y_i(A) - \bar{y}_{s_{A,j}}\right)^2, \\ v_B &= \frac{1}{\left(\frac{m}{2}-1\right)}\sum_i \delta_{is}(B)\left(y_i(B) - \bar{y}_{s_{B,j}}\right)^2. \end{aligned} \tag{3.3}$$

The t-statistic

$$\frac{e-(\theta_A-\theta_B)}{\sqrt{v(e)}} \tag{3.4}$$

is not only approximately $N(0,1)$ for large m but also is approximately $t_{(m-2)}$ for moderately large m and a large set of possible γ. Thus, a test of H_0 can be constructed having well-defined frequency properties in the sense of the randomization being repeated again and again with the same units (γ fixed), cf. the logic of Fisher's permutation test (Fisher, 1936). However, there is no guarantee that the test will be powerful in the same sense.

Roughly, powerful tests will be associated with efficient estimators e, but in analogy with sampling theory (e.g., Godambe, 1955), it can be seen that it is impossible to choose a strategy to minimize $\mathrm{Var}_R(e)$ for all γ in R^m, and that almost any strategy works well for some γ. Thus, in order to select a strategy one needs to make some assumption about the vector γ, and perhaps postulate a stochastic model for its generation. Such a model may be sufficiently general, and encompass sufficiently many distributions, that the strategy chosen may represent the best compromise.

4. GENERALIZED EXCHANGEABILITY

One simple stochastic model for γ is that the γ_i are i.i.d. with some distribution. If this is so $\gamma_1,\ldots,\gamma_m$ are symmetrically, or exchangeably, distributed, since the distribution of $\gamma_1,\ldots,\gamma_m$ jointly is invariant under permutations of the experimental units. Alternatively, the units might be separated into strata, within each of which the γ_i are i.i.d., or more generally, exchangeably distributed.

In general, if π_0 is a subgroup of the group of permutations of the experimental units, a stochastic model ξ for γ is π_0-exchangeable if the joint distribution of $\gamma_1,\ldots,\gamma_m$ is invariant under every permutation in π_0. Let ε_ξ denote expectation with respect to ξ. It is possible to show that if e is chosen among estimators such that

$$E_R(e-\theta_A+\theta_B)=0,$$

then the estimator minimizing

$$\varepsilon_\xi E_R(e-\theta_A+\theta_B)^2,$$

if it exists, will be a function of the "π_0-order statistic", suitably defined. See Section 6.

For example, if π_0 is the full permutation group, the order statistic would consist of the set of y_i values observed with the labels i removed, but the treatment used (A or B) retained. The optimal linear estimator would be

$$e = \bar{y}_s(A) - \bar{y}_s(B)$$

and for this choice of e,

$$\varepsilon_\xi \left(\bar{y}_s(A) - \bar{y}_s(B) - \theta_A + \theta_B\right)^2$$

is independent of the design obtained. Therefore

$$\varepsilon_\xi E_R \left(\bar{y}_s(A) - \bar{y}_s(B) - \theta_A + \theta_B\right)^2$$

is independent of the randomization scheme R used to assign, say, $m/2$ units to each treatment.

In this case, it can probably also be shown that (3.3) is in some sense a best estimator of

$$\varepsilon_\xi \left(\bar{y}_s(A) - \bar{y}_s(B) - \theta_A + \theta_B\right)^2,$$

and that its optimality also is independent of the randomization scheme used. If under ξ the t-statistic (3.4) has an approximately t or $N(0,1)$ distribution, then ξ-valid tests of H_0 can be based upon it, and these are independent of the randomization scheme.

However, if complete randomization is used, then $\bar{y}_s(A) - \bar{y}_s(B)$ is in fact unbiased for $\theta_A - \theta_B$ in the sense that

$$E_R \left(\bar{y}_s(A) - \bar{y}_s(B)\right) = \theta_A - \theta_B,$$

and moreover, the test of H_0 based on (3.4) has an interpretation in terms of R, as described above. Thus, if the model ξ were questionable, the tests based upon it would still have validity in terms of hypothetical repeated implementation of R. Thus, complete randomization, which mirrors exchangeability since it is generated from a single design by applying a randomly chosen permutation of the units, reinforces in a somewhat mysterious way the inference based on ξ. See Thompson (1980, 1984).

Now the test based on the t-statistic (3.4) may also be reinforced at least approximately under a restricted randomization scheme. However, schemes for which the joint allocation probabilities $\pi_{ii',rr'}$ differ from those for complete randomization will be "invalid", since under such schemes the t-statistic (3.4) will not have the proper distribution.

To take another example, suppose we have a stratification of the set of experimental units into strata S_1, S_2. If the γ_i are thought of as being

exchangeable within strata, but not across strata, there are two interesting situations (SIT1, SIT2).

In SIT1, the distribution of the γ_i is thought to be independent and different in S_1 and S_2. In particular, it might be thought that the means

$$\frac{1}{m(S_1)}\sum_{i\in S_1}\gamma_i \quad \text{and} \quad \frac{1}{m(S_2)}\sum_{i\in S_2}\gamma_i$$
$$[m(S_j) = \text{ size of } S_j; m(S_1)+m(S_2)=m] \quad (4.1)$$

are different, even on the average over many sets of m experimental units obtained in a similar way. In this situation, the model ξ is invariant under the group π_0 of permutations which leave S_1 and S_2 fixed. This group is not transitive.

If $\bar{y}_{s1}(A)$ is the mean of $y_i(A)$ over units in S_1 receiving treatment A, and the other means below are similarly defined, we may conjecture that best estimators will be expressible in terms of the order statistics for these sets. If

$$W_j = m(S_j)/m,$$

the best estimator for $\theta_A - \theta_B$ will be

$$e = W_1\bar{y}_{s1}(A) + W_2\bar{y}_{s2}(A) - W_1\bar{y}_{s1}(B) - W_2\bar{y}_{s2}(B). \quad (4.2)$$

A scheme R which amounts to complete randomization within strata is suitable, and "valid" in the sense that the t-statistic

$$\frac{e-(\theta_A-\theta_B)}{\sqrt{v(e)}},$$

where

$$v(e) = W_1^2\left(\frac{v_{1A}}{m_{1A}}+\frac{v_{1B}}{m_{1B}}\right)+W_2^2\left(\frac{v_{2A}}{m_{2A}}+\frac{v_{2B}}{m_{2B}}\right),$$
$$v_{jr} = \frac{1}{(m_{jr}-1)}\sum_{i\in S_j}\delta_{is}(r)\left(y_i(r)-\bar{y}_{sj}(r)\right)^2,$$
$$m_{jr} = \sum_{i\in S_j}\delta_{is}(r), \quad j=1,2,; r=A,B,$$

has approximately the same distribution under R as under ξ. The strata S_1 and S_2 are really treated as blocks, and a degree of freedom is "lost" thereby, though the greater efficiency of e may offset this. (In sampling, we are told to stratify as much as possible. The loss of degrees of freedom does

not worry us as much when the emphasis is on efficient point estimation rather than stable interval estimation.)

In SIT2, the two strata S_1 and S_2 are of the same size, and their γ_i configurations are thought to be interchangeable in some sense, so that the model is invariant not only under the previous π_0, but also under the larger group π_0^* of permutations which preserve but possibly interchange strata. For the given set of experimental units, the means (4.1) may again be thought to be different, but over many sets of m experimental units they would be expected to have the same average value. The group π_0^* is transitive. Since $W_1 = W_2 = \frac{1}{2}$, the estimator e of (4.2) reduces to

$$(\bar{y}_{s1}(A) + \bar{y}_{s2}(A) - \bar{y}_{s1}(B) - \bar{y}_{s2}(B))/2. \tag{4.3}$$

If $m_{1A} = m_{2A}$ and $m_{1B} = m_{2B}$, this is the same as

$$\bar{y}_s(A) - \bar{y}_s(B), \tag{4.4}$$

but not otherwise.

A randomization scheme obviously corresponding to π_0^* is to set up a design allocating roughly equal numbers of units to A and to B in each stratum, and then permute the units by a permutation randomly chosen from π_0^*.

5. SOME THOUGHTS ON UNEQUAL PROBABILITY RANDOMIZATION

In sampling theory there are two common justifications for the widely used practice of unequal probability randomization:

(i) it can be used to increase the chance of obtaining a preferred sample, while making sure that each unit has positive probability of selection; and

(ii) it can make a preferred estimator or estimators randomization unbiased.

The second justification must always be present, it seems to this author, for the practice to make sense. In Basu's (1971) example, the circus statistician comes to grief by choosing an exactly unbiased (and in a sense optimal) estimator for a sampling design satisfying only the criterion (i) above.

In Cox's (1956) example, the analogue of (ii) is brought in to justify weighting (experimental) designs with probability proportional to $\sum_u \sum_i (x_i - \bar{x}_u)^2$, where x is a concomitant variate and $\bar{x}_u$ is its uth treatment mean. As he says, to derive the randomization properties of regression estimators of response treatment means, no relationship between x and the

response y need be assumed. However, for these estimators to be *preferred* one would presumably need to have an idea that y and x were approximately linearly related for each treatment with constant residual variance.

He also remarks that this weighted randomization gives more weight to designs where treatments are balanced with respect to the mean value of x; and if $z_i = y_i(A)$ and x_i are linearly related, these designs would seem to be robustly efficient and hence to be preferred—see justification (i). For discussion in a similar vein, see Bellhouse (1986).

However, the same considerations (and their analogues for regression estimators in sampling) suggest that we can do nearly as well with an equal probability scheme, namely by stratifying with respect to x. Effectively, this reduces the "short list" of designs to one which consists of designs which are nearly balanced with respect to x. It will reduce the randomization bias of the estimators from what it would have been under complete randomization, and bring the ξ-based and R-based distributions of the estimators into closer agreement. Thus, practically speaking, a weighted randomization scheme is not necessary in this context.

In sampling theory, there are other situations where weighted randomization seems more important. Suppose $\sum_{i=1}^{m} \gamma_i = 0$ and we want to estimate θ_A from observing

$$\theta_A + \gamma_i = y_i$$

for i in a sample s of $n < m$ units. Suppose also that it is assumed that y_i/x_i are i.i.d., where $\mathbf{x} = (x_1, \ldots, x_m)$ is a known vector of positive components. That is, under ξ,

$$\theta_A = \frac{1}{m} \sum_{i=1}^{m} x_i \left(\frac{y_i}{x_i} \right)$$

is a weighted sum of realizations of i.i.d. variates. Then a natural estimator of θ_A is

$$e = \frac{1}{n} \left(\sum_{i=1}^{m} x_i \right) \sum_{i \in s} \frac{y_i}{x_i}$$

and e can be proved to be optimal under some criteria. We can show that if the probability that $i \in s$ is proportional to x_i under a randomization scheme R, the R-based and ξ-based distributions of e can be made to be approximately the same, and furthermore, $E_R(e) = \theta_A$ exactly even if the assumption of ξ is in doubt (cf. justification (ii)). If ξ is inaccurate and a randomization scheme with different inclusion probabilities is used, $E_R(e)$ may be quite different from θ_A; moments of this e are more sensitive to changes in scheme than moments of ratio or regression estimators.

Perhaps in experimental design problems analogous situations would be less likely to arise. Those which come to mind immediately seem artificial.

For example, one might have

$$y_i(A) = \theta_A x_i + \gamma_i = z_i,$$
$$y_i(B) = \theta_B x_i' + \gamma_i' = z_i',$$

where z_i/x_i are i.i.d., z_i'/x_i' are i.i.d.,

$$x_i + x_i' = \text{ const.}, \sum_i x_i = \sum_i x_i',$$

and

$$\mathbf{x} = (x_1, \ldots, x_m), \mathbf{x}' = (x_1', \ldots, x_m')$$

are known vectors of positive components.

Then

$$e = \frac{2}{m}\left(\sum_i \delta_{is}(A)\frac{y_i}{x_i} - \sum_i \delta_{is}(B)\frac{y_i}{x_i}\right)$$

would be a good estimator, which would be R-unbiased if the probability π_{iA} that i received treatment A were equal to $x_i/(x_i+x_i')$, and to accomplish this exactly might require weighted randomization.

6. AN OPTIMALITY THEOREM

The result given here is patterned on part of Theorem 5.1 of Thompson (1984), and is closely related to results of Wu (1981).

A random permutation model for $\boldsymbol{\gamma}$ is definable in terms of a subgroup Π_0 of the group of permutations or one-to-one mappings of $\{1, \ldots, m\}$ onto itself. Each $\pi \in \Pi_0$ induces a mapping g_π on the space Γ of arrays $\boldsymbol{\gamma}$, given by

$$g_\pi(\boldsymbol{\gamma}) = (\gamma_{\pi(1)}, \cdots, \gamma_{\pi(m)});$$

and for each array $\boldsymbol{\gamma}_0$ we may define an orbit relative to Π_0:

$$\text{orb}(\boldsymbol{\gamma}_0) = \{\boldsymbol{\gamma} : g_\pi(\boldsymbol{\gamma}_0) = \boldsymbol{\gamma} \text{ for some } \pi \in \Pi_0\}.$$

If Γ is closed under each g_π, $\pi \in \Pi_0$, then a *random permutation model* is a distribution on Γ under which each member of $\text{orb}(\boldsymbol{\gamma}_0)$ for some fixed $\boldsymbol{\gamma}_0$ is given equal probability.

A Π_0-*exchangeable* model on Γ is a class of distributions ξ which are invariant under $\pi \in \Pi_0$. Under each such $\boldsymbol{\gamma}$ the conditional distribution of $\boldsymbol{\gamma}$, given $\boldsymbol{\gamma} \in \text{orb}(\boldsymbol{\gamma}_0)$, may be taken to be the random permutation model associated with $\text{orb}(\boldsymbol{\gamma}_0)$.

The subgroup Π_0 is also associated with a class of invariant randomizations. Each design D_0 has an orbit:

$$\text{orb}(D_0) = \{D : D(\pi(i)) = D_0(i),\ \ i = 1, \ldots, m \text{ for some } \pi \in \Pi_0\},$$

where $D(i)$ is the treatment assigned to i under design D. Then a randomization R is invariant if for each D_0 it assigns the same probability p to every design D in $\text{orb}(D_0)$. The invariant randomization R_{D_0} *generated by* D_0 and Π_0 is the randomization which gives equal probability to all members of $\text{orb}(D_0)$ and zero probability to all other designs.

Let us call the outcome of an experiment with design D

$$\mathcal{X}_D = \left((i, y_i) : i \in s_{AD}; (i, y_i) : i \in s_{BD}\right),$$

where s_{AD} is the set of units receiving A under D, s_{BD} is defined similarly, and y_i are the response values.

Formally, we may define the Π_0-*order statistic* $\tau(\mathcal{X}_D)$ as a partition of the space of all possible values of $\mathcal{X}_D$ as γ varies in Γ and θ_A, θ_B vary in $\mathcal{R}$, where $\mathcal{R}$ is the set of real numbers. That is, we shall say that

$$\begin{aligned}&\tau\left((i, y_i) : i \in s_{AD}; (i, y_i) : i \in s_{BD}\right)\\ &= \tau\left((i', y'_{i'}) : i' \in s_{AD'}; (i', y'_{i'}) : i' \in s_{BD'}\right)\end{aligned}$$

if and only if there is some $\pi \in \Pi_0$ such that $s_{AD'} = \{\pi(i) : i \in s_{AD}\}$ and such that for every $i, i' = \pi(i) \Rightarrow y'_{i'} = y_{\pi(i)}$.

Now suppose that the model for γ is a class $\{\xi\}$ of Π_0-exchangeable distributions ξ. Let

$$S = \{(e, R)\}$$

be a class of possible strategies (strategy = estimator and randomization) for estimating $\theta_A - \theta_B$. We may seek a strategy in S to minimize

$$\varepsilon_\xi E_R(e - \theta_A + \theta_B)^2$$

for all $\xi \in \{\xi\}$. Clearly this can be done if we can find a strategy (e, R) to minimize

$$\varepsilon_{\text{orb}(\gamma_0)} E_{R|D_0}(e - \theta_A + \theta_B)^2 \tag{6.1}$$

for every D_0 and $\gamma_0 \in \Gamma$ where $\varepsilon_{\text{orb}(\gamma_0)}$ denotes expectation with respect to the random permutation distribution on orb γ_0 and $E_{R|D_0}$ denotes the randomization expectation with respect to R restricted to $\text{orb}(D_0)$.

Theorem. For each D_0 with positive probability under R for some (e, R) suppose that for every $(e, R) \in S$ and $\gamma_0 \in \Gamma$

(i) $E_{R|D_0}(e - \theta_A + \theta_B) = 0$ for all $\theta_A, \theta_B \in \mathcal{R}$, and

(ii) there exists R_0 such that $(e_0, R_0) \in S$, where $e_0 = \varepsilon_{00}(e \mid \tau(\mathcal{X}_D))$ and ε_{00} denotes expectation with respect to R_0 and the random permutation on $\text{orb}(\gamma_0)$ combined.

Then (6.1) is minimized by (e^*, R^*) in S only if e^* is a function of $\mathcal{X}_D$ only through $\tau(\mathcal{X}_D)$.

The proof is analogous to the proof of the corresponding statement of Theorem 5.1, Thompson (1984).

If e^* is unique in that $(e^*, R^*) \in S$ and e^* is a function of $\tau(\mathcal{X}_D)$, then (e^*, R^*) is optimal. (Note R^* need not be unique.) Typically e^* will be unique if Γ is sufficiently large that the order statistic $\tau(\mathcal{X}_D)$ is complete. (See Liu, 1983.)

ACKNOWLEDGMENTS

The author would like to thank D. A. Sprott, L. V. White, and W. A. Bergerud for helpful discussions.

REFERENCES

Basu, D. (1971), An essay on the logical foundations of survey sampling, Part I. *Foundations of Statistical Inference*, ed. V. P. Godambe and D. Sprott, pp. 203–233. Toronto: Holt, Rinehart and Winston.

Bellhouse, D. R. (1986), "Randomization in the analysis of covariance." *Biometrika* **73**, 207–211.

Box, J. F. (1978), *R. A. Fisher, The Life of a Scientist*. New York: Wiley and Sons.

Cochran, W. G. (1977), *Sampling Techniques*, 3rd edition. New York: Wiley and Sons.

Cox, D. R. (1956), "A note on weighted randomization." *Annals of Mathematical Statistics* **27**, 1144–1151.

Fisher, R. A. (1936), ' " The coefficient of racial likeness" and the future of craniometry.' *Journal of the Royal Anthropological Institute* **66**, 57–63.

Godambe, V. P. (1955), "A unified theory of sampling from finite populations." *Journal of the Royal Statistical Society*, Series B **17**, 269–278.

Godambe, V. P., and V. M. Joshi (1965), "Admissibility and Bayes estimation in sampling finite populations. I." *Annals of Mathematical Statistics* **36**, 1707–1722.

Liu, T. P. (1983), "A general completeness theorem in sampling theory." *Journal of the Royal Statistical Society*, Series B **45**, 369–372.

Murthy, M. N. (1967), *Sampling Theory and Methods*. Calcutta: Statistical Publishing Society.

Neyman, J. (1934) "On the two different aspects of the representative method: the method of stratified sampling and the method of purposive selection." *Journal of the Royal Statistical Society* **97**, 558–625.

Neyman, J. (1935), "Statistical problems in agricultural experimentation." *Journal of the Royal Statistical Society*, Series B supplement, 107–181.

Sukhatme, P. V., and B. V. Sukhatme (1970), *Sampling Theory of Surveys with Applications*. Rome: Food and Agriculture Organization.

Thompson, M. E. (1980), "The likelihood principle and randomization in survey sampling." University of Waterloo Faculty of Mathematics Technical Report in Statistics, 78-04.

Thompson, M. E. (1984), "Model and design correspondence in finite population sampling." *Journal of Statistical Planning and Inference* **10**, 323–334.

Wu, C. F. (1981) On the robustness and efficiency of some randomized designs. *Annals of Statistics* **9**, 1168–1177.

D. Binder, J. Kovar, S. Kumar, D. Paton and A. van Baaren [1]

ANALYTIC USES OF SURVEY DATA: A REVIEW

ABSTRACT

A brief history of the use of survey data in data analysis is given. Issues arising from the complexities of the survey design are highlighted, both from the point of view of estimation as well as for performing hypothesis tests and developing confidence intervals. Many problems such as analysis of linear models and log-linear models have been studied recently. We cite the main results. Estimation of population percentiles is also discussed.

1. INTRODUCTION

The use of survey data using scientific sampling methods can be traced back to the late 19th century. However, until the 1960's the major emphasis of sample surveys was directed toward estimation of means, totals, proportions and ratios. With the advent of high speed computers, the number of surveys increased substantially and users became more sophisticated in their requirements. Over the last 25 years there has been a flurry of activity in the use of surveys for analytic purposes rather than purely as a descriptive device. Age-old questions such as use of sampling weights and making inferences for finite populations resurfaced in this new context. Many of these questions have now been partly resolved, at least for the case of large scale surveys where asymptotic results can be applied. In this paper we review these developments.

In Section 2 we briefly summarize the developments of survey sampling up to 1970. In Section 3 we discuss the problems introduced by using surveys for analytic rather than descriptive studies. In Section 4 we discuss problems which are more particular to analysis of categorical data. Section 5 gives a brief description of problems associated with percentile estimation.

[1] Statistics Canada, Ottawa, Ontario K1A 0T6 (all authors)

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 243–264.

2. EARLY DEVELOPMENTS

The concept of generalizing from a part of the population to the whole was not considered on a scientific basis until the latter half of the 19th century. In this respect there are two main issues: [2]

1. How to select the part from the whole.
2. How to generalize from the selected part of the entire population.

Whereas the focus of this paper is on the second issue, it should, however, be borne in mind that the two issues cannot be completely separated.

The first statistician who can be credited with giving sampling a more scientific basis was A. N. Kiaer, who was the Director of the Norwegian Bureau of Statistics during the last quarter of the 19th century. It is not known whether surveys taken before that time can be called sample surveys because statisticians never gave an account of how they took their samples and what controls they used. Kiaer was the first to consider it fundamental that the accuracy of a survey depends not so much on the number of observations made, but also on the method of obtaining correct representativeness. His was the concept of the "representative method of investigations", about which he wrote several papers during the last ten years of the 19th century. It was, however, not until 1903 that his ideas were tentatively accepted by the International Institute of Statistics. Kiaer also applied the principle of stratification, which he called the "method of controls". (It should be noted that during the same period in the United States, C. D. Wright, who had a position in Massachusetts similar to Kiaer's, also applied the concept of representativeness which he independently developed, although on an even more intuitive basis than Kiaer did.) Kiaer's ideas triggered the development of a more theoretical basis for survey sampling. L. von Bortkiewitz was the first to express the idea of testing sample results for representativeness, although he was not the first to employ statistical tests in connection with sampling. (The first known application of a statistical test had already taken place about two centuries earlier by John Arbuthnot, Queen Anne's physician.) A. L. Bowley proposed to use the theory of probability in connection with survey sampling and, building on the work of K. Pearson and F. Y. Edgeworth, developed the statistical theory of sampling. [3]

A major milestone in the development of sampling was Neyman's (1934) paper, where he placed the methods of stratified and group sampling on a

[2] Actually there is a third issue "How to properly use the generalizations for practical purposes once they have been obtained". With a few notable exceptions this issue is ignored in many statistical textbooks.

[3] A bibliography of these older works is given by You Poh Seng (1951).

sound theoretical basis and criticized the method of purposive selection as described by Bowley and tested by Gini and Galvani.

Until Neyman's paper, the theory of estimation was mainly that of point estimation based on Bayes "Theorem of Inverse Probability" which requires the knowledge of the prior probabilities associated with different admissible hypotheses. Neyman described and refined the theory of "interval estimation" as suggested by R. A. Fisher with parameter estimates based on the Gauss-Markov Theorem. This method of estimation became the recognized theory of estimation. In the meanwhile, Fisher had also developed the analysis of variance, which is a technique to separate total variance into its various components. The validity of the error estimates is based on the principle of randomization. It was due to the work of A.R. Clapham that the analysis of variance also proved useful for sample surveys.

After Neyman's paper, considerable developments have taken place in sampling theory, especially with respect to sample selection and estimation. This led to modern sampling techniques, such as cluster sampling, systematic sampling, two-stage and multi-stage sampling, etc. All the developments in this respect are covered in the five "standards" which appeared in the late forties and early fifties within five years: the books by Cochran (1953), Deming (1950), Hansen *et al.* (1953), Sukhatme (1954), and Yates (1949).

An important development at this stage, which had a high impact on the analytic use of surveys in later years, is the use of supplementary information. Cochran studied this in connection with estimation leading to utilization of this information in the form of ratio or regression estimators. The supplementary information is comparable to the use of one or more covariates in experimental design. Before, the development was geared towards sampling variance models as introduced by Neyman (based on the Gauss-Markov theorem). Ratio and regression estimators were aimed at increasing the precision of the estimates. With the same objective in mind, Hansen and Hurwitz suggested the use of additional information at the sampling state leading to designs in which elements are selected with probabilities proportional to some suitable measure of size.

The earlier statistical methods were based on the assumption of simple random sampling and were developed from the concept of the hypothetical population model. The principle of randomization, as developed by Fisher for experimental design, was later adapted for the purpose of survey sampling in which it implies the use of some artificial mechanism such as a random number table. This in turn implies that the elements in the target population carry some form of label, which is the case with most populations of interest in survey sampling. The statistical methods used were still based on the original assumptions of simple random samples, although in many cases they were modified to allow for sampling without replacement from a

finite population. Estimates for regression coefficients and procedures such as testing for independence in a two-way table were relatively straightforward, especially when the sampling fractions were small, since the classical procedure for analysis seemed to apply to these situations without modification.

However, in the early 1950's because of operational and efficiency concerns, more consideration was being given to stratified sampling designs and to designs with unequal inclusion probabilities; see, for example, Horvitz and Thompson (1952). In the developments following, the sampling variance and its estimation still played a dominant role. The quantity of interest for this purpose, which was later called the design effect (deff) by Kish and Frankel (1974), is the ratio of the variance associated with a given survey design to that of simple random sampling.

The introduction and expansion of the use of electronic computers has contributed considerably to the development of methods of analysis of complex designs, whether survey designs, experimental designs or others, which were at one time considered to be too expensive computationally. An area of major development as a result of this introduction was regression and correlation analysis or more generally least-squares analysis. Although the method of least-squares was already proposed in the beginning of the previous century, development of this method of analysis was slow, mainly due to the lack of means to carry out the substantial amount of computation involved, even with a moderate number of variables. It had already been recognized that difficulties may be encountered when using regression analysis for survey data. For instance the relationship between household savings and household income using survey data was studied by Klein and Morgan (1951) who summarized the difficulties associated with: (1) weighting of observations, (2) heteroscedasticity, (3) nonlinearity, (4) the choice of alternative economic concepts and (5) errors of observation; of which (1), (2) and (5) could be associated with the use of complex surveys. Konijn (1962) discussed two models which can be used for both point and variance estimation in regression relationships, where the data have been obtained using more complex survey techniques than simple random sampling, specifically stratified and cluster sampling.

For estimating the variances of non-linear statistics such as ratios, correlations and regression coefficients, three methods are still commonly used: the delta-method or Taylor linearization (see Tepping, 1968), balanced repeated replication and jackknifing (see Section 3.3 for more details).

For analysis and summaries of categorical data, all the concepts introduced above could be equally applied to this special case. From the point of view of survey samplers little distinction was made between quantitative and qualitative data since the probability mechanism was applied to the

population labels, not the population values. Ratio estimation of population proportions was a common way to incorporate auxiliary data beyond the design variables. Tests for proportions and for differences of two proportions were relatively straight forward using Taylor linearization, balanced repeated replication or jackknifing methods. It was not until the early 1970's that detailed consideration was given to tests of independence, goodness-of-fit tests and other χ^2-type tests (see Section 4). Of course, for simple random samples, the usual χ^2 statistics were valid up to the finite population correction factor.

A major development in the analysis of categorical data from complex designs appeared in Grizzle *et al.*'s (1969) paper. They generalized tests of linear and log-linear hypotheses on the estimated proportions for categorical data, based on the Wald statistic using Taylor linearization. Many of the later developments in categorical data analysis were extensions of this fundamental contribution.

3. REGRESSION AND RELATED ANALYSIS

3.1 Descriptive vs Analytic Use of Survey Data

Because of the recent concern for tests of more complicated hypotheses, such as those described by Grizzle *et al.* (1969), a distinction between "descriptive" and "analytic" use of survey data was made. According to Kalton (1983), analytic uses refer to estimation of parameters of a causal system, ideally one of universal application. Unfortunately, in many disciplines (e.g. behavioural sciences) causal models are still in their infancy. Therefore, good predictive models, which are descriptive in nature, are sought instead. As Imrey *et al.* (1980) point out, statistical inference based on variational or structural modeling are often undertaken in several disciplines, naively assuming probability distributions based upon simple random sampling. An example of using survey data explicitly for prediction purposes is given by Cassel *et al.* (1979). They use the design information in their estimation, the underlying assumption being that any missing variables in a true causal model would behave similarly at a future time point.

