Operator related to a data matrix: a survey

Yves Escoufier

Equipe de Probabilités et Statistique, Département des Sciences mathématiques, Université de Montpellier II, Case Courrier 051,Place Eugène Bataillon, 34095 Montpellier cedex 5, France

Summary. The reading of this article will allow the readers to understand the data analysis approach which is proposed. The first paragraph gives the basic tools: the triplet (X, Q, D), the operator related to a data matrix and the coefficient RV. The two following paragraphs show how these tools are used for reading out and solving the problems of joint analysis of several data matrices and of principal component analysis with respect to instrumental variables. The conclusion recalls of the construction of this approach along the past thirty five years.

1 The initial choices

1.1 First choice: the triplet (X, Q, D)

When a researcher collects an $n \times p$ data array, X, of the values taken by n observations on p variables, he generally has two goals:

- 1. Comparison of the variables. If he chooses to conduct this comparison by way of a linear correlation coefficient, he will use a positive diagonal matrix D which defines the weights attached to each observation.
- 2. Comparison of the observations. If he chooses to compute a distance between the observations, he will need a pxp symmetric positive definite matrix Q. In the simplest case, Q is a diagonal positive pxp matrix defining the scale of the different variables. In the general case, $Q=L^tL$ where L is a pxp matrix of rank p which can be viewed as a linear transformation of X such that Y=XL will replace X.

From the preceding considerations it follows that when we speak of a data analysis, we must consider the triplet (X, Q, D) to describe the data and their use.

1.2 Second choice: the operator XQ^tXD

Consider now that we are mainly interested in the dispersion of the observations showed by the transformed data array Y. A usual way to study the dispersion is to do a principal component analysis of Y. The mapping of the observations in the space spanned by the principal components will give a way for studying the similarity of the observations. For simplicity, we suppose that $Y = (I_{nxn} - 1_n D^t 1_n) Y$, which means that the columns of Y are centred for the weights given by D. Because Y = XL, it is the same for X.

Let S= ^tYDY, the covariance matrix of Y and $\{(z_{\alpha}, \lambda_{\alpha}), \alpha = 1, p\}$ the eigenvectors and eigenvalues of S such that $Sz_{\alpha} = \lambda_{\alpha} z_{\alpha}$ with ${}^{t}z_{\alpha} z_{\beta} = \delta_{\alpha\beta}$. Then, $\{(\psi^{\alpha} = Yz_{\alpha}/\sqrt{\lambda_{\alpha}}), \alpha = 1, p\}$ are the principal components and ${}^{t}\psi^{\alpha}D\psi^{\beta} = \delta_{\alpha\beta}$.

Proposition 1.2.1

For the principal components we have: $XQ^tXD\psi^{\alpha} = \lambda_{\alpha}\psi^{\alpha}$ *Proof:* from ^tYDYz_{α} = $\lambda_{\alpha} z_{\alpha}$ we have: Y^tYD(Yz_{α}/ $\sqrt{\lambda_{\alpha}}$) = λ_{α} (Yz_{α}/ $\sqrt{\lambda_{\alpha}}$) and thus $XQ^t XD\psi^\alpha = \lambda_\alpha \psi^\alpha$

So, as long as our interest in studying the dispersion of the observations lies in the principal components of (X,Q,D), all the needed information is given by the eigenvectors and eigenvalues of the operator $WD = XQ^{t}XD$ which will be called the operator related to the study (X,Q,D).

- Proposition 1.2.2 If $\phi_{\alpha} = {}^{t} \mathrm{L}^{-1} \mathrm{z}_{\alpha}$ then:
- 1. ${}^{t}XDXQ\phi_{\alpha} = \lambda_{\alpha}\phi_{\alpha}$
- 2. ${}^{t}\phi_{\alpha}Q\phi_{\beta} = \delta_{\alpha\beta}$
- 3. $\psi^{\alpha} = XQ\phi_{\alpha}/\sqrt{\lambda_{\alpha}}$
- 4. $\phi_{\alpha} = {}^{t} \mathrm{XD} \psi^{\alpha} / \sqrt{\lambda_{\alpha}}$

Proof:

- 1. ${}^{t}YDYz_{\alpha} = \lambda_{\alpha}z\alpha \iff {}^{t}L^{t}XDXLz_{\alpha} = \lambda_{\alpha}z_{\alpha}$ ${}^{t}XDXL^{t}L({}^{t}L^{-1}z_{\alpha}) = \lambda_{\alpha}({}^{t}L^{-1}z_{\alpha})$ <=>
- 2. ${}^{t}\phi_{\alpha}Q\phi_{\beta} = {}^{t}z_{\alpha}L^{-1}(L^{t}L){}^{t}L^{-1}z_{\beta} = {}^{t}z_{\alpha}z_{\beta} = \delta_{\alpha\beta}$
- 3. $\psi^{\alpha} = Yz_{\alpha} / \sqrt{\lambda_{\alpha}} = XL {}^{t}L\phi_{\alpha} / \sqrt{\lambda_{\alpha}} = XQ\phi_{\alpha} / \sqrt{\lambda_{\alpha}}$
- 4. ${}^{t}\mathrm{XD}\psi^{\alpha} = {}^{t}\mathrm{XDXQ}\phi_{\alpha} / \sqrt{\lambda_{\alpha}} = \sqrt{\lambda_{\alpha}\phi_{\alpha}}$

The two last results of the proposition can be extended to variables and observations not used for the computation of V and W: they are named supplementary variables and observations. Let X₀ be the row of the values of such an observation (respectively X^0 the column of the values of such a variable): $X_0 Q \phi_\alpha$ will be the coordinate of this observation on the axis α (Respectively $X^0 D \psi^{\alpha}$).

Proposition 1.2.3

Let Ψ (respectively Φ) be the matrix with ψ^{α} as column α (respectively ϕ_{α}) and Λ the diagonal matrix with $\Lambda_{\alpha\alpha} = \lambda_{\alpha}$. We will note $\Psi^{[k]}$ and $\Phi^{[k]}$ the k first columns of Ψ and Φ and $\Lambda^{[k]}$ the kxk diagonal matrix constructed from the first k rows and columns of Λ . Then:

- 1. $\Psi^{[k]} \Lambda^{[k] t} \Psi^{[k]} D$ is the best approximation of XQ^tXD and $Tr[(XQ^tXD \Psi^{[k]}\Lambda^{[k] t}\Psi^{[k]}D)^2] = \sum_{i=k+1,I} \lambda_i^2$
- 2. $\Phi^{[k]} \Lambda^{[k]} t \Phi^{[k]} Q$ is the best approximation of ${}^{t} X D X Q$ and $Tr[({}^{t} X D X Q \Phi^{[k]} \Lambda^{[k]} t \Phi^{[k]} Q)^{2}] = \sum_{i=k+1,I} \lambda_{i}^{2}$
- 3. $D^{1/2} \Psi^{[k]} \Lambda^{[k]t} \Phi^{[k]} Q^{1/2}$ is the best approximation of $D^{1/2} X Q^{1/2}$ and $Tr[(D^{1/2} \Psi^{[k]} \Lambda^{[k]1/2 t} \Phi^{[k]} Q D^{1/2} X Q^{1/2})^2] = \sum_{i=k+1,I} \lambda_i$

The *proof* is a part of more general results given in (Sabatier et al. 1984). It is easy to see that the usual practices of principal components analysis on the covariance matrix and on the correlation matrix correspond respectively to the choices $Q = I_{pxp}$ and $Q = [diag(^{t}XDX)]^{-1}$

Consider now a contingency table $P = (P_{ij}, i=1,I; j=1,J)$ with the usual notations for the margins $(P_{i,j}=1,I)$ and $(P_{j,j}, j=1,J)$. With the P_{i} (respectively the P_{j}) we construct a diagonal matrix D_I (respectively D_J). Let $X = D_I^{-1}(P - D_I I_I^t I_J D_J) D_J^{-1}$. It is easy to see that $XD_J I_J = 0$ and ${}^t I_I D_I X = 0$.

The well-known correspondence analysis method can be viewed as the principal components analysis of the triplet (X, D_J, D_I) .

1.3 Third choice: the RV coefficient

Consider now two studies $E_1 = (X_1, Q_1, D)$ and $E_2 = (X_2, Q_2, D)$ for the same observations and the same D matrix. This is the usual situation when you want to study the links between two sets of variables.

The respective principal component analyses of E_1 and E_2 lead to two configurations of the observations constructed with the two sets of principal components of W_1D and W_2D . It is natural to compare these two operators.

Let S(D) be the set of the D – symmetric nxn matrices, i.e the set of matrices nxn A such that $DA = {}^{t}AD$. S(D) contains all the operators WD.

