Computational Statistics & Data Analysis 18 (1994) 97–119 North-Holland

# The ACT (STATIS method)

# Christine Lavit, Yves Escoufier

Unité de Biométrie, ENSA.M-INRA-UM II, Montpellier, France

# Robert Sabatier

Faculté de Pharmacie, Département Pharmaceutique de Physique Industrielle, Statistique et Informatique, UM I, Montpellier, France

Pierre/Traissac ORSTOM, Montpellier, France

Abstract: ACT (STATIS method) is a data analysis technique which computes Euclidean distances between configurations of the same observations obtained in K different circumstances, and thus handles three-way data as a set of K matrices. In this article, the recent developments of the ACT technique are fully described – concepts and theorems related to Euclidean scaling being discussed in the Appendix – and the software manipulation is illustrated on real data.

Keywords: Euclidean vector spaces; Spectral decomposition; RV coefficient

# 1. Introduction

The ACT (STATIS method) is an exploratory technique of multivariate data analysis based on linear algebra and especially Euclidean vector spaces (ACT stands for Analyse Conjointe de Tableaux, STATIS stands for Structuration des Tableaux A Trois Indices de la Statistique). It has been devised for multiway data situations on the basic idea of computing Euclidean distances between configurations of points (Escoufier, 1973).

At the time or writing, ACT (STATIS method) and ACT (dual STATIS method) can be obtained from CISIA as executable codes running on a PC under DOS. This package encloses also the Fortran 77 code which runs on various mainframes. A more general flexible software will be implemented at the end of 1993 in SPAD distributed by CISIA too. Besides, writing and running the ACT procedure in your own environment is quite simple since only usual

Correspondence to: C. Lavit, Unité de Biométrie, ENSA.M-INRA-UM II, Place Viala, 34060 Montpellier, France.

0167-9473/94/\$07.00 © 1994 – Elsevier Science B.V. All rights reserved SSDI 0167-9473(92)00003-A



Fonds Documentaire ORSTOM Cote: Bx-19-147 Ex: 1

97

ds

h

e A

.e

зIJ

g, al

and the second second

routines about matrix computations and eigensystems are required.

For the time being, the software ACT (STATIS method) handles input data of this sort:

- A set of K matrices  $X_1, \ldots, X_K$ , each  $X_k$  of dimension  $I \times J_k$  is a data matrix of  $J_k$  quantitative variables measured on the same I observations.

- A set of I weights  $m_1, \ldots, m_I$ .

- Parameters to specify directives of computation and output.

This program centers obligatorily each variable of each  $X_k$  according to the weights  $m_1, \ldots, m_l$ . Denoting by  $W_k$  the scalar products between observations at stage k and D the diagonal matrix

 $\begin{pmatrix} m_1 & & \\ & \ddots & \\ & & \ddots & \\ & & & m_l \end{pmatrix}$ 

rescaled to obey  $\sum m_i = 1$ , we obtain the following results:

- Euclidean distances between  $W_k$  and  $W_{k'}$  or, in other words, between configurations of observations at stages k and k'. These distances are derived from the scalar product

$$\operatorname{Tr}(W_k D W_{k'} D)$$
 or  $\frac{\operatorname{Tr}(W_k D W_{k'} D)}{\sqrt{\operatorname{Tr}[(W_k D)^2]} \sqrt{\operatorname{Tr}[(W_{k'} D)^2]}}$ .

- Trajectories which reflect the contribution of each observation to the Euclidean distance between the  $W_k$ 's.

- A compromise matrix of dummy scalar products between observations, computed as a weighted sum of the  $W_k$ 's.

The software ACT (dual STATIS method) deals with the following input data:

- A set of K matrices  $X_1, \ldots, X_K$  corresponding to the same J quantitative variables measured on K different groups of  $I_1, \ldots, I_K$  observations.

- K sets  $D_1, \ldots, D_K$  of weights and, as before, parameters to specify directives of computation and output.

If  $V_k = X'_k D_k X_k$  denotes the covariance matrix at stage k, three main results are then carried out:

- Euclidean distances between the covariance matrices  $V_k$  and  $V_{k'}$  derived from the scalar product  $Tr(V_k V_{k'})$ .

- Trajectories which reflect the contribution of each variable to the Euclidean distance between the  $V_k$ 's.

- A compromise covariance matrix computed as a weighted sum of the  $V_k$ 's.

The next version of the software will let the user work on centred scalar products (as it was the case for  $W_k$ ), non-centred scalar products (as it was the case for  $V_k$ ) or scalar products centred on one on the *I* observations, and compute scalar products of the form  $Tr(W_k SW_{k'}S)$ , *S* being any positive definite symmetric matrix.

In the following chapter, we recall well-known underlying mathematics and geometric properties of scalar products derived from usual data matrices. Chapter 3 describes the up-to-date developments of the ACT technique. The software manipulation is illustrated on real data in chapter 4. The Appendix reviews concepts and theorems related to Euclidean scaling methods from an algebraic viewpoint.

To conclude this chapter, it should be noted that, in a recent work, Franc pointed out connections between different multiway techniques by rewriting them in a multilinear algebra context (Franc, 1992). A *n*-way data matrix is considered as an element of the tensor product of *n* vector spaces. And solutions provided by the different methods (TUCKER, PARAFAC/CANDECOMP, CANDELINK among others) are expressed as sums of tensor products of vectors which obey specific constraints.

# 2. A few remarks on scalar products between observations

# 2.1. Scalar products derived from data matrices

Let  $X_{IxJ}$  be a data matrix which consists of J variables measured on I observations.

Example 1. We describe the set of observations as:

- Vectors  $x_1, x_2, ..., x_1$  of a real vector space of dimension J, on which we define the scalar product:  $(x_i | x_{i'}) = \sum_j X_{ij} X_{i'j}$ . The scalar product  $(x_i | x_{i'})$  is the element  $W_{ii'}$  of W = XX'.

- Points of a metric space since  $d^2(i, i') = \sum_i (X_{ii} - X_{i'i})^2$ .

- A J-dimensional configuration of points  $M_1, M_2, \ldots, M_I$ . The coordinates of  $M_i$  are simply the elements  $X_{i1}, \ldots, X_{iJ}$  of X. Thus we have

 $\overrightarrow{\mathrm{OM}_{i}}.\overrightarrow{\mathrm{OM}_{i'}} = W_{ii'}$  and  $\left\| \overrightarrow{\mathrm{M}_{i}}\overrightarrow{\mathrm{M}_{i'}} \right\| = \mathrm{d}(i, i').$ 

Note that  $d^2(i, i') = ||x_i - x_{i'}||^2$  where  $|| \cdot ||$  is the norm induced by the scalar product (.|.). Then

$$d^{2}(i, i') = W_{ii} + W_{i'i'} - 2W_{ii'}$$

which implies that

$$W_{ii'} = \frac{1}{2} \left[ d^2(0, i) + d^2(0, i') - d^2(i, i') \right].$$

**Example 2.** Suppose now that the columns of  $X_{I\times J}$  are centred according to the weights  $m_1, \ldots, m_I$  with the constraint  $\sum_i m_i = 1$ . That is to say  $\sum_i m_i X_{ij} = 0$  for  $j = 1, \ldots, J$ . Therefore we describe the set of variables as:

- Vectors  $x_1, x_2, \ldots, x_I$  of a real vector space of dimension I. If we want the

scalar product  $(x_j | x_{j'})$  to be the covariance between variables j and j', it is necessary that:

$$(x_j \mid x_{j'}) = \sum_{i} m_i X_{ij} X_{ij'}.$$

The scalar product  $(x_j | x_{j'})$  is the element jj' of X'DX where D denotes the diagonal matrix whose elements are  $m_1, \ldots, m_I$ .





as the matrix of  $x_j$  in an orthogonal but unstandardized basis  $(e_1, \ldots, e_I)$ assuming  $||e_i||^2 = m_i$  for  $i = 1, \ldots, I$ . Then  $x_j = \sum_i X_{ij} e_i$  implies  $(x_j | x_{j'}) = \sum_i X_{ij} X_{ij'}$   $(e_i | e_i) = \sum_i m_i X_{ij} X_{ij'}$ . Since the basis  $(e_1, \ldots, e_I)$  is unstandardized, we do not have any trivial configuration of the variables using the original coordinates  $X_{1j}, \ldots, X_{Ij}$ .

Generalization Considering that the columns of  $X_{I\times J}$  are the rows of the transpose  $X'_{J\times I}$ , the two former examples are particular cases of the following general formulation. Let  $X_{I\times J}$  be a data matrix. We describe the set of the rows as vectors  $x_1, \ldots, x_I$  of a real vector space of dimension J. We define the scalar product  $(x_i | x_{i'}) = \sum_j \sum_{j'} Q_{jj'} X_{ij} X_{i'j'}$  as the element  $W_{ii'}$  of W = XQX', Q being a positive definite symmetric matrix. Then



is the matrix of  $x_i$  in any basis  $(e_1, \ldots, e_J)$  obeying  $(e_j | e_{j'}) = Q_{jj'}$ . The rows of  $X_{I \times J}$  can be plotted as points  $M_1 \ldots M_I$  generated by the original coordinates in a set of axes neither orthogonal nor standardized. Actually this representation is unsatisfactory for our perception used to classic Euclidean geometry in which axes are assumed to be rectangular and to have unit length. It is the reason why methods based on the spectral decomposition of W calculate coordinates of the points  $M_1, \ldots, M_I$  in a new suitable set of axes.