The controversy that has arisen among survey data analysts, as it relates to regression and other linear models, extends to other analytic uses of survey data as well. The remainder of this section will concentrate on the regression framework.

3.2 Use of Sampling Design Information

For designs which are not self-weighting, the first question that faces the analyst who wishes to estimate certain model parameters is whether or not to use the sampling weights. Survey samplers are quite accustomed to

using survey weights to estimate means, totals, ratios, proportions, etc. For example,

$$\hat{Y} = \sum w_i y_i / \sum w_i$$

and

$$\hat{R} = \sum w_i y_i / \sum w_i x_i$$

are commonly used estimators of means and ratios. More complex estimators of these quantities, which are model-based but design-dependent, are given in quite general terms by Sarndal (1982).

However, for more complex parameters such as regression coefficients, the considerations on whether to use the sampling weights are more subtle. The answer seems to depend on the following points:

(a) What model is being fitted?
(b) What are the parameters of interest?
(c) How much faith can be placed on the universal application of the model?
(d) How large is the sample size?

Even for the common case of fitting regression coefficients, a number of models have been proposed in the literature. DuMouchel and Duncan (1983) studied four models for stratified random sampling. These are:

I. $$Y = X\beta + \epsilon$$

where the conditional distribution of the ϵ's (conditional on the stratum identification) is such that the ϵ's are uncorrelated, homoscedastic random variables with zero mean. Note that β is constant over all strata.

II. $$Y = X\beta_j + \epsilon$$

for stratum j, where the ϵ's have the same properties as in I.

III. $$Y = X\beta + U\gamma + \epsilon$$

where U is not, in general, observable, but has been transformed so as to be orthogonal to X; i.e. $E(X'U) = 0$. Again the ϵ's behave as in I.

IV. $$Y = X\beta^* + \epsilon^*$$

where it is simply assumed that the ϵ's and the$X$-matrix are uncorrelated and the ϵ's have mean zero.

Often, Models I, II and III are called superpopulation models. Holt *et al.* (1980) said in a more general context, that although Model I may be

true before sample selection, if after sample selection $E(\epsilon \mid X) \neq 0$ then the sample design is informative.

Porter (1973), Pfefferman and Nathan (1977) and others proposed a random coefficient regression model

$$Y_i = X_i\beta_i + \epsilon_i,$$

where a certain structure on the β_i's is imposed.

Many authors emphasize that any models implied by the analysis must be consistent with the data; see, for example, Brewer and Mellor (1973), Nathan (1981), DuMouchel and Duncan (1983) and Kalton (1983).

Under Model I, we define B as

$$\begin{aligned} B &= [E(X'X)]^{-1}E(X'Y) \\ &= \beta + O_p(N^{-1/2}), \end{aligned}$$

where the expectation operator here refers to the finite population value. Therefore, for large finite populations, the distinction between β and B can be virtually ignored. Binder (1983) extended this analogy to parameters of Generalized Linear Models and other forms of implicitly defined parameter. For Model II, DuMouchel and Duncan (1983) considered the parameter of interest to be $\sum W_j\beta_j$ where the W's are proportional to the stratum sizes and $\sum W_j = 1$. This could be extended to general W's as by Pfefferman and Nathan (1981). In Model III the parameter of interest is β. Holt *et al.* (1980) consider a model analogous to Model III, where the U's are observable (see Section 3.4). There, the parameter of interest is $V_{xy}V_{xx}^{-1}$ where V refers to the superpopulation covariance matrix. In Model IV, the parameter of interest is B given by (2.6).

We see that if the classical model (I) holds universally, then the best linear unbiased estimator for β is the usual ordinary least squares estimator, ignoring the sample design information and the sample weights. Nathan (1981) raised questions as to the relevance of B when the model does not hold. A partial answer to this quandry is given by studying Model III. First, one should ensure that the model is approximately true. This may include adding design variables to the model to reduce the correlation of the residuals. Secondly, the model may still be useful for predictive purposes, if the missing variables behave similarly at the prediction point. In this way, the analyst can view the regression coefficients as being descriptive population parameters. For example, Freeman *et al.* (1983) used the regression formulation to make an age-sex-race adjustment to their dependent variable, in order to facilitate comparisons at two different time points.

If Model I is inappropriate, but a formulation similar to Model III is appropriate, then the weighted regression coefficient estimator (using the

sampling weights) will usually provide a consistent estimator of B. Even if Model I is true, the use of the sampling weights will lead to unbiased but inefficient estimates of β. This may not be serious to the practitioner if the sample size is large. Nathan (1981), DuMouchel and Duncan (1983), and Fuller (1984) have suggested fitting models which allow for testing whether the weighted and unweighted estimates of the regression coefficients have the same expected value. Unfortunately, unless the weights are very different, this test will not be very powerful because the assumed models tend to have a high degree of multicollinearity among the independent variables.

All of the above discussions have assumed large populations with large samples. If the sample size is small, the inefficiency resulting from using the weighted estimates may be more serious when the model is in fact true. Also, if the model is only approximately true, the variance reduction resulting from using the unweighted estimates may more than compensate for the increase in bias, thus making the unweighted estimates the preferred choice. In this case, the search for all the relevant variables of the model becomes even more important.

3.3 Making Inferences

The use of the sample design information when developing confidence intervals or performing tests of hypotheses can be crucial. If the analyst has complete faith in a model such as Model I, clearly it is appropriate to apply the classical methods available for such models (including appropriate robust methods available for such models for long-tailed error distributions). However, the danger of applying such methods when the model is not strictly true has been demonstrated by Scott and Holt (1982), where a block diagonal correlated error structure can introduce serious biases into the variance estimates, even for self-weighting designs.

Also, the distinction between a superpopulation parameter, such as β, and its finite population analogue, B, is important if the sampling fractions are large. For example, in a one-way analysis of variance setup with two categories, it may be more appropriate to test the hypothesis:

$$H_0 : | \overline{Y}_2 - \overline{Y}_1 | \leq \delta$$

where $\overline{Y}_i$ is the mean of domain or category i, rather than

$$H_0 : \overline{Y}_2 - \overline{Y}_1 = 0;$$

see Nathan (1981).

Variance estimation for parameters in a design-based setting is usually performed by balanced repeated replication, jackknifing or Taylor linearization.

Taylor linearization for explicitly defined parameters was given by Tepping (1968). Woodruff (1971) showed a simpler method for computing the variances by taking total differentials of the functions to be estimated. Woodruff and Causey (1976) described a computer program for calculating these variances, where the derivatives are numerically computed.

For the case of estimating regression coefficients, Fuller (1975) gave a simpler computational formula than that given by Tepping (1968). Binder (1983) extended this to more complex situations of implicitly defined parameters; for example, parameters of Generalized Linear Models and M-estimators. Shah *et al.* (1977), and Lemeshow and Stoddard (1984) provided simulations demonstrating that the nominal significance levels for regression coefficients using Taylor linearization perform quite well even when the number of strata and the number of observations per stratum are small.

Another method used for variance estimation is the Quenouille-Tukey jackknife (Quenouille, 1956; Tukey, 1958), which was introduced in the late fifties and discussed and developed in the context of simple random sampling or sampling from infinite populations by Brillinger (1964), Miller (1964, 1968, 1974a,b) and Gray and Schucany (1972), among others. The bootstrap method, on the other hand, was introduced relatively recently by Efron (1979) and compared to the jackknife and other resampling plans by Efron (1982) for the same class of problems.

In the context of finite sampling, balanced repeated replication was discussed by Kish and Frankel (1970). In addition, McCarthy (1969), Folsom *et al.* (1971), Frankel (1971), Jones (1974) and Sharot (1976) were among the first to attempt to reuse the sample by jackknifing. Their studies were empirical in nature, considered for the most part, stratified (without replacement) designs. The results supported earlier observations of the usefulness of the jackknife and balanced repeated replication for the purpose of variance estimation and bias reduction. The parameters of concern are functions of stratum means, ratios and correlation coefficients being the most common, although weighted estimates of regression coefficients would equally apply. Further empirical extensions are given by Brillinger (1966), Kish and Frankel (1974), Bean (1975) and Lemeshow and Epp (1977), Wolter (1979) has provided a useful summary and overview.

By contrast, while the use of the bootstrap technique in the context of finite sampling is not uncommon (although infinite populations are generally assumed), the study of its properties is surprisingly rare. McCarthy and Snowden (1983) provided one of the few empirical investigations of the method as it applies to finite populations. They considered two approaches. The first, suggested by Bickel and Freedman (1984), consists of creating a superpopulation from the sample, by replicating each of its units a number of times equal to its weight. The superpopulation is then sampled with-

out replacement. McCarthy and Snowden, on the other hand, resample the sample with replacement, choosing the bootstrap sample size such that the variance of the bootstrap estimator of the mean is correct. Subsequent studies suggested, however, that, in contrast to Bickel and Freedman's method, the latter method fails to capture moments of higher order and can thus be misleading if applied to highly skewed populations.

Theoretical evaluation of sample reuse methods in the context of finite sampling has become of interest only recently and is almost exclusively confined to the study of asymptotic behaviour. Krewski (1978b) provided some insight as to the stability and efficiency of the balanced repeated replication variance estimator, as a function of the number of subsamples selected, for the case of two or more units per stratum; Royal and Cumberland (1978) justified asymptotically the jackknife variance estimator of the population total, demonstrating favourable results as compared to the best linear unbiased estimator under a linear regression model. The key results however, were put forth by Krewski (1978a), where he proved asymptotic normality and the consistency of the jackknife variance estimator for functions of U-statistics in the case of simple random sampling with replacement. Krewski's results were extended by Majumdar and Sen (1978) who proved the strong laws for the jackknife variance estimator of U-statistics. Krewski and Rao (1981) later provided some first order asymptotics in the case of stratified (with replacement) designs for both the balanced repeated replication and the jackknife variance estimators for functions of stratum means. They considered the case where the number of strata tends to infinity rather than the simpler case of large stratum sizes. Rao and Wu (1983b) provided the second order properties for this problem. A good overview of the jackknife and balanced repeated replication asymptotics is given by Rust (1984).

The asymptotic theory for the bootstrap for finite samples is scarce. Babu and Singh (1983) proved some asymptotic properties of the bootstrap variance estimator by letting the stratum sample size go to infinity. Bickel and Freedman (1984) generalized these results by considering stratified samples selected with or without replacement and by letting the total sample size tend to infinity (that is, either the number of strata, or the stratum sample sizes or both tend to infinity). They showed that the bootstrap (in their superpopulation context) and the jackknife variance estimators are asymptotically normal and consistent for the case of estimating linear combinations of stratum means. Rao and Wu (1983a) extended these first order asymptotic results for the bootstrap variance estimator to various other designs including unequal probability designs. Their method of bootstrapping, however, involves the use of adjusted values, somewhat analogous to Tukey's pseudo-values, for the jackknife.

All of the above procedures rely on asymptotics for their theoretical justi-

fication. Fuller (1984) gave the following rules of thumb for the applicability of large sample theory:

1. The mean of the Taylor deviates must be approximately normal (i.e. no influential outliers).
2. There must be sufficient effective degrees of freedom to estimate the variances well.
3. The curvature of the non-linear function of sample means or the standard error of the means must be small.

3.4 An Alternative Approach to Regression

In Section 3.2 we discussed four regression models, specific to stratified sampling designs. Here, another model, proposed by Holt *et al.* (1980) is discussed. The model, with its corresponding strategy is fundamentally different in that it is a maximum likelihood technique (using a superpopulation model) that also purports to account for the sample design. It does this, without using the sampling weights, by incorporating "design variables" in a linear superpopulation model.

The finite population is viewed as a random sample of size N from a superpopulation. The vector of variables, X, can be partitioned into

X_1: the dependent variables
X_2: the independent, carrier or explanatory variables
X_3: the design variables.

The variables are assumed to have a multivariate normal distribution in the superpopulation (this assumption can be relaxed to a set of second order conditions, as by Nathan and Holt, 1980). We let μ_i be $E(X_i)$ and V_{ij} be $E((X_i-\mu_i)(X_j-\mu_j)')$. The value of the design variable vector X_3, is known for all N units in the finite population, but X_1 and X_2 are only known for the n units in the sample.

The parameter of interest (β) is the best linear predictor of X_1 as a function of X_2, given by $V_{12}V_{22}^{-1}$.

If X_1 and X_2 were known for all the units in the population we could estimate V_{12} and V_{22}^{-1} in the usual way to give us $\hat{\beta}_1 = \hat{V}_{12}(\hat{V}_{22})^{-1}$. If X_3 was only known for the sampled units then the maximum likelihood estimate of β would be the usual ordinary least squares (OLS) estimator $\hat{\beta}_2 = S_{12}(S_{22})^{-1}$, where S_{ij} is the sample covariance matrix, based on the n sampled observations.

However the data set consists of n complete sampled observations, and $N-n$ incomplete observations consisting of those units for which only the design information is known. The maximum likelihood estimator for this problem has been discovered by a number of authors (for instance, DeMets

and Halperin, 1977):

$$\hat{\beta} = (S_{12} + S_{13}S_{33}^{-1}(\hat{V}_{33}S_{33}^{-1} - I)S_{32})(S_{22} + S_{23}S_{33}^{-1} - I)S_{32})^{-1}, \quad (3.1)$$

where $\hat{V}_{33}$ is the covariance matrix for X_3 based on the N population values.

The OLS estimate ($\hat{\beta}_2$) will be the same as $\hat{\beta}$ when $S_{32} = 0$ or $\hat{V}_{33} = S_{33}$. If S_{32} is zero, then there is no observed correlation between X_3 and X_2; that is, we observed no linear relationship between the design variables and the explanatory variables. When the survey is a simple random sample or at least approximately self-weighting, $\hat{V}_{33}$ and S_{33} will usually be approximately equal. However, if there are wide variations in the probabilities of selection and joint inclusion probabilities, S_{33} can be expected to be quite different from $\hat{V}_{33}$. Hence, while the weights are not used in the estimation of $\hat{\beta}$, they will to a large extent determine whether this estimate is different from the OLS estimate $\hat{\beta}_2$. Pfefferman and Holmes (1985) demonstrated the possible biases of the procedure under certain types of model failure.

Yet another alternative would be to use the estimator for $\hat{\beta}$ in (3.1) based on $\hat{S}_{ij}$, the weighted sample covariance matrix. This would provide design-consistent estimates of $V_{12}V_{22}^{-1}$.

4. CATEGORICAL DATA ANALYSIS

In this section we review survey data analysis, particularly as it relates to analyzing categorical data. This is an important area of application since, for many surveys, responses in categories are easier to obtain than quantitative variables. Techniques for fitting various log-linear and logistic regression models and undertaking the related analyses are described in Bishop *et al.* (1975), and also have been the subject of excellent review articles by Imrey *et al.* (1981, 1982). The treatment of Bishop *et al.* (1975) is restricted to the case of cell totals following a Poisson, multinomial or product multinomial sampling distribution. Grizzle *et al.* (1969) proposed a general approach for analyzing multivariate categorical data by using linear models. Their methodology, based theoretically on the work of Wald (1943), specified procedures for fitting linear models to functions of the unknown true cell probabilities. Subsequent work by Koch *et al.* (1975) and Shuster and Downing (1976), based on methods similar to those of Grizzle *et al.* (1969) is intended for data obtained from complex sampling designs. We give a brief summary of their methods.

Let $i = 1, 2, \ldots, s$ index the set of distinct sub-populations from which samples are drawn and $j = 1, 2, \cdots, r$ index the set of response profiles. Denoting the true proportion of the ith sub-population and the jth response

category by π_{ij}, we define

$$\boldsymbol{\pi}' = (\pi_{11}, \ldots, \pi_{1r}, \pi_{21}, \ldots \pi_{2r}, \ldots, \pi_{s1}, \ldots, \pi_{sr})$$

with $\sum_j \pi_{ij} = 1$ for each i. Suppose that a sample from each sub-population is drawn according to a specified survey design and

$$\mathbf{p}' = (p_{11}, \ldots, p_{1r}, p_{21}, \ldots, p_{2r}, \ldots, p_{s1}, \ldots, p_{sr})$$

is a design-based estimate of $\boldsymbol{\pi}'$. We are interested in functions $F_i(\boldsymbol{\pi}), (i = 1, \ldots, u)$ of $\boldsymbol{\pi}$. These functions define the relations of interest between the response categories and sub-populations. Let

$$F(\boldsymbol{\pi})' = (F_1(\boldsymbol{\pi}), F_2(\boldsymbol{\pi}), \ldots, F_u(\boldsymbol{\pi})).$$

We assume that $F_i(\boldsymbol{\pi})$'s are functionally independent so that the covariance matrix of the estimate of $F(\boldsymbol{\pi})$ is non-singular. The variation among the u elements of $F(\boldsymbol{\pi})$ may be investigated by fitting the model

$$M : F(\boldsymbol{\pi}) = X\beta,$$

where X is a design matrix of rank $v \leq u$ and β is a $v \times 1$ matrix of unknown parameters. For some problems, (e.g. homogeneity of margins) the model of interest may be $F(\boldsymbol{\pi}) = 0$.

One of several methods of estimation, such as maximum likelihood, ordinary least squares, weighted least squares (WLS), and minimum chi-square may be used for estimating β. The choice of method may depend on the statistical properties of the estimates and the computational efficiency of the associated algorithms. Koch and his co-workers advocate the use of Weighted Least Squares (WLS) methods. In that case

$$b = (X'V_F^{-1}X)^{-1}X'V_F^{-1}F,$$

where V_F is a design-based consistent estimate of the covariance matrix of $F = F(\mathbf{p})$. Note that the construction of the Wald statistic and the WLS estimate of b depend on the ability to get the estimate V_F. Goodness of fit tests are possible by defining the saturated model as $F(\pi) = X_1\beta_1 + X_2\beta_2$ and testing for $\beta_2 = 0$. In general, when the model has been found consistent with the data, statistical tests concerning linear hypothesis involving β may also be carried out. For testing $H : C\beta = 0$ where C is a known $(d \times u)$ matrix, we use the test statistic

$$Q_C = b'C'[CV_bC']^{-1}Cb,$$

where V_b is a consistent estimate of the covariance matrix of b. The statistic Q_C has an asymptotic χ^2 distribution with d d.f. under the hypothesis H. These results are easily extended to other estimates besides the WLS estimate; see Binder (1983) for the appropriate variance estimates. His general method includes estimating Generalized Linear Model parameters as described by Nelder and Wedderburn (1972).

The weighted least squares methodology, developed by Koch *et al.* (1975), has provided a useful and unified approach to the problem of analyzing and testing for $\beta_2 = 0$. However, its use is limited in some applications by the necessity to produce an estimate of the covariance matrix of F. Difficulties could arise from the required inversion of V_F when the number of cells is large or if the number of observations in some cells is small. Detailed discussion on the limitations of WLS methodology is given by Fay (1984, 1985).

Nathan (1969, 1975) has also developed asymptotic methods for testing independence in contingency tables from stratified samples. His method, based on maximum likelihood estimates, also requires estimation of the covariance matrix of the cell estimates.

For data collected by simple random samples, methods for testing the goodness-of-fit of the model, using the Pearson's chi-squared (X^2) and likelihood ratio (G^2) statistics are well known. Their use has been considerably enhanced by availability of standard computer packages. However, in the context of the complex survey design, these statistics have a serious deficiency. Unlike the Wald Statistic, X^2 (or G^2) does not usually have an asymptotic χ^2 distribution under the model of interest when clustering and stratification have been used in designing the survey. Consequently the conclusions based on these statistics may not be valid. Fellegi (1980), Rao and Scott (1981) and others have shown that clustering and stratification can have a considerable effect on the distribution of X^2 and hence its use (without any adjustment) can give misleading results in practice.

Recent work has been directed at investigating the asymptotic distribution of X^2 and G^2 under cluster sampling and other multi-stage sampling designs and adjustments to X^2 have been proposed. Cohen (1976), Altham (1976), Choi (1981) and Brier (1980) have investigated the distribution by modeling probabilities for cluster sampling. They have shown that, under several hypotheses, X^2 divided by a suitable constant has an asymptotic chi-square distribution. However, their methods impose a constraint of equal design effects of the estimates. This constraint is rarely satisfied in practice. Fellegi (1980) proposed the use of $X^2/d.$ (as having a chi-square distribution) as a test statistic, where $d.$ is the average of the design effects of the cell estimates. The computation of $d.$ requires less information about the covariance structure of sample estimates than that required by the Wald

statistic.

The asymptotic distribution of X^2, based on data from a complex survey design, has been investigated by Rao and Scott (1981, 1984) and Roberts (1985). It is shown that, for a wide class of models, the appropriate chi-squared (X^2) test statistic is asymptotically distributed as $\sum_{i-1}^{k} \delta_i Z_i$, the weighted sum of independent chi-square variables. Each Z_i is a chi-square variable with 1 degree of freedom and k depends on the hypothesis. The weights $\{\delta_i\}$ are the eigenvalues of the matrix $A_0^{-1}A_1$ where A_1 is the design based covariance matrix of a statistic used in defining X^2 and A_0 is the corresponding matrix under multinomial sampling. The quantities δ_i are called the generalized design effects and are consistently estimated by the eigenvalues of $\hat{A}_0\hat{A}_1^{-1}$, where $\hat{A}_0$ and $\hat{A}_1$ are consistent estimates of A_0 and A_1, respectively. We denote the estimate of δ_i by $\hat{\delta}_i$.

Due to the non-standard nature of the distribution of X^2, it is convenient to approximate it by some standard function. A first order approximation to the distribution of X^2 can be obtained by treating $X^2 = k\hat{\delta}.\chi_k^2$ where $\hat{\delta}. = \sum_{i=1}^{k} \hat{\delta}_i/k$ and k is the number of positive $\hat{\delta}_i$'s. Hence we may use the adjusted test statistic $X_C^2 = X^2/\hat{\delta}.$ and regard it as having a chi-square distribution. The adjusted test statistic X_C^2 (or G_C^2) provides a satisfactory correction except for the case where $\{\delta_i\}$ has a large coefficient of variation. This adjustment, like the one proposed by Fellegi (1980), requires less than full knowledge about the covariance structure of the estimates.

A better adjustment, based on Satterthwaite's approximation, treats $X_S^2 = X_C^2/(1+a^2)$ as having a χ^2 distribution with v degrees of freedom where

$$v = (k-1)/(1+a^2)$$

and

$$a^2 = \sum_i (\hat{\delta}_i - \hat{\delta}.)^2/[(k-1)\hat{\delta}.]^2.$$

Note that a^2 is the square of the coefficient of variation of the $\hat{\delta}_i$'s. This approximation is useful when a^2 is significantly different than zero. However, this approximation generally requires full knowledge of the covariance matrix. These methods have been used extensively by Hidiroglou and Rao (1983) for analysis of Canada Health Survey data. Comparative results on the significance level due to the use of X^2, $X^2/d.$, X_C^2 and X_S^2 are also provided.

The analysis of survey data using logit and other transformation models has been investigated by Roberts (1985). The methodology proposed is similar to that of Rao and Scott (1984) and has been used by Kumar and Rao (1984, 1985) for analyzing data from the Canadian Labour Force Survey.

Kumar and Rao (1984) have also developed diagnostic procedures, under a logit model based on survey data, for detecting outliers and influential points.

Fay (1985) has proposed another kind of adjustment to the standard Pearson and likelihood ratio chi-squared statistics. His approach is based on jackknifing these statistics. He proposes a new test (based on replication) called the "jackknife chi-square test" and is used for fitting a log-linear model for survey data. The original cross-classified data is split into a series of replicates. A good discussion on the choice of replication strategies is given by Fay (1983). For each replicate, X^2 (or G^2) is estimated through the solution of maximum likelihood equations appropriate to simple random sampling. The jackknife chi-squared statistics, based on these estimates, is computed. A computer program, called CPLX, for implementing jackknifed chi-square tests has also been developed by Fay (1983). The program permits three types of replication methods: the simple jackknife, the stratified jackknife and half sample methods. The choice of the replicate methods is left to the users. This method has been applied to a number of analyses done at the U.S. Bureau of Census. No comparison of the jackknife chi-squared test and those proposed by Rao and Scott has yet been conducted.

5. PERCENTILE ESTIMATION

Even for the 'standard' case of infinite population sampling, estimation of the median and other percentiles, along with associated standard errors and confidence intervals, is not an easy problem. Various alternatives include the sample median, weighted linear functions of the order statistics (Harrell and Davis, 1982), estimates based on kernel density estimates (Sheather and Maritz, 1983), and others. Standard errors of the sample median using bootstrapping (Efron, 1979, 1982; Ghosh *et al.*, 1984) or using other "smoothed" estimates (Sheather and Maritz, 1983) are available.

For survey data collected from finite populations, Woodruff (1952) described a technique for obtaining confidence intervals under a general sampling plan, by projecting the confidence interval for the binomial proportion onto the estimated distribution function. Exact intervals under simple random sampling are given by Wilks (1962) and Konijn (1973). McCarthy (1965) looked at some exact intervals under stratified sampling with proportional allocation. Sedransk and Meyer (1978) obtained exact intervals under stratified sampling in general. Gross (1980) proposed a bootstrap variance estimate for stratified samples. Bayesian methods are given by Hill (1968) and Binder (1982). The latter author obtained intervals that were asymptotically equivalent to Woodruff's (1952) intervals.

This issue is clearly one that requires much more theoretical and empirical research.

6. SUMMARY

We have concentrated here on the importance of the sample design when analyzing survey data. Although it is possible to perform quite sophisticated data analyses with the wide availability of commercially available software, these approaches are often inapplicable to data collected under complex survey designs. We have touched on a wide variety of problems, such as model parameter estimation and tests of significance. However, there are still many unresolved problems with respect to incorporating the design considerations when analyzing multivariate data from complex designs. Examples include cluster analysis, factor analysis, time series methods, multi-dimensional scaling and so on. As the users of survey data become more sophisticated and there is more awareness in the statistical community of the inherent problems, research into these areas will flourish.

REFERENCES

Altham, P. M. E. (1976), "Discrete variable analysis for individuals grouped into families." *Biometrika* **63**, 263–269.

Babu, J. A., and K. Singh (1983), "Inference on means using the bootstrap." *Annals of Statistics* **11**, 999–1003.

Bean, J. A. (1975), "Distribution and properties of variance estimators for complex multistage probability samples." *Vital and Health Statistics Series 2*, No. 65.

Bickel, P. J., and D. A. Freedman (1984), "Asymptotic normality and the bootstrap in stratified sampling." *Annals of Statistics* **12**, 470–482.

Binder, D. A. (1982), "Non-parametric Bayesian models for samples from finite populations." *Journal of the Royal Statistical Society*, Series B **44**, 388–393.

Binder, D. A. (1983), "On the variances of asymptotically normal estimators from complex surveys." *International Statistical Review* **51**, 279–292.

Bishop, Y. M. M., S. E. Fienberg, and P. W. Holland (1975), *Discrete Multivariate Analysis*. Cambridge, MA: MIT Press.

Brewer, K. R. W., and R. W. Mellor (1973), "The effect of sample structure on analytical surveys." *Australian Journal of Statistics* **15**, 145–152.

Brier, S. S. (1980), "Analysis of contingency tables under cluster sampling." *Biometrika* **67**, 591–596.

Brillinger, D. R. (1964), "The asymptotic behaviour of Tukey's general method of setting approximate confidence limits (the jackknife) when applied to maximum likelihood estimates." *International Statistical Review* **32**, 202–206.

Brillinger, D. R. (1966), "The application of the jackknife to the analysis of sample surveys." *Commentary* **8**, 74–80.

Cassel, C. M., C. E. Särndal, and J. H. Wretman (1979), "Prediction theory for finite populations when model-based and design-based principles are combined." *Scandinavian Journal of Statistics* **6**, 97–106.

Choi, J. W. (1981), "A further study on the analysis of categorical data from weighted cluster sample survey." *Proceedings of the American Statistical Association, Section on Survey Methods Research*, 15–20.

Cochran, W. G. (1953), *Sampling Techniques*. New York: Wiley and Sons.

Cohen, J. E. (1976), "The distribution of the chi-squared statistic under clustered sampling from contingency tables." *Journal of the American Statistical Association* **71**, 665–670.

DeMets, D., and M. Halperin (1977), "Estimation of a simple regression coefficient in samples arising from a sub-sampling procedure." *Biometrics* **33**, 47–56.

Deming, W. E. (1950), *Some Theory of Sampling*. New York: Wiley.

DuMouchel, W. H., and G. J. Duncan (1983), "Using sample survey weights in multiple regression analyses of stratified samples." *Journal of the American Statistical Association* **78**, 535–543.

Efron, B. (1979), "Bootstrap methods: another look at the jackknife." *Annals of Statistics* **7**, 1–26.

Efron, B. (1982), *The Jackknife, the Bootstrap and Other Resampling Plans*. Philadelphia: SIAM.

Fay, R. E. (1982), "Contingency tables for complex designs: CPLX." *Proceedings of the American Statistical Association, Section on Survey Research Methods*, 44–53.

Fay, R. E. (1983), "CPLX—Contingency Tables Analysis for Complex Sample Designs". Program documentation, unpublished report. U.S. Bureau of the Census, Washington.

Fay, R. E. (1984), "Some properties of estimates of variance based on replication methods." *Proceedings of the American Statistical Association., Section on Survey Research Methods*, 495–500.