The symmetrical bilinear form Tr(AB) is positive on S(D). Hence, it defines a scalar product on S(D).By similarity with the usual statistical vocabulary, we define:

- 1. $COVV(W_1D, W_2D) = Tr(W_1DW_2D)$
- 2. $VAV(W_1D) = Tr[(W_1D)^2]$
- 3. $RV(W_1D, W_2D) = TR(W_1DW_2D)/[Tr[(W_1D)^2]Tr[(W_2D)^2]]^{1/2}$

The following results help for the understanding of the significance of RV. Their proofs are given in (Escoufier 1986)

- 1. For any (X_1, Q_1, D) and $(X_2, Q_2, D): 0 \le RV(W_1D, W_2D) \le 1$
- 2. RV (W₁D, W₂D) = 1 if and only if W₁ = kW₂ for some non zero scalar k.
- 3. If Q_1 and Q_2 are positive definite, RV (W₁D, W₂D) = 0 if and only if ${}^{t}X_1DX_2 = 0$.

- 4. Let X_1 and X_2 be single variables and $Q_1 = Q_2 = 1$. Then: $COVV(W_1D, W_2D) = [cov(X_1, X_2)]^2$ $RV(W_1D, W_2D) = r^2(X_1, X_2)$
- 5. Let X₁ be a single variable and Q₁ = 1. Let p₂ be the number of variables in X₂. We choose Q₂ = $({}^{t}X_{2}DX_{2})^{-1}$. Then: $RV(W_{1}D, W_{2}D) = R_{X1/X2}^{2}/\sqrt{p_{2}}$ where R_{X1/X2} is the multiple correlation coefficient between X₁ and the variables in X₂.
- 6. Let $E_1 = (X_1, ({}^tX_1DX_1)^{-1}, D)$ and $E_2 = (X_2, ({}^tX_2DX_2)^{-1}, D)$ then: $RV(W_1, W_2) = \Sigma_{i=1,p2} \quad \rho_i^2/\sqrt{p_1p_2}$ where ρ_i is the canonical correlation coefficient of rank i between X_1 and X_2 .
- 7. Let X_1 be a single variable and $Q_1 = 1$. We suppose that X_2 is the nxp₂ array of indicator variables for a qualitative variable x_2 with p_2 levels. If the observation i takes the modality j, $X_{2i}^j = 1$ and $X_{2i}^k = 0$ for $k \neq j$. We choose $Q_2 = ({}^tX_2DX_2) {}^{-1} = D_2^{-1}$ the inverse of the diagonal matrix of the weights of the levels. Then:

 $RV(W_1D, W_2D) = \eta_{X1/X2}^2 / \sqrt{p_2}$

where η_{X_1/X_2}^2 is the rate of correlation between the quantitative variable X_1 and the qualitative variable x_2 .

- 8. X_1 (respectively X_2) is the array nxp_1 (respectively nxp_2) of the indicator variables of the qualitative variable x_1 (respectively x_2). We choose $Q_1 = D_1^{-1}$ and $Q_2 = D_2^{-1}$. Then:
- $RV(W_1D, W_2D) = (\chi^2/n + 1)/\sqrt{p_1p_2}$
- 9. If moreover, the columns of X₁ and X₂ are centred for D, we have: $RV(W_1D, W_2D) = \chi^2/(n\sqrt{((p_1 - 1)(p_2 - 1))}) = T^2$ where T² is the Tchuprov coefficient.

1.4 Bibliographical hints

The two concepts of operator related to a data matrix and RV coefficient were first introduced in (Escoufier 1970) and (Escoufier 1973).The distribution of the RV coefficient was studied in (Cléroux and Ducharme 1989). The study has been enlarged to rank data in (Cléroux et al. 1994).Going from matrix language to linear applications allows us to introduce the duality diagram of which the triplet (X, Q, D) can be seen a summary. We do not follow this point of view here. Interested readers will find detailed presentation of this approach either in the book written by its pioneers (Caillez and Pagès 1976) or in (Escoufier 1987). A very complete recent **R** package and courses are available at http://pbil.univ-lyon1.fr/R/enseignement.html with comments in French and in English; a large collection of sets of data is proposed. See also (Chessel et al. 2004).

2 Joint analysis of several data matrices (the STATIS method)

Consider a set of data analyses $(X_i, Q_i, D); i = 1, \dots, I$ on the same observations provided with the same weights and the family of related operators $W_i, D; i = 1, \ldots, I$. Our aim is to study the proximities and the differences between these I analyses.