# 2.2. Configuration of points

Let us consider the matrix  $W_{I \times I}$  of scalar products between *I* elements, forgetting the way it has been calculated. The problem is to plot the *I* elements in a set of orthonormal axes. We briefly note a few results, more or less known, which are detailed in the Appendix.

W is a positive semi-definite symmetrix matrix. From the spectral decomposition of W:

$$W = P_{I \times r} \Lambda_{r \times r} P'_{r \times I}$$
 with  $P'P = I_{r \times r}$  (Identity matrix),

r denoting the rank of W, we obtain an Euclidean configuration  $M_1, \ldots, M_I$  in a r-dimensional space. The r coordinates of  $M_i$  are the elements of the *i*th row of  $P\Lambda^{1/2}$ . Consequently, the scalar products  $W_{ii'}$  and the distances d(i, i') can be calculated in a classical Euclidean context since

$$\overrightarrow{\mathrm{OM}_{i}}, \overrightarrow{\mathrm{OM}_{i'}} = W_{ii'}$$
 and  $\left\| \overline{\mathrm{M}_{i}\mathrm{M}_{i'}} \right\| = \mathrm{d}(i, i').$ 

The spectral decomposition of W is a particular singular value decomposition as it is defined in the Appendix. Let S be any  $I \times I$  positive definite symmetric matrix. It will be shown that W can be written as

 $W = P_{I \times r} \Sigma_{r \times r} P'_{r \times I}$  with  $P'SP = I_{r \times r}$  (Identity matrix).

The columns of P are the eigenvectors of the self adjoint matrix WS, and  $\Sigma$  is the diagonal matrix whose elements are the corresponding eigenvalues. If we denote by r the rank of W (or WS), we obtain another set of r coordinates of  $M_i$  by taking the elements of the *i*th row of  $P\Sigma^{1/2}$ . Similarly the scalar products  $W_{ii'}$  and the distances d(i, i') can be calculated in an usual Euclidean context since

$$\overrightarrow{OM_i} \cdot \overrightarrow{OM_{i'}} = W_{ii'}$$
 and  $\|\overrightarrow{M_i} \cdot \overrightarrow{M_{i'}}\| = d(i, i').$ 

**Remark.** If the scalar products have been derived from a data matrix  $X_{I \times J}$ , and hence from J coordinates, the rank of  $W_{I \times I}$  is less than the minimum of I and J.

# 2.3. Centred scalar products

Let us consider again a matrix of I observations on J variables and suppose now that the mean of the I observations is significant. Then we can deal with the centred matrix X obeying  $\sum_i X_{ij} = 0$ , or more generally  $\sum_i m_i X_{ij} = 0$  if the observations are weighted, in order to shift the mean to the origin. This derivation is equivalent to the transformation of the original W in  $W^G$  defined by

$$W_{ii'}^G = W_{ii'} - W_{i} - W_{i'} + W_{..}$$

where  $W_{i.} = \sum_{i'} m_{i'} W_{ii'} / \sum_{i} m_{i}$  and  $W_{..} = \sum_{i} \sum_{i'} m_{i} m_{i'} W_{ii'} / (\sum_{i} m_{i})^{2}$ . The singular value decomposition of  $W^{G}$ , or  $W^{G}S$ , S being any positive definite symmetric matrix, provides a configuration  $M_1, \ldots, M_l$  in a r-dimensional space in which the origin O is the centroid G of  $M_1, \ldots, M_I$  weighted by

 $m_1, \ldots, m_I$ . The rank r of  $W^G$  (or  $W^G S$ ) is less than the minimum of I-1 and J. Note that the case

$$S = D = \begin{pmatrix} m_1 & & \\ & \ddots & \\ & & m_I \end{pmatrix}$$

with the constraint  $\sum_i m_i = 1$  gives the principal components of the PCA of the centred data matrix  $X_{I \times J}$  when the eigenvalues of  $W^G D$  are ordered in the usual way. This choise leads to the agreeable interpretation of eigenvalues as variances of principal components.

# 2.4. Scalar product-like derived from dissimilarity matrices

If the data are available in the form of an  $I \times I$  matrix  $\Delta$  of dissimilarities between pairs of observations, some results are still valid:

- Choosing the observation  $i_0$  as origin, we can calculate the scalar product-like matrix  $W^{M_{i_0}}$  of dimension I-1, defined by

 $W_{ii'}^{M_{i_0}} = \frac{1}{2} \left[ \Delta_{i_0i}^2 + \Delta_{i_0i'}^2 - \Delta_{ii'}^2 \right].$ 

And reciprocally, given W we deduce

$$\Delta_{ii'}^2 = W_{ii} + W_{i'i'} - 2W_{ii'}.$$

– On the other hand, if we suppose that the mean of the I observations is significant, we can deal with the so-called Torgerson symmetric matrix  $W^G$  defined by

$$W_{ii'}^{G} = \frac{1}{2} \Big[ \Delta_{i.}^{2} + \Delta_{ii'.}^{2} - \Delta_{ii'}^{2} - \Delta_{..}^{2} \Big]$$

where  $\Delta_{i.} = \sum_{i'} m_{i'} \Delta_{ii'} / \sum_i m_i$  and  $\Delta_{..} = \sum_i \sum_{i'} m_i m_{i'} \Delta_{ii'} / (\sum_i m_i)^2, m_1, \dots, m_I$  being the weights of the observations.

- It is well known that  $W^{M_{i_0}}$  (or  $W^G$ ) is positive semi-definite if the dissimilarities are Euclidean distances and reciprocally. In this particular case, the singular value decomposition of W or WS provides a configuration  $M_1, \ldots, M_I$  of the observations in a r-dimensional space whether W is centred or not. In both cases, the rank r of W (or WS) is less than I-1.

# 3. Strategy for ACT: Scalar products between configurations

The central idea of the ACT technique is to compare configurations of the same observations obtained in different circumstances. Thus we need to introduce a measure of similarity between two configurations. This is equivalent to define a distance between the corresponding scalar product matrices. We can use the classic Euclidean norm

$$||W_1 - W_2||^2 = \sum_i \sum_{i'} [(W_1 - W_2)_{ii'}]^2 = \operatorname{Tr}[(W_1 - W_2)^2],$$

102

ł



Figure 1. The ACT procedure

or a weighted version

$$||W_1 - W_2||^2 = \sum_i \sum_{i'} S_{ii} S_{i'i'} [(W_1 - W_2)_{ii'}]^2,$$

or, more generally

$$||W_1 - W_2||^2 = \operatorname{Tr}[(W_1S - W_2S)^2]$$

for any positive definite symmetric matrix S. Although distances between symmetric matrices have been studied for a long time, it is more convenient to argue their properties as a particular case of distances between linear mappings. Definitions and algebraic derivations are discussed in the Appendix.

According to the data and the objectives of the analysis, we have first to decide which elements have to be compared. Then, it is necessary to specify from which origin we compute the scalar products  $W_k$ 's (whereas this question does not arise when we compute distances). We will illustrate these decisive choices and their consequences on a few examples in the last section.

# 3.1. Interstructure

104

First step: which distance between the  $W_k$ 's? Properties of these distances are discussed in the Appendix. We will simply list the different choices.  $- d^2(W_k, W_{k'}) = \sum_i \sum_{i'} [(W_k - W_{k'})_{ii'}]^2$  deduced from the scalar product  $(W_k | W_{k'}) = \text{Tr}(W_k W_{k'}) = \text{Tr}(W_k S W_{k'} S)$  with S equal to the identity matrix.  $- d^2(W_k, W_{k'}) = \sum_i \sum_{i'} S_{ii} S_{i'i'} [(W_k - W_{k'})_{ii'}]^2$  deduced from  $(W_k | W_{k'}) = \text{Tr}(W_k S W_{k'} S)$  with S diagonal. Note that for  $W_k^G$  centred on a weighted centroid G with weights  $m_1, \ldots, m_I$ , the matrix S can be any diagonal matrix and not necessarily

 $\begin{pmatrix} m_1 & & \\ & \ddots & \\ & & & m_I \end{pmatrix}.$ 

-  $d^2(W_k, W_{k'}) = Tr[(W_k S - W_{k'}S)^2]$  deduced from the scalar product  $(W_k | W_{k'})$ =  $Tr(W_k S W_{k'}S)$  where S is any positive definite symmetric matrix.