Fay, R. E. (1985), "A jackknifed chi-squared test for complex samples." *Journal of the American Statistical Association* **80**, 148–157.

Fellegi, I. P. (1980), "Approximate tests of independence and goodness of fit based on stratified multistage samples." *Journal of the American Statistical Association* **75**, 261–268.

Folsom, R., D. L. Bayless, and B. V. Shah (1971), "Jackknifing for variance components in complex sample survey designs." Invited paper at the American Statistical Association Meetings, Fort Collins, Colorado.

Frankel, M. R. (1971), *Inference from Survey Samples*. Ann Arbor: Institute for Social Research, University of Michigan.

Freeman, J. L., D. H. Freeman, Jr., and A. M. Ostfeld (1983), "Analysis of data from successive complex sample surveys, with an example of hypertension prevalence from the United States Health Examination Survey." *International Journal of Epidemiology* **12**, 230–237.

Fuller, W. A. (1975), "Regression analysis for sample survey." *Sankhya*, Series C **37**, 117–132.

Fuller, W. A. (1984), "Least squares and related analyses for complex survey designs." *Survey Methodology* **10**, 97–118.

Ghosh, M., W. C. Parr, K. Singh, and G. J. Babu (1984), "A note on bootstrapping the sample median." *Annals of Statistics* **12**, 1130–1135.

Gray, H. L., and W. R. Schucany (1972), *The Generalized Jackknife Statistic.* New York: Marcel Dekker.

Grizzle, J. E., C. F. Starmer, and G. G. Koch (1969), "Analysis of categorical data by linear models." *Biometrics* **25**, 489–504.

Gross, S. T. (1980), "Median estimation in sample surveys." *Proceedings of the American Statistical Association., Section on Survey Research Methods,* 181–184.

Hansen, M. H., W. N. Hurwitz, and W. G. Madow (1953), *Sample Survey Methods and Theory,* Vol. I and II. New York: Wiley.

Harrell, F. E., and C. E. Davis (1982), "A new distribution-free quantile estimator." *Biometrika* **69**, 635–640.

Hidiroglou, M. A., and J. N. K. Rao (1983), "Chi-squared test for the analysis of three way contingency tables from the Canada Health Survey." Technical report, Statistics Canada.

Hill, B. M. (1968), "Posterior distribution of percentiles: Bayes' theorem for sampling from a population." *Journal of the American Statistical Association* **63**, 677–691.

Holt, D., T. M. F. Smith, and P. D. Winter (1980), "Regression analysis of data from complex surveys." *Journal of the Royal Statistical Society* Series A **143**, 474–487.

Horvitz, D. G., and D. J. Thompson (1952), "A generalization of sampling without replacement from a finite universe." *Journal of the American Statistical Association* **47**, 663–685.

Imrey, P. B., G. G. Koch, and M. E. Stokes (1981, 1982), "Categorical data analysis: Some reflections on the log linear model and logistic regression: Parts I and II." *International Statistical Review* **49**, 265–283, and **50**, 35–64 (in collaboration with J. N. Darroch, D. H. Freeman, Jr., and H. D. Tolley).

Imrey, P. B., E. Sobel, and M. Francis (1980), "Modelling contingency tables from complex surveys." *Proceedings of the American Statistical Association, Section on Survey Research Methods,* 212–217.

Jones, H. L. (1974), "Jackknife estimation of functions of stratum means." *Biometrika* **61**, 343–348.

Kalton, G. (1983), "Models in the practice of survey sampling." *International Statistical Review* **51**, 175–188.

Kish, L., and M. R. Frankel (1970), "Balanced repeated replications for standard errors." *Journal of the American Statistical Association* **65**, 1071–1094.

Kish, L., and M. R. Frankel (1974), "Inference from complex samples." *Journal of the Royal Statistical Society,* Series B **36**, 1–37.

Klein, L. R., and J. N. Morgan (1951), "Results of alternative statistical treatments of sample survey data." *Journal of the American Statistical Association* **46**, 442–460.

Koch, G. G., D. H. Freeman, Jr., and J. L. Freeman (1975), "Strategies in the multivariate analysis of data from complex surveys." *International Statistical*

Review **43**, 59–78.

Konijn, H. S. (1962), "Regression analysis in sample surveys." *Journal of the American Statistical Association* **57**, 590–606.

Konijn, H. S. (1973), *Statistical Theory of Sample Survey Design and Analysis.* Amsterdam: North-Holland.

Krewski, D. (1978a), "Jackknifing U-statistics in finite populations." *Communications in Statistics A, Theory and Methods* **7**, 1–12.

Krewski, D. (1978b), "On the stability of some replication variance estimators in the linear case." *Journal of Statistical Planning and Inference* **2**, 45–51.

Krewski, D., and J. N. K. Rao (1981), "Inference from stratified samples: properties of the linearization, jackknife and balanced repeated replication methods." *Annals of Statistics* **9**, 1010–1019.

Kumar, S., and J. N. K. Rao (1984), "Logistic regression analysis of Labour Force Survey data." *Survey Methodology* **10**, 62–81.

Kumar, S., and J. N. K. Rao (1985), "Fitting Box-Cox transformation models to Labour Force Survey data." *Survey Methodology*, to appear.

Lemeshow, S., and R. Epp (1977), "Properties of the balanced half-sample and jackknife variance estimation techniques in the linear case." *Communications in Statistics A, Theory and Methods* **6**, 1259–1274.

Lemeshow, S., and A. M. Stoddard (1984), "A comparison of alternative variance estimation strategies for estimating the slope of a linear regression in sample surveys." *Communications in Statistics B, Simulation and Computation* **13**, 153–168.

Majumdar, H., and P. K. Sen (1978), "Invariance principles for jackknifing U-statistics for finite population sampling and some applications." *Communications in Statistics A, Theory and Methods* **7**, 1007–1025.

McCarthy, P. J. (1965), "Stratified sampling and distribution-free confidence intervals for a median." *Journal of the American Statistical Association* **60**, 772–783.

McCarthy, P. J. (1969), "Pseudo-replication: half samples." *International Statistical Review* **37**, 239–264.

McCarthy, P. J., and C. B. Snowden (1983), "The bootstrap and finite population sampling." Unpublished manuscript.

Miller, R. G. (1964), "A trustworthy jackknife." *Annals of Mathematical Statistics* **35**, 1594–1605.

Miller, R. G. (1968), "Jackknifing variances." *Annals of Mathematical Statistics* **39**, 567–582.

Miller, R. G. (1974a), "An unbalanced jackknife." *Annals of Statistics* **2**, 880–891.

Miller, R. G. (1974b), "The jackknife—a review." *Biometrika* **61**, 1–15.

Nathan, G. (1969), "Tests of independence in contingency tables from stratified samples." In *New Developments in Survey Sampling*, ed. N. L. Johnson and H. Smith, pp. 578–600. New York: Wiley and Sons.

Nathan, G. (1975), "Tables of independence in contingency tables from stratified samples." *Sankhya*, Series C **37**, 77–87.

Nathan, G. (1981), "Notes on inference based on data from complex sample designs." *Survey Methodology* **7**, 77–87.

Nathan, G., and D. Holt (1980), "The effect of survey design on regression analysis." *Journal of the Royal Statistical Society*, Series B **42**, 377–386.

Nelder, J. A., and R. W. M. Wedderburn (1972), "Generalized linear models." *Journal of the Royal Statistical Society*, Series A **135**, 370–384.

Neyman, J. (1934), "On the two different aspects of the representative method: the method of stratified sampling and the method of purposive selection." *Journal of the Royal Statistical Society* **97**, 558–625.

Pfefferman, D., and D. Holmes (1985), "Robustness considerations in the choice of a method of inference for regression analysis of survey data." *Journal of the Royal Statistical Society*, Series A **148**, 268–278.

Pfefferman, D., and G. Nathan (1981), "Regression analysis of data from a cluster sample." *Journal of the American Statistical Association* **76**, 681–689.

Porter, R. D. (1973), "On the use of survey sampling weights in the linear model." *Annals of Economic and Social Measurement* **2**, 141–158.

Quenouille, M. H. (1956), "Notes on bias in estimation." *Biometrika* **43**, 353–360.

Rao, J. N. K., and M. A. Hidiroglou (1981), "Chi-squared tests for the analysis of categorical data from complex surveys." *Bulletin of the International Statistical Institute* **49**, 699–718.

Rao, J. N. K., and A. J. Scott (1979), "Chi-squared tests for analysis of categorical data from complex surveys." *Proceedings of the American Statistical Association, Section on Survey Research Methods*, 58–66.

Rao, J. N. K., and A. J. Scott (1981), "The analysis of categorical data from complex sample surveys: chi-squared tests for goodness of fit and independence in two-way tables." *Journal of the American Statistical Association* **76**, 221–230.

Rao, J. N. K., and A. J. Scott (1984), "On chi-squared tests for multiway contingency tables with cell proportions estimated from survey data." *Annals of Statistics* **12**, 46–60.

Rao, J. N. K., and C. F. J. Wu (1983a), "Bootstrap inference with stratified samples." Laboratory for Research in Statistics and Probability, Technical Report No. 19.

Rao, J. N. K., and C. F. J. Wu (1983b), "Inference from stratified samples: Second order analysis of three methods for non-linear statistics." Laboratory for Research in Statistics and Probability, Technical Report No. 7.

Roberts, G. R. (1985), "Contributions to chi-squared tests with survey data." Ph.D. Thesis, Carleton University.

Royall, R. M., and W. G. Cumberland (1978), "Variance estimation in finite population sampling." *Journal of the American Statistical Association* **73**, 351–358.

Rust, K. F. (1984), "Techniques for estimating variances for sample surveys." Ph.D. Thesis, University of Michigan.

Särndal, C. E. (1982), "Implication of survey design for generalized regression estimation of linear functions." *Journal of Statistical Planning and Inference* **7**, 156–170.

Scott, A. J., and D. Holt (1982), "The effect of two-stage sampling on ordinary least squares methods." *Journal of the American Statistical Association* **77**, 848–854.

Scott, A. J., and J. N. K. Rao (1981), "Chi-squared tests for contingency tables with proportions estimated from survey data." In *Current Topics in Survey Sampling*, ed. D. Krewski, R. Platek and J. N. K. Rao, pp. 247–265. New York: Academic Press.

Sedransk, J., and J. Meyer (1978), "Confidence intervals for the quantiles of a finite population: simple random and stratified simple random sampling." *Journal of the Royal Statistical Society*, Series B **40**, 239–252.

Seng, Y. P. (1951), "Historical survey of the development of sampling theories and practice". *Journal of the Royal Statistical Society*, Series A **114**, 214–231.

Shah, B. V., M. M. Holt, and R. E. Folsom (1977), "Inference about regression models from sample survey data." *Bulletin of the International Statistical Institute* **41**(3), 43–57.

Sharot, T. (1976), "The generalized jackknife: finite samples and subsample sizes." *Journal of the American Statistical Association* **25**, 109–122.

Sheather, S. J., and J. S. Maritz (1983), "An estimate of the asymptotic standard error of the sample median." *Australian Journal of Statistics* **25**, 109–122.

Shuster, J. J., and D. J. Downing (1976), "Two-way contingency tables for complex sampling schemes." *Biometrika* **63**, 271–276.

Sukhatme, P. V. (1953), *Sampling Theory of Surveys with Applications*. Ames, Iowa: Iowa State College Press.

Tepping, B. J. (1968), "Variance estimation in complex surveys." *Proceedings of the American Statistical Association., Social Statistics Section*, 11–18.

Tukey, J. W. (1958), "Bias and confidence in not-quite large samples." Abstract. *Annals of Mathematical Statistics* **29**, 614.

Wald, A. (1943), "Tests of statistical hypothesis concerning general parameters when the number of observations is large." *Transactions of the American Mathematical Society* **54**, 426–482.

Wilks, S. S. (1962), *Mathematical Statistics*, 2nd edition. New York: Wiley and Sons.

Wolter, S. S. (1962), "Variance estimation." U. S. Bureau of the Census, Course Notes.

Woodruff, R. S. (1952), "Confidence intervals for medians and other position measures." *Journal of the American Statistical Association* **47**, 635–646.

Woodruff, R. S. (1971), "A simple method for approximating the variance of a complicated estimate." *Journal of the American Statistical Association* **66**, 411–414.

Woodruff, R. S., and B. D. Causey (1976), "Computerized method for approximating the variance of a complicated estimate." *Journal of the American Statistical Association* **71**, 315–321.

Yates, F. (1949), *Sampling Methods for Censuses and Surveys*. London: Griffin.

Wayne A. Fuller [1]

ESTIMATORS OF THE FACTOR MODEL FOR SURVEY DATA

ABSTRACT

Limiting properties of estimators of the parameters of the factor model computed from an estimated covariance matrix are presented. Construction of the estimators and of the estimated covariance matrix of the estimators is computationally feasible for data collected in surveys of complex design.

1. INTRODUCTION

We assume that the p-dimensional row vector $\mathbf{Z}_t$ is observed for a sample of n observations selected from a finite population. We assume that there is a sequence of samples and designs such that estimators of the population covariances, normalized by $n^{1/2}$, converge in distribution to a normal random vector.

We shall say that the factor model holds if the population matrix of second moments satisfies

$$\Sigma_{ZZ} = \mathbf{A}\Sigma_{xx}\mathbf{A}' + \Sigma_{\epsilon\epsilon}, \tag{1}$$

where Σ_{xx} is a $k \times k$ nonsingular covariance matrix , $\mathbf{A} = (\beta, \mathbf{I})'$, β is a $k \times r$ matrix, $p = k + r$, and $\Sigma_{\epsilon\epsilon}$ is a diagonal covariance matrix. The unknown parameters of the model are β, $\Sigma_{\epsilon\epsilon}$, and Σ_{xx}. We let

$$\gamma = [(\text{vec } \beta)', \sigma_{\epsilon\epsilon 11}, \sigma_{\epsilon\epsilon 22}, \ldots, \sigma_{\epsilon\epsilon pp}, (\text{vech } \Sigma_{xx})']'$$

denote the vector of parameters, where vec β is the $(k \times r)$ -column obtained by listing the columns of β one beneath another and vech Σ_{xx} is the $\frac{1}{2}k(k+1)$-column vector composed of the elements on and below the diagonal of

[1] Statistical Laboratory, Iowa State University, Ames, Iowa 50011

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 265–284.

Σ_{xx}. We may write $\Sigma_{ZZ}(\gamma)$ to denote the fact that the covariance matrix of $\mathbf{Z}_t$ is a function of the q-dimensional vector γ. Let

$$\sigma(\gamma) = \text{vech } \Sigma_{ZZ}(\gamma)$$

be the $\frac{1}{2}p(p+1)$ vector of unique elements of $\Sigma_{ZZ}(\gamma)$ obtained by listing the elements on and below the diagonal of $\Sigma_{ZZ}(\gamma)$ in a column.

There are at least two approaches to the problem of estimating the parameters from a sample covariance matrix constructed from data collected in a sample survey of complex design. In the first, the sample moment matrix and the estimated covariance matrix of the sample moment matrix are used to construct generalized least squares estimators of the parameters. We call these estimators the generalized least squares estimators. Note that the least squares procedure is applied to the elements of the sample moment matrix, not to the original sample elements. The least squares method has been discussed by Jöreskog and Goldberger (1972), Anderson (1973), Browne (1974, 1984), and Dahm and Fuller (1985). The covariance matrix of these estimators is given by the generalized least squares formulas. In the second approach, the estimators are those values that maximize the Wishart likelihood function. While the conditions required for the proper application of the likelihood procedure are not met, we call the estimators constructed in this way the likelihood estimators. The covariance matrix of the likelihood estimators will be estimated using the sample covariance matrix of the sample moment matrix.

The generalized least squares procedure will be shown to have a limiting distribution with smaller covariance matrix than that of the likelihood method. However, the calculations associated with the generalized least squares method increase rapidly as the dimension p of $\mathbf{Z}_t$ increases. Therefore, one may well choose the likelihood estimators for moment matrices of medium size ($p > 8$). For large problems ($p > 25$) the calculation of the covariance matrix for the likelihood estimators also becomes very expensive.

This is generally true in the construction of nonlinear estimates for survey data. The estimators that are asymptotically efficient require additional computation. Also a minimum number of primary sampling units is required for the computation of a nonsingular estimated covariance matrix for the basic statistics. Generally speaking, the number of primary sampling units must considerably exceed the minimum number before one feels comfortable with the generalized least squares estimated variances of the generalized least squares estimators.

2. ESTIMATION

The least squares and likelihood procedures can be applied to any estimated covariance matrix of $\mathbf{Z}$. We denote the estimator of $\mathbf{\Sigma}_{ZZ}$ by $\mathbf{m}_{ZZ}$. We assume that

$$n^{1/2}(\text{vech } \mathbf{m}_{ZZ} - \text{vech } \mathbf{\Sigma}_{ZZ}) \tag{2}$$

converges in distribution to a normal random vector with mean zero and covariance matrix $\mathbf{D}_{ZZ}$. One choice for $\mathbf{m}_{ZZ}$ in the survey sampling context is the normal model estimator discussed by Anderson (1957), Holt *et al.* (1980), and Skinner (1983). The variance of the estimator can be estimated by likelihood methods or by regression methods described by Fuller (1982).

A second choice for $\mathbf{m}_{ZZ}$ is the design consistent estimator

$$\mathbf{m}_{ZZ} = \sum_{i=1}^{n} w_i(\mathbf{Z}_i - \overline{\mathbf{Z}})'(\mathbf{Z}_i - \overline{\mathbf{Z}}), \tag{3}$$

where the sum is over all elements in the sample, the w_i are proportional to the inverse of the sampling rates, $\sum_{i=1}^{n} w_i = 1$, and

$$\overline{\mathbf{Z}} = \sum_{i=1}^{n} w_i \mathbf{Z}_i. \tag{4}$$

The estimator can also be written as

$$\mathbf{m}_{ZZ} = \sum_{i=1}^{n} w_i \mathbf{Z}_i'\mathbf{Z}_i - \overline{\mathbf{Z}}'\overline{\mathbf{Z}}. \tag{5}$$

We are using a single subscript for $\mathbf{Z}_i$, but multistage and stratified samples are in our domain of discussion. From expression (5), we see that

$$E\{\mathbf{m}_{ZZ}\} = \mathbf{\Sigma}_{ZZ} - \mathbf{V}\{\overline{\mathbf{Z}}\}. \tag{6}$$

Under mild assumptions for a sequence of designs and populations, the variance of the limiting distribution of

$$n^{1/2}(\text{vech } \mathbf{m}_{ZZ} - \text{vech } \mathbf{\Sigma}_{ZZ})$$

is

$$\begin{aligned} \mathbf{D}_{ZZ} &= \mathbf{V}\{n^{1/2}\text{vech } \mathbf{m}_{ZZ}\} \\ &= n\mathbf{V}\{\text{vech } [\sum_{i=1}^{n} w_i \mathbf{Z}_i'\mathbf{Z}_i - \boldsymbol{\mu}'\overline{\mathbf{Z}} - \overline{\mathbf{Z}}'\boldsymbol{\mu}]\} \\ &= n\mathbf{V}\{\text{vech } [\sum_{i=1}^{n} w_i(\mathbf{Z}_i - \boldsymbol{\mu}_Z)'(\mathbf{Z}_i - \boldsymbol{\mu}_Z)]\}. \end{aligned} \tag{7}$$

Given a consistent estimator of $\mathbf{D}_{ZZ}$, one can estimate the parameters of the model by applying the generalized least squares method to vech $\mathbf{m}_{ZZ}$. Thus the generalized least squares estimator of γ is the γ that minimizes

$$[\text{vech } \mathbf{m}_{ZZ} - \sigma(\gamma)]'\hat{\mathbf{D}}_{ZZ}^{-1}[\text{vech } \mathbf{m}_{ZZ} - \sigma(\gamma)]$$

where $\hat{\mathbf{D}}_{ZZ}$ is a consistent estimator of $\mathbf{D}_{ZZ}$. In Theorem 1 we state conditions under which the least squares estimator $\tilde{\gamma}$ has a normal distribution in the limit.

Theorem 1. Let $\mathbf{m}_{ZZ}$ be an estimator of the positive definite covariance matrix $\mathbf{\Sigma}_{ZZ}$ such that

$$n^{1/2}\text{vech}(\mathbf{m}_{ZZ} - \mathbf{\Sigma}_{ZZ}) \xrightarrow{L} \text{N}(\mathbf{0}, \mathbf{D}_{ZZ})$$

as $n \to \infty$, where $\xrightarrow{L}$ denotes convergence in distribution. Let $\sigma(\gamma)$ be a continuous function of γ with continuous first and second derivatives. Let $\tilde{\gamma}$ be the generalized least squares estimator. Then

$$n^{\frac{1}{2}}(\tilde{\gamma} - \gamma) \xrightarrow{L} \text{N}\{\mathbf{0}, (\mathbf{F}_Z'\mathbf{D}_{ZZ}^{-1}\mathbf{F}_Z)^{-1}\},$$

where $\mathbf{F}_Z$ is the matrix of partial derivatives of $\sigma(\gamma)$ with respect to γ evaluated at the true γ.

The least squares estimator has considerable theoretical appeal in the sampling situation where it is difficult to specify the distributional structure for $\mathbf{Z}_t$. However, the computation of the estimator can be burdensome for problems of large dimension. The $\frac{1}{2}p(p+1)$ matrix $\hat{\mathbf{D}}_{ZZ}$ must be inverted and a nonlinear algorithm for the q-dimensional vector γ must be developed. In many nonlinear algorithms a q-dimensional inverse will be required at every step of the iteration. Therefore, alternative estimators requiring less computation deserve discussion. We consider the estimator of γ constructed as if the sample were a sample of normal independent vectors.

Fuller *et al.* (1985) have derived the limiting distribution of the likelihood estimators of the factor model under general conditions. We state a theorem that follows from their results.

Theorem 2. Let $\mathbf{m}_{ZZ}$ be an estimator of the positive definite covariance matrix $\mathbf{\Sigma}_{ZZ}$ with the property

$$n^{1/2}\text{vech}(\mathbf{m}_{ZZ} - \mathbf{\Sigma}_{ZZ}) \xrightarrow{L} \text{N}(\mathbf{0}, \mathbf{D}_{ZZ}) \tag{8}$$

as $n \to \infty$. Let $\boldsymbol{\Sigma}_{ZZ} = \boldsymbol{\Sigma}_{ZZ}(\boldsymbol{\gamma})$ be a continuous function of the q-dimensional vector $\boldsymbol{\gamma}$ with continuous first and second derivatives. Let $\boldsymbol{\gamma}$ be identified and let $\hat{\boldsymbol{\gamma}}$ be the estimator of $\boldsymbol{\gamma}$ obtained by minimizing

$$\log | \boldsymbol{\Sigma}_{ZZ}(\boldsymbol{\gamma}) | + \operatorname{tr}\{\mathbf{m}_{ZZ}\, \boldsymbol{\Sigma}_{ZZ}^{-1}(\boldsymbol{\gamma})\}. \tag{9}$$

Then

$$n^{1/2}(\hat{\boldsymbol{\gamma}} - \boldsymbol{\gamma}) \xrightarrow{L} \mathrm{N}(\mathbf{0}, \mathbf{G}),$$

where

$$\mathbf{G} = (\mathbf{F}_Z' \boldsymbol{\Omega}_{ZZ}^{-1} \mathbf{F}_Z)^{-1} \mathbf{F}_Z' \boldsymbol{\Omega}_{ZZ}^{-1} \mathbf{D}_{ZZ} \boldsymbol{\Omega}_{ZZ}^{-1} \mathbf{F}_Z (\mathbf{F}_Z' \boldsymbol{\Omega}_{ZZ}^{-1} \mathbf{F}_Z)^{-1}, \tag{10}$$

$\mathbf{F}_Z$ is the matrix of partial derivatives of vech $\boldsymbol{\Sigma}_{ZZ}(\boldsymbol{\gamma})$ with respect to $\boldsymbol{\gamma}$ evaluated at the true $\boldsymbol{\gamma}$,

$$\begin{aligned} \boldsymbol{\Omega}_{ZZ} &= \mathbf{V}\{\text{vech } \mathbf{a}'\mathbf{a}\} = 2\boldsymbol{\psi}(\boldsymbol{\Sigma}_{ZZ} \otimes \boldsymbol{\Sigma}_{ZZ})\boldsymbol{\psi}', \\ \boldsymbol{\Omega}_{ZZ}^{-1} &= \boldsymbol{\Phi}'(\boldsymbol{\Sigma}_{ZZ}^{-1} \otimes \boldsymbol{\Sigma}_{ZZ}^{-1})\boldsymbol{\Phi}/2, \end{aligned} \tag{11}$$

$\mathbf{a}$ is a vector distributed as $\mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma}_{ZZ})$,

$$\boldsymbol{\psi} = (\boldsymbol{\Phi}'\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}'$$

and $\boldsymbol{\Phi}$ is the matrix such that

$$\text{vec } \boldsymbol{\Sigma}_{ZZ} = \boldsymbol{\Phi} \text{ vech } \boldsymbol{\Sigma}_{ZZ}.$$

Fuller and Pantula (1982) give explicit expressions for $\mathbf{F}_Z$ and

$$(\mathbf{F}_Z' \boldsymbol{\Omega}_{ZZ}^{-1} \mathbf{F}_Z)^{-1}.$$

It is sometimes computationally convenient to transform expression (10) from an expression in the moments of $\mathbf{Z}$ to an expression in the moments of the vector

$$\boldsymbol{\delta}_t = (\mathbf{v}_t, \mathbf{X}_t), \tag{12}$$

where

$$\mathbf{v}_t = \mathbf{Y}_t - \boldsymbol{\beta}_0 - \mathbf{X}_t\boldsymbol{\beta}_1. \tag{13}$$

With no loss of generality let $\boldsymbol{\beta}_0 = 0$, so that we can write

$$\boldsymbol{\delta}_t = \mathbf{Z}_t\mathbf{H}, \tag{14}$$

where

$$\mathbf{H} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ -\boldsymbol{\beta} & \mathbf{I} \end{pmatrix}.$$

Then

$$\begin{aligned}\text{vech } \mathbf{m}_{\delta\delta} &= \boldsymbol{\psi}(\mathbf{H}' \otimes \mathbf{H}') \text{ vech } \mathbf{m}_{ZZ} \\ &= \boldsymbol{\psi}(\mathbf{H}' \otimes \mathbf{H}')\, \boldsymbol{\Phi} \text{ vech } \mathbf{m}_{ZZ} \\ &= \mathbf{L} \text{ vech } \mathbf{m}_{ZZ}\end{aligned} \tag{15}$$

and the variance expression in (10) becomes

$$\mathbf{G} = (\mathbf{F}_\delta' \boldsymbol{\Omega}_{\delta\delta}' \mathbf{F}_\delta)^{-1} \mathbf{F}_\delta' \boldsymbol{\Omega}_{\delta\delta}' \mathbf{D}_{\delta\delta} \boldsymbol{\Omega}_{\delta\delta}^{-1} \mathbf{F}_\delta (\mathbf{F}_\delta' \boldsymbol{\Omega}_{\delta\delta}^{-1} \mathbf{F}_\delta)^{-1}, \tag{16}$$

where

$$\begin{aligned}\mathbf{L} &= \boldsymbol{\psi}(\mathbf{H}' \otimes \mathbf{H}')\, \boldsymbol{\Phi}, \\ \mathbf{F}_\delta' &= \mathbf{F}_Z' \mathbf{L}, \\ \boldsymbol{\Omega}_{\delta\delta} &= \mathbf{L}' \boldsymbol{\Omega}_{ZZ}\, \mathbf{L}.\end{aligned}$$

Assume that $\mathbf{m}_{ZZ}$ is given by (3) and that $\hat{\boldsymbol{\gamma}}$ is the $\boldsymbol{\gamma}$ that minimizes (9). A consistent estimator of $\mathbf{D}_{\delta\delta}$ can be constructed using

$$\hat{\boldsymbol{\delta}}_t = (\hat{v}_{t1}, \hat{v}_{t2}, \cdots, \hat{v}_{tp}, X_{t1} - \overline{X}_2, \cdots, X_{tk} - \overline{X}_k), \tag{17}$$

where

$$\begin{aligned}\hat{v}_{ti} &= Y_{ti} - \overline{Y}_i - \textstyle\sum_{j=1}^{k} \hat{\beta}_{ji}(X_{tj} - \overline{X}_j), && i = 1, 2, \ldots, r, \\ \overline{X}_j &= \textstyle\sum_{t=1}^{n} w_t\, X_{tj}, && i = 1, 2, \ldots, k, \\ \overline{Y}_i &= \textstyle\sum_{t=1}^{n} w_t\, Y_{ti}, && i = 1, 2, \ldots, r,\end{aligned}$$

and $\hat{\beta}_{ji}$ are the appropriate elements of $\hat{\boldsymbol{\gamma}}$. The covariance matrix $\mathbf{D}_{\delta\delta}$ is estimated by employing the ordinary sampling formulas to estimate the covariance matrix of the vector vech $\hat{\mathbf{m}}_{\delta\delta}$, where

$$\text{vech } \hat{\mathbf{m}}_{\delta\delta} = \sum_{t=1}^{n} w_t \text{ vech } \hat{\boldsymbol{\delta}}_t' \hat{\boldsymbol{\delta}}_t.$$

For example, if the sample is a simple random sample of n observations, the first entry in $\hat{\mathbf{D}}_{\delta\delta}$ is

$$n^{-1}(n-1) \sum_{t=1}^{n} (\hat{\delta}_{t1}^2 - m_{\delta\delta 11})^2, \tag{18}$$

where

$$\begin{aligned}\hat{\delta}_{t1} &= \hat{v}_{t1}, \\ m_{\delta\delta 11} &= (n-1)^{-1} \sum_{t=1}^{n} \hat{v}_{t1}^2.\end{aligned}$$

Let $\hat{\gamma}$ denote the q-dimensional vector of likelihood estimators. Then the variance of the limiting distribution of $n^{1/2}(\hat{\gamma} - \gamma)$ is estimated by

$$\hat{\mathbf{G}} = (\hat{\mathbf{F}}_\delta \hat{\mathbf{\Omega}}_{\delta\delta} \hat{\mathbf{F}}_\delta)^{-1} \hat{\mathbf{F}}_\delta' \hat{\mathbf{\Omega}}_{\delta\delta}^{-1} \hat{\mathbf{D}}_{\delta\delta} \hat{\mathbf{\Omega}}_{\delta\delta}^{-1} \hat{\mathbf{F}}_\delta (\hat{\mathbf{F}}_{\delta\delta}' \hat{\mathbf{\Omega}}_{\delta\delta}^{-1} \hat{\mathbf{F}}_\delta)^{-1}, \tag{19}$$

where

$\hat{\mathbf{F}}_\delta = \hat{\mathbf{L}}' \hat{\mathbf{F}}_Z$,

$\hat{\mathbf{\Omega}}_{\delta\delta} = 2\, \boldsymbol{\psi}(\hat{\mathbf{m}}_{\delta\delta} \otimes \hat{\mathbf{m}}_{\delta\delta})\boldsymbol{\psi}'$,

$\mathbf{L}$ is defined by (14) and (15),

$\hat{\mathbf{D}}_{\delta\delta}$ is a consistent estimator of $\mathbf{D}_{\delta\delta}$ (such as that defined in (18)),

$\mathbf{F}_Z$ is the $\frac{1}{2}p(p+1)$ by q matrix of partial derivatives of $\operatorname{vech}\mathbf{\Sigma}_{ZZ}(\gamma)$ with respect to γ,

$(n-1)^{-1}\mathbf{\Omega}_{\delta\delta}$ is the $\frac{1}{2}p(p+1)$ by $\frac{1}{2}p(p+1)$ covariance matrix of vech $\mathbf{m}_{\delta\delta}$ for a sample of n observations that are $\mathrm{NI}(\mathbf{0}, \mathbf{\Sigma}_{\delta\delta})$,

and the hat ($\hat{\cdot}$) is used throughout to denote a consistent estimator. In practice $\hat{\mathbf{F}}_\delta$ is computed directly using the expressions of Fuller and Pantula (1982).