2.1 Global comparison of the data analyses (Intrastucture)

Let C be the IXI matrix with elements $C_{ij} = COVV$ (W_iD, W_jD). Let r be the rank of C ($r \leq I$). We note Γ the Ixr matrix of the eigenvectors of C and Θ the rxr diagonal matrix of the eigenvalues. By the spectral decomposition theorem, we have: $C = \Gamma \Theta^t \Gamma$ with ${}^t \Gamma \Gamma = I_{rxr}$.

So there exists a configuration of points $(P_i; i=1,I)$ in \mathbb{R}^r such that each data analysis is represented by a point. The coordinates of P_i are the elements of the ith row of $\Gamma \Theta^{1/2}$. In this configuration the distance between P_i and P_j is $d(P_i, P_j) = (C_{ii} + C_{jj} - 2C_{ij})^{1/2}$. Of course practical thought leads to limit the representation to two or three eigenvectors of C associated with the largest eigenvalues. The quality of the approximation is evaluated by the usual tools: rate between the extracted eigenvalues and Tr(C) for example.

If the norms of the operators are very different, it could be better to conduct the same analysis with the matrix R with elements RV (W_id, W_jD). In this case the distance between P_i and P_j is $(2(1 - RV (W_i d, W_j D))^{1/2}$.

2.2 Looking for a summary (the compromise)

We have seen that the quantities COVV are always non negative. So, the matrix C has a first eigenvector, γ_1 , the elements of which can be chosen non negative. Let $(\gamma_{1i}, i=1, I)$ these elements.

Proposition 2.2.1

For all $(\beta_i, i=1,I)$ such that $\beta_i \geq 0$ and $\sum_{i=1,I} \beta_i^2 = \sum_{i=1,I} \gamma_{1i}^2 = 1$, we have:

 \leq

- $$\begin{split} 1. \ VAV(\sum_{i=1,I} \beta_i W_i D) &\leq VAV(\sum_{i=1,I} \gamma_{1i} W_i D) = \theta_1 \\ 2. \ \sum_{i=1,I} [COVV(\sum_{j=1,I} \beta_j W_j D, W_i D)]^2 \\ \Sigma_{i=1,I} [COVV(\sum_{j=1,I} \gamma_{1j} W_j D, W_i D)]^2 &= \theta_1^2 \end{split}$$

The *proof* comes from the two following equalities:

- 1. $VAV(\sum_{i=1}^{J} \beta_i W_i D) = Tr[(\sum_{i=1}^{J} \beta_i W_i D)^2] = {}^t \beta C \beta$
- 2. $\sum_{i=1,I} [COVV(\sum_{j=1,I} \beta_j W_j D, W_i D)]^2 = {}^t \beta C^2 \beta$

These results look like the results obtained in principal component analysis for the first component. As a matter of fact, they are analogous. In principal

component analysis, the objects are the variables and the inner product is the usual covariance. Here, the objects are the operators related to the statistical studies and the inner product is *COVV*.

 $WD = \sum_{i=1,I} \gamma_{1i} W_i D$ which has the largest norm and which maximizes the sum of squares of the inner products with the initial operators is named the compromise of the I studies. As a non negative linear combination of semi definite positive operators, WD is semi definite positive. So let ν be the number of non zero eigenvalues of WD and let Ψ the $n \times \nu$ matrix of its eigenvectors such that ${}^{t}\Psi D\Psi = I_{\nu \times \nu}$ and Λ the $\nu \times \nu$ diagonal matrix of its eigenvalues. The $\Psi \Lambda^{1/2}$ coordinates give a representation of n points. One point represents one initial observation. The proximity of two points is interpreted as an average similarity of the associated observations.

2.3 Comparison of the initial studies with the compromise (Interstructure)

2.3.1 Representation of the observations

Let $\lambda_{\alpha}^{1/2} \Psi^{\alpha} = WD\Psi^{\alpha}/\sqrt{\lambda_{\alpha}}$ the coordinates of the observations on the axis α in the representation associated to the compromise.

We define $\lambda_{\alpha}^{1/2} \Psi_k^{\alpha} = W_k D \Psi^{\alpha} / \sqrt{\lambda_{\alpha}}$. If $W_k D = WD$ then $\Psi_k^{\alpha} = \Psi^{\alpha}$ and the representation of the observations given by W_kD is exactly similar to the representation obtained from the compromise WD . When W_kD goes away from WD, the similarity of the representations decreases.

