Appendix A
A Euclidean Viewpoint on Statistics

This appendix gives the main algebraic and geometric principles used in the descriptive statistic methods presented in this book.

A.1 Inner and Dot Products

Let us consider two vectors $\mathbf{x}$ and $\mathbf{y}$ of $\mathbb{R}^n$. The inner product is a function that associates a real number to the pair of vectors $\mathbf{x}$ and $\mathbf{y}$:

$$\langle \,|\, \rangle : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$$

with the following properties:

- **Symmetric:** $\langle \mathbf{x}|\mathbf{y}\rangle = \langle \mathbf{y}|\mathbf{x}\rangle, \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$
- **Bilinear:**
  - $\langle \mathbf{x}|\mathbf{y}+\mathbf{z}\rangle = \langle \mathbf{x}|\mathbf{y}\rangle + \langle \mathbf{x}|\mathbf{z}\rangle, \forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^n$
  - $\langle \mathbf{x}|\alpha\mathbf{y}\rangle = \alpha \langle \mathbf{x}|\mathbf{y}\rangle, \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and $\forall \alpha \in \mathbb{R}$
- **Positive definite:** $\langle \mathbf{x}|\mathbf{x}\rangle \geq 0, \forall \mathbf{x} \in \mathbb{R}^n$
- **Non-degenerate:** $\langle \mathbf{x}|\mathbf{x}\rangle = 0 \Rightarrow \mathbf{x} = \mathbf{0}, \forall \mathbf{x} \in \mathbb{R}^n$

In $\mathbb{R}^n$, the dot product is the inner product defined in the standard basis by:

$$\langle \mathbf{x}|\mathbf{y}\rangle = \sum_{i=1}^{n} x_i y_i = \mathbf{y}^\top \mathbf{x}$$

If $\mathbf{A}$ is an $n \times n$ symmetric positive definite matrix, then the bilinear form $\mathbf{y}^\top \mathbf{A}\mathbf{x}$ satisfies the four properties and defines thus an inner product denoted:

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$$\langle \mathbf{x}|\mathbf{y}\rangle_{\mathbf{A}} = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij} x_j y_i$$

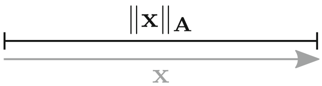
In $\mathbb{R}^n$, the usual dot product defined in the standard basis is obtained by setting $\mathbf{A}$ to the identity matrix $\mathbf{I}_n$. More generally, given a basis $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ of $\mathbb{R}^n$, the matrix $\mathbf{A}$ defined by $a_{ij} = \langle \mathbf{v}_i|\mathbf{v}_j\rangle_{\mathbf{A}}$ is the unique matrix representing the dot product $\langle \mathbf{x}|\mathbf{y}\rangle_{\mathbf{A}}$. Indeed, we have $\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{v}_i$ and $\mathbf{y} = \sum_{i=1}^{n} y_i \mathbf{v}_i$, $\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, and:

$$\begin{aligned}\langle \mathbf{x}|\mathbf{y}\rangle_{\mathbf{A}} &= \left\langle \sum_{i=1}^{n} x_i \mathbf{v}_i \middle| \sum_{j=1}^{n} y_j \mathbf{v}_j \right\rangle_{\mathbf{A}} = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i \langle \mathbf{v}_i|\mathbf{v}_j\rangle_{\mathbf{A}}\, y_j \\ &= \sum_{i=1}^{n}\sum_{j=1}^{n} x_i a_{ij} y_j = \mathbf{y}^\top \mathbf{A}\mathbf{x}\end{aligned}$$

A.2 Length, Projection, Angle and Distance

The norm (or length) of a vector $\mathbf{x}$ is defined by:

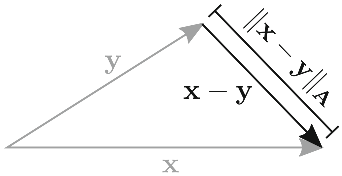
$$\|\mathbf{x}\|_{\mathbf{A}} = \sqrt{\langle \mathbf{x}|\mathbf{x}\rangle_{\mathbf{A}}}$$



Note that $\|\alpha\mathbf{x}\|_{\mathbf{A}} = |\alpha|\, \|\mathbf{x}\|_{\mathbf{A}}$.

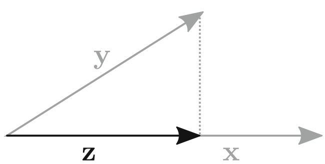
The distance between two vectors $\mathbf{x}$ and $\mathbf{y}$ is the norm of their difference:

$$d_{\mathbf{A}}(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_{\mathbf{A}}$$



The projection of $\mathbf{y}$ on the nonzero vector $\mathbf{x}$ is a vector $\mathbf{z}$ parallel to $\mathbf{x}$ so that $\mathbf{y} - \mathbf{z}$ is orthogonal to $\mathbf{x}$. It is given by:

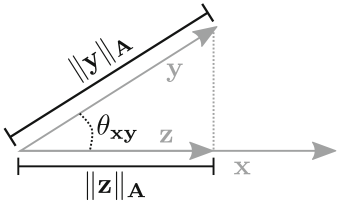
$$\mathbf{z} = \frac{\langle \mathbf{x}|\mathbf{y}\rangle_{\mathbf{A}}}{\langle \mathbf{x}|\mathbf{x}\rangle_{\mathbf{A}}}\mathbf{x}$$



It follows that

$$\cos(\theta_{\mathbf{xy}}) = \frac{\|\mathbf{z}\|_{\mathbf{A}}}{\|\mathbf{y}\|_{\mathbf{A}}} = \frac{\langle\mathbf{x}|\mathbf{y}\rangle_{\mathbf{A}}}{\|\mathbf{x}\|_{\mathbf{A}}\,\|\mathbf{y}\|_{\mathbf{A}}}$$

$$0 \leq \theta_{\mathbf{xy}} \leq \pi$$



and thus

$$\langle\mathbf{x}|\mathbf{y}\rangle_{\mathbf{A}} = \|\mathbf{x}\|_{\mathbf{A}}\,\|\mathbf{y}\|_{\mathbf{A}}\cos(\theta_{\mathbf{xy}})$$