It is often of interest to test the hypothesis that the number of factors is k against the alternative of the unrestricted model. If the generalized least squares method is used to construct the estimator, the generalized residual sum of squares is approximately distributed as a chi-square random variable. In the usual normal likelihood theory, the likelihood ratio statistic

$$2 \log R = -\log |\, \mathbf{\Sigma}_{ZZ}^{-1}(\hat{\gamma})\, \mathbf{m}_{ZZ} \,| + \operatorname{tr} \mathbf{m}_{ZZ}\, \mathbf{\Sigma}_{ZZ}^{-1}(\hat{\gamma}) - p \tag{20}$$

is used for this test.

If one has a sample in which the usual likelihood theory does not hold for the moment matrix $\mathbf{m}_{ZZ}$, several approaches to the testing problem are possible. We first consider a least squares approach using the sample moment matrix of the estimated residuals

$$\hat{\mathbf{v}}_t = \mathbf{Y}_t - \overline{Y} - (\mathbf{X}_t - \overline{X})\hat{\boldsymbol{\beta}}. \tag{21}$$

Under the model

$$\mathbf{Z}_t = \mathbf{x}_t(\boldsymbol{\beta}, \mathbf{I}) + \mathbf{e}_t$$

and

$$\mathbf{v}_t = \mathbf{Z}_t(\mathbf{I}, -\boldsymbol{\beta}')' = \mathbf{Z}_t\, \mathbf{C}.$$

Let

$$\mathbf{m}_{vv} = \mathbf{C}'\, \mathbf{m}_{ZZ}\, \mathbf{C},$$
$$\hat{\mathbf{m}}_{vv} = \hat{\mathbf{C}}'\, \mathbf{m}_{ZZ}\, \hat{\mathbf{C}}.$$

From the model definition

$$\begin{aligned}\mathrm{m}_{ZZ} &= \mathrm{m}_{xx} + \mathrm{m}_{x\epsilon} + m_{\epsilon x} + \mathrm{m}_{\epsilon\epsilon} \\ &= (\boldsymbol{\beta}, \mathrm{I})'\mathrm{m}_{xx}(\boldsymbol{\beta}, \mathrm{I}) + (\boldsymbol{\beta}, \mathrm{I})'\mathrm{m}_{x\epsilon} + \mathrm{m}_{\epsilon x}(\boldsymbol{\beta}, \mathrm{I}) + \mathrm{m}_{\epsilon\epsilon}\end{aligned}$$

and

$$\begin{aligned}\hat{\mathrm{C}}'\,\mathrm{m}_{ZZ}\,\hat{\mathrm{C}} &= (\boldsymbol{\beta}' - \hat{\boldsymbol{\beta}}')\mathrm{m}_{xx}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) + (\boldsymbol{\beta}' - \hat{\boldsymbol{\beta}}')\mathrm{m}_{x\epsilon}(\mathrm{I}, -\hat{\boldsymbol{\beta}}')' \\ &\quad + \hat{\mathrm{C}}'\mathrm{m}_{\epsilon x}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) + \hat{\mathrm{C}}' m_{\epsilon\epsilon}\hat{\mathrm{C}} \\ &= \hat{\mathrm{C}}'\,\mathrm{m}_{\epsilon\epsilon}\hat{\mathrm{C}} + O_p(n^{-1}) \\ &= \hat{\mathrm{C}}'\boldsymbol{\Sigma}_{\epsilon\epsilon}\hat{\mathrm{C}} + \hat{\mathrm{C}}'(\mathrm{m}_{\epsilon\epsilon} - \boldsymbol{\Sigma}_{\epsilon\epsilon})\hat{\mathrm{C}} + O_p(n^{-1}),\end{aligned} \tag{22}$$

where we have used

$$\begin{aligned}\hat{\mathrm{C}} - \mathrm{C} &= O_p(n^{-\frac{1}{2}}), \\ \mathrm{m}_{x\epsilon} &= O_p(n^{-\frac{1}{2}}).\end{aligned}$$

If we write

$$\begin{aligned}\mathrm{s}_v = \operatorname{vech} \hat{\mathrm{m}}_{vv} &= \hat{\mathrm{L}}\,\boldsymbol{\gamma}_\epsilon + \mathrm{a} \\ &= \hat{\mathrm{L}}\,\boldsymbol{\gamma}_\epsilon + \boldsymbol{\psi}(\hat{\mathrm{C}}' \otimes \hat{\mathrm{C}})\operatorname{vech}(\mathrm{m}_{\epsilon\epsilon} - \boldsymbol{\Sigma}_{\epsilon\epsilon}) + O_p(n^{-1}),\end{aligned} \tag{23}$$

where $\boldsymbol{\gamma}_\epsilon = (\sigma_{\epsilon\epsilon 11}, \sigma_{\epsilon\epsilon 22}, \cdots, \sigma_{\epsilon\epsilon pp})'$, then

$$\begin{aligned}\hat{\boldsymbol{\gamma}}_\epsilon &= [\hat{\mathrm{L}}'\hat{\mathrm{V}}^{-1}\{\mathrm{s}_v\}\hat{\mathrm{L}}]^{-1}\hat{\mathrm{L}}'[\hat{\mathrm{V}}^{-1}\{\mathrm{s}_v\}]\mathrm{s}_v \\ &= \boldsymbol{\gamma}_\epsilon + \hat{\mathrm{L}}'[\hat{\mathrm{V}}^{-1}\{\mathrm{s}_v\}][\boldsymbol{\psi}(\hat{\mathrm{C}}' \otimes \hat{\mathrm{C}})\operatorname{vec}(\mathrm{m}_{\epsilon\epsilon} - \boldsymbol{\Sigma}_{\epsilon\epsilon})] + O_p(n^{-1}) \\ &= \boldsymbol{\gamma}_\epsilon + \mathrm{L}'[\mathrm{V}^{-1}\{\mathrm{s}_v\}][\operatorname{vech}(\mathrm{C}\,\mathrm{m}_{\epsilon\epsilon}\,\mathrm{C}' - \mathrm{C}\,\boldsymbol{\Sigma}_{\epsilon\epsilon}\,\mathrm{C}')] + O_p(n^{-1}).\end{aligned} \tag{24}$$

It then follows, by the application of generalized least squares theory, that the generalized residual sum of squares

$$(\mathrm{s}_v - \hat{\mathrm{s}}_v)'[\hat{\mathrm{V}}^{-1}\{\mathrm{s}_v\}](\mathrm{s}_v - \hat{\mathrm{s}}_v) \xrightarrow{L} \chi^2_{\frac{1}{2}r(r+1)-p}, \tag{25}$$

as $n \to \infty$, where

$$\hat{\mathrm{s}}_v = \hat{\mathrm{L}}\hat{\boldsymbol{\gamma}}_\epsilon.$$

The computation of this test statistic requires the inverse of the matrix $\hat{\mathrm{V}}\{\mathrm{s}_v\}$ which is of dimension $\frac{1}{2}r(r+1)$. The computation of the test statistic is a considerable task if r is large. Therefore, one may prefer to use the approximate distribution of the likelihood ratio statistic. This statistic is

$$\begin{aligned}2\log R &= -\log\,\mathrm{m}_{ZZ}\,\boldsymbol{\Sigma}_{ZZ}^{-1}(\hat{\boldsymbol{\gamma}}) + \operatorname{tr}\{\mathrm{m}_{ZZ}\,\boldsymbol{\Sigma}_{ZZ}^{-1}(\hat{\boldsymbol{\gamma}})\} - p \\ &= -\log\,\hat{\mathrm{m}}_{vv}\,\boldsymbol{\Sigma}_{vv}^{-1}(\hat{\boldsymbol{\gamma}}) + \operatorname{tr}\{\hat{\mathrm{m}}_{vv}\,\boldsymbol{\Sigma}_{vv}^{-1}(\hat{\boldsymbol{\gamma}})\} - p,\end{aligned} \tag{26}$$

where $\hat{\mathbf{m}}_{vv}$ is the sample moment matrix of $\hat{\mathbf{v}}_t$ and $\boldsymbol{\Sigma}_{vv}(\hat{\boldsymbol{\gamma}})$ is the likelihood estimator of $\boldsymbol{\Sigma}_{vv}$. The limiting distribution of $2\log R$ is the same as that of

$$(\mathbf{s}_Z - \hat{\mathbf{s}}_Z)'\hat{\boldsymbol{\Omega}}_{ZZ}^{-1}(\mathbf{s}_Z - \hat{\mathbf{s}}_Z) \tag{27}$$

where $\hat{\mathbf{s}}_Z = \operatorname{vech} \boldsymbol{\Sigma}_{ZZ}(\hat{\boldsymbol{\gamma}})$. Therefore we consider the limiting distribution of (27) which is the same as the limiting distribution of

$$(\mathbf{s}_Z - \hat{\mathbf{s}}_Z)'\boldsymbol{\Omega}_{ZZ}^{-1}(\mathbf{s}_Z - \hat{\mathbf{s}}_Z). \tag{28}$$

By our earlier results

$$n^{\frac{1}{2}}(\mathbf{s}_Z - \hat{\mathbf{s}}_Z) \xrightarrow{L} \mathrm{N}(\mathbf{0}, \mathbf{A}_{ss}), \tag{29}$$

where

$$\begin{aligned}\mathbf{A}_{ss} = {} & \mathbf{D}_{ZZ} - \mathbf{F}_Z(\mathbf{F}_Z'\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{F}_Z)^{-1}\mathbf{F}_Z'\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{D}_{ZZ} \\ & - \mathbf{D}_{ZZ}\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{F}_Z(\mathbf{F}_Z'\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{F}_Z)^{-1}\mathbf{F}_Z' \\ & + \mathbf{F}_Z(\mathbf{F}_Z'\boldsymbol{\Omega}_{ZZ}^{-1}\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{F}_Z)^{-1}\mathbf{F}_Z'\boldsymbol{\Omega}_{ZZ}^{-1} \\ & \times \mathbf{D}_{ZZ}\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{F}_Z(\mathbf{F}_Z'\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{F}_Z)^{-1}\mathbf{F}_Z'.\end{aligned} \tag{30}$$

It follows that the mean of the limiting distribution of the statistic (28) is

$$\begin{aligned}&\operatorname{tr}\{\mathbf{A}_{ss}\boldsymbol{\Omega}_{ZZ}^{-1}\} \\ &= \operatorname{tr}[\mathbf{D}_{ZZ}\boldsymbol{\Omega}_{ZZ}^{-1} - (\mathbf{F}_Z'\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{F}_Z)^{-1}\mathbf{F}_Z'\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{D}_{ZZ}\boldsymbol{\Omega}_{ZZ}^{-1}\mathbf{F}_Z]\end{aligned} \tag{31}$$

and the variance of the limiting distribution is

$$\operatorname{tr}\{(\mathbf{A}_{ss}\boldsymbol{\Omega}_{ZZ}^{-1})^2\}. \tag{32}$$

The mean and variance of the limiting distribution can be estimated by replacing the matrices with consistent estimators. The computations require only matrix multiplications because the component matrices can be constructed directly. The limiting distribution is that of a linear combination of chi-square random variables.

3. ILLUSTRATION

To illustrate the application of the theory we use a created data set. The data set is composed of 200 observations on a vector of five variables arranged in forty clusters of size five. The data vectors

$$\mathbf{Z}_{ij} = [Y_{1ij}, Y_{2ij}, Y_{3ij}, X_{1ij}, X_{2ij}]$$

were generated by the model

$$\mathbf{Z}_{ij} = \mathbf{x}_{ij}(\boldsymbol{\beta}, \mathbf{I}) + \epsilon_{ij},$$
$$\epsilon_{ij} = \mathbf{a}_i + \mathbf{d}_{ij},$$

where

$$\mathbf{x}_{ij} = (x_{1ij}, x_{2ij}) = (\mathbf{g}_i + \mathbf{h}_{ij}),$$
$$\boldsymbol{\beta} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \end{pmatrix},$$
$$\mathbf{g}_i' \sim \mathrm{NI}[\mathbf{0}, \mathrm{diag}(0.5, 1.0)],$$
$$\mathbf{h}_{ij} \sim \mathrm{NI}\left[\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 4.25 & -1.00 \\ -1.00 & 4.00 \end{pmatrix}\right],$$
$$\mathbf{a}_i' \sim \mathrm{NI}[\mathbf{0}, \mathrm{diag}(0.49, 0.49, 0.25, 0.49, 0.49)],$$
$$\mathbf{d}_{ij}' \sim \mathrm{NI}[\mathbf{0}, \mathrm{diag}(1.00, 1.96, 1.00, 1.00, 2.89)],$$
$$i = 21, 22, \ldots, 40,$$
$$\mathbf{d}_{ij}' \sim \mathrm{NI}[\mathbf{0}, \mathrm{diag}(4.00, 7.84, 4.00, 11.56)],$$
$$i = 1, 2, \ldots, 20.$$

Thus the marginal covariance matrix of $\mathbf{Z}_{ij}$ satisfies the factor structure. Cluster effects enter the data generation in two ways. First, the x-variables and the error vector satisfy the usual "components of variance" additive model and, second, the within cluster variances are not constant over clusters. It is the second source of variation that contributes the largest portion of the cluster component in the variance of the estimated moment matrices. See Skinner (1982).

The likelihood estimators are given in Table 1. The standard errors of the estimators computed by equation (19) are given in the third column of the table. The standard errors computed under the assumption of the classical normal (independently identically distributed) model are given in column four of the table. On the average, the standard errors computed recognizing the cluster structure of the data are about 20% larger than those computed under the assumption of independent identically distributed observations. The ratios range from 1.56 to 0.91. It is interesting that both the largest and smallest ratios are associated with estimators of the error variances $\sigma_{\epsilon\epsilon ii}$. It should be remembered that the estimators of the standard errors are themselves subject to considerable sampling variance. The estimated variances of the elements of $\mathbf{m}_{\delta\delta}$ are given in Table 2. The cluster variances were estimated as the variance of the sample mean of the variables

$$[\hat{v}_{1ij}^2, \hat{v}_{1ij}\hat{v}_{2ij}, \ldots, (X_{1ij} - \overline{X}_1)^2, (X_{1ij} - \overline{X}_1)(X_{2ij} - \overline{X}_2), (X_{2ij} - \overline{X}_2)^2],$$

Table 1. *Parameters and Estimates for a Sample of 200 Observations*

Parameter	Population Value	Sample Estimate	Sample Standard Error	Normal Standard Error	Ratio of s.e.
β_{11}	1.00	0.893	0.173	0.168	1.03
β_{21}	1.00	0.928	0.272	0.206	1.32
β_{12}	1.00	1.184	0.235	0.196	1.20
β_{22}	−1.00	−0.977	0.245	0.211	1.16
β_{13}	1.00	1.145	0.134	0.131	1.02
β_{23}	0.00	0.004	0.133	0.109	1.22
σ_{xx11}	4.75	3.373	0.750	0.648	1.16
σ_{xx12}	−1.00	−0.225	0.649	0.576	1.13
σ_{xx22}	5.00	4.243	1.572	1.202	1.31
$\sigma_{\varepsilon\varepsilon 11}$	2.99	3.258	1.144	0.984	1.16
$\sigma_{\varepsilon\varepsilon 22}$	5.39	5.980	1.277	1.312	0.97
$\sigma_{\varepsilon\varepsilon 33}$	2.75	2.856	0.448	0.490	0.91
$\sigma_{\varepsilon\varepsilon 44}$	2.99	3.118	0.681	0.436	1.56
$\sigma_{\varepsilon\varepsilon 55}$	7.72	7.424	1.608	1.088	1.48

using the cluster sample option of SUPER CARP. The variances in the column headed "variance normal" were computed as

$$\hat{V}\{\hat{\sigma}_{ij}\} = (199)^{-1}(\hat{\sigma}_{ii}\hat{\sigma}_{jj} + \hat{\sigma}_{ij}^2).$$

With one exception (σ_{XX11}) the variances estimated by the cluster sample formulas are considerably larger than the variances estimated under the assumption that the sample is composed of normal independent vectors. For the method used to generate the example, the variance of the cluster sample estimator of σ_{XX11} is 0.723. For a sample of normal independent vectors the variance of the estimator of σ_{XX11} is 0.602. The average of the ratios of the standard errors is 1.38. Thus the estimated average effect of clustering is larger for the elements of the sample moment matrix than for the parameters of the factor model.

Table 2. *Estimated Variances of Elements of Sample Covariance Matrix*

Element	Sample Estimate	Variance Normal	Variance Cluster	Ratio of s.e.
σ_{vv11}	12.15	1.50	4.12	1.66
σ_{vv12}	-3.44	1.14	2.09	1.35
σ_{vv13}	3.22	0.48	1.07	1.49
σ_{vX11}	-2.79	0.44	0.65	1.22
σ_{vX12}	-6.89	0.96	1.78	1.36
σ_{vv22}	17.44	3.09	5.31	1.31
σ_{vv23}	4.20	0.70	1.34	1.35
σ_{vX21}	-3.69	0.64	0.77	1.10
σ_{vX22}	7.26	1.30	2.26	1.32
σ_{vv33}	6.95	0.49	1.22	1.58
σ_{vX31}	-3.57	0.29	0.47	1.27
σ_{vX32}	-0.03	0.41	0.47	1.07
σ_{XX11}	6.49	0.43	0.39	0.95
σ_{XX12}	-0.22	0.38	0.44	1.08
σ_{XX22}	11.67	1.38	2.32	1.30

4. LANGUAGE EXAMPLE

In November 1983 the Intensive English and Orientation Program of the Department of English at Iowa State University conducted a study in which members of the general university faculty were asked to evaluate two essays. The essays were presented to the faculty as essays prepared as part of a placement examination by two foreign graduate students that were nonnative speakers of English. Three pairs of essays were used in the study: a pair containing errors in the use of articles, a pair containing errors in spelling and a pair containing errors in verb tense. The faculty members were asked to read the essays and to score them using a five point scale for eleven items. The study is described by Vann and Lorenz (1985).

We analyze the responses for six items. The six items are divided into two groups: three items pertaining to the essay and three items pertaining to the language used. The low and high points of the scale for the six items are described as follows:

A. The essay is
   $\mathbf{Z}_1$: poorly developed – well developed
   $\mathbf{Z}_2$: difficult to understand – easy to understand
   $\mathbf{Z}_3$: illogical – logical
B. The writer uses language which is
   $\mathbf{Z}_3$: inappropriate – appropriate
   $\mathbf{Z}_5$: unacceptable – acceptable
   $\mathbf{Z}_6$: irritating – not irritating

For our purposes the sample can be considered to be a self weighting stratified sample, where the strata were the following subdivisions of the faculty.

1. Humanities and Social Science Men
2. Humanities and Social Science Women
3. Physical Sciences, Mathematics and Engineering
4. Biological and Agricultural Sciences

Table 3 contains a summary of the data for 219 respondents. The observation for each item is the sum of the scores on that item for the two essays scored by the faculty member. Thus the possible values for a response are the integers from two to ten. The moment matrix was computed as

$$\mathbf{m}_{ZZ} = (n-1)^{-1}\sum_{t=1}^{n}(\mathbf{Z}_t - \overline{\mathbf{Z}})'(\mathbf{Z}_t - \overline{\mathbf{Z}}),$$

where $\mathbf{Z}_t$ is a vector of dimension six.

The normal standard errors for the elements of $\mathbf{m}_{ZZ}$ are computed as square roots of the diagonal elements of

$$(n-1)^{-1}\hat{\mathbf{\Omega}}_{ZZ} = 2(n-1)^{-1}\boldsymbol{\psi}(\mathbf{m}_{ZZ} \otimes \mathbf{m}_{ZZ})\boldsymbol{\psi}'.$$

For the covariance matrix of $(\overline{\mathbf{Z}}, [\text{vech } \mathbf{m}_{XX}]')$, the simple random sampling estimator is computed as

$$\hat{\mathbf{V}}_{bb} = n^{-1}(n-1)^{-1}\sum_{t=1}^{n}(\mathbf{b}_t - \overline{\mathbf{b}})'(\mathbf{b}_t - \overline{\mathbf{b}}),$$

where

$$\mathbf{b}_t = \{\mathbf{Z}_t, [\text{vech}(\mathbf{Z}_t - \overline{\mathbf{Z}})'(\mathbf{Z}_t - \overline{\mathbf{Z}})]'\}.$$

Table 3. *Statistics for 219 Respondents to Language Evaluation*

Statistic	Estimate	Standard error mult. by 10			Ratio of Variances
		Normal	SRS	Stratified	SRS/Normal
$\overline{Z}_1$	6.42	1.16	1.16	1.16	1.00
$\overline{Z}_2$	7.27	1.14	1.14	1.14	1.00
$\overline{Z}_3$	6.80	1.25	1.25	1.24	1.00
$\overline{Z}_4$	6.78	1.27	1.27	1.25	1.00
$\overline{Z}_5$	7.00	1.08	1.08	1.08	1.00
$\overline{Z}_6$	7.60	1.17	1.17	1.15	1.00
m_{ZZ11}	2.95	2.83	2.58	2.58	0.83
m_{ZZ21}	1.85	2.32	2.25	2.26	0.93
m_{ZZ31}	1.61	2.42	2.56	2.57	1.12
m_{ZZ41}	1.52	2.42	2.48	2.49	1.05
m_{ZZ51}	2.08	2.33	2.18	2.18	0.88
m_{ZZ61}	1.44	2.23	2.26	2.26	1.03
m_{ZZ22}	2.83	2.71	2.38	2.39	0.77
m_{ZZ32}	1.72	2.41	2.24	2.25	0.86
m_{ZZ42}	1.66	2.42	2.40	2.41	0.98
m_{ZZ52}	1.90	2.23	2.05	2.06	0.85
m_{ZZ62}	1.50	2.21	2.15	2.17	0.95
m_{ZZ33}	3.43	3.29	3.08	3.08	0.88
m_{ZZ43}	2.63	2.96	3.06	3.05	1.07
m_{ZZ53}	1.55	2.26	2.23	2.24	0.98
m_{ZZ63}	2.09	2.59	2.91	2.92	1.27
m_{ZZ44}	3.54	3.39	3.28	3.29	0.93
m_{ZZ54}	1.43	2.25	2.35	2.35	1.09
m_{ZZ64}	2.14	2.63	3.03	3.04	1.33
m_{ZZ55}	2.54	2.43	2.09	2.09	0.74
m_{ZZ65}	1.40	2.09	2.03	2.03	0.95
m_{ZZ66}	2.98	2.83	3.09	3.10	1.17

The estimated covariance matrix for stratified sampling was computed in the analogous way by applying the stratified formulas to the vector $\mathbf{b}_t$.

The estimates are given in the first column of Table 3, the standard errors computed under the three assumptions are given in the next three columns and the ratio of the variance computed by the moment method for

simple random sampling to the variance computed under normality is given in the last column. In this example stratification had almost no effect, giving essentially the same standard errors as simple random sampling.
Under normality the variance of the ratio

$$(2\mathrm{m}_{ZZii}^2)^{-1}(n-1)^{-1}\sum_{t=1}^{n}[(\mathbf{Z}_{ti}-\overline{\mathbf{Z}}_i)^2-\mathrm{m}_{ZZii}]^2$$

is about $6(n-1)^{-1}$. Thus, if the sample is a random sample from a normal distribution, about 95% of such ratios should fall in the interval (0.67, 1.33). None of the six ratios of this type in Table 3 fall outside the interval. The average of the six ratios is 0.89, suggesting that the variance of the squares is less than that for normal variables. This is reasonable because the variables are restricted to the interval (2,10). The average of the ratios for the variances of 15 covariances is 1.02. On the basis of this table, one might well conclude that use of normal formulas would be reasonable and, in fact, might overestimate the true variance.

We assume the data satisfy the factor model in two factors and let

$$\mathbf{Z}_t=(\mathbf{Y}_{t1},\mathbf{Y}_{t2},\mathbf{Y}_{t3},\mathbf{Y}_{t4},\mathbf{X}_{t1},\mathbf{X}_{t2})$$

where $\mathbf{Y}_{t1}$ = developed, $\mathbf{Y}_{t2}$ = understand, $\mathbf{Y}_{t3}$ = appropriate, $\mathbf{Y}_{t4}$ = acceptable, $\mathbf{X}_{t1}$ = logical and $\mathbf{X}_{t2}$ = irritating. The model can be written in the form

$$\mathbf{Z}_t=(\boldsymbol{\beta}_0,\mathbf{0})+\mathbf{x}_t(\boldsymbol{\beta},\mathbf{I})+\boldsymbol{\epsilon}_t,$$
$$\mathbf{X}_t=(x_{t1},x_{t2})+(u_{t1},u_{t2}),$$

where $\mathbf{Z}_t$ is the observed vector, (x_{t1},x_{t2}) are the true values of the factor vector $\boldsymbol{\epsilon}_t$ is the 6-dimensional vector of errors and $(\epsilon_{t5},\epsilon_{t6})=(u_{t1},u_{t2})$. Then the population covariance matrix of $\mathbf{Z}_t$ can be written as

$$\boldsymbol{\Sigma}_{ZZ}=(\boldsymbol{\beta},\mathbf{I})'\boldsymbol{\Sigma}_{xx}(\boldsymbol{\beta},\mathbf{I})+\boldsymbol{\Sigma}_{\epsilon\epsilon},$$

where $\boldsymbol{\Sigma}_{\epsilon\epsilon}$ is a diagonal covariance matrix.