Moreover, $WD = \sum_{k=1,I} \gamma_{1k} W_k D$ and thus $\lambda_{\alpha}^{1/2} \Psi^{\alpha} = \sum_{k=1,I} \gamma_{1k} \lambda_{\alpha}^{1/2} \Psi^{\alpha}$.

The coordinate of one observation given by the compromise is the barycentre of the coordinates of this observation given by the different studies on the same axis. When the index of the initial studies is the time, it is usual to speak of the trajectories of the observations in the representation obtained by the compromise.

2.3.2 Representation of the variables

All the variables of the initial studies and all the linear combinations of these variables (for instance the principal components of the initial variables) can be represented as supplementary variables in the compromise. As in principal component analysis, the proximity between one variable's projection and one axis is used to interpret the axis. The coordinate of a variable X^{j} on the axis α is given by the covariance $c_{\alpha j} = {}^{t} X^{j} D \Psi^{\alpha}$ between X^{j} and Ψ^{α} .

From a practical point of view we must keep in mind that at this step the number of points in the representations is very large: nx(I+1) for the observations only .Careful algorithmic and numerical choices have to be made for method to be feasible.

2.4 Bibliographical hints

The first publication on this topic is (Escoufier 1977). The two following papers consider the situation of a set of similarity or covariance matrices (Escoufier and L'Hermier 1978), (Escoufier 1980). A very detailed approach of the practical problems can be found in (Lavit et al. 1994); in an application , we must choose between the COVV approach and the RV approach; but choices are also necessary for the representations: they could be centred or not. All the situations are explained carefully .The book written by (Lavit 1988) gives many examples and suggest some software. An application in the field of sensometrics is the subject of the paper by (Schlich 1996). STATIS has been developed for a family of data array. This means that in STATIS we have three indices: one for each array, one for the observations and one for the variables. So, we can use the term of three – way multiblock for the data. (Vivien and Sabatier 2003) and (Sabatier and Vivien 2004) explore extension of STATIS to the joint analysis of two three – way multiblocks or for a four – way multiblock.

3 Principal component analysis with respect to instrumental variables

3.1 The problem and its linear solution

We are interested here with situations in which we have two sets of data observed on the same observations provided with the same weights. We suppose that the two sets do not play the same role. One of them is a reference, a target. The objective is to know if the variables of the second set can reconstruct the principal component analysis of the target set. We will note (Y, Q, D) the target study where Y is nxp .The pxp Q matrix is known. Let $W_yD =$ YQ^tYD the operator related to this study. From the second set, we only know the data array X, nxq, and we use the same diagonal matrix of the weights D. We consider the following problem:

Find M a $q \times q$ semi definite symmetric matrix such that:

 $Tr[(YQ^tYD - XM^tXD)^2]$ is minimum.

Proposition 3.1.1

Let $R = ({}^{t}XDX)^{-1} t^{X}DYQ^{t}YDX({}^{t}XDX)^{-1}$ then:

 $Tr[(YQ^{t}YD - XM^{t}XD)^{2}] =$ $Tr[(YQ^{t}YD - XR^{t}XD)^{2}] + Tr[(YR^{t}YD - XM^{t}XD)^{2}]$

The proof is given in (Bonifas et al. 1984). The result shows that the discrepancy between YQ^tYD and XM^tXD is the sum of two terms. The first one

does not depend on M. It assesses the part of the representation of the observations given by (Y, Q, D) which will never be reconstructed from a study based on X. The second term depends of the selected M. It shows obviously that the best choice for M is R.

Let $P_X = X(^t X D X)^{-1 t} X D$ the *D*-orthogonal projector on the subspace of R^n spanned by the columns of X.We have:

$$XR^tXD = P_XYQ^t(P_XY)D$$

Thus, the operators related to the studies (X, R, D) and $(P_X Y, Q, D)$ are identical .They give the same representation of the observations. This means that the best reconstruction of the representation of the observations given by (Y, Q, D) is obtained when applying the same Q matrix to the projections of the variables Y on the subspace of \mathbb{R}^n spanned by the variables in X.

3.2 Quality of the linear solution

From the properties of the projectors and of the trace, we obtain:

Proposition 3.2.1

- 1. $Tr(^{t}YDYQ) = Tr(^{t}(P_XY)D(P_XY)Q) + Tr(^{t}((I_{n\times n} P_X)Y)D((I_{n\times n} P_X)Y)Q)$
- 2. $Tr(YQ^tYD) = Tr((P_XY)Q^t(P_XY)D) + Tr(((I_{n\times n} P_X)Y)Q^t((I_{n\times n} P_X)Y)D)$

The proposition shows that the total inertia of the study (Y, Q, D) can be cut in two parts, one given by the projections of the variables Y on the subspace of \mathbb{R}^n spanned by the variables X and one part given by the projections in the orthogonal sub-space.