Hence, two vectors $\mathbf{x}$ and $\mathbf{y}$ are orthogonal if $\langle\mathbf{x}|\mathbf{y}\rangle_{\mathbf{A}} = 0$. Moreover, we have

$$\left|\langle\mathbf{x}|\mathbf{y}\rangle_{\mathbf{A}}\right| \leq \|\mathbf{x}\|_{\mathbf{A}}\,\|\mathbf{y}\|_{\mathbf{A}} \text{ (Cauchy-Schwartz inequality)}$$

and

$$\|\mathbf{x}+\mathbf{y}\|_{\mathbf{A}} \leq \|\mathbf{x}\|_{\mathbf{A}} + \|\mathbf{y}\|_{\mathbf{A}} \text{ (triangular inequality)}$$

A.3 Mean and Variance

The observed values of a quantitative variable for n individuals are stored in $\mathbf{x} = (x_1, \cdots, x_n)^\top$, a vector of $\mathbb{R}^n$. The mean of $\mathbf{x}$ is equal to

$$\mathrm{m}(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} x_i$$

and its variance is

$$\mathrm{v}(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} (x_i - \mathrm{m}(\mathbf{x}))^2$$

Let us consider the uniform inner product of $\mathbb{R}^n$ associated to the diagonal matrix $\frac{1}{n}\mathbf{I}_n$. In a geometric viewpoint, the standard mean is computed by an inner product and corresponds to a Euclidean projection (Fig. A.1):

$$\mathrm{m}(\mathbf{x}) = \langle\mathbf{x}|\mathbf{1}_n\rangle_{\frac{1}{n}\mathbf{I}_n}$$

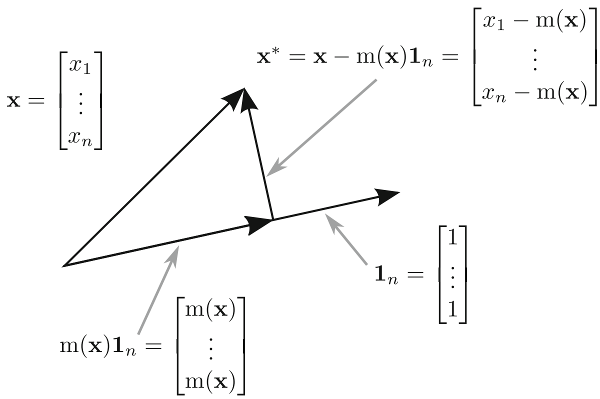


Fig. A.1 Centring a variable seen as an orthogonal projection.

The variance is equal to the squared norm of the centred vector $\mathbf{x}^*$

$$\mathrm{v}(\mathbf{x}) = \|\mathbf{x} - \mathrm{m}(\mathbf{x})\mathbf{1}_n\|^2_{\frac{1}{n}\mathbf{I}_n} = \left\|\mathbf{x}^*\right\|^2_{\frac{1}{n}\mathbf{I}_n}$$

A.4 Weighted Mean and Varianc

A weighting function can be defined to give some individuals more influence on the result than other individuals. Weights for the n individuals are stored in a vector $\mathbf{w}$ of $\mathbb{R}^n$. They are positive and their sum is equal to 1:

$$\mathbf{w} = (w_1 \cdots w_n)^\top \text{ with } \sum_{i=1}^{n} w_i = 1 \text{ and } w_i > 0$$

Using $\mathbf{w}$, the weighted mean of $\mathbf{x}$ is

$$\mathrm{m}_{\mathbf{w}}(\mathbf{x}) = \sum_{i=1}^{n} w_i x_i$$

and the weighted variance equals

$$\mathrm{v}_{\mathbf{w}}(\mathbf{x}) = \sum_{i=1}^{n} w_i \left(x_i - \mathrm{m}_{\mathbf{w}}(x)\right)^2$$

Considering the diagonal matrix $\mathbf{D}_{\mathbf{w}} = \mathrm{diag}(\mathbf{w})$ as the inner product of $\mathbb{R}^n$, the weighted mean and variance are given by:

$$\mathrm{m}_{\mathbf{w}}(\mathbf{x}) = \langle \mathbf{x} | \mathbf{1}_n \rangle_{\mathbf{D_w}}$$

and

$$\mathrm{v}_{\mathbf{w}}(\mathbf{x}) = \| \mathbf{x} - \mathrm{m}_{\mathbf{w}}(\mathbf{x}) \mathbf{1}_n \|^2_{\mathbf{D_w}}$$

The standard mean and variance (m($\mathbf{x}$), v($\mathbf{x}$)) correspond to the particular cases of weighted statistics ($\mathrm{m}_{\mathbf{w}}(\mathbf{x})$, $\mathrm{v}_{\mathbf{w}}(\mathbf{x})$) when uniform weights $w_i = \frac{1}{n}$ are chosen. From a geometric viewpoint, computing standard or weighted statistics corresponds to the same operation (i.e., a projection) but using different inner products.

A.5 Covariance and Correlation

The values of two quantitative variables are stored in the vectors $\mathbf{x}$ and $\mathbf{y}$. This information can be considered either as n points (individuals) in $\mathbb{R}^2$ or as 2 points (variables) of $\mathbb{R}^n$. In the first case, data centring corresponds to moving the origin of the system of axes (Fig. A.2a). In the second case, it corresponds to two orthogonal projections on the vector $\mathbf{1}_n$ (Fig. A.2b).