Second step: do we compare the  $W_k$ 's or the normed  $W_k$ 's? A large distance  $d(W_k, W_{k'})$  points out a strong difference between  $W_k$  and  $W_{k'}$ . Difference in shape or difference in size? To eliminate the second effect, we can compare the normed scalar products

$$\frac{W_k}{\|W_k\|} = \frac{W_k}{\sqrt{\mathrm{Tr}(W_k S)^2}}$$

and thus calculate

$$\left(\frac{W_k}{\|W_k\|} \left\|\frac{W_{k'}}{\|W_{k'}\|}\right) = \frac{\operatorname{Tr}(W_k S W_{k'} S)}{\sqrt{\operatorname{Tr}(W_k S)^2} \sqrt{\operatorname{Tr}(W_{k'} S)^2}} \right)^2$$

Graphical representation of the interstructure. Let  $W_{K\times K}$  be the interstructure matrix whose elements are the scalar products  $(W_k | W_{k'})$ . To plot the K stages in a two or three-dimensional space, say a h-dimensional space, we use the least squares approximation  $W_h$  of W, equal to the h first elements of the spectral decomposition  $\sigma_1 p_1 p'_1 + \cdots + \sigma_r p_r p'_r = P \Sigma P'$  of W, with P'P = I. Stage k is plotted as point  $M_k$  whose coordinates are the h first elements of the kth row of  $P \Sigma^{1/2}$ . The points  $M_1, \ldots, M_K$  satisfy  $\overline{OM}_k \cdot \overline{OM}_{k'} = (W_h)_{kk'}$ . And the loss function is

$$||W - W_h||^2 = \sum_{k} \sum_{k'} \left[ (W - W_h)_{kk'} \right]^2 = \sum_{l=h+1}^{r} \sigma_l^2.$$

On this graph, scalar products are not easily readable, except for the norm  $||W_k||$  approximated by the length of vector  $\overrightarrow{OM}_k$ , and for the scalar product between normed  $W_k$  and normed  $W_{k'}$  approximated by the cosine of  $(\overrightarrow{OM}_k, \overrightarrow{OM}_{k'})$ .

Distances  $d(W_k, W_{k'})$  can also be readable on a graph using the first elements of the spectral decomposition of the interstructure matrix  $W^G$ , centred on the

centroid G of the K stages, in a similar way. On these two graphs, the projected distance induced by least squares approximation is systematically lower than  $d(W_k, W_{k'})$ . Besides, it is possible to distort Euclidean distances  $d(W_k, W_{k'})$  into ultrametric distances and build a dendrogram, or use another technique of visual information.

# 3.2. Compromise

In this section, the  $W_k$ 's are required to be positive semi-definite whereas this restrictive assumption was not necessary in the interstructure derivations.

**Property 1.** Let  $W_1 = \sigma_1 p_1 p'_1$  be the first element of the spectral decomposition of the interstructure matrix W. Components of  $p_1$  can be chosen positive.

To establish this particular case of the Frobenius theorem, see Property 8 in the Appendix which implies that all the elements of W are positive. Consequently, in the configuration of the K stages, cosines are positive and angles  $(\overrightarrow{OM}_k, \overrightarrow{OM}_{k'})$  acute. Thus the points  $M_k$  are situated inside a convex cone.

**Definition 1.** The  $I \times I$  compromise matrix W is defined as a weighted sum  $\sum_k \alpha_k W_k$ . The coefficient  $\alpha_k$  is the coordinate of stage k in the one-dimensional plot deduced from the first element  $W_1$  of the spectral decomposition of W.

**Property 2.** As the  $W'_k$ 's are positive semi-definite and the  $\alpha'_k$ 's are positive, the compromise matrix W is positive semi-definite. Thus W will be considered as a scalar product matrix which induces a compromise configuration of the I elements.

**Property 3.** The compromise matrix W is the linear combination of the  $W_k$ 's the most related to each  $W_k$ . In other words, W maximizes

$$\sum_{l} \left( \sum_{k} \alpha_{k} W_{k} \mid W_{l} \right)^{2} / \sum_{k} \alpha_{k}^{2}.$$

Recalling that  $W_{kl}$  equals  $(W_k | W_l)$ , we develop the numerator into

$$\sum_{k} \sum_{k'} \alpha_k \alpha_{k'} \sum_{l} (W_k \mid W_l) = \sum_{k} \sum_{k'} \alpha_k \alpha_{k'} (W^2)_{k'k}.$$

In the spectral decomposition of W,  $p_1$  is the eigenvector of  $WW^* = W^2$  associated to the largest eigenvalue (see Property 7 of the Appendix). Thus the quotient can be written as the Rayleigh quotient

$$\frac{x'WW^*x}{\|x\|^2} \quad \text{with} \quad x = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_K \end{pmatrix},$$

which is maximum for  $x = p_1$ .

**Constraints on the**  $\alpha_k$ 's. If the  $W'_k$ 's are centred on a centroid G, or a particular element  $i_0$ , the compromise matrix W will obviously be centred in the same way. Similarly, if the origin is equidistant from the I elements at each stage k, this property holds for W. However when the  $W'_k$ 's are correlation matrices, it is necessary to rescale the  $\alpha'_k$ 's with the constraint  $\sum_k \alpha_k = 1$  in order to obtain a compromise of the same nature. If the  $W'_k$ 's are normed, the compromise will be rescaled to be normed too.

Interpreting the compromise. If  $W_k$  and  $W_{k'}$  correspond to similar configurations in shape and size, the angle  $(\overrightarrow{OM}_k, \overrightarrow{OM}_{k'})$  is small and the lenghts  $\|\overrightarrow{OM}_k\|, \|\overrightarrow{OM}_{k'}\|$  are nearly the same. This case leads to identical values for  $\alpha_k$ and  $\alpha_{k'}$ . On the other hand, a large difference between the two configurations induces either a large angle  $(\overrightarrow{OM}_k, \overrightarrow{OM}_{k'})$  or unequal lenghts for  $\overrightarrow{OM}_k$  and  $\overrightarrow{OM}_{k'}$ , and different values for  $\alpha_k$  and  $\alpha_k$  in both cases. Consequently W gives relatively less weight to outliers, and leads to a compromise configuration which reflects the inter-element distances as they are seen by the majority.

Graphical representation of the compromise. To plot the *I* elements according to the compromise in a *h*-dimensional space, we use the least squares approximation  $W_h$  of W, equal to the *h* first elements of the singular value decomposition  $\sigma_1 p_1 p'_1 + \cdots + \sigma_r p_r p'_r = P \Sigma P'$  of W, with P'SP = I. Element *i* is plotted as point  $M_i$  whose coordinates are the *h* first elements of the *i*th row of  $P \Sigma^{1/2}$ .

The points  $M_1, \ldots, M_I$  satisfy  $\overrightarrow{OM}_i \cdot \overrightarrow{OM}_{i'} = (W_h)_{ii'}$  and the loss function is

$$||W - W_h||^2 = \operatorname{Tr}[(WS - W_hS)^2] = \sum_{l=h+1}^r \sigma_l^2.$$

Note that it is logical, but not necessary, to take the same matrix S as the one used in the computation of the distances  $d(W_k, W_{k'})$ . Think, for example, to the case where S is not diagonal.

# 3.3. Trajectories

In this section, S is required to be diagonal. Then  $d^2(W_k, W_{k'})$  can be written element by element, as the sum  $\sum_i S_{ii}(\sum_{i'} S_{i'i'}[(W_k - W_{k'})_{ii'}]^2)$  and split into contributions of the different elements. This decomposition leads to an  $I \times [\frac{1}{2}K(K-1)]$  matrix from which we can detect which elements are strongly perturbed from one configuration to another.

However knowing the direction of the perturbation needs further investigations. We consider the  $W_k$ 's and the compromise W as matrices of linear mappings between an Euclidean vector space F and its dual  $F^*$  (see Appendix, Section 6).

$$w_k^i = \begin{pmatrix} (W_k)_{i1} \\ \vdots \\ (W_k)_{iI} \end{pmatrix}$$

is a vector of  $F^*$  which appears in the decomposition of  $d^2(W_k, W_{k'}) = \sum_i S_{ii} ||w_k^i - w_k^i \cdot ||^2$ . It is now of interest to know the direction of the different vectors  $w_k^i - w_{k'}^i$ . Eigenvectors  $p_1, \ldots, p_r$  of WS which occur in the singular value decomposition  $\sigma_1 p_1 p'_1 + \cdots + \sigma_r p_r p'_r$  of W, can be completed to form a s-orthonormal basis of  $F^*$ . The idea is to express  $w_k^i$  in this new basis.

**Graphical representation of the trajectories.** Unfortunately, if we want to plot the *I* elements as they are seen by the different stages in a unique two-dimensional space, it is obvious that none of the subspaces spanned by  $p_1, \ldots, p_r$  corresponds to the best choice. Nevertheless, we decide to restrict  $w_k^i$  to its projection on the two-dimensional space spanned by  $p_1$  and  $p_2$ .