The second result of the proposition says that the decomposition is true for each diagonal element of YQ^tYD which is the norm of this element multiplied by its weight. This quantity is the inertia of the observation with respect to the origin.

The first result shows that, when Q is diagonal, an analogous decomposition is available for the variances and this is well-known.

The ratio $Tr({}^t(P_XY)D(P_XY)Q)/Tr({}^tYDYQ)$ can be used for appreciating the quality of the reconstruction. When $Q = I_{p \times p}$, this ratio is the coefficient of Stewart and Loeve. It can be used as a basis for a permutation test of significance for the reconstruction. The following proposition shows that $RV(YQ{}^tYD, (P_XY)Q{}^t(P_XY)D)$ can be also used for such an evaluation.

Proposition 3.2.2

$$TR((YQ^{t}YD - (P_{X}Y)Q^{t}(P_{X}Y)D)^{2}) = Tr((YQ^{t}YD)^{2}) \times$$
$$\times (1 - (RV(YQ^{t}YD, (P_{X}Y)Q^{t}(P_{X}Y))^{2})$$
(1)

Let Z be a third data array observed on the same observations provided with the same weights. We can do for P_Z and $(I_{n\times n} - P_X)Y$ what we did for P_X and Y. We will obtain a decomposition of the inertia contained in the subspace orthogonal to the space spanned by the variables in X. It is clear that all the results traditionally used in analysis of variance for the decomposition of the variance with respect to factors, orthogonal or not, can be developed here for the decomposition of the inertia of (Y, Q, D).

3.3 Non linear solution

We consider a finite set of functions $(b_k; k = 1, ..., l)$ and F the set of the linear combinations of these functions. Let B^j the matrix $n \times l$ in which $B_i^{jk} = b_k(X_i^j)$ where X_i^j is the value taken by the observation i for the variable j. Let t_j a vector with l elements. We consider the non linear transformation of X^j defined by: $f(X^j) = \sum_{k=1,...,l} t_{jk} B^{jk} = B^j t_j$.

Let B the $n \times (q \times l)$ matrix obtained by the juxtaposition of the matrices B^j and T, the $(q \times l) \times q$ matrix constructed with the $(t_j; j = 1, q)$ in such a way that the column j of BT is $B^j t_j$.

We can look for the solution of the following problem: Find T and R such that $Tr((YQ^tYD - BTR^tT^tBD)^2)$ is minimum.

For a given T, we obtain from the preceding paragraphs an explicit solution for R. When R is known, T can be computed through a numerical algorithm. The solution will be obtained by an iterative algorithm based on these two steps.

3.4 Bibliographical hints

The method of principal components with respect to instrumental variables is a part of the basic paper by (Rao 1965). It has been presented through the use of the RV coefficient in (Robert and Escoufier 1976). Canonical analysis and discriminant analysis are also presented in that paper as an RV optimisation problem. Here we have followed the presentation published in (Bonnifas et al. 1984). For the paragraph 3.2, we recommend (Fraile et al. 1993) which gives the details of an application in the correspondence analysis context and also the paper by (Kazi – Aoual et al. 1995) which gives the explicit first three moments for the distribution of the permutation test. The non linear approach is mainly based on the work of (Durand 1992, 1993). (Imam et al. 1998; Schlich and Guichard 1989) are applications. In the beginning of the research on RV, the choice of variables in principal components analysis was the main goal. This topic has been presented as a contributed paper in Compstat 1974 in Vienna (Escoufier et al. 1974).See also (Escoufier and Robert 1979).

We have considered before the operator $(I_{n\times n} - P_X Y)Q^t(I_{n\times n} - P_X Y)D$ related to the study $((I_{n\times n} - P_X)Y, Q, D)$. In such a study, all the information orthogonal to the X variables is deleted. Consider Z a $qx \times r$ matrix and $P_Z = Z(^tZQZ)^{-1}ZQ$. The array $(I_{n\times n} - P_X)Y^t(I_{q\times q} - P_Z)$ has its columns D – orthogonal to X and its rows Q – orthogonal to Z. Some authors use these results in correspondence analysis to avoid linear, quadratic or cubic components. They introduce suitable constraint matrices X and Z (Beh 1997), (D'Ambra et al. 2002).