The vectors $\mathbf{x}^*$ and $\mathbf{y}^*$ contain centred data. The standard covariance is equal to

$$\begin{aligned} \mathrm{cov}(\mathbf{x}, \mathbf{y}) &= \mathrm{cor}(\mathbf{x}, \mathbf{y}) \sqrt{\mathrm{v}(\mathbf{x})} \sqrt{\mathrm{v}(\mathbf{y})} \\ &= \frac{1}{n} \sum_{i=1}^{n} (x_i - \mathrm{m}(\mathbf{x}))(y_i - \mathrm{m}(\mathbf{y})) = \frac{1}{n} \sum_{i=1}^{n} x_i^* y_i^* \end{aligned}$$

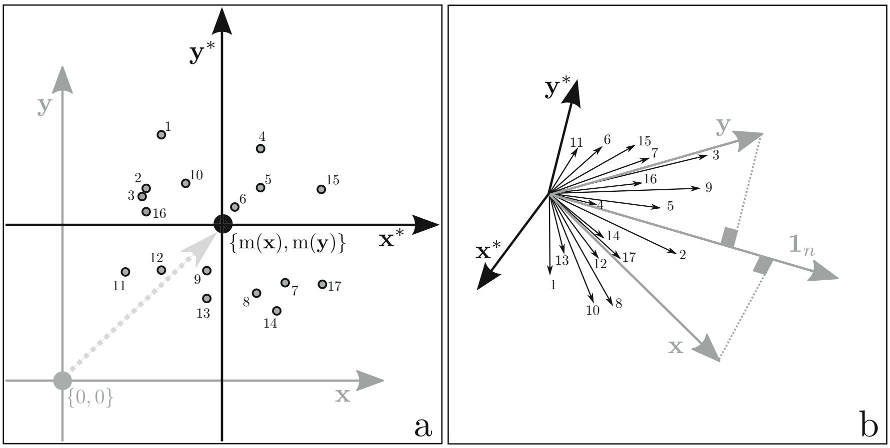


Fig. A.2 Two geometric viewpoints on centring (example with 2 variables and 17 individuals). It corresponds to (**a**) move the origin in $\mathbb{R}^2$ and to (**b**) two orthogonal projections in $\mathbb{R}^{17}$.

It can be rewritten as:

$$\begin{aligned}\mathrm{cov}(\mathbf{x},\mathbf{y}) &= \langle \mathbf{x}^*|\mathbf{y}^*\rangle_{\frac{1}{n}\mathbf{I}_n} \\ &= \|\mathbf{x}\|_{\frac{1}{\mathbf{n}}\mathbf{I_n}}\,\|\mathbf{y}\|_{\frac{1}{\mathbf{n}}\mathbf{I_n}}\cos(\theta_{\mathbf{xy}})\end{aligned}$$

As $\|\mathbf{x}\|_{\frac{1}{\mathbf{n}}\mathbf{I_n}} = \sqrt{\mathrm{v}(\mathbf{x})}$ and $\|\mathbf{y}\|_{\frac{1}{\mathbf{n}}\mathbf{I_n}} = \sqrt{\mathrm{v}(\mathbf{y})}$, it follows that:

$$\mathrm{cor}(\mathbf{x},\mathbf{y}) = \cos(\theta_{\mathbf{xy}})$$

Hence, the covariance is equal to the dot product between the two vectors whereas the correlation is the cosine of the angle formed by the two vectors. Note that weighted covariance and correlation could be obtained by using the appropriate inner product $\mathbf{D_w}$.

A.6 Linear Regression

The linear model that aims to explain the variation of $\mathbf{y}$ by the dependent variable $\mathbf{x}$ can be written as:

$$\mathbf{y} = \beta\mathbf{x} + \alpha\mathbf{1}_n + \boldsymbol{\epsilon}$$

Estimates of α and β are chosen to minimise the sum of squared residuals $\sum_{i=1}^{n}\epsilon_i^2 = \sum_{i=1}^{n}(y_i - \alpha - \beta x_i)^2$ (Fig. A.3a). The least squares estimates of parameters are given by:

$$\hat{\alpha} = \mathrm{m}(\mathbf{y}) - \hat{\beta}\mathrm{m}(\mathbf{x}) \text{ and } \hat{\beta} = \frac{\mathrm{cov}(\mathbf{x},\mathbf{y})}{\mathrm{v}(\mathbf{x})}$$

Considering the centred variables $\mathbf{x}^*$ and $\mathbf{y}^*$, the estimate of the slope can be rewritten as:

$$\hat{\beta} = \frac{\langle \mathbf{x}^*|\mathbf{y}^*\rangle_{\frac{1}{n}\mathbf{I}_n}}{\|\mathbf{x}^*\|^2_{\frac{1}{n}\mathbf{I}_n}}$$

Thus, the vector of predicted values $\hat{\mathbf{y}}$ can be decomposed as follows:

$$\begin{aligned}\hat{\mathbf{y}} &= \hat{\beta}\mathbf{x} + (\mathrm{m}(\mathbf{y}) - \hat{\beta}\mathrm{m}(\mathbf{x}))\mathbf{1}_n \\ &= \hat{\beta}(\mathbf{x}^* + \mathrm{m}(\mathbf{x})\mathbf{1}_n) + (\mathrm{m}(\mathbf{y}) - \hat{\beta}\mathrm{m}(\mathbf{x}))\mathbf{1}_n \\ &= \hat{\beta}\mathbf{x}^* + \mathrm{m}(\mathbf{y})\mathbf{1}_n\end{aligned}$$

$$= \frac{\langle \mathbf{x}^* | \mathbf{y}^* \rangle_{\frac{1}{n}\mathbf{I}_n}}{\|\mathbf{x}^*\|^2_{\frac{1}{n}\mathbf{I}_n}} \mathbf{x}^* + \langle \mathbf{y} | \mathbf{1}_n \rangle_{\frac{1}{n}\mathbf{I}_n} \mathbf{1}_n$$

The previous equation shows that the vector of predicted values $\mathbf{y}$ can be computed as the sum of two vectors (Fig. A.3b). The first vector corresponds to the projection of the centred variable $\mathbf{y}^*$ on $\mathbf{x}^*$. The second vector corresponds to the projection of $\mathbf{y}$ on $\mathbf{1}_n$.