In this space, we know that a least squares approximation of the compromise configuration is provided by the points  $M_1, \ldots, M_I$  whose coordinates are the components of  $\sigma_1^{1/2} p_1 = \sigma_1^{-1/2} WSp_1$  (namely the projections on  $p_1$  rescaled by  $\sigma_1^{-1/2}$ ) and  $\sigma_2^{1/2} p_2 = \sigma_2^{-1/2} WSp_2$ . In order to draw the trajectory of element *i* around its compromise position  $M_i$ , we rescale the projections of the  $w_k^i$ 's for  $k = 1, \ldots, K$ , in the same way. More precisely, we plot the *I* elements, as they are seen by stage *k*, by the points  $M_1^k, \ldots, M_I^k$  whose coordinates are the *I* components of  $\sigma_1^{-1/2} W_k Sp_1$  on the first axis and  $\sigma_2^{-1/2} W_k Sp_2$  on the second axis. In spite of this obvious lack of optimality, numerous examples show that, in practice, the vector  $\overline{M_i^k M_i^{k'}}$  gives a good idea of the importance and the direction of the change of position of element *i* between the stages *k* and *k'*.

# 3.4. Some applications of the ACT technique

**Example 1.** The first set of data, fully discussed in Chapter 4 consists of K matrices  $X_1, \ldots, X_K$  of I rows and J columns, corresponding to the judgment of K students on I of their professors according to J criteria. In this particular case, we decide to work on the matrices  $W_k^G = X_k X'_k$  after having centred each column of  $X_k$ . In other words we compare the configurations of the I professors as they are seen by each student, after having standardized severe and generous students to the same level of notation. Distances  $d(W_k, W_{k'})$  are interpreted as disagreements between judgments. The compromise matrix W provides a configuration of the I professors reflecting the majority opinion. And the trajectories point out who are the professors on which students are not in agreement.

On the other hand we can decide to study the correlation matrices  $V_k = (1/I)X'_kX_k$  (the columns of  $X_k$  being standardized to have mean 0 and unit variance). The objectives are then different. Forgetting the configurations of professors, we are now interested in associations or oppositions between criteria. Are they different from one student to another? Which criteria make the difference? Answers are given by the interstructure and the trajectories, whereas the compromise correlation matrix summarizes the  $V_k$ 's.

**Example 2.** Let us consider a set of five sociological data matrices  $X_{54}$ ,  $X_{62}$ ,  $X_{68}$ ,  $X_{75}$ ,  $X_{82}$  describing the evolution of the working population of I communes

around Montpellier in the last forty years. It happens that the definition of occupation groups changed from 1975 to 1982. Thus, the population has been classified into nine occupation groups for the four first census returns and only eight groups for the last one. Nevertheless the five configurations of the I communes can be compared through the matrices  $W_k^G$  (where the centroid G, weighted or not, represents a dummy average commune) or through  $W_k^{i_0}$  (if we take Montpellier, indexed by  $i_0$ , as a reference).

**Example 3.** The third set of data consists of J variables characterizing different stages of the sleep, collected on  $I_1$  narcoleptics and  $I_2$  persons in good health, after 16 hours, 20 hours and 24 hours of wakefulness. Comparing the six correlation matrices by means of the interstructure and the trajectories can be a first approach to understand how this disease disturbs the distribution of the different stages of the sleep, whereas the compromise matrix is not of interest here.

**Example 4.** The last set of data concerns I sites described by three specialists: a botanist, a pedologist and a biologist. The botanist describes the floristic composition of the sites by an  $I \times J_1$  presence-absence data matrix. The pedologist provides an  $I \times J_2$  data matrix of chemical characteristics of the soil, and the biologist gives an  $I \times J_3$  data matrix concerning the abundance of various earthworms.

If two sites are claimed similar by the biologist, are they found similar by the pedologist or the botanist? To deal with such a situation, we have to discuss with each specialist which dissimilarity or distance is appropriate, then derive scalar product-like matrices  $W_1$ ,  $W_2$  and  $W_3$  centred on a reference site  $i_0$ , and compare them by means of the interstructure for which the positivity of the  $W_k$ 's is not required. Further information can be extracted from the decomposition of the squared distance  $d^2(W_k^{i_0}, W_k^{i_0})$  between specialists into contributions of the different sites.

Suppose now that the data are available in the form of K dissimilarity matrices, each matrix corresponding to a dissimilarity coefficient  $\delta_k$  whose square root is an Euclidean distance as Rogers and Tanimoto, Russel and Rao or Ochiaï coefficients (Fichet and Le Calvé, 1984). In this case, instead of performing only the first step of ACT on the scalar product-like matrices straightforward derived from the  $\delta'_k$ s, we can operate the whole procedure on the positive semi-definite  $W_k$ 's derived from the square roots  $\sqrt{\delta_k}$  as follows:

$$(W_k^{i_0})_{ii'} = \frac{1}{2} [\delta_k(i_0, i) + \delta_k(i_0, i') - \delta_k(i, i')].$$

The compromise matrix W induces Euclidean distances between sites which satisfy  $d^2(i, i') = \sum_k \alpha_k \delta_k(i, i')$ . And, all things considered, as  $\sqrt{\delta}$  is a monotonic function of  $\delta$ , performing ACT on  $\sqrt{\delta}$  instead of  $\delta$  turns out to be a useful insight into the structure of the original dissimilarity matrices.

# 4. Input and output of the 01.90 version of ACT (STATIS method)

**Input.** K = 8 students judge I = 11 professors by means of J = 7 criteria: competence, lucid explanation, pedagogy, cheerfulness, is the professor dynamic? accessible? does the student find the subject interesting? The data are given in Table 1.

"Practice" having missing values, is considered as a supplementary row and ignored when we compute the  $W_k$ 's and the compromise. The other active rows have identical weights  $m_i = 1/10$ . Practice has weight 0. The preprocessing of the data consists of centering each column of each  $X_k$  according to those weights. Thus we compare the  $10 \times 10$  matrices  $W_k^G$  centred on the centroid G of the ten active rows,  $W_4^G$  being derived from only six criteria.

**Interstructure output.** The norms of the  $W_k$ 's are derived from the scalar product  $(W_k | W_{k'}) = \text{Tr}(W_k S W_{k'} S)$  where S is diagonal and equal to



These norms are equal to 119, 151, 87, 78, 101,117, 137 and 102. Since they are different, we decide to compute the Euclidean distances between the normed  $W_k$ 's deduced from the RV-coefficients (Definition 9 of the Appendix). We note that the opinion of judges no. 2 and no. 8 fairly differs from the others.

**Compromise output.** The compromise matrix W is defined as the linear combination  $\sum_k \alpha_k W_k$  of normed  $W_k$ 's with  $\alpha_k$  equal to the coordinate of judge k on the first axis of Figure 2. W gives relatively less weight to judges nr. 2 and nr. 8, and leads to a configuration of the professors which reflects principally the opinion of the six judges left.

$\alpha_k$	0.18	0.08	0.17	0.17	0.22	0.20	0.21	0.11
$d^2(W, W_k)$	0.46	1.32	0.60	0.61	0.19	0.33	0.27	1.06

Since the  $W_k$ 's are centred on the centroid G of the active rows, the compromise W is centred in the same way. In addition, as the data are available in the form of observations × variables matrices, we have  $J_1 + \ldots + J_8$  variables at our disposal. We can then compute their correlations with the coordinates of the compromise points in order to explain the position of the different professors.

**Trajectories output.** In the interstructure output, we noted that the distances between judge no. 2 and the others were quite important. It is interesting to