The first column of Table 4 contains the maximum likelihood estimates of the parameters of the factor model constructed under the assumption of random sampling from a normal distribution. The ratio of estimated variances of the estimated parameters in the last column is much different from the corresponding column of Table 3. The estimated $\boldsymbol{\beta}$'s fall into two groups. In the group for $\mathbf{Y}_1$ and $\mathbf{Y}_2$, the ratio of the moment estimator of variance to the estimator of variance based on normality is about 1.5. In the group for $\mathbf{Y}_3$ and $\mathbf{Y}_4$, the ratio is about 2.5. Although the variances of the original moments looked similar to the variances for a normal distribution,

Table 4. *Factor Model Estimates*

Parameter	Normal Estimate	Standard errors mult. by 10			Ratio of Variances
		Normal	SRS	Stratified	SRS/Normal
β_{01}	−0.648	4.82	4.64	4.64	0.93
β_{02}	0.130	5.01	4.74	4.74	0.90
β_{03}	−2.274	7.59	8.43	8.45	1.24
β_{04}	−2.383	8.28	9.21	9.18	1.25
μ_{x1}	7.005	1.08	1.08	1.08	1.00
μ_{x2}	7.598	1.17	1.17	1.15	1.00
β_{11}	0.869	1.23	1.44	1.44	1.37
β_{21}	0.130	1.16	1.35	1.35	1.35
β_{12}	0.651	1.07	1.33	1.33	1.54
β_{22}	0.340	1.10	1.41	1.40	1.67
β_{13}	−0.146	1.40	2.21	2.22	2.52
β_{23}	1.330	1.62	2.52	2.53	2.44
β_{14}	−0.295	1.58	2.53	2.54	2.57
β_{24}	1.477	1.85	2.95	2.96	2.56
σ_{ee11}	0.956	1.38	1.51	1.51	1.20
σ_{ee22}	1.086	1.24	1.33	1.33	1.15
σ_{ee33}	0.875	1.54	1.68	1.68	1.19
σ_{ee44}	0.805	1.80	2.19	2.19	1.50
σ_{ee55}	0.350	1.36	1.51	1.51	1.24
σ_{ee66}	1.248	1.42	2.01	2.01	2.03
σ_{xx11}	2.186	2.75	2.60	2.60	0.90
σ_{xx12}	1.402	2.08	2.03	2.02	0.95
σ_{xx22}	2.727	2.71	3.18	3.18	1.39

the variances for the functions of the moments giving the factor estimates are much different from those based on normality.

The reason for the difference between the moment estimator and the normal estimator is illustrated in Figure 1. In this figure

$$\hat{v}_{t4} = Y_{t4} - \hat{\beta}_{04} - \hat{\beta}_{14}X_{t1} - \hat{\beta}_{24}X_{t2}$$

is plotted against

$$\hat{x}_{t1} = X_{t1} - (\hat{v}_{t1}, \hat{v}_{t2}, \hat{v}_{t3}, \hat{v}_{t4})\hat{\Sigma}_{vv}^{-1}\hat{\Sigma}_{vu1}),$$

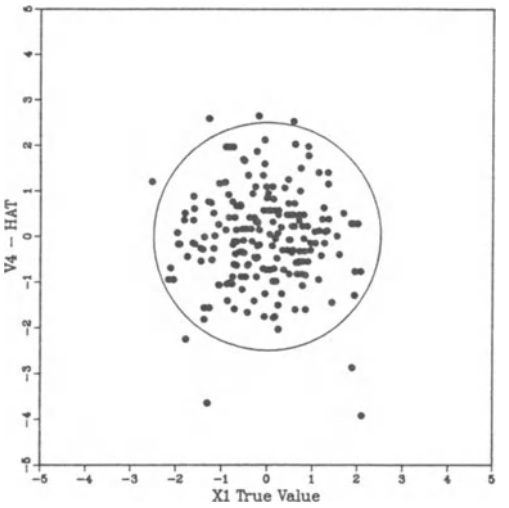

Figure 1. *Plot of* $\hat{v}_{t4}$ *against* $\hat{x}_{t1}$.

where $\hat{v}_{ti}$ is analogous to a regression residual, $\hat{x}_{ti}$ is the estimated true value of x_{ti}, $\hat{\Sigma}_{vv}$ is the estimated covariance matrix of the four dimensional factor v_t, $\hat{\Sigma}_{vu1}$ is the estimated covariance between v_t and u_{t1}, and

$$X_{ti} = x_{ti} + u_{ti}, \qquad i = 1, 2.$$

Under normality

$$\ddot{x}_{ti} = X_{ti} - (v_{t1}, v_{t2}, v_{t3}, v_{t4})\Sigma_{vv}^{-1}\Sigma_{vu1}$$

and v_{tj} are independent. The estimators display a similar property in that the maximum likelihood estimators satisfy

$$\sum_{t=1}^{n} \hat{x}_{ti}\hat{v}_{tj} = 0$$

for i = 1, 2, and j = 1, 2, 3, 4. The $\hat{x}_{ti}$ and $\hat{v}_{tj}$ in the figure have been standardized by dividing by the appropriate standard errors. The departure of $\hat{v}_{t4}$ from normality is apparent in the figure. The probability is about 0.02 that three or more observations in a sample of 219 from a normal distribution

Table 5. *Properties of Empirical Distribution of Ratio of Two Estimated Variances (SRS/Normal)*

Parameter	Standard Error of Ratio	Percentiles of Empirical Dist.	
		0.05	0.95
β_{01}	0.14	0.81	1.24
β_{02}	0.13	0.76	1.24
β_{03}	0.13	0.80	1.23
β_{04}	0.15	0.80	1.27
μ_{x1}	0.00	1.00	1.00
μ_{x2}	0.00	1.00	1.00
β_{11}	0.11	0.77	1.20
β_{21}	0.13	0.76	1.21
β_{12}	0.15	0.82	1.28
β_{22}	0.13	0.84	1.24
β_{13}	0.14	0.77	1.26
β_{23}	0.15	0.81	1.33
β_{14}	0.14	0.80	1.21
β_{24}	0.14	0.77	1.23
σ_{ee11}	0.15	0.75	1.31
σ_{ee22}	0.16	0.79	1.32
σ_{ee33}	0.16	0.75	1.34
σ_{ee44}	0.14	0.83	1.33
σ_{ee55}	0.14	0.79	1.23
σ_{ee66}	0.21	0.73	1.33
σ_{xx11}	0.14	0.78	1.22
σ_{xx12}	0.14	0.79	1.22
σ_{xx22}	0.16	0.76	1.28

will differ from the mean by more than 2.5σ. Six of the observed standardized $\hat{v}_{t4}$ exceed $2.5\hat{\sigma}_{v4}$ in absolute value.

One step of a Gauss-Newton procedure was used to approximate the nonlinear generalized least squares estimates of the parameters. All differences between the likelihood estimates and the one step generalized least squares estimates were less than one standard error. In fact, all differences were less than 75% of the normal likelihood standard errors.

The generalized least squares residual sum of squares defined in (25) is

3.92. If the model holds, the sum of squares is approximately distributed as a chi-square random variable with four degrees of freedom. Therefore, the model is easily accepted. In this example, the usual likelihood ratio statistic yields a similar value of 4.12.

To obtain an idea of how the ratios of the two types of estimated variances vary due to sampling, 100 samples of size 219 were generated from a 6-dimensional multivariate normal distribution. The mean of the population was equal to the sample mean and the covariance matrix was equal to $\hat{\Sigma}_{ZZ}$, where $\hat{\Sigma}_{ZZ}$ is the factor covariance matrix of the form (1) constructed with the estimates of Table 4.

Properties of the sample of ratios of estimated variances are given in Table 5. The variance of the ratio

$$s^{-4}(n-1)^{-1}\sum_{t=1}^{n}(e_t^2 - s^2)^2$$

is $6(n-1)^{-1}$, where

$$s^2 = (n-1)\sum_{t=1}^{n}(e_t - \bar{e})^2 \quad \text{and} \quad e_t \sim \text{NI}(0, \sigma^2).$$

The standard errors of the ratios in Table 5, for statistics that are functions of second moments, are generally slightly less than $[6(n-1)^{-1}]^{\frac{1}{2}}$. There is little doubt that estimated variances based on normality seriously underestimate the true variances of the factor estimators for the language data.

ACKNOWLEDGMENTS

This manuscript was prepared while the author was a Visiting Research Fellow in the Faculty of Mathematics at the University of Southampton. Research was supported by Grant Number HR 7152 of the Social Science Research Council (UK); Statistical Procedures for Analytic Surveys. Appreciation is expressed to Dr. Sastry Pantula and Mr. Stephen Miller who carried out the calculations for the illustration and for the language data, respectively. The language data were used through the courtesy of Professor Roberta Vann and Professor Fred Lorenz.

REFERENCES

Anderson, T. W. (1957), "Maximum likelihood estimates for a multivariate normal distribution when some observations are missing." *Journal of the American Statistical Association* **52**, 200–203.

Anderson, T. W. (1973), "Asymptotically efficient estimation of covariance matrices with linear structure." *Annals of Statistics* **1**, 135–141.

Browne, M. W. (1974), "Generalized least squares estimators in the analysis of covariance structures." *South African Statistical Journal* **8**, 1–24.

Browne, M. W. (1984), "Asymptotically distribution-free methods for the analysis of covariance structures." *British Journal of Mathematical and Statistical Psychology* **37**, 62–83.

Dahm, P. F., and W. A. Fuller. (1985), "Generalized least squares estimation of the functional multivariate linear errors-in-variables model." *Journal of Multivariate Analysis.* To appear.

Fuller, W. A. (1975), "Regression analysis for sample survey." *Sankhya*, Series C **37**, 117–132.

Fuller, W. A. (1982), " Regression estimation of regression equations". Department of Statistics, Iowa State University, Ames Iowa.

Fuller, W. A., and S. G. Pantula (1982), "A computational algorithm for the factor model". Unpublished Report. Department of Statistics, Iowa State University, Ames, Iowa.

Fuller, W. A., S. G. Pantula, and Y. Amemiya (1985), "The covariance matrix of estimators for the factor model." *Journal of Multivariate Analysis.* To appear.

Holt, D., T. M. F. Smith, and P. D. Winter (1980), "Regression analysis of data from complex surveys." *Journal of the Royal Statistical Society*, Series A **143**, 474–487.

Jöreskog, K. G., and A. S. Goldberger (1972), "Factor analysis by generalized least squares." *Psychometrika* **37**, 243–260.

Skinner, C. J. (1981), "Estimation of the variance of a finite population for cluster samples." *Sankhya*, Series B **43**, 1–7.

Skinner, C. J. (1983), "Multivariate prediction from selected samples". *Biometrika* **70**, 289–292.

Vann, R., and F. Lorenz (1985), "Faculty evaluation of foreign student language errors". Unpublished manuscript. Department of English, Iowa State University, Ames, Iowa.

M. A. Hidiroglou and D. G. Paton [1]

SOME EXPERIENCES IN COMPUTING ESTIMATES AND THEIR VARIANCES USING DATA FROM COMPLEX SURVEY DESIGNS

ABSTRACT

Many large scale surveys have designs that are complex, incorporating stratification and perhaps more than one stage of selection. Data from these surveys are used for a considerable amount of analysis, involving the computation of statistics ranging from simple totals and means, to those required for the comparison of domains, linear and logistic regression analysis and contingency table analysis. These analyses are usually done using computer software which does not take the design into account. This paper focuses on the development and use of computer programs which take the design into account for such analyses.

1. INTRODUCTION

Many large scale sample surveys have designs that are complex, incorporating stratification and perhaps more than one stage of selection. These designs are favoured by survey taking organizations because they offer cost and operational advantages in their design and implementation. However, the analysis of data and particularly the calculation of variances from such surveys is considerably more difficult than from simple random samples. The major statistical computing packages such as SAS, BMDP and SPSS do not as yet include procedures that calculate variances from complex survey data, so the analyst is forced to use more specialized packages or to write specialized programs for the analysis of complex survey data.

The Canada Health Survey, conducted in 1978 and 1979, and the Labour Force Survey, an ongoing monthly survey, have similar complex designs, with stratification and several stages of selection. The data from these surveys have been used for a considerable amount of analysis, involving the computation of statistics ranging from simple totals and means to those required for the comparison of domains, linear and logistic regression analysis and

[1] Statistics Canada, Ottawa, Ontario K1A 0T6 (both authors)

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 285–308.

contingency table analysis. These analyses have involved the calculation of variances that account for the survey design using the methods developed by Kish and Frankel (1974), Fuller (1975), Binder (1983) and Rao and Scott (1984). Some of these analyses have been discussed by Binder *et al.* (1983) and Hidiroglou and Rao (1985); these papers highlight the effect of the survey design on the analysis.

Several methods for estimating sampling variances of statistics calculated from complex survey data have been developed. The four most generally accepted and frequently used techniques are independent replications, "Balanced Repeated Replication" (BRR), "jackknife" and Taylor series linearization. Our experience has been with the Taylor series method, using SUPER CARP (a specialized survey analysis package) and custom programs written in SAS which take advantage of its capabilities as a statistical programming language. In this paper we will discuss our approach and experiences in using these programs for post-stratification, ratio estimation, linear and logistic regression and contingency table analysis, and will include a general discussion of computational considerations and desirable features of a variance estimation program and statistical programming language.

2. VARIANCE COMPUTATION FOR COMPLEX SURVEY DESIGNS

A typical complex survey design involves stratification and several stages of selection, the selection at each stage usually being without replacement. The information collected from each responding unit will most likely be multivariate in nature. The simplest estimators derived from such a data set are totals and means. The resulting analysis can be complicated because statistical methods beyond the estimation of these simple descriptive parameters may be applied to the data set. These will include domain estimation and comparison, linear regression, logistic regression and contingency table analysis.

Notwithstanding the complexity of the analysis, an important aspect for inference is that an estimator of variance be associated with each estimator. The total is a simple linear function of the observations and it is possible to derive explicit algebraic expressions for estimating variances of such linear functions. It must be noted that for the type of complex design mentioned above, an estimator of variance for the total must take into account all stages of selection, requiring as well the computation of joint probabilities of selection for all sampled units throughout the stages. The general theory for the computation of these variances, taking into account each stage, has been provided by Des Raj (1966) and Rao (1975). A computer program specified by Bellhouse (1980) has been produced experimentally in order to

implement the rules given by Rao (1975). In large scale surveys, it is often assumed that the first stage clusters have been selected with replacement even though the actual selection scheme may have been without replacement. This assumption enables one to compute only the first stage variance (Des Raj, 1968, p. 210). This assumption will be the one that will be used throughout this paper.

For nonlinear functions of the vector of observations, the previously mentioned variance approximation methods are available. A brief description of these methods is provided next. The method of independent replication requires the drawing of several independent samples from the same population in order to obtain independent estimates of the same statistic $\hat{\theta}$, for example $\hat{\theta}_1, \hat{\theta}_2, \ldots, \hat{\theta}_M$.

The mean estimate is $\tilde{\theta} = \sum_{i=1}^{M} \hat{\theta}_i / M$ and an estimate of its variance is

$$v_r(\tilde{\theta}) = \sum_{i=1}^{M} (\hat{\theta}_i - \tilde{\theta})^2 / [M(M-1)].$$

In practice $\tilde{\theta} \neq \hat{\theta}$ and it is necessary to assume that $v_R(\hat{\theta}) = v_R(\tilde{\theta})$. This technique places several restrictions on the sample design, since each independent sample is much smaller than the "total sample" feasible. The number of replications will be small (2–8) and hence the estimate of variance will have few degrees of freedom and tend to be unstable.

The balanced half-sample replication method suggested by McCarthy (1966) is designed for surveys with exactly 2 primary sampling units per stratum in the sample. For a design with L strata, an orthogonal subset of half-samples amongst the possible 2^L half-samples is chosen, with each half of the sample selected by choosing randomly a primary sampling unit in each stratum. An estimate $\hat{\theta}_i$ is formed from each member of the orthogonal subset and the variance is computed as $v_B(\hat{\theta}) = \sum_{i=1}^{S} (\hat{\theta}_i - \hat{\theta})^2 / S$, where $L+1 \leq S \leq L+4$. This method places restrictions on the sample design as well.

The jackknife approach originally suggested by Quenouille (1956) and so named by Tukey (1958) is another sample reuse method applicable to with replacement sampling. It is computed as follows in the stratified context. Let θ be a non-linear parameter of interest and $\hat{\theta}$ be its estimator from the full sample. Let $\hat{\theta}_{(hi)}$ be the estimator of θ after omitting the ith unit within the hth stratum. Let $\hat{\theta}_{(h)} = \sum_{i=1}^{n_h} \hat{\theta}_{(hi)} / n_h$ (where n_h is the number of sampled primary sample units within the hth stratum). Then the jackknife variance estimator of $\hat{\theta}$ is $v_j(\hat{\theta}) = \sum_{h=1}^{L} \frac{n_h - 1}{n_h} \sum_{i=1}^{n_h} (\hat{\theta}_{(hi)} - \hat{\theta})^2$.

The linearization (Taylor) method expresses the statistic $\hat{\theta}$ as a function $g(\mathbf{y})$ of $\mathbf{y} = (Y_1, \ldots, Y_p)$ where Y_j is the total of a given variable in the

population. A consistent estimator of $g(\mathbf{y})$ is $g(\hat{\mathbf{y}})$ where $\hat{\mathbf{y}} = (\hat{Y}_1, \ldots, \hat{Y}_p)$ is the design estimator of $\mathbf{y}$. Now assuming that $\hat{Y}_j = \sum_{h=1}^{L} \sum_{i=1}^{n_h} w_{hi} y_{hij}$, we have that

$$\begin{aligned}
\mathrm{Var}[g(\hat{\mathbf{y}})] &= V\left[\sum_{j=1}^{p} \left(\hat{Y}_j - Y_j\right) g^{(j)}(\mathbf{y})\right] \\
&= V\left[\sum_{j=1}^{p} \hat{Y}_j g^{(j)}(\mathbf{y})\right] \\
&= \sum_{h=1}^{L} V\left[\sum_{i=1}^{n_h} w_{hi} z_{hi}\right],
\end{aligned}$$

where $z_{hi} = \sum_{j=1}^{p} y_{hij} g^{(j)}(\hat{\mathbf{y}})$ and $g^{(j)}(\hat{\mathbf{y}}) = \frac{\partial g(\mathbf{y})}{\partial \hat{Y}_j} \mid \hat{Y}_j = Y_j$.

A consistent estimator of $V[g(\hat{\mathbf{y}})]$ is $\sum_{h=1}^{L} v(\hat{z}_h)$ where $\hat{z}_h = \sum_{i=1}^{n_h} w_{hi} \hat{z}_{hi}$ and $\hat{z}_{hi} = \sum_{j=1}^{p} y_{hij} g^{(j)}(\hat{\mathbf{y}})$. This formulation of the Taylorized variance was given by Woodruff (1971). Computationally more efficient methods have been given by Fuller (1975) in the case of regression in finite sampling by appealing to the Central Limit Theorem and Binder (1983) for general functions of totals using implicit differentiation. The advantages of Taylorized deviations over the other methods is that it places no restrictions on the sample design, it is computationally not difficult, and it can be used for variance components. It requires the existence of the first $(2 + \delta)$ moments in order to apply the general central limit theorem. Computationally, only the linear combination given by $\hat{z}_{hi}$ need be calculated, and the usual variances for the algorithms of totals can then be applied for designs with several stages of selection.

Since all the methods involve approximations in the case of non-linear statistics, the biases as well as the precisions of the variances should be examined when comparing these methods in terms of their potential for estimating well the variances of interest. Their small sample properties have been investigated through empirical studies: see Frankel (1971), Hidiroglou (1974), Kish and Frankel (1974), Woodruff and Causey (1976), Bean (1975), and Mellor (1973). The findings of these studies indicated that all the methods yield good estimators of variance for several statistics: ratio and post-stratified means, regression coefficients, simple and partial correlation coefficients. Large sample properties given by Krewski and Rao (1981) yield similar conclusions. It also appears from these studies that the methods give reasonable results, with none being markedly superior to the others. The choice of method is dependent on flexibility of sample design, computing economy and availability of programs. The program developed by Woodruff and Causey (1976), which allows automatic computation of the

partial derivatives for the Taylor method, has encouraged the use of this method.

For the types of statistics that will be discussed here (ratio estimation, post-stratification, regression, logistic regression and contingency table analysis), SUPER CARP (1980) or extensions have been used to obtain variance estimates for all the aforementioned statistics except logistic regression. SAS programs have been developed by Paton to estimate variances for all previously mentioned statistics for stratified sample designs assuming that the primary sampling units had been selected with replacement. The SUPER CARP and SAS programs share the property that Taylor methods were used to compute the variances.

If we take the case of the ratio estimate given by

$$r = \sum_h \sum_i w_{hi} y_{hi} / \sum_h \sum_i w_{hi} x_{hi},$$

its Taylorized variance estimator is given by

$$v(r) = \sum_h \frac{n_h}{n_h - 1} \sum_i (z_{hi} - \bar{z}_h)^2,$$

where $z_{hi} = w_{hi}(y_{hi} - r x_{hi})$ and $\bar{z}_h = \sum_i z_{hi}/n_h$ for a stratified survey design with the primary sampling units selected with replacement. For this design, the number of required computations to estimate the variance of r is given in Table 1. From this table, for 2 p.s.u.'s per stratum, it can be observed that the replication methods require the fewest computations and the jackknife requires the most computations. The Taylor linearization method is intermediate in terms of number of computations. Comparisons of computer times, for variance estimation of domain totals, were carried out by Maurer *et al.* (1978). Their study, for this particular type of estimation, showed that either the B.R.R. or Taylorized variance estimation procedures could win in terms of computer time, the critical factor being the number of cells contained in each published table. With a higher number of cells within a table, the B.R.R. became more time efficient.

Large surveys such as the Labour Force or the Canada Health Survey are post-stratified to known population totals $({}_aN)$ according to age and sex $(a = 1, \ldots, A)$. This adjustment will greatly improve the efficiency of the estimates if the published variables of interest are highly correlated with age and sex. The variances of such adjusted estimates must properly take into account the post-stratification in order to reflect properly the estimation procedure. The Taylorized method is easy to compute and can be derived as a straight forward extension of the variance given for the ratio estimator. For example, the estimator of variance for the ratio of two post-stratified

Table 1. *Number of Required Computations for Different Variance Estimation Procedures (2 p.s.u.'s/stratum) for Combined Ratio Estimation*

Operation	Replication 1	Replication 2	Balanced Repeated Replication (B.R.R.)	Jackknife	Taylor Linearization
Variance	$\sum_{i=1}^{2}(\hat{r}_i - \tilde{r})^2/2$	$\sum_{h=1}^{L}\sum_{i=1}^{2}(\hat{r}_{hi} - \hat{r}_h)^2/2$	$\sum_{i=1}^{S}(\hat{\hat{r}}_i - \hat{r})^2/S$ $L+1 \le S \le L+4$	$\sum_{h=1}^{L}\sum_{i=1}^{2}(r_{(hi)} - \hat{r})^2/2$	$2\sum_{h=1}^{L}\sum_{i=1}^{2}(z_{hi} - \bar{z}_h)^2/\hat{X}^2$
	$\hat{r}_i = \frac{\sum_{h=1}^{L} w_{hi}y_{hi}}{\sum_{h=1}^{L} w_{hi}x_{hi}}$	$\hat{r}_{hi} = y_{hi}/x_{hi}$	$\hat{\hat{r}}$ obtained using B.R.R.	$\hat{r}_{(hi)}$ is like $\hat{r}$ omitting the ith unit/hth stratum	$z_{hi} = w_{hi}(y_{hi} - \hat{r}x_{hi})$
					$\bar{z}_h = \sum_{i=1}^{2} z_{hi}/2$
	$\tilde{r} = (\hat{r}_1 + \hat{r}_2)/2$	$\hat{r}_h = (\hat{r}_{h1} + \hat{r}_{h2})/2$	$\hat{r} = \frac{\sum_{h=1}^{L}\sum_{i=1}^{2} w_{hi}y_{hi}}{\sum_{h=1}^{L}\sum_{i=1}^{2} w_{hi}x_{hi}}$		
Addition	$4L+3$	$3L$	$4L + S(2L+1)$	$8L^2 + 2L$	$8L$
Subtraction	2	$2L$	S	$2L$	$4L$
Multiplication	$4L+2$	–	$2L + 2SL$	$8L^2$	$8L$
Division	3	$3L+1$	$S+2$	$2L+3$	$L+2$
Squaring	L	$2L$	S	$2L$	$2L+1$
Total	$8L+12$	$10L+1$	$(4L+4)S + 8L + 2$	$16L^2 + 8L + 3$	$23L+3$

estimators in the context of a stratified design (with the strata indexed by $h = 1, 2, \ldots, L$, with the p.s.u.'s $i = 1, \ldots, n_h$ in stratum h assumed to have been selected with replacement) can be obtained, using double application of the Taylor linearization method. Denoting the basic sampling weight as

$$w_{hik}(a = 1, \ldots, A;\ h = 1, \ldots, L;\ i = 1, \ldots, n_h;\ k = 1, \ldots, m_{hi}),$$

${}_a y_{hik} = y_{hik}\ {}_a 1_{hik}$, ${}_a x_{hik} = x_{hik}\ {}_a 1_{hik}$, where ${}_a 1_{hik}$ is an indicator variable equal to one if the hikth sampled unit belongs to the ath post-stratum and zero otherwise, the estimator for the population ratio is

$$r_{POST} = \hat{Y}_{POST} / \hat{X}_{POST},$$

where $\hat{Y}_{POST} = \sum_a [({}_a N / {}_a \hat{N})\ {}_a \hat{Y}]$, ${}_a \hat{Y} = \sum_h \sum_i \sum_k w_{hik}\ {}_a y_{hik}$, ${}_a \hat{N} = \sum_h \sum_i \sum_k w_{hik}\ {}_a 1_{hik}$, with ${}_a N$ being known counts for the ath post-stratum. The estimator of variance for r_{POST} is

$$v(r_{POST}) = \sum_h \frac{n_h}{n_h - 1} \sum_i (z_{hi} - \bar{z}_h)^2, \tag{2.1}$$

where

$$z_{hi} = \sum_k w_{hik} \frac{\left[(y_{hik} - r_{POST} x_{hik}) - \sum_a ({}_a \hat{Y} - r_{POST}\ {}_a \hat{X})\ {}_a 1_{hik} / {}_a \hat{N}\right]}{\hat{X}_{POST}}$$

and

$$\bar{z}_h = \sum_i z_{hi} / n_h.$$

The effect of using a post-stratified ratio estimator on the variance estimation has been a double application of the Taylorized method: the first application reflecting the ratio estimation and second application reflecting the post-stratification. Formula (2.1) is one which can be adapted for several types of estimation (linear regression, logistic regression, and log-linear models) by suitably modifying the "z_{hi}" term. This term, as it will be seen in the following section, can be made to reflect the type of estimation procedure as well as any post-stratification by using the Taylorized method.

3. GENERALIZED LINEAR MODELS

Nelder and Wedderburn (1972) described a class of models which they named the generalized linear models and showed that maximum likelihood

estimates for models in this class can be calculated using a general algorithm related to linear least squares regression. The class includes many of the most commonly used statistical models; linear regression, logistic regression, and log-linear models for categorical data are all examples of generalized linear models.

While these are superpopulation models and hence unacceptable to some survey analysts, we can view the maximum likelihood estimate that would be obtained if a census were taken to be a finite population parameter and concern ourselves with the estimation and sampling variability of this descriptive parameter. This strategy has been suggested by a number of authors, for instance Fuller (1975) and Binder (1983). Thus from the usual superpopulation model for linear regression:

$$y_i = \mathbf{x}_i'\boldsymbol{\beta} + e_i, \quad e_i \text{ are i.i.d. } N(0, \sigma^2)$$

with

$$\mathbf{X}_N = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)'$$
$$\mathbf{y}_N = (y_1, y_2, \ldots, y_N)'$$
(the $\mathbf{x}$ and y values for the population of size N)

we have $\mathbf{b} = (\mathbf{X}_N'\mathbf{X}_N)^{-1}\mathbf{X}_N'\mathbf{y}_N$ as the census based m.l.e. of $\boldsymbol{\beta}$ and now consider $\mathbf{b}$ as a finite population parameter.

Binder (1983) described a method of estimating variances for a class of finite population parameters that includes those that correspond to the generalized linear models. This method is based on Taylor linearization and has been used in the SAS programs we have developed for estimation and variance calculation for linear regression, logistic regression, and log-linear models.

Details of the theoretical background to the design based variance estimate have been given by Binder (1983), and more detail on generalized linear models has been given by Nelder and Wedderburn (1972).

Briefly, generalized linear models have density functions of the form:

$$p(y; \theta, \phi) = \exp[\alpha(\phi)\{y\theta - g(\theta) + h(y)\} + \gamma(\phi, y)],$$

where $\alpha(\phi) > 0$. Note that $E(Y) = g'(\theta) = \mu(\theta)$, and $V(Y) = \mu'(\theta)/\alpha(\phi)$ and $\theta = f(\mathbf{x}'\boldsymbol{\beta})$, where $f(\cdot)$ is a known differentiable function and $\boldsymbol{\beta}$ is unknown.

Then, based on observations $\{(y_i, \mathbf{x}_i'),\ i = 1, 2, \ldots, N\}$ the m.l.e. for $\boldsymbol{\beta}$ is the solution to the equation

$$\sum_{k=1}^{N} [y_k - \mu(f(\mathbf{x}_k'\boldsymbol{\beta}))]\, f'(\mathbf{x}_k'\boldsymbol{\beta})\, \mathbf{x}_k = \mathbf{0}.$$

For linear regression, logistic regression and log-linear models, $f(\mathbf{x}'\boldsymbol{\beta})$ is $\mathbf{x}'\boldsymbol{\beta}$ with μ defined as follows:

linear regression–	$\mu(\mathbf{x}_k'\boldsymbol{\beta}) = \mathbf{x}_k'\boldsymbol{\beta}$;
logistic regression–	$\mu(\mathbf{x}_k'\boldsymbol{\beta}) = \exp(\mathbf{x}_k'\boldsymbol{\beta})/[1+\exp(\mathbf{x}_k'\boldsymbol{\beta})]$;
log-linear model–	$\mu(\mathbf{x}_k'\boldsymbol{\beta}) = \exp(\mathbf{x}_k'\boldsymbol{\beta})$.