As $\mathbf{x} = \mathbf{x}^* + \mathrm{m}(\mathbf{x})\mathbf{1}_n$, the three vectors $\mathbf{x}$, $\mathbf{x}^*$ and $\mathbf{1}_n$ are linearly dependent and thus lie in the same plane. It follows that vector of fitted values $\hat{\mathbf{y}}$ corresponds to the orthogonal projection of $\mathbf{y}$ on the plane spanned by the vectors $\mathbf{x}$ and $\mathbf{1}_n$. Applying the Pythagorean theorem to the triangle formed by the vectors $\mathbf{y}$, $\hat{\mathbf{y}}$ and $\boldsymbol{\epsilon} = \mathbf{y} - \hat{\mathbf{y}}$, we obtained the well-known decomposition of variance (Fig. A.4):

$$\|\mathbf{y}\|^2_{\frac{1}{n}\mathbf{I}_n} = \underbrace{\|\hat{\mathbf{y}}\|^2_{\frac{1}{n}\mathbf{I}_n}}_{\text{explained variance}} + \underbrace{\|\mathbf{y} - \hat{\mathbf{y}}\|^2_{\frac{1}{n}\mathbf{I}_n}}_{\text{residual variance}}$$

The coefficient of determination, $R^2_{\mathbf{y}|\mathbf{x}}$ measures the proportion of variance of the dependent variable $\mathbf{y}$ explained by the explanatory variable $\mathbf{x}$. Geometrically, it is the cosine of the angle formed by the vectors $\hat{\mathbf{y}}$ and $\mathbf{y}$ (Fig. A.4):

$$R^2_{\mathbf{y}|\mathbf{x}} = \frac{\|\hat{\mathbf{y}}\|^2_{\frac{1}{n}\mathbf{I}_n}}{\|\mathbf{y}\|^2_{\frac{1}{n}\mathbf{I}_n}} = \cos(\theta_{\hat{\mathbf{y}}\mathbf{y}})$$

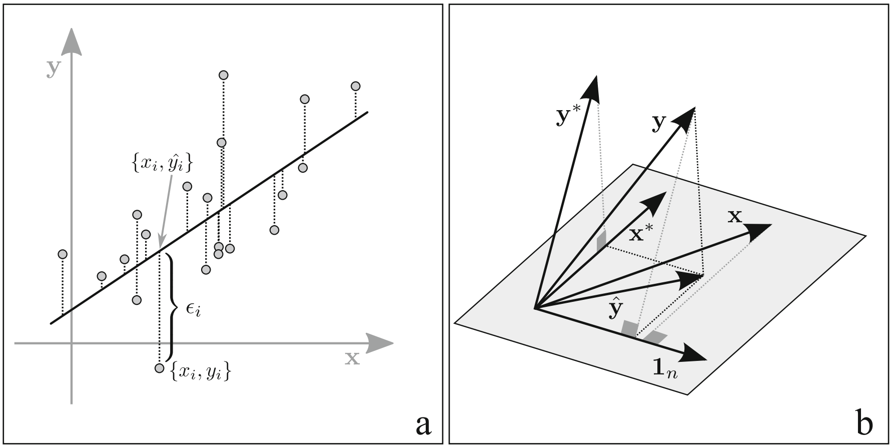


Fig. A.3 Two geometric viewpoints on linear regression with intercept (example with one explanatory variable and 20 individuals). In $\mathbb{R}^2$ (**a**), the usual representation shows that the regression line minimises the residual sum of squares. In $\mathbb{R}^{20}$ (**b**), fitted values are obtained by orthogonal projection of $\mathbf{y}$ on the plane spanned by vectors $\mathbf{x}$ and $\mathbf{1}_n$.

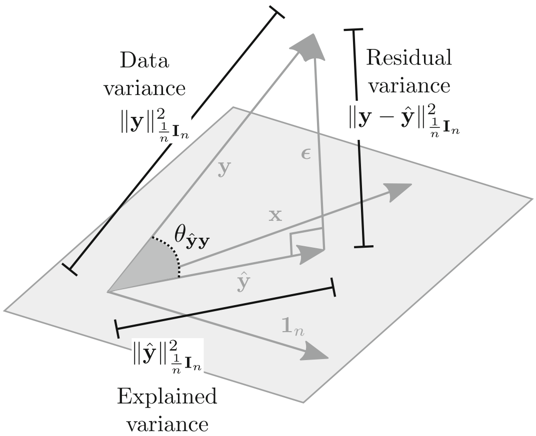


Fig. A.4 Geometric decomposition of the variance using the Pythagorean theorem.

A.7 Categorical Variables

A categorical variable is a variable that can take one of a finite number of possible values, each individual being assigned to a particular group (category, level or class). If we consider a categorical variable with m categories measured for n individuals, the information can be coded as a vector $\mathbf{q}$ of integers. An $n \times m$ table $\mathbf{X} = [\mathbf{x}_1 | \ldots | \mathbf{x}_m]$ of dummy variables can be built. For the k-th category, the dummy variable $\mathbf{x}_k$ is equal to 1 if the individual belongs to this category and 0 otherwise:

$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ \vdots \\ n \end{array} \begin{array}{c} \text{Category} \\ \begin{bmatrix} \text{blue} \\ \text{red} \\ \text{blue} \\ \text{green} \\ \vdots \\ \text{black} \end{bmatrix} \end{array} \rightarrow \begin{array}{c} \mathbf{q} \\ \begin{bmatrix} 1 \\ 2 \\ 1 \\ 3 \\ \vdots \\ m \end{bmatrix} \end{array} \rightarrow \begin{array}{c} \begin{array}{ccccc} \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \cdots & \mathbf{x}_m \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix} \end{array}$$

Whereas a quantitative variable corresponds to a vector, a categorical variable defines a subspace spanned by vectors $\mathbf{x}_1, \ldots, \mathbf{x}_m$. If we consider a diagonal matrix of weights $\mathbf{D_w}$, the dummy variables are orthogonal by definition (i.e., $\langle \mathbf{x}_i | \mathbf{x}_j \rangle_{\mathbf{D_w}}$ for $i \neq j$). The weight w_k^+ associated to the k-th category is equal to the sum of the weights of the individuals belonging to this category. It is equal to the squared norm of the associated dummy variable, $w_k^+ = \|\mathbf{x}_k\|^2_{\mathbf{D_w}}$.