# Table 1

computer science	judge nr. 1	judge nr. 2	judge nr. 3	judge nr. 4
architecture	13 18 8 1 13 3 20	18 18 10 2 14 12 18	15 18 10 4 10 0 18	14 17 7 12 2 10
theory	121053957	6 4 8 2 4 12 16	12 5 4 8 10 8 10	6 5 7 5 10 7
languages	410 6 6 610 2	2 2 2 4 2 20 10	10 12 5 6 5 3 10	3 2 3 2 4 3
practice	17 16 17 17 17 18 18	18 20 18 12 14 18 18	14 13 15 12 12 10 13	14 12 14 10 15 13
economics	15 12 13 14 13 18 9	14 16 14 12 10 18 10	13 12 12 12 12 11 11	767 4165
accounting	16 18 15 11 13 15 15	18 18 18 12 16 16 18	17 15 15 14 12 14 14	16 16 14 12 12 13
management	1212911179	18 20 18 10 12 18 14	19 16 18 13 15 12 16	16 14 10 7 3 12
information system design	$10\ 18\ 0\ 2\ 12\ 2\ 17$	16 18 18 16 14 18 16	$16\ 2\ 2\ 2\ 2\ 2\ 12$	555 269
statistics	17 12 16 19 20 19 13	18 16 18 12 12 18 14	15 6 14 12 15 10 5	10 11 10 5 14 12
operations research	11 8 5 1 8 1 15 ,	$18\ 16\ 14\ 0\ 14\ 6\ 16$	$15\ 13\ 8\ 2\ 2\ 2\ 10$	13 13 7 10 3 14
English	17 18 15 10 13 15 15	10 4 2 0 4 4 8	$15\ 10\ 10\ 0\ 12\ 5\ 4$	17 13 10 13 10 9
computer science	judge nr. 5	judge nr. 6	judge nr. 7	judge nr. 8
architecture	14 15 0 0 7 0 15	19 18 5 3 15 1 18	15 15 0 0 11 5 13	18 14 11 17 15 15 16
theory	12 8 8 8 15 16 9	11 14 13 8 17 15 17	12 15 12 11 14 15 13	18 18 17 12 17 18 15
languages	5200280	8412111	10 0 5 5 1 5 1	17 18 18 10 12 14 15
practice	16 15 16 14 10 14 16	14 12 13 15 17 18 17	20 15 14 13 16 14 18	
economics	12 10 15 15 10 15 7	9 12 15 17 16 14 15	15 12 15 16 15 18 14	16 15 15 12 17 18 17
accounting	16 15 15 12 14 13 14	19 17 18 15 17 3 15	16 13 15 11 14 14 14	16 16 12 5 10 14 16
management	814 9 215 8 3	15 13 15 12 17 5 15	12 15 12 10 12 6 18	14 10 11 9 14 10 16
information system design	12 7 5 7 5 10 14	12 5 3 2 10 15 13	$15\ 10\ \ 0\ 15\ 12\ 15\ 10$	19 18 19 17 17 14 12
statistics	18 10 18 14 15 15 8	12 15 15 10 18 17 15	20 20 20 20 20 20 20 20	1 2 4 2 2 9 2
operations research	10 8 5 2 11 8 10	14 10 10 5 12 10 17	10 11 13 4 2 5 12	15 11 12 7 14 14 16
English	14 13 15 5 10 10 12	18 15 17 15 17 12 17	17 17 15 12 14 14 15	13 15 10 11 12 10 17

C. Lavit et al. / The ACT (STATIS Method)

Table 2 RV-coe	fficients		
1			
0.17	1	-	
	0.00		

1.78

1.39

1.55

1.17

. :

0.17	1	-						
0,45	0.28	1						
0.43	0.30	0.42	1					
0.69	0.22	0.53	0.54	1				
0.48	0.16	0.54	0.63	0.76	1			
0.63	0.18	0.49	0.41	0.87	0.73	1		
0.42	0.11	0.31	0.23	0.29	0.19	0.40	1	
			۲	*พุธ	ž.			
Table 3 d²( <i>k</i> , <i>k'</i> )	= 2(1 - RV)	)						
0					······			
1.65	0							
1.10	1.44	0						
1.15	1.39	1,16	0					
0.62	1.56	0,94	0.92	0				
1.04	1.68	0.92	0.74	0.48	0 •			
0.75	1.64	1.03	1.17	0.26	0.54	0		

1.42

1.62

1.20

0

 $\sigma_2^2 = 1.01$   $M_1$   $M_1$   $M_1$   $M_5$   $M_5$   $\sigma_2$   $\sigma_1^2 = 17.43$   $M_6$   $M_3$   $M_4$   $M_4$   $M_4$ 





Fig. 3. Graphical representation of the compromise. Loss function:  $||W - W_h||^2 = \text{Tr}((W - W_h)S)^2$ =  $(\frac{1}{10})^2 \text{Tr}(W - W_h)^2 = \sigma_3^2 + \cdots + \sigma_9^2 = 0.09$ 

split those distances into contributions  $\frac{1}{10} \| w_2^i - w_k^i \|^2$  of the different elements *i* to detect who are the professors on which the opinion of judge no. 2 differs from the others. Table 4 shows that the difference comes essentially from languages, English, statistics and information system design.

For sake of readibility, only three trajectories are drawn on Figure 4: languages, architecture and the supplementary element practice. The star corresponds to the compromise point. Recall that the vector between judges no. 2 and no. 6 is the projection of  $w_6^i - w_2^i$  on the two-dimensional space spanned by eigenvectors  $p_1$  and  $p_2$  of the compromise. (For practice, we compute the centred scalar products between this supplementary row and the active ones and

Table 4

decomposition of the squared distance between judge no. 2 and judge no. k in parts  $\frac{1}{10} || w_2^i - w_k^i ||^2 / d^2(2, k)$  explained by professor *i* 

squared distance $d^2(2, k)$							
between judge no. 2 and	no. 1	по. З	no. 4	no. 5	по. б	по. 7	no. 8
	1.65	1.44	1.39	1.56	1.68	1.64	1.78
contributions (percentage)							
architecture	2.51	3.01	3.36	9.47	2.41	5.70	2.56
theory	7.97	7.56	9.51	9.61	10.48	9.50	8.06
languages	10.41	14.53	16.94	18.62	27.26	22.84	12.48
economics	6.24	2.58	7.07	4.70	3.36	2.84	3.64
accounting	8.41	9.38	11.64	8.08	8.69	5.47	5.53
management	6.94	11.41	7.09	7.20	4.62	4.22	3 54
inf. sys. design	12.85	27.80	15.87	8.93	14.35	6.71	2.47
statistics	16.66	6.65	3.37	10.78	4.93	16.89	37.07
operations research	6.82	6.68	1.14	3.99	2.57	6.41	1.55
English	21.19	10.39	24.01	18.64	21.31	19.41	12.99

Fig. 4. Graphical representation of the trajectories.

project this vector in the same way). Keeping this distortion in mind, we note that all the vectors  $w_k^i - w_{k'}^i$ , have significant norms for languages. It means that languages contributes for a large part to any distances  $d^2(k, k')$  between judges (and not only between judge no. 2 and the others), and between judges and the compromise. It seems on the contrary, that disagreements between judgments are less crucial for architecture and practice.

# Appendix: Euclidean distances between scalar product matrices

We review definitions and properties of linear mappings associated with Euclidean scaling methods. See Rao (1973, 1980), Robert and Escoufier (1976), Sabatier (1987) and Lavit (1988) for proofs and complements.

# 1. Euclidean vector space

**Definition 1.** An Euclidean vector space  $(E, s_J)$  is the association of a *J*-dimensional real vector space *E* and a scalar (or inner) product  $s_J$ .  $(x | y)_{s_J}$  denotes the scalar product of x and y.

**Definition 2** (Dual of an euclidean vector space). The dual  $E^*$  of an euclidean vector space E is the set  $L(E, \mathbb{R})$  of linear mappings between E and the set of

# C. Lavit et al. / The ACT (STATIS Method)

real numbers. Note that elements of  $E^*$  correspond simply to vectors of E written as row matrices.

and the second secon

This supplementary mathematical concept will appear to be an appropriate tool later.

**Property 1.** It is convenient to consider the scalar product on E as an one to one linear correspondence  $\mathscr{S}$  between E and  $E^*$  (which implies that  $\mathscr{S}^{-1}$  does exist).  $\forall x \in E, \ \mathscr{S}(x) \in E^*$  is defined as the row vector which, applied to y, gives

$$(\mathscr{S}(x))(y) = (x \mid y)_{s}.$$

**Definition 3.**  $s^*$  is defined as follows:

 $\forall u \quad \forall v \in E^* \quad (u \mid v)_{s^*} = v(\mathscr{S}^{-1}(u))$ 

is a scalar product on  $E^*$ , called dual scalar product of s.

2. Adjoint of a linear mapping

Notation. E and F being two vector spaces, L(E, F) denotes the vector space of linear mappings between E and F.

**Definition 4** (Transpose of a linear mapping). Let  $\mathscr{A}$  be any element of L(E, F). The transpose of  $\mathscr{A}$  is the element  $\mathscr{A}'$  of  $L(F^*, E^*)$  defined as:

 $\forall x \in E \quad \forall v \in F^* \quad (\mathscr{A}'(v))(x) = v(\mathscr{A}(x)).$ 

**Definition 5** (Adjoint of a linear mapping). Let  $\mathscr{A}$  be any linear mapping between  $(E, s_I)$  and  $(F, s_I)$ . The adjoint of  $\mathscr{A}$  is the element  $\mathscr{A}^*$  of L(F, E) defined as:

 $\forall x \in E \quad \forall y \in F \quad (x \mid \mathscr{A}^*(y))_{s_I} = (\mathscr{A}(x) \mid y)_{s_I}$ 

or  $\mathscr{A}^* = \mathscr{S}_J^{-1} \mathscr{A}' \mathscr{S}_I$ .

# 3. Self adjoint operator

**Definition 6.** An element of L(E, E) is called operator of E.

**Definition 7.** An operator of (E, s) is self adjoint if  $\mathscr{A} = \mathscr{A}^*$ , or  $\mathscr{S}\mathscr{A} = \mathscr{A}'\mathscr{S}$ .

**Property 2** (Spectral decomposition of a self adjoint operator  $\mathscr{A}$  of (E, s)). x is an eigenvector of  $\mathscr{A}$  if there exists a real number  $\sigma$  such that  $\mathscr{A}(x) = \sigma x$ . It can be shown that there exists a s-orthonormal basis of eigenvectors. In other words, the matrix A can be written as  $A = P\Sigma P'$  with P'SP = I.  $\Sigma$  is diagonal and its elements are the eigenvalues of A, the columns of P are the corresponding eigenvectors, S is the matrix of s and I is the identity matrix.