The finite population parameter of interest is thus the vector $\mathbf{b}$ that satisfies:

$$\mathbf{R}(\mathbf{b}) = \sum_{k=1}^{N} \mathbf{r}_k = \mathbf{0}, \tag{3.1}$$

where $\mathbf{r}_k = (y_k - \mu(f(\mathbf{x}_k'\mathbf{b})))\, f'(\mathbf{x}_k'\mathbf{b})\, \mathbf{x}_k$.

We estimate $\mathbf{b}$ by $\hat{\mathbf{b}}$, the solution to the equation

$$\hat{\mathbf{R}}(\hat{\mathbf{b}}) = \sum_{k=1}^{n} w_k \hat{\mathbf{r}}_k = \mathbf{0},$$

where the sum is over the n individuals in the sample and w_k is the sampling weight for individual k.

The estimate $\hat{\mathbf{b}}$ can be obtained by the Newton-Raphson method in a manner differing from that described by Nelder and Wedderburn (1972) only in the inclusion of the sampling weights. Hence each iteration in the solution can be viewed as a weighted least squares estimation, with dependent variable

$$y^* + \frac{[y - \mu(f(y^*))]}{\frac{d\mu(f(t))}{dt}\big|_{t=y^*}},$$

where $y^* = \mathbf{x}'\mathbf{b}^*$ ($\mathbf{b}^*$ is the current estimate of $\mathbf{b}$), and weight

$$w \frac{\left[\frac{d\mu(f(t))}{dt}\big|_{t=y^*}\right]^2}{\frac{d\mu(t)}{dt}\big|_{t=f(y^*)}} = w^*(\mathbf{x}'\mathbf{b}^*),$$

where w is the sampling weight.

The variance of $\hat{\mathbf{b}}$ is estimated by

$$\hat{\mathbf{V}}(\hat{\mathbf{b}}) = \hat{\mathbf{J}}^{-1}(\hat{\mathbf{b}})\hat{\boldsymbol{\Sigma}}(\hat{\mathbf{b}})\hat{\mathbf{J}}^{-1}(\hat{\mathbf{b}}),$$

where

$$\hat{\mathbf{J}}(\hat{\mathbf{b}}) = \mathbf{X}_n'\, \mathbf{D}\, \mathbf{X}_n$$

and $\mathbf{D} = \text{diag}(w^*(\mathbf{x}_1'\hat{\mathbf{b}}),\ w^*(\mathbf{x}_2'\hat{\mathbf{b}}), \ldots, w^*(\mathbf{x}_n'\hat{\mathbf{b}}))$. $\hat{\Sigma}(\hat{\mathbf{b}})$ is a consistent estimator of the covariance matrix of $\hat{\mathbf{R}}(\hat{\mathbf{b}})$ (see equation (3.1)).

A program for estimation and variance calculation can thus be constructed in three parts, the first of which estimates $\mathbf{b}$, $\mathbf{J}(\mathbf{b})$ and creates the $\mathbf{r_k}$ (or $w_k\mathbf{r}_k$) vectors and the third combines $\hat{\mathbf{J}}$ and $\hat{\Sigma}$ to give $\hat{\mathbf{V}}(\hat{\mathbf{b}})$. The second and third parts are the same for all generalized models so that, once a modular program has been written, only the first module needs to be changed to adapt to another model.

The linear regression model is the simplest of the generalized linear models and presents few problems when programming it in SAS. PROC REG can be used to perform a weighted regression and to output datasets containing the residuals, the parameter estimates and the sum of squares and cross products matrix. Three DATA steps are used in our program to extract these from the datasets output by PROC REG and to calculate $(y - \mathbf{x}'\hat{\mathbf{b}})\mathbf{x}'\mathbf{w}$ for each observation. This is the most convenient place to apply the sampling weight w.)

The second part of the program consists of a module that estimates the variance-covariance matrix for a vector of totals. Since $\hat{\mathbf{R}}(\hat{\mathbf{b}})$ is a vector of totals we obtain $\sigma(\hat{\mathbf{b}})$ by applying this module to the $(y - \mathbf{x}'\hat{\mathbf{b}})\mathbf{x}'\mathbf{w}$ vectors.

For the stratified, multistage surveys we have worked with, the formula for the variance of the estimated total for the vector of variables $\mathbf{z}$ is:

$$\hat{\mathbf{V}}(\mathbf{z}) = \sum_h \frac{n_h}{n_h - 1} \sum_i (\mathbf{z}_{hi} - \bar{\mathbf{z}}_h)(\mathbf{z}_{hi} - \bar{\mathbf{z}}_h)', \tag{3.2}$$

where $\mathbf{z}_{hi} = \sum_k w_{hik}\mathbf{z}_{hik}$ and $\bar{\mathbf{z}}_h = \frac{1}{n_h}\sum_i \mathbf{z}_{hi}$.

This formula is easily translated into a series of SAS procedures (PROC MEANS followed by PROC CORR followed by PROC MATRIX; details are presented in Appendix 1). It should perhaps be emphasized here that it is in this part of the program that the survey design must be taken into account. A different design, or a post-stratification adjustment to the weights would necessitate the use of a different variance formula (see, for example, equation 2.1) and hence a different series of SAS procedures. Since the estimation of a vector of totals is a common task during the tabulation and analysis of survey data this module is useful in other contexts.

The third part consists of a PROC MATRIX step which combines the results of the first two parts to yield the variance estimate of the parameter and to perform the hypothesis tests.

Programming these procedures in SAS is quite simple, highlighting the power of this package as a statistical programming language. We make use of the SAS macro language to simplify using the resulting program with new sets of variables or subsets of the data. ARRAY statements make it

easy to treat groups of variables as vectors in DATA steps. SAS has a few idiosyncrasies, the most striking one that affects this program being that the sum of squares and cross products matrix produced by PROC REG is not symmetric. This problem can be easily solved by rearranging the columns to make the matrix symmetric.

The program for logistic regression proved to be more difficult. We initially programmed the estimation phase in PROC MATRIX, but discovered that for the data sets and models we were using (10,000–20,000 observations and up to 25–30 variables), the estimation consumed large amounts of CPU time. By programming the estimation in PL/1, we reduced the amount of CPU time required at the cost of making the program more cumbersome to use. The PL/1 step passes the parameter estimates and the $\hat{\mathbf{J}}(\hat{\mathbf{b}})$ matrix to the SAS step, which then calculates the vectors $\{y_k - \exp(\mathbf{x}_k'\hat{\mathbf{b}})/[1+\exp(\mathbf{x}_k'\hat{\mathbf{b}})]\}\mathbf{x}_k' w_k$. The remainder part of the program is the same as that for the linear regression case.

4. LOG-LINEAR ANALYSIS OF CATEGORICAL DATA

Log-linear models are generalized linear models, but they are conceptually quite different from the linear and logistic models as the data consist of category counts of proportions (the categories often correspond to cells in a contingency table) rather than individual values for each respondent. The carrier or independent variables are a set of design variables that characterize the categories.

The method of computing the Wald statistic described by Binder (1983) and Rao and Scott (1984) presents a few problems but can be relatively easily implemented in SAS. Two key quantities are $\hat{\mathbf{n}}' = (\hat{n}_1, \hat{n}_2, \ldots, \hat{n}_q)$ and $\hat{\mathbf{V}}(\hat{\mathbf{n}})$, the vector of estimated category totals its variance-covariance matrix (q is the number of categories). These can be calculated using the same group of SAS procedures that was used in the second part of the linear and logistic regression programs to estimate the covariance matrix of a vector of totals. The appropriate vector at the respondent level is $\mathbf{d}' = (d_1, \ldots, d_q)$, with $d_i = 1$ if the respondent is in category "i" and $d_i = 0$ otherwise. It has proved useful to save $\hat{\mathbf{n}}$ and $\hat{\mathbf{V}}(\hat{\mathbf{n}})$ in a permanent dataset rather than to recompute them for each new model.

The estimation step and the matrix manipulations to calculate the estimated variances of the parameters are easily programmed in PROC MATRIX, but the real difficulty is in creating the design matrix and in labelling its columns in a meaningful way.

The solution we used was to generate the design matrix for the saturated model and then to delete the columns that do not correspond to the

null hypothesis. In this solution it is essential that the vector representation of the table be in the correct order. We represent the three-way table (n_{ijk}): $i = 1,2,\ldots,A_1$; $j = 1,2,\ldots,A_2$; $k = 1,2,\ldots,A_3$ as the vector $(n_{111}, n_{112}, \ldots, n_{11A_3}, n_{121}, \ldots, n_{A_1A_2A_3})$.

In the general case of a m-way table with dimensions $A_1, A_2, \ldots, A_m$, if $n_{i_1i_2\ldots i_m}$ is in category i_j of dimension j, $j = 1,2,\ldots,m$, then $n_{i_1i_2\ldots i_m} = n^*_\ell$, where $\mathbf{n}^*$ is the vector representation of the table $\mathbf{n}^* = (n^*_1, n^*_2, \ldots, n^*_{A_1A_2\ldots A_M})$ and $\ell = \sum_{j=1}^{m-1}(i_j - 1)\left\{\prod_{k=j+1}^{m} A_k\right\} + i_m$.

For the three-way table a saturated model design $\mathbf{X}$ matrix for representation can be easily constructed in PROC MATRIX of SAS as the Kronecker product:

$$\mathbf{X} = \mathbf{B}_1 \otimes \mathbf{B}_2 \otimes \mathbf{B}_3,$$

where

$$\mathbf{B}_i = \begin{bmatrix} \mathbf{1}_{A_i-1} & | & \mathbf{I}_{A_i-1} \\ --- & -- & ----- \\ 1 & | & -\mathbf{1}'_{A_i-1} \end{bmatrix},$$

$$\mathbf{1}_{A_i-1} = \text{ vector of ones of length } (A_i - 1),$$

and

$$\mathbf{I}_{A_i-1} = \text{ identity matrix of size } (A_i - 1) \text{ by } (A_i - 1).$$

A useful labelling of the columns of $\mathbf{X}$ can also be generated using the Kronecker product:

$$\mathbf{c} = \mathbf{c}_1 \otimes \mathbf{c}_2 \otimes \mathbf{c}_3$$

with

$$\mathbf{c}_i = (1 \mid p_i \cdot \mathbf{1}'_i), \qquad p_1 = 2, \quad p_3 = 3, \quad p_3 = 5.$$

Then each element of $\mathbf{c}$ is of the form $2^d3^e5^f$, with d, e, and f being 0 or 1. The intercept column corresponds to $d = e = f = 0$; the main effect columns for the second dimension correspond to $d = f = 0$, $e = 1$; the two way interactions between the first and third dimension effects correspond to columns where $d = e = 1$, and $f = 0$, etc. With the columns labelled in this way, it becomes relatively easy to select the groups of columns that correspond to the hypothesis of interest. This algorithm can easily be extended to higher dimension tables.

This approach tests hypotheses using Wald statistics, but we have used SAS to implement the statistics suggested by Rao and Scott (1981, 1984). The ease of writing the programs to perform this analysis were a striking demonstration of the power and convenience of the matrix manipulations available within PROC MATRIX. Marginal totals can be easily extracted

from the vector representation of the table using manipulation by matrices of the form (for the 3-way case):

$$\begin{array}{c} \\ A_1 \\ A_2 \\ A_3 \end{array} \begin{array}{c} \begin{array}{ccccc} A_1 & & A_2 & & A_3 \end{array} \\ \begin{pmatrix} \mathbf{1} & \otimes & \mathbf{1} & \otimes & \mathbf{I}_{A_1} \\ \mathbf{1} & \otimes & \mathbf{I}_{A_2} & \otimes & \mathbf{1} \\ \mathbf{I}_{A_3} & \otimes & \mathbf{1} & \otimes & \mathbf{1} \end{pmatrix} \end{array}.$$

These marginals and their covariance matrix form the basis for calculating $\hat{\delta}$. used as one of the corrections to the χ^2 statistic suggested by Rao and Scott (1981, 1984). The eigenvalues needed to make the Satterthwaite adjustment are easily calculated from the design based covariance matrix and the multinomial based one using the HALF, INV and EVAL functions. Complex matrix operations can generally be translated quickly and directly from the notation in a theoretical paper into a working algorithm in PROC MATRIX.

5. COMPUTATIONAL CONSIDERATIONS

Means, sums, variances and covariances are the basic ingredients that become parts of the required computations for the statistics described in Section 2. Notwithstanding the particular variance estimation procedure chosen to associate a measure of uncertainty with these statistics, the choice of algorithms for computing these statistics should take into account precision, speed and storage requirements. Beaton *et al.* (1976) have noted that a "concern about highly accurate computational methods must be tempered with a concern for whether the data are accurate enough to make the results meaningful". Although this concern is well taken, there is no reason not to use good computational techniques in any event. For the computations of sums of corrected cross-products (variances or covariances), one-pass or two-pass algorithms may be used. A one-pass algorithm updates the sum of corrected cross-products by using a recursive relationship between the current and previous sum. A two-pass algorithm requires the computations of means appearing in the cross-products in a separate pass. The one-pass algorithm is computationally more efficient in terms of time than the two-pass algorithm. The question between the choice of the algorithms is in terms of precision. Ling (1974) studied different variations of one-pass and two-pass algorithms. Ling's conclusion was that there was no universally best algorithm. The best algorithm for a given data set depends on the particular number composition of that data set. One of his recommendations was to use double precision arithmetic. For SUPER CARP, one-pass recursive algorithms programmed in double precision have been chosen to compute the

means and the sums of corrected cross-products.

Matrix inversion is required for regression and contingency table analysis. The choice for inversion algorithms is quite important in packages. Longley (1967) examined the accuracy of some inversion algorithms and found serious computational inaccuracies. He reported that the most accurate results were obtained by using the orthonormalization procedure. Kopitze *et al.* (1975) have recommended the use of the Cholesky decomposition as an inverting algorithm. They pointed out that as compared to the Gaussian elimination schemes, it does not require pivoting to stabilize symmetric positive definite matrices. This means less time for inverting. The Cholesky decomposition does not need much core storage and is easier to program than the Gaussian elimination scheme. One of its other advantages, as Wilkinson's (1975) analysis shows, is that it is quite accurate. Another of its advantages is that it can be readily put to use to find eigenvalues for systems of equations of the form $Ax = Bx$, where A is a positive matrix and B is a positive semi-definite matrix. Computations of eigenvalues are required to establish the stability of the inversion process. A condition number defined as the ratio of the maximum eigenvalue of a matrix to its minimum eigenvalue, will be the indicator of matrix inversion stability. In the case of the Wald statistic, which requires an inversion of the covariance matrix of the observed cross-classification cells, this condition number will be very high when there is a large number of cells. The condition number is therefore a good diagnostic to have at hand in order to indicate if the estimated regression parameters or Wald test are usable.

Data are either read from cards, tapes or input directly into the computer via terminals. These data are then stored on a disk drive awaiting further instructions. If the dataset is large, the number of different passes required to produce different statistics can become a critical factor in terms of time efficiency. The number of rewinds over the dataset must therefore be kept to a minimum by writing programs that can perform operations in as few passes as possible. For example, in the contingency table context, an $r \times s$ table defines rs different domains. If domain totals and their associated variances are required for such a table, rs passes over the data set is the extreme. If the program has been efficiently written, with the ability to handle multidimensional contingency tables, one pass over the data set would be sufficient to produce the required cross-tabular statistics. In the case of regression one pass would be sufficient to produce the largest required matrix and vector to compute the regression coefficients. If the best fit were to be found, backward elimination procedures could then operate on subsets of the computed matrix and vector, in order to obtain the regression coefficients for the reduced model. Iterative procedures for computing the associated variances for the regression coefficients would then have to be applied. In

the context of contingency table analysis, all the required marginal and cell probabilities as well as the associated design effects could be computed in one pass in order to allow the user to fit the best log-linear model. Users interested in linear contrasts of statistics must have the variances of these statistics as well as their covariances computed, in order to conduct valid tests of hypotheses. If such contrasts are not required, the computation of covariances will add significantly to computer time: for a p-dimensional vector, $p(p-1)/2$ covariances have to be computed.

6. EXAMPLES

In order to illustrate the analytical methods previously mentioned, three examples from the Canada Health Survey (1978–79) are presented.

Example 1: Regression

In Table 2 we present the results of three linear regressions using Canada Health Survey data. The dependent variable is a derived health status index (HEALTHRD) which takes on values between zero and one. The first of the regressions is an unweighted OLS; the second and third both use the sampling weights and so share the same estimates, but they differ in that the third uses the design in the estimation of variances.

While the estimates change from the unweighted to the weighted case, the most striking differences between the three regressions are found in the t statistics, with all nine variables deemed significant by the OLS analysis, only seven by the simple weighted analysis and only five by the design based analysis.

In general, the design based variances lead to a smaller t statistics, but this is not consistent, reflecting the variable-to-variable differences in design effects. It is clear, however, that inference based on the analysis which ignored the design would differ significantly from the design based inference.

Example 2: Logistic Regression

Similar results for logistic regression can be seen in Table 3. These are the results of a regression investigating the relationship between physician use in terms of income and age groupings. It is apparent that design based inference would be somewhat different from that which might be made if the design were ignored.

Example 3: Contingency Table Analysis

In Table 4, we give a 3×5 table from the Canada Health Survey, which cross-classifies smoking habits (Current, Past, Never) and diastolic blood

Table 2. *Estimates and t Statistics for Three Linear Regression Techniques Applied to the Same Data*

	Unweighted OLS		Weighted Least Squares		
	Estimate	"t"	Estimate	Weighted OLS "t"	Design Based "t"
INTERCEPT	.822	16.69	.883	17.50	14.34
REGION 5	.082	3.19	.114	4.27	3.59
RETIRED	.100	1.99	.138	2.20	3.96
LANGFR	−.041	2.30	−.030	1.73	1.36
WHTGH	.047	2.29	.041	1.96	1.41
LIFEEVNT	.040	2.51	.028	1.71	1.50
SMKLOT	.072	2.49	.094	3.13	2.86
NEGABS	−.030	7.77	−.037	9.31	7.86
MHEART	.041	2.24	.044	2.27	1.77

Dependent Variable: HEALTHRD (derived from activity limitation, chronic health problem, and health opinion variables).

Sample Size: 1186

Carrier Variables:

REGION 5 = 1 if respondent lives in B.C.
= 0 otherwise

RETIRED = 1 if major activity is retired
= 0 otherwise

LANGFR = 1 if language normally spoken is French
= 0 otherwise

WTHGH = 1 if more than 30% overweight
= 0 otherwise

LIFEEVNT = 1 if a major life event in the past year
= 0 otherwise

SMKLOT = 1 if smokes more than 20 cigarettes per day
= 0 otherwise

NEGABS = 1 negative affect balance score

MHEART = 1 if mother had a heart related problem
= 0 otherwise

Degrees of freedom for design based variance calculation: 22.

Table 3. *Unweighted and Design Based Logistic Regressions Compared*

	Unweighted OLS		Weighted Design Based Variances	
	Estimate	t	Estimate	t
INTERCEPT	.662	12.87	.712	12.35
QUINT 1	.031	.57	.155	2.10
QUINT 2	−.184	3.49	−.104	1.94
QUINT 3	−.102	1.94	−.052	.76
QUINT 4	−.072	1.39	.026	.40
QUINTUNK	−.406	5.59	−.426	3.34
AGE 2	.619	9.98	.613	5.80
AGE 3	.622	13.17	.517	10.97
AGE 4	.640	12.79	.570	8.80
AGE 5	1.082	16.02	1.040	10.55

Dependent Variable: PHYSUSE = 1 if visited a physician in the past 12 months

Sample Size: 20748

Carrier Variables:

QUINT 1 to QUINT 4 — 0–1 variables indicating family income quintile

QUINTUNK — = 1 if family income unknown; = 0 otherwise

AGE 2 — = 1 if $20 \leq$ age ≤ 24; = 0 otherwise

AGE 3 — = 1 if $25 \leq$ age ≤ 44; = 0 otherwise

AGE 4 — = 1 if $45 \leq$ age ≤ 64; = 0 otherwise

AGE 5 — = 1 if age ≥ 65; = 0 otherwise

Degrees of freedom for design based variance calculation: 45.

Table 4. *Diastolic Blood Pressure by Type of Cigarette Smoker (in thousands); Counts Adjusted by Age-Sex Distribution*

	Type of Smoker		
Blood Pressure	Current Cells 1–5	Past Cells 6–10	Never Cells 11–15
55–64	82[a] (9.6%)[b]	38 (10.0%)	47 (13.6%)
65–74	187 (5.5%)	107 (10.8%)	142 (6.6%)
75–84	208 (5.4%)	157 (11.6%)	182 (7.2%)
85–94	94 (9.0%)	83 (9.8%)	88 (6.4%)
95–104	36 (19.5%)	25 (17.7%)	29 (16.1%)

a – Counts, b – Coefficients of Variation %.

pressure (55–64, 65–74, 75–84, 85–94, 95–104). The sample size is $n = 4007$.

The statistics provided in Table 4 have been adjusted by known Age-Sex counts at the provincial level. This post-stratification adjustment has reduced the estimated coefficients of variation considerably. For example, for the current smokers group with diastolic pressure in the 55-64 range, the estimated coefficient of variation with no post-stratification adjustment is 13.6% as opposed to 9.6% with the post-stratification adjustment. Next, adjusted (for post-stratification) and unadjusted design effects are provided in the lexicographical order given in Table 4.

Adjusted design effects (Unadjusted)

2.19	(5.30)	1.12	(2.85)	2.41	(5.06)
1.92	(6.03)	3.99	(9.07)	1.78	(5.59)
2.03	(2.97)	5.53	(13.92)	2.36	(8.28)
2.38	(5.09)	1.98	(3.92)	1.11	(2.29)
3.72	(8.12)	2.07	(5.50)	2.10	(4.74)

As evidenced from the above design effects, post-stratification has also reduced the effect of the stratification and clustering inherent to the Canada Health Survey. The null hypothesis of interest is whether type of smoking is independent of diastolic blood pressure. The unadjusted for design chi-square test based on the usual Pearson statistic yields a value of 31 while for the corresponding Wald statistic, which takes the survey design and post-stratification into account, the value is 36. The Wald value is larger than the upper 5% point of χ^2_8 ($\chi^2_{8;0.05} = 15.5$) so that the null hypothesis is not tenable. The modifications to the Pearson statistic suggested by Fellegi (1980) which deflates it by the average of the design effects (2.45) yields a value of 12.65: this modification's estimated significance level is conservative

(0.02 for a nominal level of 0.05). The modification based on the mean of the eigenvalues (1.61) as suggested by Rao and Scott (1984) between the covariance matrix under the complex design and assuming multinominal sampling brings the Pearson value down to 19.2. The Satterthwaite approximation based on the eigenvalues as suggested by Rao and Scott (1984) brings the Pearson value down to 15.3 which is not significant at the 5% level. It must be noted that either the Wald or the Pearson would reject the null hypothesis. Standardized residuals (taking the design into account) provide an effective tool for isolating cells which depart from the null hypothesis of interest (in our case, independence). As can be noted from the residual plot given in Figure 1, there are relatively more current smokers with a diastolic blood pressure 55–64 and fewer current smokers with a diastolic blood pressure 85–94. Individuals who used to smoke (past) and who have never smoked (never) have diastolic blood pressure distributions which are quite similar.

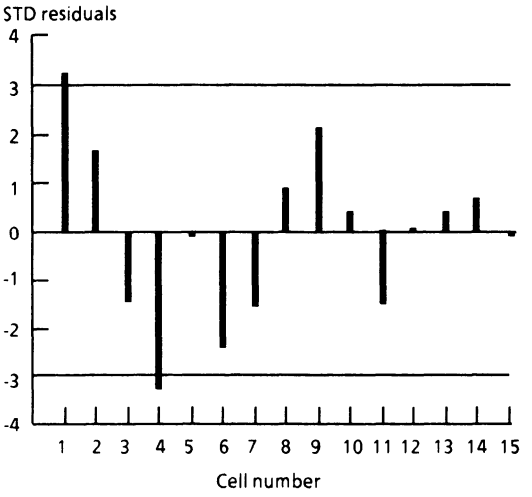

Figure 1. *Standardized residuals.*

7. CONCLUSION

The analysis of data collected via complex surveys is not a straightforward matter of using existing software packages such as SAS. There currently exists some software for this specialized analysis, including CPLX and SUPER CARP to name only two. These are basically stand-alone programs that perform their assigned tasks of estimation and variance computation, but lack the data management facilities of the comprehensive packages such as SAS or SPSS.

Ideally, an integrated software package for survey data analysis would contain the following features. It would be "user-friendly" in the sense that the control statements would allow English-like procedures and commands. It would contain powerful data management options such as data transformation, separation, combination, deletion and sorting. It should have the flexibility of creating data files containing the results of analyses, and allow the use of these for further analysis. A wide spectrum of survey designs should be acceptable (it should be able to handle more than one-stage stratified designs with sampling proportional to size). Its analytical and explanatory usefulness would be enhanced by plotting facilities.

Its procedural statements, statements linked to the particular type of analysis being performed, should be connectable to every part of the system. Additions to procedural statements should be easy for the specialists responsible for the development of the integrated software. The algorithms for computing the required statistics called by the procedural statements should be interconnectable, valid in terms of precision and efficiency. The resulting output should summarize key features of the survey design such as the number of observations, primary sampling units, stages and strata. The impact of survey design on the various resulting statistics could be measured in terms of design effect factors based on the design and the particular estimators.

APPENDIX 1

We translated equation (3.2) into SAS in the following way, assuming that the weights have already been applied to the data.

```
% LET NSTRATA = 44;
% LET NVAR =10;
PROC MEANS SUM NOPRINT
   DATA =
BY STRATUM CLUSTER;
  VAR X1 - X&NVAR;
OUTPUT OUT = TBYCLUST
     SUM = X1 - X&NVAR;
PROC CORR COV NOCORR NOPRINT
    DATA = TBYCLUST
    OUT = STRATCOV (TYPE = COV);
BY STRATUM;
VAR X1 - X&NVAR;
PROC MATRIX;
    POPCOV = J (&NVAR, &NVAR, 0);
    NPLUS3 = &NVAR + 3;
    DO I = 1 TO &NSTRATA;
      FETCH SCOV NPLUS3 DATA = STRATCOV;
      NCLUST = SCOV (NPLUS3, 2);
     POPCOV = POPCOV + SCOV (1: &NVAR, 2: &NVAR + 1)
        # NCLUST;
      END;
```

PROC MEANS calculates $\mathbf{X}_{hi} = \sum_k w_{hik}\mathbf{x}_{hik}$

PROC COV calculates $\mathbf{v}_h = \frac{1}{n_h}\sum_i (\mathbf{x}_{hi} - \bar{\mathbf{x}}_h)(\mathbf{x}_{hi} - \bar{\mathbf{x}}_h)'$

PROC MATRIX calculates $\sum_h n_h \mathbf{V}_h$

APPENDIX 2: DESCRIPTION OF THE CANADA HEALTH SURVEY

The Canada Health Survey, 1978–79 was a national household survey, conducted jointly by Statistics Canada and Health and Welfare Canada to provide information on the health status of Canadians. The Canada Health Survey may be described as a multi-stage stratified cluster sample design. For the purpose of variance estimation, it was assumed that the primary sampling units within strata were selected with replacement. There are a total of 44 strata and 100 primary sampling units. Each stratum contained 2, 3 or 4 primary sampling units.

The information collected was made up of two main components. The first, known as the Interview Component, used two types of questionnaires. The first questionnaire covered items which in general required probing by an interviewer and could be obtained for the entire household from a suitable member, such as questions relating to accidents or injuries, chronic conditions, hearing and disability days. The second questionnaire (the self administered questionnaire) was restricted to the population of persons 15 years of age or older. This questionnaire included queries on tobacco use, alcohol use and health related activities. The second component, known as the Physical Measures Component was also divided into two parts. The first part included physical masurements of blood pressure, cardiorespiratory fitness, height, weight, and skinfolds on persons aged two years and over. The second part involved taking of blood samples from persons three years and over in order to determine immune status as well as biochemical and trace metal levels.

REFERENCES

Bean, J. A. (1975), "Distributions and properties of variance estimators for complex multistage probability samples. An empirical distribution". *Vital and Health Statistics*, Series 2, No. 65, U.S. Department of Health, Education, and Welfare. Washington: U.S. Government Printing Office.

Beaton, A. E., D. B. Rubin, and J. L. Barone (1976), "The acceptability of regression solutions: another look at computational accuracy". *Journal of the American Statistical Association* **71**, 315–321.

Bellhouse, D. R. (1980), "Computation of variance-covariance estimates for general multi-stage designs". In *COMSTAT: Processing in Computation Statistics*, ed. M. M. Barritt and D. Wishart, pp. 57–63. Vienna: Physica-Verlag.