Let us consider a quantitative variable $\mathbf{y}$. The projection of $\mathbf{y}$ on the k-th dummy variable is equal to:

$$\mathcal{P}_{\mathbf{x}_k}(\mathbf{y}) = \frac{\langle \mathbf{y} | \mathbf{x}_k \rangle_{\mathbf{D_w}}}{\|\mathbf{x}_k\|^2_{\mathbf{D_w}}} \mathbf{x}_k = \frac{\sum\limits_{i/q_i=k} w_i y_i}{w_k^+} \mathbf{x}_k = \mathrm{m}_{\mathbf{w}/k}(\mathbf{y}) \mathbf{x}_k$$

The value $\mathrm{m}_{\mathbf{w}/k}(\mathbf{y})$ is the conditional mean of $\mathbf{y}$ given k (i.e., the weighted mean of the variable $\mathbf{y}$ computed only on the individuals belonging to the k-th category). Hence, the vector $\mathcal{P}_{\mathbf{x}_k}(\mathbf{y})$ takes the value $\mathrm{m}_{\mathbf{w}/k}(\mathbf{y})$ for the individuals of the k-th category and 0 otherwise.

It follows that the projection of the centred variable $\mathbf{y}^* = \mathbf{y} - \mathrm{m}_{\mathbf{w}}(\mathbf{y})\mathbf{1}_n$ on $\mathbf{x}_k$ is simply given by:

$$\mathcal{P}_{\mathbf{x}_k}(\mathbf{y}^*) = (\mathrm{m}_{\mathbf{w}/k}(\mathbf{y}) - \mathrm{m}_{\mathbf{w}}(\mathbf{y}))\mathbf{x}_k$$

As the dummy variables are orthogonal, the projection on the subspace spanned by the vectors $\mathbf{x}_1, \dots, \mathbf{x}_m$ is simply the sum of the individual projections on each vector $\mathbf{x}_k$:

$$\mathcal{P}_{\mathbf{X}}(\mathbf{y}^*) = \sum_{k=1}^{m} \mathcal{P}_{\mathbf{x}_k}(\mathbf{y}^*)$$

After some substitutions, the squared norm of this projection can be rewritten as:

$$\left\|\mathcal{P}_{\mathbf{X}}(\mathbf{y}^*)\right\|^2_{\mathbf{D_w}} = \sum_{k=1}^{m} w_k^+ (\mathrm{m}_{\mathbf{w}/k}(\mathbf{y}) - \mathrm{m}_{\mathbf{w}}(\mathbf{y}))^2 = b(\mathbf{y})$$

The quantity $b(\mathbf{y})$ is the between-group variance that measures the differences among categories. Using the Pythagorean theorem, the within-group variance is defined by

$$w(\mathbf{y}) = \left\|\mathbf{y}^* - \mathcal{P}_{\mathbf{X}}(\mathbf{y}^*)\right\|^2_{\mathbf{D_w}}$$

and we obtain the standard ANOVA decomposition of variance:

$$\left\|\mathbf{y}^*\right\|^2_{\mathbf{D_w}} = \underbrace{\left\|\mathcal{P}_{\mathbf{X}}(\mathbf{y}^*)\right\|^2_{\mathbf{D_w}}}_{\text{between-group variance}} + \underbrace{\left\|\mathbf{y}^* - \mathcal{P}_{\mathbf{X}}(\mathbf{y}^*)\right\|^2_{\mathbf{D_w}}}_{\text{within-group variance}}$$

The correlation ratio $\eta^2(\mathbf{q}, \mathbf{y}) = \frac{b(\mathbf{y})}{\mathrm{v}_{\mathbf{w}}(\mathbf{y})}$ measures the proportion associated to the between-group variance. It varies between 0 and 1. Geometrically, it is the cosine of the angle formed by the vectors $\mathcal{P}_{\mathbf{X}}(\mathbf{y}^*)$ and $\mathbf{y}^*$.

A.8 Weighted Multiple Regression

Multiple regression aims to explain the variation of a response variable $\mathbf{y}$ by several dependent variables $\mathbf{x}_1, \dots, \mathbf{x}_p$ stored in column in an $n \times p$ table $\mathbf{X}$

($\mathbf{X} = [\mathbf{x}_1|\dots|\mathbf{x}_p] = [x_{ij}]$). For a given weighting matrix $\mathbf{D_w}$, the aim of multiple regression is to predict the observation y_i by a linear model:

$$\hat{y}_i = \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \alpha = y_i - \epsilon_i$$

The weighted least-squares estimation leads to minimise the residual sum of squares:

$$RSS = \sum_{i=1}^{n} w_i(\hat{y}_i - y_i)^2 = \|\mathbf{y} - \hat{\mathbf{y}}\|^2_{\mathbf{D_w}}$$

The minimisation of the RSS is provided by the orthogonal projection of $\mathbf{y}$ on the subspace spanned by the vectors $\mathbf{x}_1, \dots, \mathbf{x}_p, \mathbf{1}_n$. The vector $\mathbf{1}_n$ is added to consider the intercept in the model so that

$$\hat{\mathbf{y}} = \beta_1\mathbf{x}_1 + \cdots + \beta_p\mathbf{x}_p + \alpha\mathbf{1}_n$$

The vector of predicted values $\hat{\mathbf{y}}$ exists and is unique. The uniqueness of the coefficients $\beta_1, \cdots, \beta_p, \alpha$ is ensured only if the vectors $\mathbf{x}_1, \dots, \mathbf{x}_p, \mathbf{1}_n$ are independent (i.e., no multicollinearity). This independence is obtained if and only if the centred vectors $\mathbf{x}_1^*, \dots, \mathbf{x}_p^*$ are independent, with $\mathbf{x}_i^* = \mathbf{x}_i - \mathrm{m}_{\mathbf{w}}(\mathbf{x}_i)\mathbf{1}_n$. If the centred vectors are independent, the covariance matrix $\mathbf{X}^{*\top}\mathbf{D_w}\mathbf{X}^*$ is invertible (with $\mathbf{X}^* = [\mathbf{x}_1^*|\dots|\mathbf{x}_p^*]$). In this case, we have:

$$\begin{aligned}\hat{\mathbf{y}} &= \mathcal{P}_{\mathbf{X}^*}(\mathbf{y}) + \mathcal{P}_{\mathbf{1}_n}(\mathbf{y}) \\ &= \mathcal{P}_{\mathbf{X}^*}(\mathbf{y}^*) + \mathcal{P}_{\mathbf{1}_n}(\mathbf{y}^*) + \mathcal{P}_{\mathbf{X}^*}(\mathrm{m}_{\mathbf{w}}(\mathbf{y})\mathbf{1}_n) + \mathcal{P}_{\mathbf{1}_n}(\mathrm{m}_{\mathbf{w}}(\mathbf{y})\mathbf{1}_n)\end{aligned}$$