4 Conclusions

It could be useful in this survey to recall the construction of the results along the years.

- 1. First Steps: The initial work (Escoufier 1970) focussed on sampling of variables in a family of variables. The aim was to quantify the discrepancy between the principal component analysis of the family and the principal component analysis of the sample of variables. The not yet called RV coefficient was proposed. The immediate consequence was an interest for the choice of variables in principal component analysis (Escoufier et al. 1974). We stress the applied focus of this approach.
- 2. Then two theoretical orientations appeared. The first was the use of the *RV* coefficient as a unifying tool for the presentation of the different methods of multivariate analysis (Robert and Escoufier 1976). They were presented as solutions of optimization problems under various constraints. The second orientation sprang to mind from collaboration with JP. Pagés and F. Caillez. It appeared that the operator related to a data matrix found a natural place in the duality diagram which was at the centre of their own work on data analysis. All the work accomplished after that to present the different multivariate analysis methods through a particular triplet (X, Q, D) have their beginning in this convergence.
- 3. STATIS came from another convergence. Two topics were often discussed in statistical literature: multidimensional scaling and joint analysis of several data matrices. The operators related to data matrices and their scalar product COVV gave a very straightforward solution for the global comparison of the studies. The property of the solution (the compromise is also an operator) has been exploited for the definition of the two other steps of the method.
- 4. In France, the use of supplementary observations and supplementary variables was frequent in principal component analysis and correspondence analysis. This practice which uses at the end of a study information known at its beginning is rather questionable from a logical point of view even if it is useful. The principal component analysis with respect to instrumental variables method allows one to take into account the instrumental variables from the beginning of the study and moreover gives a quantification of their effects. This is the reason for its development.

The reader will recognize three types of references in this article. The oldest, often in French, are given for historical reasons. They had opened

the field. The second, in English, can be found more easily. They have been chosen for the interested readers who want to go further in this approach of data analysis. The third, the most recent, are by colleagues younger than me, who have been actors of this story and who are always very active. When I name them, I know that I commit two injustices: One towards them because their works do not find in my article a sufficient place and one towards other researchers who made important contributions to the topic. I hope that they will forgive me.

Acknowledgements

I wish to thank the scientific committee of Compstat 2006 and its president, Professor Alfredo Rizzi, who invited me for this contribution. They have given to me the opportunity to go back over what has been written about operator related to a data matrix. This exercise has been a pleasure for me. Several colleagues helped me find appropriate references: I thank them very much. I am most grateful to Susan Holmes for her judicious comments and suggestions.

References

[Beh97]	Beh E.J (1997) Simple correspondence analysis of ordinal cross - clasifi-
	cations using orthogonal polynolials. Biometrical Journal 39, 589 – 613
[BEG84]	Bonifas L, Escoufier Y, Gonzalez P.L, Sabatier R (1984) Choix de vari-
	ables en analyse en composantes principales. Rev. Statistique Appliquée
	XXXII(2) 5 – 15
[CP76]	Caillez F, Pages J.P (1976) Introduction á l'analyse des données SMASH,
	Paris
[CDT04]	Chessel D, Dufour A.B, Thioulouse J (2004) The ade4 package – I: One-
	table methods. R News 4: 5–10
[CD89]	Cléroux R, Ducharme G (1989) Vector correlation for elliptical distribu-
	tion. Comm. Stat. A, 18, 1441 – 1454.
[CLL95]	Cléroux R, Lazraq A, Lepage Y (1995) Vector correlation based on ranks
	and a nonparametric test of no association between vectors. Communica-
	tions in Stat., 24, 713 – 733.
[DBA05]	D'Ambra L, Beh E.J, Amenta P (2005) Catanova for two – way contin-
	gency tables with ordinal variables using orthogonal polynomials. Com-
	munications in statistics, theory and methods, 34, 1755 – 1770.
[Dur92]	Durand J.F (1992) Additive spline discriminant analysis. In: Y. Dodge
	and J.C. Whittakers (eds) Computational Statistics, Heidelberg: Physica
	– Verlag,I, 145–150.
[Dur93]	Durand J.F (1993) Generalized principal component analysis with respect
	to instrumental variables via univariate spline transformations. Compu-
	tational Statistics and Data Analysis, 16, 423 – 440.
[Esc70]	Escoufier Y (1970) Echantillonnage dans une population de variables aléa-
	toires réelles.Publl. Inst.Statist. Univ. Paris 19, 4, 1 – 47.