Binder, B. A., M. Gratton, M. A. Hidiroglou, and J. N. K. Rao (1983), "Analysis of categorical data from surveys with complex designs". Paper presented at the *Seminar on Recent Developments in the Analysis of Large Scale Data Sets*,

sponsored by the Statistical Offices of European Communities, Luxemburg.

Binder, B. A. (1983), "On the variances of asymptotically normal estimation from complex surveys". *International Statistical Review* **51**, 279–292.

Clogg, C. C. (1982), "Some models for the analysis of association in multiway cross-classifications having ordered categories". *Journal of the American Statistical Association* **77**, 803–815.

Fay, R. E. (1982), "Contingency tables for complex designs, CPLX". *Proceedings of the American Statistical Association, Section on Survey Research Methods*, pp. 44–53.

Fay, R. E. (1983), "CPLX — Contingency tables analysis for complex sample designs, program documentation". Unpublished report. U.S. Bureau of the Census, Washington.

Fay, R. E. (1985), "A jackknifed chi-square test for complex samples". *Journal of the American Statistical Association* **90**, 148–157.

Fellegi, I. P. (1980), "Approximate tests of independence and goodness of fit based on stratified multistage samples". *Journal of the American Statistical Association* **71**, 665–670.

Frankel, M. R. (1971). *Inference from Survey Samples*. Ann Harbor: Institute for Social Research, University of Michigan.

Fuller, W. A. (1975), "Regression analysis for sample surveys". *Sankhyā* **37**, 117–132.

Hidiroglou, M. A. (1974), "Estimation of regression parameters for finite populations". Ph.D. Thesis, Iowa State University.

Hidiroglou, M. A., W. A. Fuller, and R. D. Hickman (1980), "SUPER CARP", Survey Section, Iowa State University, Ames, Iowa.

Hidiroglou, M. A., and J. N. K. Rao (1985), "On chi-squared tests with categorical data from the Canada health survey". Statistics Canada report.

Jones, H. L. (1974), "Jackknife estimation of functions of stratum means". *Biometrika* **62**, 343–348.

Kish, L., and M. R. Frankel (1974), "Inference from complex samples". *Journal of the Royal Statistical Society*, Series B **36**, 1–37.

Kopitze, R., T. J. Boardman, and F. A. Graybill (1975), "Least square programs. A look at the square root procedure". *The American Statistician* **29**, 64–66.

Krewski, D., and J. N. K. Rao (1981), "Inference from stratified samples: properties of the linearization, jackknife and balanced repeated replication methods". *Annals of Statistics* **9**, 1010–1019.

Ling, R. G. (1974), "Comparison of several algorithms for computing sample means and variances". *Journal of the American Statistical Association* **69**, 859–866.

Longley, J. (1967), "An appraisal of least squares programs for the electronic computer from the point of view of the use". *Journal of the American Statistical Association* **62**, 819–841.

Maurer, K., G. Jones, and E. Bryant (1978), "Repeated computational efficiency of the linearized and balanced repeated replication procedures for computing sampling variances". *Proceedings of the American Statistical Association, Section on Survey Research Methods*, 388–391.

McCarthy, P. J. (1966), "Replication: An approach to the analysis of data from complex surveys". NCHS report, Series 2, No. 14, U.S. Dept. of Health, Education and Welfare.

Mellor, R. W. (1973), "Subsample replication variance estimators". Ph.D. Thesis, Harvard University.

Nelder, J. A., and R. W. M. Wedderburn (1972), "Generalized linear models". *Journal of the Royal Statistical Society*, Series A **135**, 370–384.

Quenouille, M. H. (1956), "Notes on bias estimation". *Biometrika* **43**, 353–360.

Raj, D. (1966), "Some remarks on a simple procedure of sampling without replacement". *Journal of the American Statistical Association* **61**, 393–397.

Raj, D. (1968), *Sampling Theory*. New York: McGraw-Hill.

Rao, J. N. K. (1975), "Unbiased variance estimation for multi-stage design". *Sankhya*, Series C **37**, 133–139.

Rao, J. N. K., and A. J. Scott (1984), "On chi-square tests for multiway contingency tables with cell proportions estimated from survey data". *Annals of Statistics* **12**, 46–60.

Shah, B. V. (1978), "SUDAAN: Survey data analysis software". *Proceedings of the American Statistical Association, Statistical Computation Section*, pp. 146–151.

The Health of Canadians (1981). *Report of the Canada Health Survey*, Health and Welfare and Statistics Canada Publication, Catalogue 82–538E.

Tukey, J. W. (1958), "Bias and confidence in not-quite large samples". *Annals of Mathematical Statistics* **29**, 614.

Wilkinson, J. H. (1975), *The Algebraic Eigenvalues Problem*. Oxford: Clarendon Press, 229–233.

Woodruff, R. W. (1971), "A simple method for approximating the variance of a complicated estimate". *Journal of the American Statistical Association* **6**, 411–414.

Woodruff, R. S., and B. D. Causey (1976), "Computerized method for approximating the variance of a complicated estimate". *Journal of the American Statistical Association* **71**, 315–321.

A. R. Sen [1] and P. K. Sen [2]

ESTIMATION OF THE CHARACTERISTICS OF RARE ANIMALS BASED ON INVERSE SAMPLING AT THE SECOND OCCASION

ABSTRACT

Theory has been developed to provide current estimates of the mean measurement (along with their sampling errors) on a characteristic of a rare animal in successive sampling using the (without replacement) inverse sampling method (at the second occasion) in the usual capture-mark-recapture situation. Relative efficiency results (with respect to other modes of sampling) are also studied in detail.

1. INTRODUCTION

In sampling on repeated occasions (with replacement of parts of the sample on each occasion), we consider a population of N units over a period of time, where N is large relative to the sizes of the samples to be drawn. A simple random sample (SRS) of size n_1 is selected and measured (e.g., weighed) on the first occasion. On the second occasion, m (m for *matched*) of the units in the first occasion are retained and measured on the second occasion; also a new selection of u ($= n-m$, u for unmatched) units is made on the second occasion. Assume a positive correlation between measurements on the two occasions.

However, in sampling for moving populations which are rare, inverse sampling using capture-mark-recapture (CMR) is employed in which a sample (of size n_1) is selected on the first occasion; these are marked, measured and released. The members in the sample are then allowed to mix and on the

[1] Department of Mathematics and Statistics, The University of Calgary, Calgary, Alberta T2N 1N4

[2] Department of Biostatistics, School of Public Health, The University of North Carolina at Chapel Hill, Chapel Hill, North Carolina 27514

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 309–322.

next occasion, the second sample (of size n) is continued without replacement (WOR) till a prescribed number of marked animals ($m < n_1$) have been recovered; we assume that the population is closed. In this setup, generally, m is fixed and n ($\geq m$) is a positive integer valued random variable (r.v.). This method provides an unbiased estimator of N with an exact expression of its sampling variance and a coefficient of variation (CV) which is almost independent of N. Hence, instead of taking a given number of marked animals in the sample, an alternative scheme is to continue the second sample until N is estimated with a given CV. Amongst humans, considerations of cost and of patients' welfare may dictate the use of such a sampling procedure. At the second stage, measurements are made on the m marked animals as well as on the u ($= n - m$) extra (unmarked) animals selected to provide the m marked ones. It is shown that the information contained in the measurements on both the occasions for the marked units when incorporated in the estimation scheme leads to a better estimator (than based on the n observations alone at the second stage).

To avoid assumption of constant probability of capture, which may not generally hold in practice, a less common situation has been considered in which members of the second sample are caught one at a time, marked, measured and returned immediately to the population, and sampling is continued until a prescribed number of previously marked units appear. Theory has also been developed for this inverse sampling scheme in which the second sample is selected with replacement (WR). The efficiency of this CMR method is compared with (i) SRS, with and without replacement, ignoring selection by CMR, and (ii) using CMR without replacement of the second sample units.

It is shown that inverse sampling with replacement is more efficient than sampling with replacement ignoring CMR, but its efficiency with respect to sampling without replacement (SRS) would depend on the relative sizes of the first and second samples and on the correlation in the measurements on the occasions. Also, inverse sampling with CMR in which the second sample is SRS is more efficient than inverse sampling in which the second sample is selected with replacement. The results have been illustrated with numerical examples in different situations.

2. THE PROPOSED ESTIMATORS: THEORY

Let N be the size of the unknown population (assumed to be the same on both the occasions), and let $Y_1^{(j)}, \ldots, Y_N^{(j)}$ be the population values at the jth occasion, for $j = 1, 2$. For the first sample of size n_1, let $y_{11}, \ldots, y_{1n_1}$ be the realizations (recorded); these units are all marked and released. Finally,

let n be the second sample size (SRS) containing exactly m marked units, where m is a non-random positive integer.

In this setup, n is a random variable and its probability law is given by the negative hypergeometric distribution:

$$p_{N,n_1}(n \mid m) = \binom{n_1}{m-1}\binom{N-n_1}{n-m}(n-m+1)\Big/\left\{\binom{N}{n-1}(N-n+1)\right\}$$
$$= m\binom{n_1}{m}\binom{N-n_1}{n-m}\Big/\left\{\binom{N}{n}\right\},$$
$$\text{for } n = m, m+1, \ldots, N-n_1+m. \tag{1}$$

For the m matched units in the second sample, we denote the sample values on the first occasion by $y_1^{(1)}, \ldots y_m^{(1)}$ and on the second occasion by $y_1^{(2)}, \ldots, y_m^{(2)}$, respectively, so that we have actually m pairs $(y_i^{(1)}, y_i^{(2)})$, $i = 1, \ldots, m$, of observations for these matched units. In the second sample, for the unmatched u $(= n - m)$ units, the sample observations are denoted by $y_{m+1}^{(2)}, \ldots, y_n^{(2)}$. Though not all are observed on the second occasion, for the first sample n_1 units, we denote the pair of values on the two occasions by $(y_{11}, y_{21}), \ldots, (y_{1n_1}, y_{2n_1})$. Then let

$$\bar{y}_{jm} = m^{-1}\sum_{i=1}^{m} y_i^{(j)},$$
$$\bar{y}'_{jn_1} = n_1^{-1}\sum_{i=1}^{n_1} y_{ji}$$

and

$$\bar{Y}^{(j)} = N^{-1}\sum_{i=1}^{N} Y_i^{(j)}, \qquad j = 1, 2. \tag{2}$$

For the $N - n_1$ units in the population not drawn in the first sample, we denote the mean value of the characteristic (at the second occasion) by $\bar{y}''_{2n_1}$, so that $\bar{y}''_{2n_1} = \left(N\bar{Y}^{(2)} - n_1\bar{y}'_{2n_1}\right)/(N - n_1)$; note that $\bar{y}'_{1n_1}$, $\bar{y}'_{2n_1}$ and $\bar{y}''_{2n_1}$ are all random variables. Also, let

$$s_{jj'}^{(m)} = m^{-1}\sum_{i=1}^{m} y_i^{(j)} y_i^{(j')} - \bar{y}_{jm}\bar{y}_{j'm}, \quad j, j' = 1, 2; \quad b_m = s_{12}^{(m)}/s_{11}^{(m)}, \tag{3}$$

$$s_{jj'}^{(n_1)} = n_1^{-1}\sum_{i=1}^{n_1} y_{ji} y_{j'i} - \bar{y}_{jn_1}\bar{y}_{j'n_1}, \quad j, j' = 1, 2; \quad b_{n_1}^{*} = s_{12}^{(n_1)}/s_{11}^{(n_1)}, \tag{4}$$

$$S_{jj'} = N^{-1}\sum_{i=1}^{N} Y_i^{(j)}Y_i^{(j')} - \overline{Y}^{(j)}\overline{Y}^{(j')}, \quad j,j' = 1,2; \quad B^* = S_{12}/S_{11}, \tag{5}$$

$$s_{22}^* = (N-n_1)^{-1}\sum_{i>n_1}\left(y_{2i} - \overline{y}''_{2n_1}\right)^2, \tag{6}$$

and

$$\overline{y}_{2u} = u^{-1}\sum_{i=m+1}^{m+u} y_i^{(2)}, \qquad \text{for } u \geq 1. \tag{7}$$

Consider then the two estimators of $\overline{Y}^{(2)}$ (derived from the matched and unmatched parts of the second sample, respectively):

$$Z_1 = \overline{y}_{2m} - b_m\left(\overline{y}_{1m} - \overline{y}'_{1n_1}\right), \tag{8}$$

$$Z_2 = \begin{cases} 0, & \text{if } n = m, \\ \overline{y}_{2u}, & \text{if } n = m+u, \quad u \geq 1. \end{cases} \tag{9}$$

Now, disregarding CMR, one may estimate $\overline{Y}^{(2)}$ by $\overline{y}_n^{(2)} = n^{-1}\sum_{i=1}^{n} y_i^{(2)}$ (where we need to keep in mind that in this inverse sampling scheme n is random and the measurements on the y_{1i} and $y_i^{(1)}$ are not taken into account). Our primary goal is to consider an improved estimator which incorporates this additional information. Toward this, we denote $\tilde{E}$ and $\tilde{V}$ and (and $\widetilde{\mathrm{Cov}}$), the mean, variance (and covariance), conditional on the $y_{11},\ldots,y_{1n_1}$ (in the first sample). Also, we may rewrite (8) as

$$Z_1 = \overline{y}_{2m} - b^*_{n_1}\left(\overline{y}_{1m} - \overline{y}'_{1n_1}\right) + \left(b^*_{n_1} - b_m\right)\left(\overline{y}_{1m} - \overline{y}'_{1n_1}\right) \tag{10}$$

and note that, as m increases,

$$|\, b^*_{n_1} - b_m \,| = O_p(m^{-1/2}) \qquad \text{and} \qquad |\, \overline{y}_{1m} - \overline{y}'_{1n_1} \,| = O_p(m^{-1/2}). \tag{11}$$

Consequently, the last term on the right hand side of (10) is $O_p(m^{-1})$. Hence,

$$\tilde{E}(Z_1) = \overline{y}'_{2n_1} - 0 + O_p(m^{-1}) = \overline{y}'_{2n_1} + O_p(m^{-1}) \tag{12}$$

$$\tilde{V}(Z_1) = \left\{ s_{22}^{(n_1)} - \left(s_{12}^{(n_1)}\right)^2 \right\}\{(n_1-m)/m(n_1-1)\} + O_p(m^{-2}), \tag{13}$$

and, similarly,

$$\begin{aligned}\tilde{E}(Z_2) &= \tilde{E}\left[\tilde{E}(Z_2 \mid n)\right] \\ &= 0 \cdot p_{N,n_1}(m \mid m) + \sum_{u \geq 1} \overline{y}''_{2n_1} p_{N,n_1}(m+u \mid m) \\ &= \overline{y}''_{2n_1}\left\{1 - p_{N,n_1}(m \mid m)\right\} \\ &= \overline{y}''_{2n_1}\left\{1 - \binom{n_1}{m} \Big/ \binom{N}{m}\right\}, \end{aligned} \tag{14}$$

$$\begin{aligned}\tilde{V}(Z_2) &= \tilde{E}\left[\tilde{V}(Z_2 \mid n)\right] + \tilde{E}\left[\tilde{E}(Z_2 \mid n) - \tilde{E}(Z_2)\right]^2 \\ &= s^*_{22} \sum_{u \geq 1} \left[(N - n_1 - u)/u\,(N - n_1 - 1)\right] p_{N,n_1}(m+u \mid m) \\ &\quad + \left(\overline{y}''_{2n_1}\right)^2 p_{N,n_1}(m \mid m)\left[1 - p_{N,n_1}(m \mid m)\right], \end{aligned} \tag{15}$$

$$\begin{aligned}\widetilde{\mathrm{Cov}}(Z_1, Z_2) &= \tilde{E}[\widetilde{\mathrm{Cov}}(Z_1, Z_2 \mid n)] \\ &\quad + \tilde{E}\{[\tilde{E}(Z_1 \mid n) - \tilde{E}(Z_1)][\tilde{E}(Z_2) \mid n) - \tilde{E}(Z_2)\} \\ &= 0 + O_p\left(m^{-1} p_{N,n_1}(m \mid m)\right). \end{aligned} \tag{16}$$

At this stage, we let

$$n_1 = \alpha N, \quad m = \beta n_1 = \alpha\beta N \quad \text{where} \quad 0 < \alpha < 1 \quad \text{and} \quad 0 < \beta < 1. \tag{17}$$

Then, by using the Stirling approximation for factorials, we have

$$\begin{aligned} p_{N,n_1}(m \mid m) &= \{(1 - \alpha\beta)/(1 - \beta)\}^{1/2} \\ &\quad \cdot \left[\alpha^{\alpha\beta}(1 - \alpha\beta)^{1-\alpha\beta}/(1 - \beta)^{\alpha(1-\beta)}\right]^N \left\{1 + O(N^{-3})\right\} \end{aligned}$$

which converges to zero at an exponential rate as N increases. Hence, we may set

$$p_{N,n_1}(m \mid m) = O(N^{-3}). \tag{18}$$

From the above formulae, we obtain that

$$\begin{aligned} E(Z_1) &= E[\tilde{E}(Z_1)] = \overline{Y}^{(2)} + O(N^{-2}), \\ E(Z_2) &= E[\tilde{E}(Z_2)] = \overline{Y}^{(2)} + O(N^{-2}), \end{aligned} \tag{19}$$

and

$$\begin{aligned} V(Z_1) &= E[\tilde{V}(Z_1)] + E[\tilde{E}(Z_1) - E(Z_1)]^2 \\ &= \{(n_1 - m)/[m(n_1 - 1)]\}\, E\left\{ s_{22}^{(n_1)} - \left(s_{12}^{(n_1)}\right)^2 / s_{11}^{(n_1)} \right\} \\ &\quad + E\left(\bar{y}'_{2n_1} - \bar{Y}^{(2)}\right)^2 + O(N^{-2}) \\ &= S_{22}\left\{(1-\rho^2)(n_1 - m)/[m(n_1 - 1)] + (N - n_1)/[n_1(N-1)]\right\} \\ &\quad + O(N^{-2}), \end{aligned} \tag{20}$$

where $\rho^2 = S_{12}^2/(S_{11}S_{22})$; we use the results on functions of U-statistics in finite population sampling (Nandi and Sen, 1963) after noting that the $s_{ij}^{(n_1)}$ are all U-statistics and the first sample is drawn in a SRS scheme. In a similar manner, we obtain that

$$\begin{aligned} V(Z_2) &= E[\tilde{V}(Z_2)] + E[\tilde{E}(Z_2) - E(Z_2)]^2 \\ &= S_{22}\Bigg\{ \sum_{u \geq 1} \{(N - n_1 - 1)/[u(N - n_1 - 1)]\}\, p_{N,n_1}(m + u \mid m) \\ &\quad + \{n_1/[(N - n_1)(N-1)]\} \Bigg\} + O(N^{-2}), \end{aligned} \tag{21}$$

$$\begin{aligned} \mathrm{Cov}(Z_1, Z_2) &= E\left[\widetilde{\mathrm{Cov}}(Z_1, Z_2)\right] + E\left\{\left[\tilde{E}(Z_1) - E(Z_1)\right]\left[\tilde{E}(Z_2) - E(Z_2)\right]\right\} \\ &= E\left\{\left(\bar{y}'_{2n_1} - \bar{y}^{(2)}\right)\left(\bar{y}''_{2n_2} - \bar{Y}^{(2)}\right)\right\} + O(N^{-2}) \\ &= -n_1(N - n_1)^{-1} E\left(\bar{y}'_{2n_1} - \bar{Y}^{(2)}\right)^2 + O(N^{-2}) \\ &= -(N-1)^{-1} S_{22} + O(N^{-2}). \end{aligned} \tag{22}$$

Thus, for large N and given α, β, we have

$$E\left\{N^{1/2}\left(Z_1 - \bar{Y}^{(2)},\ Z_2 - \bar{Y}^{(2)}\right)\right\} = \mathbf{O}(N^{-1/2}) \to \mathbf{0} \tag{23}$$

and

$$\begin{aligned} &NE\left[\left(Z_1 - \bar{Y}^{(2)},\ Z_2\bar{Y}^{(2)}\right)'\left(Z_1 - \bar{Y}^{(2)},\ Z_2 - \bar{Y}^{(22)}\right)\right] \\ &\quad \to \mathbf{A}S_{22};\ \ \mathbf{A} = ((a_{ij})), \end{aligned} \tag{24}$$

where

$$a_{11} = (1-\beta)(1-\rho^2)/[\alpha\beta] + (1-\alpha)/\alpha, \qquad a_{12} = a_{21} = -1,$$
$$a_{22} = \alpha/(1-\alpha) + (1-\beta)/[\beta(1-\alpha)] = 1/[\beta(1-\alpha)] - 1. \tag{25}$$

Note that β, m and n_1 are given, but α and N are unknown quantities. However, in this context, the CMR technique (in an inverse sampling setup) provides an estimator of N (Chapman, 1952):

$$\hat{N} = \{n(n_1+1)/m\} - 1, \tag{26}$$

so that an estimator of α is given by $\hat{\alpha} = n_1/\hat{N}$. Let then $\hat{A} = ((\hat{a}_{ij}))$ be defined by

$$\hat{a}_{11} = (1-\beta)\left(1-\hat{\rho}_m^2\right)/[\hat{\alpha}\beta] + \hat{\alpha}^{-1} - 1$$
$$\hat{a}_{12} = \hat{a}_{21} = -1,$$
$$\hat{a}_{22} = \{\beta(1-\hat{\alpha})\}^{-1} - 1, \tag{27}$$

where

$$\hat{\rho}_m^2 = (s_{12}^{(m)})^2/(s_{11}^{(m)} s_{22}^{(m)}). \tag{28}$$

Now, using a variant form of the *weighted least squares method,* wherein we employ the estimated covariance matrix instead of the actual one (Rao, 1966), we may propose the following (combined) estimator of $\overline{Y}^{(2)}$:

$$\hat{\overline{Y}}^{(2)} = \{(\hat{a}_{22} - \hat{a}_{21})\, Z_1 + (\hat{a}_{11} - \hat{a}_{12})\, Z_2\} \,/\, (\hat{a}_{11} + \hat{a}_{22} - 2\hat{a}_{12})$$

$$= \frac{Z_1/[\beta(1-\hat{\alpha})] + [(1-\beta)(1-\hat{\rho}_m^2) + \beta] Z_2/[\hat{\alpha}\beta]}{1/[\beta(1-\hat{\alpha})] + [(1-\beta)(1-\hat{\rho}_m^2) + \beta]/[\hat{\alpha}\beta]}$$

$$= \frac{\hat{\alpha} Z_1 + (1-\hat{\alpha})\left[(1-\beta)(1-\hat{\rho}_m^2) + \beta\right] Z_2}{\hat{\alpha} + (1-\hat{\alpha})\left[(1-\beta)(1-\hat{\rho}_m^2) + \beta\right]}$$

$$= \frac{Z_1\hat{\alpha} + (1-\hat{\alpha})\left\{1 - \hat{\rho}_m^2(1-\beta)\right\} Z_2}{1 - (1-\hat{\alpha})(1-\beta)\hat{\rho}_m^2}. \tag{29}$$

An alternative estimator of $\overline{Y}^{(2)}$ ignoring CMR (but adapted to the inverse sampling scheme) is given by

$$\tilde{\overline{Y}}^{(2)} = n^{-1} \sum_{i=1}^{n} y_i^{(2)} \qquad \text{(where } n \text{ is itself a r.v.).} \tag{30}$$

Whereas in (29), the repeated measurements on the matched part of the second sample provides additional information, in (30), this being ignored, we expect (at least intuitively) some loss of efficiency, and we shall study this in the next section.

3. SAMPLING VARIANCES AND RELATIVE EFFICIENCY RESULTS

We intend to study the large sample expressions for the sampling variance of the proposed estimators in (29) and (30). Towards this, we write $U_j = N^{1/2}(Z_j - \overline{Y}^{(2)})$, $j = 1,2$, where the Z_j are defined by (8) and (9). Then, we have

$$N^{1/2}(\hat{\overline{Y}}^{(2)} - \overline{Y}^{(2)}) = \frac{\hat{\alpha}U_1 + (1-\hat{\alpha})\left(1 - \hat{\rho}_m^2(1-\beta)\right)U_2}{1-(1-\hat{\alpha})(1-\beta)\hat{\rho}_m^2}. \tag{31}$$

Side by side, we let

$$\check{\overline{Y}}^{2} = \left\{\alpha Z_1 + (1-\alpha)\left(1-\rho^2(1-\beta)\right)Z_2\right\} / \left\{1-(1-\alpha)(1-\beta)\rho^2\right\}, \tag{32}$$

so that

$$N^{1/2}(\check{\overline{Y}}^{(2)} - \overline{Y}^{(2)}) = \frac{\alpha U_1 + (1-\alpha)\left(1-\rho^2(1-\beta)\right)U_2}{1-(1-\alpha)(1-\beta)\rho^2}. \tag{33}$$

Since (U_1, U_2) has a non-degenerate distribution (as N increases), while $\hat{\alpha} \to \alpha$ and $\hat{\rho}_m \to \rho$, in probability, as m increases, we may appeal to the Slutzky Theorem (Cramér, 1946, p. 254), and conclude that the large sample distributions of $N^{1/2}(\hat{\overline{Y}}^{(2)} - \overline{Y}^{(2)})$ and $N^{1/2}(\check{\overline{Y}}^{(2)} - \overline{Y}^{(2)})$ are the same. On the other hand, for the right hand side of (33), we may use (20), (21) and (22), and conclude that

$$\begin{aligned}
&V(N^{1/2}(\check{\overline{Y}}^{(2)} - \overline{Y}^{(2)})) \\
&= S_{22}\frac{\{a_{11}(a_{22}-a_{12})^2 + a_{22}(a_{11}-a_{12})^2 + 2a_{12}(a_{11}-a_{12})(a_{22}-a_{12})\}}{(a_{11}+a_{22}-2a_{12})^2} \\
&= S_{22}\left\{\left(a_{11}a_{22} - a_{12}^2\right) / (a_{11}+a_{22}-2a_{12})\right\} \\
&= S_{22}\beta^{-1}(1-\beta)\left[1-\rho^2\left(1-\beta(1-\alpha)\right)\right] / \left[1-(1-\alpha)(1-\beta)\rho^2\right].
\end{aligned} \tag{34}$$

Hence, the *asymptotic variance* of $N^{1/2}(\hat{\overline{Y}}^{(2)} - \overline{Y}^{(2)})$ may be taken as

$$\left\{\beta^{-1}(1-\beta)\left[1-\rho^2\left(1-\beta(1-\alpha)\right)\right] / \left[1-(1-\alpha)(1-\beta)\rho^2\right]\right\} S_{22}. \tag{35}$$

For the computation of the asymptotic variance of the estimator in (30), in view of the fact that n is itself a random variable, additional considerations are necessary. In this context, we note that

$$E(n) \sim N[\beta(1-\alpha)+\alpha\beta] = N\beta = n^* \quad \text{(say)}, \tag{36}$$

and the probability law in (1) may be used to verify easily that

$$n/n^* \to 1, \quad \text{in probability, as } m \text{ increases.} \tag{37}$$

Given (37), the large sample distribution of $N^{1/2}(\tilde{\bar{Y}}^{(2)} - \bar{Y}^{(2)})$ may be approximated by that of a similar statistic computed for the sample size n^* (which is non-stochastic), provided the classical Anscombe (1952) condition of uniform continuity in probability is verified. Verification of this Anscombe condition for finite population sampling can easily be made by an appeal to Theorem 3.3.3 of Sen (1981), so that the asymptotic variance of $N^{1/2}(\tilde{\bar{Y}}^{(2)} - \bar{Y}^{(2)})$ is given by

$$S_{22}\{(N-n^*)N/[n^*(N-1)]\} \sim S_{22}\beta^{-1}(1-\beta). \tag{38}$$

Comparing (35) and (38), we conclude that the *asymptotic relative efficiency* (ARE) of the proposed estimator $\hat{\bar{Y}}^{(2)}$ with respect to $\tilde{\bar{Y}}^{(2)}$ is given by

$$\begin{aligned}
&\{1-\rho^2(1-\alpha-\beta+\alpha\beta)\}/\{1-\rho^2(1-\beta+\alpha\beta)\} \\
&= \{1-\rho^2(1-\beta+\alpha\beta)+\alpha\rho^2\}/\{1-\rho^2(1-\beta+\alpha\beta)\} \\
&= 1+\alpha\rho^2/\{1-\rho^2(1-\beta+\alpha\beta)\} \\
&\geq 1, \quad \text{for all} \quad \alpha>0, \quad \beta>0 \quad \text{and} \quad \rho^2 \geq 0,
\end{aligned} \tag{39}$$

and the strict equality sign holds when $\rho = 0$; note that α and β are both positive. It may be noted that for small β (close to 0), the penultimate expression in (39) reduces to

$$1+\alpha\rho^2(1-\rho^2)^{-1}, \tag{40}$$

and this is also an upper bound (over $\beta > 0$). There is considerable gain in efficiency with increasing α and ρ^2, though the gain is negligible for small values of α or ρ^2. For given α and ρ^2, the gain in efficiency is a decreasing function of β $(0 < \beta < 1)$. For some numerical values, we may refer to Table 1. Consider next the inverse sampling scheme in which (at the second occasion) sampling (with replacement) is continued until a prescribed number (m) of marked animals have been captured (marked and released). Using

the same notation as for the negative hypergeometric model, the probability law for n (the second sample size) is given by the negative binomial law:

$$p'_{N,n_1}(n \mid m) = \binom{n-1}{m-1}(n_1/N)^m(1-n_1/N)^{n-m}, \quad n = m, m+1, \ldots \tag{41}$$

Parallel to (35), for this negative binomial model, the asymptotic variance of $N^{1/2}(\hat{\overline{Y}}_*^{(2)} - \overline{Y}^{(2)})$ (where $\hat{\overline{Y}}_*^{(2)}$ is analogous to (29) but for the with replacement model) is

$$S_{22}\frac{\beta^{-1}(1-\beta)\left[(1+\beta)-\rho^2(1+\alpha\beta)\right]}{(1-\beta^2)-\rho^2(1-\alpha-\beta+\alpha\beta)}. \tag{42}$$

Comparing (35) and (42), the ARE of $\hat{\overline{Y}}^{(2)}$ with respect to $\hat{\overline{Y}}_*^{(2)}$ is obtained as

$$\left\{\frac{(1+\beta)-\rho^2(1+\alpha\beta)}{(1-\beta^2)-\rho^2(1-\alpha)(1-\beta)}\right\}\left\{\frac{1-\rho^2(1-\alpha)(1-\beta)}{1-\rho^2(1-\beta+\alpha\beta)}\right\}$$
$$=\left\{\frac{1-\rho^2(1-\alpha-\beta+\alpha\beta)}{(1-\beta^2)-\rho^2(1-\alpha-\beta+\alpha\beta)}\right\}\left\{\frac{(1+\beta)-\rho^2(1+\alpha\beta)}{1-\rho^2(1-\beta+\alpha\beta)}\right\}. \tag{43}$$

Since $\beta \in (0,1)$, the first factor on the right hand side of (43) is greater than 1 for every $\beta > 0$. Also, note that $(1+\beta)-\rho^2(1+\alpha\beta)-1+\rho^2(1+\alpha\beta-\beta) = \beta(1-\rho^2) \geq 0$, so that the second factor is also greater than 1, and it is equal to one only in the degenerate case where $\beta = 0$ or $\rho^2 = 1$. This gain in efficiency is small for small values of β irrespective of the values of α and ρ (see Table 2). An estimator parallel to that in (30) [ignoring CMR and using sampling with replacement] is denoted by $\tilde{\overline{Y}}_*^{(2)}$. Verification of (36) and (37) can be made on using (41) and some routine steps, and parallel to (38), the asymptotic variance of $N^{1/2}(\tilde{\overline{Y}}_*^{(2)} - \overline{Y}^{(2)})$ is given by

$$\beta^{-1}S_{22}. \tag{44}$$

Hence, the ARE of $\tilde{\overline{Y}}_*^{(2)}$ with respect to $\hat{\overline{Y}}_*^{(2)}$ is given by

$$\{(1+\beta)-\rho^2(1-\alpha)\} / \{(1+\beta)-\rho^2(1+\alpha\beta)\} > 1, \tag{45}$$

as $[(1+\beta)-\rho^2(1-\alpha)] - [(1+\beta)-\rho^2(1+\alpha\beta)] = \alpha\rho^2(1+\beta) > 0$, for every $\alpha > 0$, $\rho^2 > 0$ and $\beta \geq 0$.