By definition, the centred vectors $\mathbf{x}_1^*, \dots, \mathbf{x}_p^*, \mathbf{y}^*$ are orthogonal to $\mathbf{1}_n$ so that the previous equation simplifies to

$$\hat{\mathbf{y}} = \mathcal{P}_{\mathbf{X}^*}(\mathbf{y}^*) + \mathcal{P}_{\mathbf{1}_n}(\mathrm{m}_{\mathbf{w}}(\mathbf{y})\mathbf{1}_n)$$

In the standard basis, the projection operator $\mathcal{P}_{\mathbf{X}^*}(.)$ is simply equal to $\mathbf{X}^*(\mathbf{X}^{*\top}\mathbf{D_w}\mathbf{X}^*)^{-1}\mathbf{X}^*\mathbf{D_w}$ and the previous equation can be rewritten as:

$$\hat{\mathbf{y}} = \mathbf{X}^*(\mathbf{X}^{*\top}\mathbf{D_w}\mathbf{X}^*)^{-1}\mathbf{X}^*\mathbf{D_w}\mathbf{y}^* + \mathrm{m}_{\mathbf{w}}(\mathbf{y})\mathbf{1}_n$$

The estimates of the parameters are then obtained by

$$\begin{bmatrix}\hat{\beta}_1 \\ \vdots \\ \hat{\beta}_p\end{bmatrix} = (\mathbf{X}^{*\top}\mathbf{D_w}\mathbf{X}^*)^{-1}\mathbf{X}^*\mathbf{D_w}\mathbf{y}^*$$

and

$$\hat{\alpha} = \mathrm{m}_{\mathbf{w}}(\mathbf{y}) - \hat{\beta}_1 \mathrm{m}_{\mathbf{w}}(\mathbf{x}_1^*) - \cdots - \hat{\beta}_p \mathrm{m}_{\mathbf{w}}(\mathbf{x}_p^*)$$

As in simple regression, the part of variance explained by the model is equal to the ratio of two squared norms (and thus the cosine of the angle formed by these two vectors):

$$R^2_{\mathbf{y}|\mathbf{X}} = \frac{\|\hat{\mathbf{y}}\|^2_{\mathbf{D_w}}}{\|\mathbf{y}\|^2_{\mathbf{D_w}}}$$

Appendix B
Graphical User Interface

Abstract This chapter is a short presentation of **ade4TkGUI**, a Tcl/Tk Graphical User Interface (GUI) package for some basic functions of **ade4**. The **ade4TkGUI** package tries to mix the advantages of a GUI (ease of use, no need to learn numerous commands) with the possibility to use **R** expressions in the dialog boxes, to generate understandable **R** commands, and to manage a session `.Rhistory` file.

B.1 Introduction

This chapter is based on the paper by Thioulouse and Dray (2007), but only the most interesting features of **ade4TkGUI** are detailed here. The **ade4** package is a part of a previous software that was written in C. This software was mainly used by ecologists, and it had a rich and very useful GUI, written in HyperTalk and based successively on HyperCard, WinPlus and MetaCard (see Chapter 1, Thioulouse et al. 1997).

Switching to **R** and to the command line interface of **ade4** was a hard task for many users, and we decided to make it easier by providing them with a GUI. The first aim of **ade4TkGUI** was to give the users of "Classical ADE-4" an easy access to the main functions of **ade4**. As most users would also be new to **R**, we wanted it to be easy to install, and using **Tcl/Tk** was a guarantee of easiness and multi-platform compatibility.

Only one-table and two-table methods are currently available in **ade4TkGUI** and graphical functions are limited to the basic classes. *K*-table methods are not included.

We decided to use the **Tcl/Tk** language to implement **ade4TkGUI** because the **tcltk** package is available in **R**, and included by default in the base distribution. Many other GUI development systems are available, but they do not offer the same level of availability and platform independence as **tcltk**.

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B.2 Overview of the ade4TkGUI Package

It is not possible to give here a detailed description of all the functions of **ade4TkGUI**, and only the main characteristics will be presented. The core of the package is the `ade4TkGUI()` function, which opens the main GUI window (Fig. B.1).

In the main GUI window, buttons are grouped in 6 rows, according to their function: Data sets, One table analyses, One table analyses with groups, Two tables analyses, Graphic functions, and Advanced graphics. To avoid cluttering this window, only a limited subset of functions is displayed. Less frequently used functions are available through the menus of the menu bar, located at the top of the window. Right-clicking the buttons opens the **ade4** help window for the corresponding function. The question-head button opens the help window of **ade4TkGUI**.

The `ade4TkGUI()` function takes two boolean arguments, `show` and `history`. The first one determines whether the **R** commands generated by the GUI

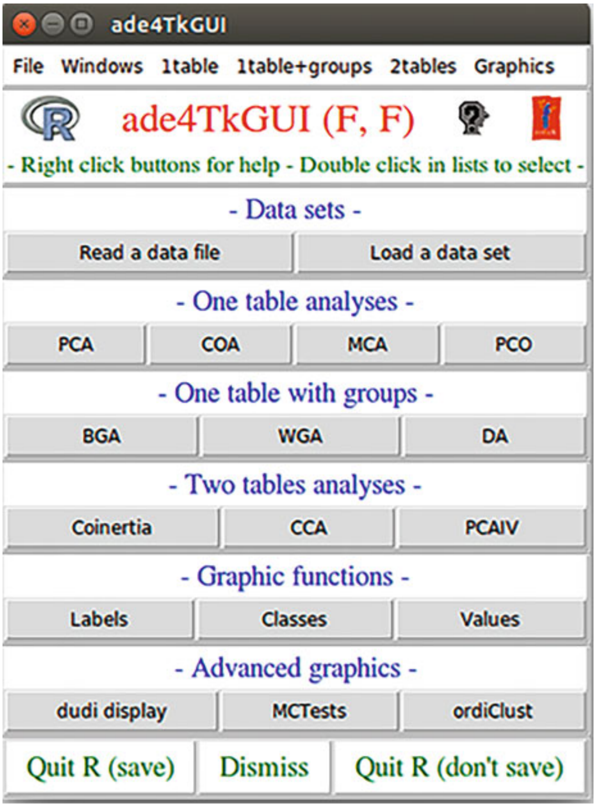

Fig. B.1 The main **ade4TkGUI** window.