- [Esc73] Escoufier Y (1973) Le traitement des variables vectorielles. Biometrics 29, 751 760.
- [Esc77] Escoufier Y (1977) Operators related to a data matrix. In: J.R. Barra (ed) Recents developpements in Statistics: North – Holland Publishing Company, 125 – 131.
- [Esc80] Escoufier Y (1980) Exploratory data analysis when data are matrices. In:
 K. Matusita (ed) Recent developments in Statistical inference and data analysis: North Holland Publishing Company
- $\begin{array}{ll} \mbox{[Esc86]} & \mbox{Escoufier Y (1986) A propos du choix de variables en analyse des données.} \\ & \mbox{Metron XLIV, } 31-47. \end{array}$
- [Esc87] Escoufier Y (1987) The duality diagramm : a means of better practical applications. In: Legendre P. and Legendre L (eds) Development in numerical ecology, Nato ASI series, Vol.G14, Springer – Verlag, Berlin Heidelberg, 139–156.
- [EL78] Escoufier Y, L'Hermier H (1978) A propos de la comparaison graphique des matrices de variance. Biom.J. vol.20, 477 – 483.
- [ER79] Escoufier Y, Robert P (1979) Choosing variables and metrics by optimizing the RV coefficient. In: Optimizing methods in Statistics: Academic Press, Inc.
- [ERC74] Escoufier Y, Robert P, Cambon J (1974) Construction of a vector equivalent to a given vector from the point of view of the analysis of principal components: Compstat, Vienne.
- [FER93] Fraile L, Escoufier Y, Raibaut A (1993) Analyse des correspondances de données planifiées: étude de la chémotaxie de la larve infestante d'un parasite. Biometrics 49, 1142 – 1153.
- [Hol06] Holmes S (2006) Multivariate Statistics: The French Way In: D.Nolan and T. Speed (eds) Festschrift for David Freedman, IMS Lectures Notes – Monograph Series, Ohio.To appear.
- [IAE98] Iman W, Abdelkbir S, Escoufier Y (1998) Quantification des effets spatiaux linéaires et non linéaires dans l'explication d'un tableau de données concernant la qualité des eaux souterraines. Rev. Statistique Appliquée, XLVI (3) 37 – 52.
- [Lav88] Lavit Ch (1988) Analyse conjointe des tableaux quantitatifs: Masson, Paris
- [LES94] Lavit Ch, Escoufier Y, Sabatier R, Traissac P (1994) The ACT (STATIS method). Computational Statistics & Data Analysis 18, 97 – 119.
- [KHS95] Kazi-Aoual F, Hitier S, Sabatier R, Lebreton J.D (1995) Refined approximations to permutation tests for multivariate inference. Computational Statistics & Data Analysis 20, 643 – 656.
- [Rao65] Rao C.R (1965) The use and interpretation of principal component analysis in applied research. Sankhya A 26, 329 – 358
- $[{\rm RE76}] \qquad {\rm Robert \ P, \ Escoufier \ Y \ (1976) \ A \ unifying \ tool \ for \ linear \ multivariate \ statistical \ methods: \ the \ RV \ \ coefficient. \ Appl.Statist. \ 25, \ 257-265 \ }$
- [SV04] Sabatier R, Vivien M (2004) A new linear method for analyzing four way multibloks tables: STATIS – 4 submitted to Computational Statistics & Data analysis
- [SJE] Sabatier R, Jan Y, Escoufier Y (1984) Approximations d'applications linéaires et analyse en composantes principales In: E.Diday et al.(eds) Data Analysis and informatics III. Elsevier Science Publishers B.V. (North-Holland)

- [Sch96] Schlich P (1996) Defining and validating assessor compromises about product distances and attributes correlations. In: Naes T. and Risvik E (eds) Multivariate analysis of data in sensory science. Elesevier Science B.V.
- $\begin{array}{lll} [{\rm Sch89}] & {\rm Schlich \ P,\ Guichard \ E\ (1989)\ Selection\ and\ classification\ of\ volatile\ compounds\ of\ abricot\ using\ the\ RV\ coefficient.\ Journal\ of\ Agricultural\ and\ Food\ Chemistry,\ 37,\ 142-150 \end{array}$
- [VS04] Vivien M, Sabatier R (2004) A generalization of STATIS ACT strategy: Do ACT for multiblocks tables. Computational Statistics & data Analysis 46, 155–171