Table 1. *Relative efficiency of* $\hat{\bar{Y}}^{(2)}$ *with respect to* $\tilde{\bar{Y}}^{(2)}$ *for some typical values of* α, β, *and* ρ.

	$\rho = 0.9$				$\rho = 0.8$				$\rho = 0.6$			
$\alpha \backslash \beta$	0.10	0.20	0.25	0.33	0.10	0.20	0.25	0.33	0.10	0.20	0.25	0.33
0.10	1.31	1.24	1.22	1.19	1.15	1.13	1.13	1.12	1.05	1.05	1.05	1.05
0.20	1.64	1.51	1.46	1.40	1.31	1.28	1.26	1.24	1.11	1.10	1.10	1.10
0.25	1.81	1.65	1.59	1.52	1.29	1.25	1.33	1.31	1.13	1.13	1.13	1.12
0.33	2.11	1.91	1.83	1.73	1.53	1.48	1.46	1.42	1.18	1.17	1.17	1.17

Table 2. *Relative efficiency of* $\hat{\bar{Y}}^{(2)}$ *with respect to* $\hat{\bar{Y}}_*^{(2)}$ *for some typical values of* α, β *and* ρ.

	$\rho = 0.9$				$\rho = 0.8$				$\rho = 0.6$			
$\alpha \backslash \beta$	0.10	0.20	0.25	0.33	0.10	0.20	0.25	0.33	0.10	0.20	0.25	0.33
0.10	1.11	1.23	1.31	1.49	1.11	1.24	1.32	1.48	1.11	1.25	1.33	1.50
0.20	1.10	1.22	1.29	1.44	1.11	1.24	1.32	1.47	1.11	1.25	1.33	1.50
0.25	1.10	1.22	1.29	1.43	1.11	1.24	1.32	1.47	1.11	1.25	1.33	1.49
0.33	1.10	1.21	1.28	1.42	1.11	1.24	1.31	1.47	1.11	1.25	1.33	1.49

Table 3. *Relative efficiency of* $\hat{\bar{Y}}_*^{(2)}$ *with respect to* $\tilde{\bar{Y}}^{(2)}$ *for some typical values of* α, β *and* ρ.

	$\rho = 0.9$				$\rho = 0.8$				$\rho = 0.6$			
$\alpha \backslash \beta$	0.10	0.20	0.25	0.33	0.10	0.20	0.25	0.33	0.10	0.20	0.25	0.33
0.10	1.18	1.01	0.93	0.81	1.04	0.91	0.85	0.75	0.95	0.84	0.79	0.70
0.20	1.49	1.23	1.13	0.97	1.18	1.03	0.96	0.84	1.00	0.88	0.83	0.73
0.25	1.64	1.36	1.24	1.06	1.26	1.09	1.01	0.89	1.02	0.90	0.85	0.75
0.33	1.92	1.57	1.43	1.22	1.38	1.20	1.11	0.97	1.06	0.94	0.88	0.78

Finally, the ARE of $\hat{\bar{Y}}_*^{(2)}$ with respect to $\tilde{\bar{Y}}^{(2)}$ is obtained as

$$\{(1-\beta)[(1+\beta)-\rho^2(1-\alpha)]\}/\{(1+\beta)-\rho^2(1+\alpha\beta)\}$$
$$=1+\{\rho^2(\alpha+\beta)-\beta(1+\beta)\}/\{(1+\beta)-\rho^2(1+\alpha\beta)\} \tag{46}$$

and this is greater than one when $\rho^2 > \beta(1+\beta)/(\alpha+\beta)$; this is generally realized when β is small and α is large (see Table 3).

4. ESTIMATION OF TOTAL

An estimate of the total $Y^{(2)}(=N\bar{Y}^{(2)})$ based on $\hat{\bar{Y}}^{(2)}$ and $\hat{N}$ (in (26)) is

$$\hat{Y}^{(2)} = \hat{N}\hat{\bar{Y}}^{(2)}. \tag{47}$$

Note that by simple steps,

$$E[\hat{Y}^{(2)}-Y^{(2)}]^2 = N^2E(\hat{\bar{Y}}^{(2)}-\bar{Y}^{(2)})^2+(\bar{Y}^{(2)})^2E(\hat{N}-N)^2$$
$$+E[(\hat{\bar{Y}}^{(2)}-\bar{Y}^{(2)})^2(\hat{N}-N)^2], \tag{48}$$

where $E(\hat{N}-N)^2$ may be taken as $\{(n_1-m+1)(N+1)(N-n_1)\}/[m(n_1+2)]$, (see Chapman, 1952) and for $NE(\hat{\bar{Y}}^{(2)}-\bar{Y}^{(2)})^2$, (35) may be used. Further, using the arguments in (35) through (38) and proceeding on parallel lines, it can be shown that the last term on the right hand side of (48), for large m, can be expressed as the product of $NE(\hat{\bar{Y}}^{(2)}-\bar{Y}^{(2)})^2$ and $NE(\hat{N}/N-1)^2$; other terms are of lower order magnitudes. Since under (17), $(n_1-m+1)(N+1)(N-n_1)/[m(n_1+1)] \approx N(m)^{-1}$, we may provide the following asymptotic expression for $N^{-1}E[\hat{Y}^{(2)}-Y^{(2)}]^2$:

$$(\bar{Y}^{(2)})^2(\alpha\beta)^{-1}+(26)\{1+(\alpha\beta)^{-1}\}, \tag{49}$$

where (26) refers to the expression in (26). Similar asymptotic expressions can be obtained for the sampling variance of the estimators of $Y^{(2)}$ based on other estimators of $\bar{Y}^{(2)}$ and $\hat{N}$. Note that if N were known, in (47), we would have used N instead of $\hat{N}$, and this would lead to (26) instead of (49). Thus, $(\alpha\beta)^{-1}\{(\bar{Y}^{(2)})^2+(26)\}$ relates to the increase in the variability due to the unknown N (and its estimate due to the CMR technique). Generally, $(\alpha\beta)^{-1}$ is large, and this explains why the estimation of the total (with unknown N) we have generally a much higher asymptotic variance. Similar results hold for small sample sizes as well.

5. SUMMARY

The theory developed here pertains particularly to the situation where the population size N is unknown and inverse sampling with CMR is prescribed for the simultaneous estimation of N, and the average characteristic value (at the second stage) can be much more efficient than simple random sampling based on the second sample only. The relative efficiency picture depends on the first and second sample sizes as well as on the correlation of the measurements on successive occasions. The above sampling scheme is more efficient than inverse sampling in which the second sample is selected with replacement, i.e., when members of the second sample are caught one at a time, measured and returned immediately after measurement, sampling being continued until a prescribed number of marked animals have been caught. This plan is also realized when the proportion (n/N) is small. The plan avoids the assumption of constant catchability which is inherent in the former scheme though the situation in which it is applicable is less common.

It is shown that the gain in efficiency using inverse sampling without replacement over one with replacement in the second sample is small (Table 2) if the proportion of marked animals in the second sample (β) is small, irrespective of α and ρ. The relative efficiency of inverse sampling with replacement with respect to simple random sampling units from the second sample only increases with the increase in α and ρ^2 and it decreases with the increase in β. Finally, one has to pay a generally high price (in terms of the asymptotic variance) for estimating the total $Y^{(2)}$ when N is not precisely known. This case may typically arise with mobile populations of rare animals, and hence, needs more detailed examinations. We intend to pursue this line of research in a subsequent study.

REFERENCES

Anscombe, F. J. (1952), "Large sample theory of sequential estimation". *Proceedings of the Cambridge Philosophical Society* **48**, 600–607.

Chapman, D. G. (1952), "Inverse, multiple and sequential sample censuses". *Biometrics* **8**, 286–306.

Cramér, H. (1946), *Mathematical Methods of Statistics*. New Jersey: Princeton University Press.

Nandi, H. K., and P. K. Sen (1963), "On the properties of U-statistics when the observations are not independent. Part II: Unbiased estimation of the parameters of a finite population". *Calcutta Statistical Association Bulletin* **12**, 125–148.

Rao, C. R. (1966), "Least squares theory using an estimated dispersion matrix and its application to measurement of signals". *Proceedings of the Fifth Berkeley*

Symposium on Mathematical Statistics and Probability **1**, 355–372.
Sen, P. K. (1981), *Sequential Nonparametrics: Invariance Principles and Statistical Inference*. New York: Wiley and Sons.

Stanley L. Warner [1]

IDENTIFYING RATIONAL OPINION-FORMATION WITH THE OVERLAPPING INFORMATION MODEL

1. INTRODUCTION

The overlapping information model introduced by Warner (1984) provides an estimating scheme for concepts of interest when a summary of information is presented to a number of persons. Required for the estimates are measurements of each person's before-summary and after-summary beliefs that some proposition is true, with the measurements expressed as personal probabilities. For possible applications in monitoring summaries upon which policy decisions might be based, the model is interpreted as if the person preparing the summary tries to present impartially both points of view and the persons receiving the information act as a test population for the purpose of analyzing the summary. In particular, the members of the test population try to process rationally the information presented.

The introductory paper and some previously presented extensions set out the basic model. In general, the analogy of ordinary Bayesian processing of statistical information, implying the coherent adjusting of prior beliefs to posterior beliefs on the basis of sample information, is used to suggest measurements for concepts such as the balance and completeness of a summary.

This paper considers the possible use of the model to measure the relative ability of different persons to process summary information rationally. Since the method for measuring summary information is based on the before and after opinions of a group assumed to be reasonably rational in their processing of information, it is of interest to consider estimating which persons in the test population appear to be the relatively more rational in the sense that they are more able to avoid being additionally influenced by information which has already influenced them before. Persons influenced by the simple repetition of slogans, for example, are illogically processing

[1] Administrative Studies, York University, Downsview, Ontario M3J 2R6

I. B. MacNeill and G. J. Umphrey (eds.),
Applied Probability, Stochastic Processes, and Sampling Theory, 323-329.

information when measured against the Bayesian standard where beliefs are modified only by new information. An approach to identifying irrationality associated with over-influence of the order of argument is discussed by Warner (1975, 1981).

The next section summarizes the basic model and considers its possible use for estimating which of those in the test-population appear to be relatively better at discounting information which overlaps with that which they have seen before. A final section illustrates the concepts and the operation of the model through a simple simulation related to the standard problem of modifying probabilistic belief in which of two normal distributions generated a given set of data.

2. THE MODEL

In analogy with finite sampling procedures the collection of relevant facts and arguments to be summarized is considered as if it were a hypothetical population of data, with each piece of data influencing positively or negatively the probability that the hypothesis is thought to be true by a person who sees that piece of data. Since the information summarizer is assumed to select a subset from the population of data in as representative and impartial a fashion as possible, and since randomized selection represents a widely accepted standard for judging impartiality in selection, the model considers implications suggested by randomized selection of summary data from the hypothetical population of data. In an application the summary is necessarily purposefully chosen but is intended to satisfy criteria for balance suggested by randomized selection.

To represent the procedure the ith person's opinion prior to receiving the summary is expressed by P_i, and after receiving the summary by Q_i, $i = 1, 2, \ldots, n$. The net influence of the summary on the ith person is measured by

$$I_i = \ln(Q_i/(1 - Q_i)) - \ln(P_i/(1 - P_i)). \tag{1}$$

All relevant facts and arguments are viewed as if conceptually combined into a population of N pieces of data, each of the N pieces being so constituted as to be a relatively independent piece of influence regarding the proposition. The influence of data in information terms is thus additive so that, regarding Y_{ij} as the information seen by the ith person in the jth piece of data, the prior ln odds of person i is represented as

$$Z_i = \ln(P_i/(1 - P_i)) = \sum_{j \text{ in } A(i)} Y_{ij}, \tag{2}$$

where "j in $A(i)$" refers to the k_i pieces of data that have been seen by person i before the summary.

Similarly, with S_i representing the sum of the Y_{ij} over the m units presented in the summary, and V_i representing the sum of the Y_{ij} over the x_i overlapping units that are both in the summary and in the set seen before by person i, the basic identity for the model is given by

$$I_i = S_i + D_i V_i \tag{3}$$

with $D_i \geq -1$. Defining $\overline{Z}_i = Z_i/k_i$, $\overline{V}_i = V_i/x_i$, $r_i = x_i/k_i$, and $U_i = k_i(\overline{Z}_i - \overline{V}_i)$, expression (3) can also be written as

$$I_i = S_i + D_i r_i (Z_i - U_i), \tag{4}$$

where U_i is interpreted as a measurement error relating the unobservable $k_i\overline{V}_i$ to the observable Z_i.

The introductory development of Warner (1984) considered inferences from the simple regression model implied by assuming all $D_i = -1$, noting randomized selection implies all $E(r_i) = m/N$, and ignoring differences in Y_{ij} for different i as well as all bias due to complications such as measurement errors. This provides the most transparent form for interpretation of the model. In particular, the values S_i would be the same for each i and would be an approximation to $m\overline{Y}$, under the random sampling analogy, where $\overline{Y}$ is the average of the Y_j over the N pieces in the data population. Similarly, under random sampling, the coefficient of Z_i could be interpreted to have an expected value of $-(m/N)$, thus suggesting a first-approximation least squares estimating equation of

$$I_i = m\overline{Y} - (m/N)Z_i + e_i. \tag{5}$$

In this form the implied estimate of the vertical intercept, $m\overline{Y}$, is evidently interpretable as the estimated effect the summary would have on a person with no previous relevant knowledge and thus whose initial value of Z_i was zero. The estimate of the horizontal intercept, an approximation of $(N/m)(m\overline{Y}) = Y$, is similarly interpretable as an estimate of the ultimate effect of the entire population of data if it were seen, and the estimate of the slope coefficient, (m/N), is a measure of the completeness of the summary with values between zero and 1. Finally, some evidence of the balance of the information could be provided by seeing if the coefficients of the Z_i, reflecting the sampling proportion, tended to be estimated the same in separate regressions using first observations with small values of Z_i and then observations with large values of Z_i.

While the assumptions leading to the simple interpretation for (5) are useful to illustrate the approach, they are likely to be too restrictive for most purposes. Less stringent assumptions that still allow useful inferences are given by allowing the Y_{ij} to differ for different i, Z_i to be positively correlated with U_i, S_i to be positively correlated with Z_i but not correlated with U_i or $D_i r_i$, and considering $D_i r_i$ independent of Z_i and U_i with D_i independent of r_i. In particular, defining

$$\text{LSB} = \text{Cov}(I, Z)/\text{Var}(Z) - E(D)E(r), \tag{6}$$

$$\beta_i = D_i r_i + \text{LSB}, \tag{7}$$

and

$$\alpha_i = S_i - D_i r_i U_i - (\text{LSB}) Z_i, \tag{8}$$

the random coefficients model

$$I_i = \alpha_i + \beta_i Z_i \tag{9}$$

is shown by Warner (1985) to be consistently estimated by conventional methods such as that of Hildreth and Houck (1968).

While the direct interpretation of estimated coefficients implied by (4) are obviously no longer possible, since among other complications estimates of the expected values of α_i and β_i do not equal $E(S_i)$ and $E(D_i)E(r_i)$, it can be shown the assumptions still allow bounds to be estimated for some of the concepts of interest. In particular, the assumptions provide that the parameter $E(D_i)E(r_i)$ is bounded from below by -1, and in large samples can be estimated to be bounded above by the estimate of the expected value of the β_i, because under the assumptions LSB tends to be positive. Estimates of parameters such as $E(r_i) = (m/N)$, the measure of completeness, are no longer directly estimable without additional assumptions, but, as for the example of $E(r_i)$, at least the relative values of some parameters for different summaries may be estimated through presenting different summaries to random samples from the same test population.

The problem of estimating which of those in the test population appear to discount more rationally overlapping information is the problem of estimating which members of the test population have values of D_i that are relatively closer to -1. Under the assumptions, the D_i are independent of the r_i, and since the β_i are defined by (7), an estimated ordering of the D_i is possible through estimating the ordering of the β_i. In this paper the simple procedure of Griffiths (1972) is used to estimate the β_i, and the ordering of the β_i is estimated to be the ordering of the D_i.

While identification of those with relatively lower D_i is necessarily imprecise for any given person in any given application, information can accrue

if the same person participates as a member of other test populations for other summaries. For the somewhat easier problem of simply identifying a relatively preferred group in the test population, the estimated ordering from a single application may be helpful in itself. This suggests the possibility of improving estimates of some parameters through re-estimates based on that part of the original test population estimated to process information more rationally.

3. ILLUSTRATION WITH SIMULATED DATA

The familiar problem of using independent sample observations to modify prior beliefs regarding which of two normal distributions is appropriate provides the basis for a simple illustration. In particular, a sample of $N = 100$ observations was drawn from a distribution approximately normal with expected value 1 and standard deviation 3, and the choice considered was whether the observations came from this distribution or from a distribution approximately normal with expected value 0 and standard deviation 3.

The data representing the population of N pieces of information were thus alike for all i, and were constituted by the 100 values formed by recording the logarithms of the relative densities evaluated for each of the 100 drawn observations. The density of the generating distribution was the density in the numerator, and the sum of the 100 pieces of information resulted in a total which converted to a probability of .954 for the distribution with mean 1, assuming zero initial knowledge and thus .5 as a prior probability.

The number n in the test population was set equal to 200, with each member provided an initial endowment of some of the information in the population. While these pieces are not required to be random by the model, they were randomly selected for convenience. For each of the 200 members, each of the 100 pieces was independently drawn with probability .1, so that each person had somewhat more or less than 10 pieces before the summary.

The summarizer is presumed to collect and present information impartially, and for the model discussed, the notion of impartiality is that implied by random sampling. Unlike an actual application, in this simulation the influence of the summary actually was established by drawing each of the possible 100 pieces with probability .5, thus determining $E(r_i) = 5$, and the resulting pieces were then presented as the summary to each member in the test population.

For the discounting parameters D_i, each was determined by drawing from a uniform distribution defined between -1 and 0, so that $E(D_i) = -.5$. For each member of the test population, the prior probability was computed

according to the data seen before the summary. Then the information for the posterior probability was calculated by adding the information in the summary to the initial information and subtracting the effect of the overlapping information according to D_i.

The least squares and generalized least squares estimates of $E(D_i)E(r_i)$ were respectively $-.20$ and $-.19$, with estimated standard errors of approximately .02 in each case. Since the true value of the estimated quantity is $(-.5)(.5) = -.25$, this illustrates the effect of the positive bias of LSB. The estimate of the intercept, made easy by the uniformity of the information values for each i and an average value for Z_i near 0, provided an estimated posterior probability of .78, virtually the exact true value for a person with zero initial information who might be exposed to the summary.

The estimated β_i were significantly but only weakly correlated with the true D_i with $r = +.25$. There is thus little information regarding the relative performance of any particular test population member even in this example where conditions are both known and favorable. On the other hand, for the group predicted to have D_i below the mean, 66% were below, while for the group predicted to have D_i above the mean, only 40% were below. This illustrates the better possibility of ordering the rationality of groups rather than that of individuals.

It should be emphasized that the results of the simulation are only illustrative and imply little for the abstract applications for which the model is intended. Until many actual experiments are accomplished it is by no means clear that even the key slope parameter represented by $E(D_i)E(r_i)$ will be estimated to be negative often enough to make estimates of much interest. At least for the first actual experiment, however, reported in more detail by Warner (1985) the results are encouraging. This experiment, accomplished through a February 1985 telephone survey in which 400 students were provided a summary of a debate regarding an elected Senate, resulted in an estimate of $-.25$ for the key slope parameter and .03 for its standard error.

REFERENCES

Griffiths, W. E. (1972), "Estimating actual response coefficients in the Hildreth-Houck random coefficient model." *Journal of the American Statistical Association* **67**, 628–632.

Hildreth, C., and J. P. Houck (1968), "Some estimators for a linear model with random coefficients." *Journal of the American Statistical Association* **63**, 584–595.

Warner, S. L. (1975), "Advocate scoring for unbiased information." *Journal of the American Statistical Association* **70**, 15–22.

Warner, S. L. (1981), "Balanced information: the Pickering Airport experiment."

The Review of Economics and Statistics **63**, 256–262.

Warner, S. L. (1984), "The overlapping information model for evaluating summary information." *Proceedings of the Social Statistics Selection of the American Statistical Association Meetings*, August 1984, Philadelphia, 581–584.

Warner, S. L. (1985), "Applications of the overlapping information model." *Proceedings of the Survey Research Section of the American Statistical Association Meetings*, August 1985, Las Vegas, 401–403.

THE UNIVERSITY OF WESTERN ONTARIO SERIES IN PHILOSOPHY OF SCIENCE

A Series of Books in Philosophy of Science, Methodology, Epistemology, Logic, History of Science, and Related Fields

1. J. Leach, R. Butts, and G. Pearche (eds.), *Science, Decision and Value.* 1973, vii + 219 pp.
2. C. A. Hooker (ed.), *Contemporary Research in the Foundations and Philosophy of Quantum Theory.* 1973, xx + 385 pp.
3. J. Bub, *The Interpretation of Quantum Mechanics.* 1974, ix + 155 pp.
4. D. Hockney, W. Harper, and B. Freed (eds.), *Contemporary Research in Philosophical Logic and Linguistic Semantics.* 1975, vii + 332 pp.
5. C. A. Hooker (ed.), *The Logico-Algebraic Approach to Quantum Mechanics.* 1975, xv + 607 pp.
6. W. L. Harper and C. A. Hooker (eds.), *Foundations of Probability Theory, Statistical Inference, and Statistical Theories of Science.* 3 Volumes. Vol. I: *Foundations and Philosophy of Epistemic Applications of Probability Theory.* 1976, xi + 308 pp. Vol. II: *Foundations and Philosophy of Statistical Inference.* 1976, xi + 455 pp. Vol. III: *Foundations and Philosophy of Statistical Theories in the Physical Sciences.* 1976, xii + 241 pp.
7. C. A. Hooker (ed.), *Physical Theory as Logico-Operational Structure.* 1979, xvii + 334 pp.
8. J. M. Nicholas (ed.), *Images, Perception, and Knowledge.* 1977, ix + 309 pp.
9. R. E. Butts and J. Hintikka (eds.), *Logic, Foundations of Mathematics, and Computability Theory.* 1977, x + 406 pp.
10. R. E. Butts and J. Hintikka (eds.), *Foundational Problems in the Special Sciences.* 1977, x + 427 pp.
11. R. E. Butts and J. Hintikka (eds.), *Basic Problems in Methodology and Linguistics.* 1977, x + 321 pp.
12. R. E. Butts and J. Hintikka (eds.), *Historical and Philosophical Dimensions of Logic, Methodology and Philosophy of Science.* 1977, x + 336 pp.
13. C. A. Hooker (ed.), *Foundations and Applications of Decision Theory.* 2 volumes. Vol. I: *Theoretical Foundations.* 1978, xxiii + 442 pp. Vol. II: *Epistemic and Social Applications.* 1978, xxiii + 206 pp.
14. R. E. Butts and J. C. Pitt (eds.), *New Perspectives on Galileo.* 1978, xvi + 262 pp.
15. W. L. Harper, R. Stalnaker, and G. Pearce (eds.), *Ifs. Conditionals, Belief, Decision, Chance, and Time.* 1980, ix + 345 pp.
16. J. C. Pitt (ed.), *Philosophy in Economics.* 1981, vii + 210 pp.
17. Michael Ruse, *Is Science Sexist?* 1981, xix + 299 pp.

18. Nicholas Rescher, *Leibniz's Metaphysics of Nature.* 1981, xiv + 126 pp.
19. Larry Laudan, *Science and Hypothesis.* 1981, x + 258 pp.
20. William R. Shea, *Nature Mathematized.* Vol. I, 1983, xiii + 325 pp.
21. Michael Ruse, *Nature Animated.* Vol. II, 1983, xiii + 274 pp.
22. William R. Shea (ed.), *Otto Hahn and the Rise of Nuclear Physics.* 1983, x + 252 pp.
23. H. F. Cohen, *Quantifying Music.* 1984, xvii + 308 pp.
24. Robert E. Butts, *Kant and the Double Government Methodology.* 1984, xvi + 339 pp.
25. James Robert Brown (ed.), *Scientific Rationality: The Sociological Turn.* 1984, viii + 330 pp.
26. Fred Wilson, *Explanation, Causation and Deduction.* 1985, xviii + 385 pp.
27. Joseph C. Pitt (ed.), *Change and Progress in Modern Science.* 1985, viii + 398 pp.
28. Henry B. Hollinger and Michael John Zenzen, *The Nature of Irreversibility.* 1985, xi + 340 pp.
29. Kathleen Okruhlik and James Robert Brown (eds.), *The Natural Philosophy of Leibniz.* 1985, viii + 342 pp.
30. Graham Oddie, *Likeness to Truth.* 1986, xv + 218 pp.
31. Fred Wilson, *Laws and Other Worlds.* 1986, xv + 328 pp.
32. John Earman, *A Primer on Determinism.* 1986, xiv + 273 pp.
33. Robert E. Butts (ed.), *Kant's Philosophy of Physical Science.* 1986, xii + 363 pp.
34. Ian B. MacNeill and Gary J. Umphrey (eds.), Vol. I, *Applied Probability, Stochastic Processes, and Sampling Theory.* 1987, xxv + 329 pp.
35. Ian B. MacNeill and Gary J. Umphrey (eds.), Vol. II, *Foundations of Statistical Inference.* 1987, xvii + 287 pp.
36. Ian B. MacNeill and Gary J. Umphrey (eds.), Vol. III, *Time Series and Econometric Modelling.* 1987, xix + 394 pp.
37. Ian B. MacNeill and Gary J. Umphrey (eds.), Vol. IV, *Stochastic Hydrology.* 1987, xv + 225 pp.
38. Ian B. MacNeill and Gary J. Umphrey (eds.), Vol. V, *Biostatistics.* 1987, xvi + 283 pp.
39. Ian B. MacNeill and Gary J. Umphrey (eds.), Vol. VI, *Actuarial Science.* 1987, xvi + 250 pp.