4. Singular value decomposition

**Property 3.** Let  $\mathscr{A}$  be any linear mapping between  $(E, s_J)$  and  $(F, s_I)$ . Then  $\mathscr{A}^*\mathscr{A}$  and  $\mathscr{A}\mathscr{A}^*$  satisfy the following statements:

 $-\mathscr{A}^*\mathscr{A}$  is a self adjoint operator of E, and it is positive, that is to say:

$$\forall x \in E \quad (\mathscr{A}^*\mathscr{A}(x) \mid x)_{s_j} \ge 0.$$

 $\mathscr{A}\mathscr{A}^*$  is a positive self adjoint operator of F, as well.

- Ker  $(\mathscr{A}^*\mathscr{A}) = \text{Ker}(\mathscr{A}).$ 

-  $\mathscr{A}^*\mathscr{A}$  and  $\mathscr{A}\mathscr{A}^*$  have the same eigenvalues. If x is an eigenvector of  $\mathscr{A}^*\mathscr{A}$  obeying  $||x||_{s_I} = 1$ , and  $\sigma$  the corresponding eigenvalue, then  $y = \sigma^{-1/2} \mathscr{A}(x)$  is the corresponding eigenvector of  $\mathscr{A}\mathscr{A}^*$  obeying  $||y||_{s_I} = 1$ . -  $\mathscr{A}, \mathscr{A}^*, \mathscr{A}\mathscr{A}^*$  and  $\mathscr{A}^*\mathscr{A}$  have identical rank.

**Property 4** (Singular value decomposition of  $\mathscr{A}$ ). Let r be the rank of  $\mathscr{A}$ . The operator  $\mathscr{A}^*\mathscr{A}$  being self adjoint and positive, have positive eigenvalues  $\sigma_1^2, \ldots, \sigma_r^2$ . The square roots  $\sigma_1, \ldots, \sigma_r$  are called singular values of  $\mathscr{A}$ . Let  $p_1, \ldots, p_r$  be a set or  $s_I$ -orthonormal eigenvectors of  $\mathscr{A}\mathscr{A}^*$ , and  $q_1, \ldots, q_r$  a set of  $s_J$ -orthonormal eigenvectors of  $\mathscr{A}^*\mathscr{A}$ , corresponding to the eigenvalues  $\sigma_1^2, \ldots, \sigma_r^2$ . Then, the matrix  $A_{IxJ}$  can be written as the sum

 $A = \sigma_1 p_1 q'_1 S_J + \cdots + \sigma_r p_r q'_r S_J,$ 

or as the matrix product

 $A = P \Sigma Q' S_I$  with  $P' S_I P = I$  and  $Q' S_I Q = I$ .

 $\Sigma_{rxr}$  is a diagonal matrix whose elements are the singular values  $\sigma_1, \ldots, \sigma_r$  and the columns of  $P_{Ixr}$  (respectively  $Q_{Jxr}$ ) are the eigenvectors  $p_1, \ldots, p_r$  (respectively  $q_1, \ldots, q_r$ ) of  $\mathscr{A}\mathscr{A}^*$  (respectively  $\mathscr{A}^*\mathscr{A}$ ).

5. Euclidean distances between linear mappings

**Definition 8** (Scalar product on L(E, F)). Let  $\mathscr{A}$  and  $\mathscr{B}$  two linear mappings between  $(E, s_I)$  and  $(F, s_I)$ . Then

 $(\mathscr{A} \mid \mathscr{B}) = \mathrm{Tr}(\mathscr{A}\mathscr{B}^*) = \mathrm{Tr}(\mathscr{A}\mathscr{S}_I^{-1}\mathscr{B}'\mathscr{S}_I)$ 

defines a scalar product on L(E, F). The induced norm is  $d^2(\mathscr{A}, \mathscr{B}) = ||\mathscr{A} - \mathscr{B}||^2 = Tr((\mathscr{A} - \mathscr{B})\mathscr{S}_I^{-1}(\mathscr{A} - \mathscr{B})'\mathscr{S}_I).$ 

**Property 5** (Approximation of a linear mapping). Let  $\mathscr{A}$  be any linear mapping of rank r between E and F. Let us consider its singular value decomposition with singular values  $\sigma_1, \ldots, \sigma_r$  in decreasing order. Then

 $\min_{\substack{\mathscr{B} \in L(E,F) \\ \text{rank of } \mathscr{B} \leq h}} \| \mathscr{A} - \mathscr{B} \|^2 = \| \mathscr{A} - \mathscr{A}_h \|^2 = \sum_{l=h+1}^r \sigma_l^2,$ 

where  $\mathscr{A}_h$  is the sum of the h first elements of the singular value decomposition of  $\mathscr{A}$ .

# 6. Embedding W into an Euclidean vector space

Let us consider again a matrix  $W_{IxI}$  of scalar products (or scalar product-like) between I elements.

(a) W can be viewed as an element of  $L(F, F^*)$ . Let F be an I-dimensional vector space, and  $(f_1, \ldots, f_i)$  a basis of F, each vector  $f_i$  being associated to one of the I elements. The symmetric matrix W can be regarded as the matrix of a bilinear mapping w between  $F \times F$  and the set of real numbers  $\mathbb{R}$ , defined on the basis vectors by  $w(f_i, f_{i'}) = W_{ii'}$ .

Now, as it has been done for a scalar product in Property 1, we associate to w the following element  $\mathcal{W}$  of  $L(F, F^*)$ . For any vector x of F,  $\mathcal{W}(x)$  is the element of  $F^*$ , which, applied to any vector y of F, gives

$$(\mathscr{W}(x))(y) = w(x, y).$$

(b) Euclidean structure of F. To calculate euclidean distances between the w's as we did in Section 5 between linear mappings, we need to enrich the structure of F with a scalar product denoted  $\mathcal{S}^{-1}$  instead of the straightforward designation  $\mathcal{S}$  for a simple question of notation. Thus, the dual scalar product on  $F^*$  corresponds to  $\mathcal{S}$  and the adjoint mapping of  $\mathcal{W}$  is simply  $\mathcal{SWS}$  (and not  $\mathcal{S}^{-1}\mathcal{WS}^{-1}$ ).

(c) Euclidean structure of  $L(F, F^*)$ . Suppose that  $W_1$  and  $W_2$  are two matrices of scalar products (or scalar product-like) between the same I elements. We associate to  $W_1$  and  $W_2$  the corresponding linear mappings  $\mathcal{W}_1$  and  $\mathcal{W}_2$ between  $(F, s^{-1})$  and  $(F^*, s)$ . Then the scalar product

$$(\mathscr{W}_1 \mid \mathscr{W}_2) = \operatorname{Tr}(\mathscr{W}_1 \mathscr{W}_2^*) = \operatorname{Tr}(W_1 S W_2 S)$$

induces the Euclidean distance

 $d^{2}(W_{1}, W_{2}) = Tr[(W_{1} - W_{2})S(W_{1} - W_{2})S].$ 

This general formulation includes two usual distances: - If S is the identity matrix I, then  $d^2(W_1, W_2) = \sum_i \sum_{i'} [(W_1 - W_2)_{ii'}]^2$ . The

basis  $(f_1, \ldots, f_I)$  is required to be s-orthonormal. - If S is diagonal, then  $d^2(W_1, W_2) = \sum_i \sum_{i'} S_{ii'} S_{i'i'} [(W_1 - W_2)_{ii'}]^2$ . The basis  $(f_1, \ldots, f_I)$  is required to be s-orthogonal but not necessarily standardized. In other words, weights of the elements are taken into account in the calculation of  $d(W_1, W_2)$ .

The more general case where S is not diagonal can be interpreted as some exogenous constraint of contiguity between elements, which should be taken into consideration in the calculation of  $d(W_1, W_2)$ .

7. Special case of positive semi-definite W's.

**Property 6.** If  $\mathcal{W}$  is p.s.d., then  $\mathcal{WS}$  is a positive self adjoint operator of  $F^*$ .

**Property** 7 (Singular value decomposition of  $\mathcal{W}$ ). If  $\mathcal{W}$  is p.s.d., the singular value decomposition of  $\mathcal{W}$  is deduced from the spectral decomposition of the self-adjoint operator  $\mathcal{WS}$ . Namely  $W = \sigma_1 p_1 p'_1 + \cdots + \sigma_r p_r p'_r = P \Sigma P'$  with P'SP = I, where the singular values  $\sigma_1, \ldots, \sigma_r$  are the eigenvalues of  $\mathcal{WS}$ , and  $p_1, \ldots, p_r$  are eigenvectors of  $\mathcal{WS}$ .

It can be shown that eigenvectors  $p_1, \ldots, p_r$  of  $\mathscr{W}\mathscr{W}^*$  are eigenvectors of  $\mathscr{W}\mathscr{S}$ and  $q_1 = \mathscr{S}(p_1), \ldots, q_r = \mathscr{S}(p_r)$  are eigenvectors of  $\mathscr{W}^*\mathscr{W}$ . Then the singular value decomposition of  $W = P\Sigma Q'S^{-1}$  turns out to  $P\Sigma P'$ .