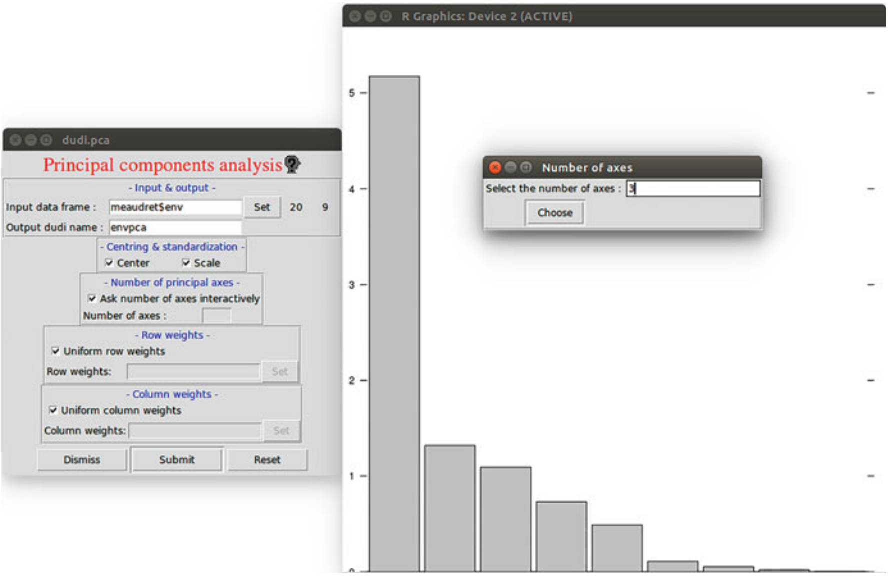

Fig. B.2 The `dudi.pca` function GUI window (left), the eigenvalues barchart (right) and the selection of the number of axes by the user (top-right).

should be printed in the console. When users interact with the GUI, they modify the status of **tcltk** widgets, and when they click on the "`Submit`" button, an **R** command is generated from the status of these widgets. This command is executed and can optionally be displayed in the console. If the `history` argument is set to TRUE, the commands generated by the GUI are also stored in the `.Rhistory` file, where they can easily be retrieved by users. The state of the two parameters is recalled in the main window heading "`ade4TkGUI(T,T)`".

The "`Read a data file`" button opens a dialog window that can be used to set the parameters of the `read.table` command to read a data text file. The "`Load a data set`" just displays the list of **ade4** data sets. This list can be used to choose a particular data set and to load it in memory using the `data` command.

When the "`PCA`" button is clicked, a new window appears (Fig. B.2): this is the GUI window of the `dudi.pca` function.

In this new window, the "`Set`" button can be used to choose the PCA input data frame through a listbox showing the list of data frames in the user global environment. After the "`Input data frame`" text field has been filled by the user, the number of rows and columns (20, 9) are displayed next to it. The output of the `dudi.pca` function is an object of class `dudi` and the user can type the name of this object in the "`Output dudi name`" field. If this field is left empty, the name "`Untitled1`" is used automatically.

The remaining widgets can be used to set particular options for the PCA: centring and standardisation, number of principal axes used to compute row and column coordinates, and row and column weights.

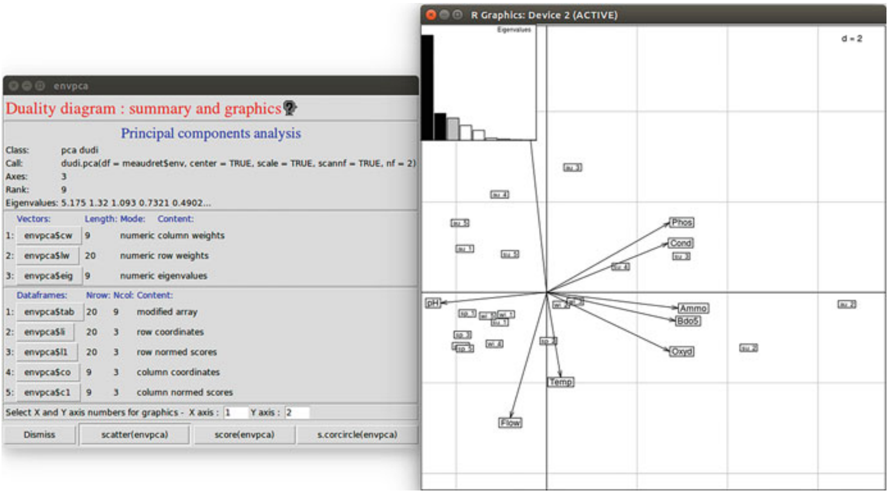

Fig. B.3 The `dudi` object display window (left) and the biplot obtained by clicking on the "`scatter`" button (right).

Most of the windows created by **ade4TkGUI** are non-blocking, which means that the user can do other things in the GUI or in the **R** console before taking the action required by this window. This was designed to make the interface more flexible and easier to use.

Clicking the "`Submit`" button starts the PCA computations. When they are completed, the barplot of eigenvalues is displayed (right of Fig. B.2) and, if this option was chosen in the previous dialog window, the user is asked to select the number of axes on which the row and column scores should be computed.

After scores are computed, the `dudi` window is displayed (Fig. B.3, left). This window shows a summary of the analysis, and displays the elements of the `dudi` object under the form of buttons. All these buttons can be used to draw graphs of the corresponding elements. For example, the row and column coordinates buttons draw the classical factor maps. In the lower part of the window, the user can choose which axes are used to draw these graphs.

The last row of buttons gives access to special graphs, according to the particular properties of the `dudi` that is displayed. For example, in the case of a normed PCA, the "`s.corcircle`" button allows to draw a correlation circle. The "`scatter`" button draws a biplot, with a small barchart for eigenvalues (Fig. B.3, right). These additional buttons are adapted to the type of `dudi` that is displayed, and they allow to draw graphs that illustrate particular properties of this `dudi`.

An example of GUI for one of the graphical functions of **adegraphics** is given in Fig. B.4. This is the `s.class` function, which allows to draw factor maps with groups of individuals. The user can choose the data frame containing the row scores (here they come from the "`envpca`" `dudi`), and the factor that should be used

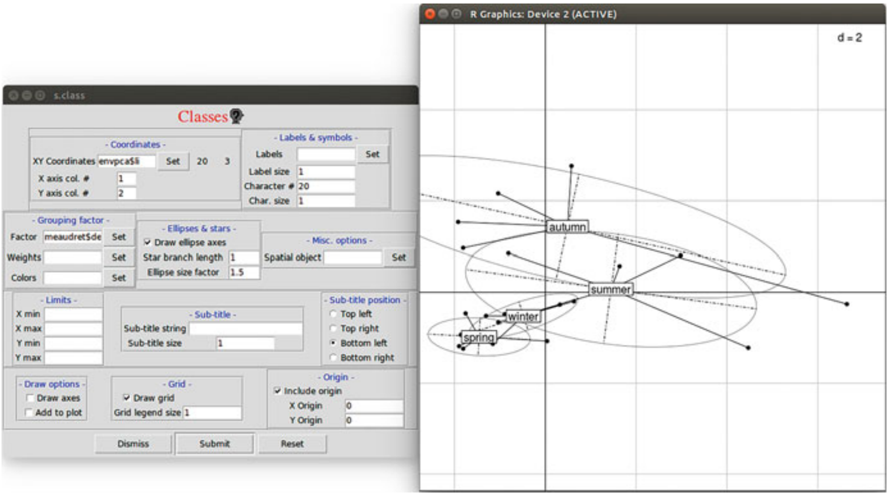

Fig. B.4 The `s.class` GUI window (left) and the corresponding graph (right).

to draw the groups on the factor map. Many other options can be set to enrich the graphs.

B.3 Conclusion

The main advantage of a GUI is the ease of use for beginners, occasional users, or teachers and students. It makes easier learning how to use a software by making the learning curve smoother, or to get back to work after a long period. This is particularly important in the case of **ade4** in ecological data analysis, because ecologists are mostly occasional users of **R**.

An important feature in **ade4** is the `dudi`, a complex **R** object containing all the information relating to a duality diagram. The `dudi` GUI window (Fig. B.3) was designed to display all the components of a `dudi`, and to draw automatically default graphs for each of these components. Therefore, it offers a centralised and synthetic view of an analysis, and it allows to see rapidly and interactively many graphs. In command line mode, the user must know all the components of a `dudi`, and remember which one is needed to draw a particular graph; this is particularly difficult for occasional users.

The **ade4TkGUI** package also facilitates the use of **ade4** by pre-selecting the type of objects that are proposed to users when they must do a selection. For example, in the `dudi.pca` dialog window (Fig. B.2), when the user clicks on the “`Set`” button to select a data frame, the dialog box contains only data frames present in the global environment (or in lists present in the global environment). In the same window, if the user wants to set non-uniform row weights, the “`Set`” button for row weights displays only vectors of length equal to the number of rows of the data frame. More generally, lists are filtered to propose only objects with properties consistent with the aim of the action. In the same way, in the `dudi` window, the buttons and their functions are coherent with the type of `dudi` and with the mathematical properties of its components.

Obviously, a GUI is not well adapted to scripting, and even to simple repetitive tasks. It is also not good for batch, online or remote use, and it is not easy to integrate into Sweave or R Markdown documents and vignettes. This is probably the main drawback of GUIs: they are made for *personal* and *instant* use, while the command line interface (CLI) allows many operations like scripting, re-doing the same analysis later, sharing pieces of code among colleagues, and batch use for time-consuming computations.

GUIs and CLIs should not be opposed, but considered as complementary. GUIs make the learning curve smoother for beginners, and can be used in education to introduce students to CLI mode. CLI mode is more powerful, it allows to build more complex analyses, particularly when using several packages jointly. When possible, the joint use of both CLI and GUI is attractive, as the user gets the benefits of the two approaches. Joint use can be very intimate: for example, it is possible to use **R** expressions in the GUI dialogs, and the GUI can return **R** expressions that can be copied and pasted in the console. In the case of **ade4TkGUI**, the strings typed by the user in the text fields of the GUI are parsed, and it is therefore possible to use **R** expressions, for example, to specify a subset of a data frame in a PCA.

When `ade4TkGUI` is called with argument "`show = TRUE`", **R** commands built by the GUI are echoed to the console. It is then possible to copy/paste these commands and execute them when needed in the console. This is also an effective way for beginners to learn how to use elaborate **R** function calls. Occasional users can thus analyse these command lines and possibly adapt them to their needs, with the additional benefit of gradually learning the **R** language.

In addition to this **Tcl/Tk** GUI, we are developing a new Shiny application to use the main `ade4` functionalities through a Web application. Shiny is an **R** package that makes very easy building interactive Web Apps in **R**. The main advantage is that users do not have to install **R** and multiple packages: they only need a web browser. As an example, a first piece of this "in progress" work is deployed on the *shinyapps.io* web site. It can be used to perform a PCA at this URL: https://ade4.shinyapps.io/ShinyPCA. We plan to develop this approach in the near future and hope to be able to propose a complete Shiny GUI to the `ade4` package.

Appendix C
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C.1 Chapter 3: The `dudi` Class

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