If S is the identity matrix, the singular value decomposition of W is simply designated as spectral decomposition of  $W: P\Sigma P'$  with P'P = I.

**Property 8.** If  $\mathcal{W}$  is p.s.d.,  $(\mathcal{W}_1 \mid \mathcal{W}_2) = \operatorname{Tr}(\mathcal{W}_1 \mathcal{W}_2^*)$  is a positive real number.

**Property 9.** Suppose that  $\mathcal{W}_1$  p.s.d. has rank r and  $\mathcal{W}_2$  p.s.d. has rank h less than r. If  $\sigma_1, \ldots, \sigma_r$  denote the singular values of  $\mathcal{W}_1$  in decreasing order, then the scalar product between  $\mathcal{W}_1/||\mathcal{W}_1||$  and  $\mathcal{W}_2/||\mathcal{W}_2||$  verify

$$0 \le \frac{\left(\mathcal{W}_{1} \mid \mathcal{W}_{2}\right)}{\|\mathcal{W}_{1}\| \| \|\mathcal{W}_{2}\|} \le 1 - \frac{\sum_{l=h+1}^{r} \sigma_{l}^{2}}{2\sum_{l=1}^{r} \sigma_{l}^{2}}.$$

To establish this inequality, apply Property 5 to  $\mathscr{A} = \mathscr{W}_1 / || \mathscr{W}_1 ||$  and  $\mathscr{B} = \mathscr{W}_2 / || \mathscr{W}_2 ||$  recalling that  $(\mathscr{A} | \mathscr{B}) = \frac{1}{2} (|| \mathscr{A} ||^2 + || \mathscr{B} ||^2 - || \mathscr{A} - \mathscr{B} ||^2)$ . This property must be kept in mind while interpreting the ACT's results on Example 4 of Chapter 3, as the number of flower species might be five times greater than the number of variables measured by the pedologist.

# 8. Special case of matrices W = XQX'.

Let  $X_1$  be an  $I \times J_1$  matrix of I observations on  $J_1$  variables, and  $X_2$  an  $I \times J_2$  matrix of the same observations on  $J_2$  variables. The  $J_1$  columns of  $X_1$  are centred according to weights  $m_1, \ldots, m_I$ , with the constraint  $\sum m_i = 1$ , and  $J_2$  columns of  $X_2$  are likewise centred according to the same weights.

Thus  $W_1 = X_1Q_1X_1'$  and  $W_2 = X_2Q_2X_2'$  are two matrices, obtained in two different circumstances, of centred scalar products between the *I* elements. If, in addition, we choose *S* equal to the diagonal matrix

 $\begin{pmatrix} m_1 & & \\ & \ddots & \\ & & \ddots & \\ & & & m_I \end{pmatrix}$ 

usually denoted D, the scalar product  $Tr(\mathcal{W}_1 \mathcal{W}_2^*) = Tr(W_1 D W_2 D)$  have the following interesting statistical interpretation.

**Property 10.**  $Tr(W_1DW_2D)$  is the sum of the squared covariances between each variable of  $X_1$  and each variable of  $X_2$ . If each column of  $X_1$  and  $X_2$  is standardized to have unit variance,  $Tr(W_1DW_2D)$  is the sum of the squared correlations.

**Definition 9.** The scalar product between normed W's

$$\frac{\operatorname{Tr}(W_1 D W_2 D)}{\sqrt{\operatorname{Tr}(W_1 D)^2} \sqrt{\operatorname{Tr}(W_2 D)^2}}$$

is known as Rv-coefficient [Robert and Escoufier, 1976].

**Remark.** Whether S is equal to D with  $m_1 = \cdots = m_l$  or equal to the identity matrix, the scalar product

$$\frac{\operatorname{Tr}(W_1 S W_2 S)}{\sqrt{\operatorname{Tr}(W_1 S)^2} \sqrt{\operatorname{Tr}(W_2 S)^2}}$$

has the same value.

### References

Carlier, A., Ch. Lavit, M. Pages, M.O. Pernin and J.Ch. Turlot, A comparative review of methods which handle a set of indexed data tables, Coppi and Bolasco, (ed.), in: Multiway Data Analysis, (North-Holland, Amsterdam, 1989) 85-101.

Escoufier, Y., Le traitement des variables vectorielles, Biometrics, 29 (1973) 751-760.

Escoufier, Y., Operators related to a data matrix, in: Barra et al. (ed.), Recent Developments in Statistics, (North-Holland, Amsterdam, 1977) 125-131.

Fichet, B. and G. Le Calve, Structure géométrique des principaux indices de dissimilarité sur signes de présence-absence, Statistique et Analyse de Données, 9 (3) (1984) 11-44.

Franc, A., Etude algébrique des multi-tableaux. Apports de l'algèbre tensorielle, doctoral thesis, University of Montpellier II, 1992.

Lavit, Ch., Analyse Conjointe de Tableaux Quantitatifs, (Masson, Paris, 1988).

Rao, C.R., Linear Statistical Inference and its Applications, (Wiley, New York, 1973).

Rao, C.R., Matrix approximations and reduction of dimensionality in multivariate statistical analysis, in: Krishnaiah, (ed.), *Multivariate Analysis*, (North-Holland, Amsterdam, 1980) 3-22.

Robert, P. and Y. Escoufier, A unifying tool for linear multivariate statistical methods: the RV coefficient, *Applied Statistics C*, **25** (3) (1976) 257–265.

Sabatier, R., Méthodes factorielles en analyse des données, doctoral thesis, University of Montpellier II, 1987.

## Availability of the software

**Distributor:** CISIA, 1, Avenue Herbillon, 94160 Saint Mandé France. Tel.: (1) 43 74 20 20. Fax: (1) 43 74 17 29

การการสาวสาวสาวสาวสาวสาวสาวสาวสาวสาวสาวสาว

Author: Christine Lavit, Unité de Biométrie, ENSA.M.-INRA-UM II, Place Viala - 34060 Montpellier, France.

**Release for IBM-compatible micro-computers:** User's guide + executable code for ACT (STATIS method) and ACT (dual STATIS method) + source code written in portable FORTRAN 77 on floppy disks. Minimal hardware required to run the executable code: 512 K RAM.

Other computers: The source code is available for implementing the software on other kind of computers, work stations under UNIX and mainframes as IBM, VAX, UNIVAC...

Cost: 1500 FF.

# 

.



.

• •

.

# COMPUTATIONAL STATISTICS & DATA ANALYSIS

### Instructions to Authors

### A. Journal Portion (Sections I-III)

Four copies of contributions (including one original of the figures) should be submitted to the appropriate Co-Editor. Manuscripts from Europe, Asia and Africa should be sent to Peter Naeve, Ph.D., Department of Statistics and Computing, University of Bielefeld, Post Box 100131, D-33501 Bielefeld, Germany. Manuscripts from North-, Central and South America, as well as the rest of the world should be sent to Stanley Azen, Ph.D., Department of Preventive Medicine, University of Southern California, 1420 San Pablo St., PMB B1010, Los Angeles, CA 90033, USA. Although the submission of papers is regionally divided, the reviewing process is standardized between the CoEditors.

Submission of accepted papers as electronic manuscripts, i.e., on disk with accompanying manuscript, is encouraged. Electronic manuscripts have the advantage that there is no need for rekeying of text, thereby avoiding the possibility of introducing errors and resulting in reliable and fast delivery of proofs. The preferred storage medium is a 5.25 or 3.5 inch disk in MS-DOS format, although other systems are welcome, e.g., Macintosh (in this case, save your file in the usual manner; do not use the option "save in MS-DOS format"). Do not submit your original paper as electronic manuscript but hold on the disk until asked for this by the Editor (in case your paper is accepted without revisions). Do submit the accepted version of your paper as electronic manuscript. Make absolutely sure that the file on the disk and the printout are identical. Please use a new and correctly formatted disk and label this with your name; also specify the software and hardware used as well as the title of the file to be processed. Do not convert the file to plain ASCII. Ensure that the letter "I" and digit "1", also the letter "O" and digit "0" are used properly, and format your article (tabs, indents, etc.) consistently. Characters not available on your word processor (Greek letters, mathematical symbols, etc.) should not be left open but indicated by a unique code (e.g., gralpha, < alpha > , @, etc., for the Greek letter  $\alpha$ ). Such codes should be used consistently throughout the entire text; a list of codes used should accompany the electronic manuscript. Do not allow your word processor to introduce word breaks and do not use a justified layout. Please adhere strictly to the general instructions below on style, arrangement and, in particular, the reference style of the journal.

1. All contributions should be written in English and contain an abstract of approximately 200 words plus a list of key words.

2. The manuscript must be typed on one side of the paper in double spacing (including footnotes, references and abstracts) with wide margins.

3. All mathematical symbols which are not typewritten should be listed and explained on a separate sheet. The numbers identifying displayed mathematical expressions should be placed in parentheses at the right margin. Parts of text should not be subject to this numbering.

4. Special care should be given to the preparation of the drawings for the figures and diagrams. Except for a reduction in size, they will appear in the final printing in exactly the same form as submitted by the author; normally they will not be redrawn by the printer. In order to make a photographic reproduction possible, all drawings should be on separate sheets, with wide margins, drawn large size, in India ink, and carefully lettered. Exceptions are diagrams only containing formulae and a small number of straight lines (or arrows): these can be typeset by the printer. 5. References should be listed alphabetically in the same way as the following examples:

Rao, C.R., *Linear statistical inference and its applications* (Wiley, New York, 1973) 14–32.

Bock, R.D. and D. Brandt, Comparison of some computer programs for univariate and multivariate analysis of variance, in: P.R. Krishnaiah (Ed.), *Handbook of statistics*, Vol. 1 (North-Holland, Amsterdam, 1980) 703-744.

Ghosh, S., Robustness of BIBD against the unavailability of data, J. Statist. Plann. Inference, 6(1) (Dec. 1982) 29-32.

Pillai, K.C.S. and B. Saweris, Asymptotic formulae for the distribution of Hotelling's trace for equality of two covariance matrices, Mimeo. (Dept. of Statistics, Purdue University, Lafayette, IN, 1983).

6. Papers reporting results based on computation should provide enough information so that readers can evaluate the quality of the results. Such information includes estimated accuracy of results, as well as descriptions of pseudo-random-number generators, numerical algorithms, computer(s), programming language(s), and major software components that were used

Submission of a paper will be held to imply that it contains original unpublished work and is not being submitted for publication elsewhere.

Upon acceptance of an article, the author(s) will be asked to transfer copyright of the article to the publisher. This transfer will ensure the widest possible dissemination of information. Please ensure that the paper is submitted in its final form. Correction in the proof stage, other than printer's errors, should be avoided; cost arising from such extra corrections will be charged to the authors. Otherwise, no page charges will be made. A reprint order form will be sent to the principal author together with the proofs. Twenty-five reprints of each contribution to Sections I-III are available free of charge. Additional reprints can be ordered from the Publisher.

### B. Statistical Software Newsletter (Section IV)

Three copies of informational articles and news items (including one original of the figures) should be submitted to one of the SSN Editors: Allmut Hörmann (Managing Editor), GSF Medis-Institut, Neuherberg, Postfach 1129, 85758 Oberschleissheim, Germany; Joyce Niland, Ph.D., Department of Biostatistics, City of Hope National Medical Centre, 1500 E. Duarte Road, Duarte, CA 91010, USA; Andrew Westlake, Department of Epidemiology, London School of Hygiene and Tropical Medicine, Keppel Street, London WC1E 7HT, UK.

Books and other relevant literature for consideration should be submitted to the Book Review Editor, Walter Krämer, Lehrstuhl für Wirtschafts- und Sozialstatistik, FB Statistik der Universität Dortmund, Postfach 500, D-44221 Dortmund, Germany.

1. All contributions must be in English. Informational articles must follow the specifications for Sections I-III.

2. In order to expedite publication, the editors would welcome material on diskette, e.g. texts favouritely as Word for Windows files. Word for MS-DOS, Word for Apple Macintosh (only DOS formatted), WordPerfect, and ASCII files will always be accepted. Additional specific details can be obtained in advance from the Managing Editor.

3. If figures, tables, and computer output cannot be included on the diskette, material must be presented in a format to permit direct reproduction.

4. The Managing Editor will have the final responsibility for each issue of the SSN.

# COMPUTATIONAL STATISTICS & DATA ANALYSIS

Computational Statistics & Data Analysis 18 (1994) 97–119 North-Holland

# The ACT (STATIS method)

# Christine Lavit, Yves Escoufier

Unité de Biométrie, ENSA.M-INRA-UM II, Montpellier, France

# Robert Sabatier

Faculté de Pharmacie, Département Pharmaceutique de Physique Industrielle, Statistique et Informatique, UM I, Montpellier, France

Pierre Traissac ORSTOM, Montpellier, France



# **COMPUTATIONAL STATISTICS & DATA ANALYSIS**

## Aims and Scope of CSDA

 $\mathcal{X}$ 

Computational Statistics & Data Analysis ("CSDA") the official journal of the International Association of Statistical Computi ("IASC"), is an international journal dedicated to the dissemination of methodological research and applications in the areas computational statistics and data analysis. The Journal consists of three refereed sections, and a fourth section dedicated news on statistical computing. The refereed sections are divided into the following subject areas: I) Data Analytic Methodolc and Procedures (e.g., density estimation, robust procedures, design of experiments, classification, model free data explorat and pattern recognition); II) Applications and Comparative Studies (e.g. simulation experiments, data exploration, utilization survey data, graphical tools, comparison of statistical methodology, strategies for analysis of data sets arising from the physi behavioral or natural sciences); and III) Computational Statistics (e.g. design of statistical systems (data structures, languag or user interfaces], statistical algorithms [numerical aspects, parallelization, complexity, or semantics], graphical metho evaluation and quality assurance of statistical software, databases and statistics, statistical workstations, knowledge-ba [expert systems]. The fourth section, the Statistical Software Newsletter ("SSN"), promotes the rapid exchange of information articles and news items. Although not peerreviewed, contributions to the SSN are screened for appropriateness and edited accuracy, Informational articles may include statistical software development (e.g., new techniques, software standa innovative applications) and comparative evaluations of software. Book and package reviews, announcements and repormeetings and conference, as well as short and timely notes concerning the statistical computing profession may also contributed to this section. On occasion, special events or topics will be published as a Special Issue of CSDA, prepared Guest Editor.

Publication information: COMPUTATIONAL STATISTICS & DATA ANALYSIS (ISSN 0167-9473). For 1994 volumes 17 ar are scheduled for publication. Subscription prices are available upon request from the publisher. Subscriptions are acce on a prepaid basis only and are entered on a calendar year basis. Issues are sent by surface mail except to the folic countries where air delivery via SAL is insured: Argentina, Australia, Brazil, Canada, Hong Kong, India, Israel, Japan, Mala Mexico, New Zealand, Pakistan, PR China, Singapore, South Africa, South Korea, Taiwan, Thailand, USA. For all countries airmail rates are available upon request. Claims for missing issues must be made within six months of our public (mailing) date. Please address all your requests regarding orders and subscription queries to: Elsevier Science B.V., Jc Department, P.O. Box 211, 1000 AE Amsterdam, The Netherlands. Tel.: 31-20-5803642, fax: 31-20-5803598.

US mailing notice – Computational Statistics & Data Analysis (ISSN 0167-9473) is published monthly except in April and J-Elsevier Science B.V. (Molenwerf 1, Postbus 211, 1000 AE Amsterdam). Annual subscription price in the USA US\$ 712.0C price valid in North, Central and South America only), including air speed delivery. Second class postage rate is p Jamaica, NY 11431.

USA POSTMASTERS: Send address changes to Computational Statistics & Data Analysis Publications Expediting, Inc Meacham Avenue, Elmont, NY 11003. Airfreight and mailing in the USA by Publication Expediting.

### © 1994, Elsevier Science B.V. All rights reserved

No part of this publication may be reproduced, stored in a retrieval system or transmitted in any form or by any relectronic, mechanical, photocopying, recording or otherwise, without the prior permission of the publisher, Elsevier & B.V., Copyright & Permissions Department, P.O. Box 521, 1000 AM Amsterdam, The Netherlands.

No responsibility is assumed by the Publisher for any injury and / or damage to persons or property as a matter of perliability, negligence or otherwise, or from any use or operation of any methods, products, instructions or ideas contained material herein. Although all advertising material is expected to conform to ethical standards, inclusion in this publicatic not constitute a guarantee or endorsement of the quality or value of such product or of the claims made of it manufacturer.

Special regulations for authors – Upon acceptance of an article by the journal, the author(s) will be asked to transfer ce of the article to the publisher. This transfer will ensure the widest possible dissemination of information.

Special regulations for readers in the USA – This journal has been registered with the Copyright Clearance Cen Consent is given for copying of articles for personal or internal use, or for the personal use of specific clients. This co given on the condition that the copier pays through the Center the per-copy fee stated in the code on the first page article for copying beyond that permitted by Sections 107 or 108 of the US Copyright Law. The appropriate fee st forwarded with a copy of the first page of the article to the Copyright Clearance Center, Inc., 27 Congress Street, Se 01970, USA. If no code appears in an article, the author has not given broad consent to copy and permission to copy obtained directly from the author. The fee indicated on the first page of an article in this issue will apply retroactiv articles published in the journal, regardless of the year of publication. This consent does not extend to other kinds of such as for general distribution, resale, advertising and promotion purposes, or for creating new collective works written permission must be obtained from the publisher for such copying.

(a) The paper used in this publication meets the requirements of ANSI/NISO 239.48-1992 (Permanence of Paper).

Published ten times a year