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Multi-way principal components analysis of a complex data array resulting from physicochemical characterization of natural waters

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Abstract

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Multi-way principal components analysis (MPCA) is an efficient tool for reducing higher dimensional data arrays. Using the Kroonenberg algorithm — which originally was developed for three-dimensional data arrays but may be generalized to arbitrary dimensions in a straightforward manner — MPCA is applied to a complex example from the chemistry of waters. The data originated from the measurements of fifteen physicochemical parameters (variables) at ten different locations (objects) within some specific area of the Niger delta. These measurements were consistently recorded 22 times (occasions) in the course of a year. MPCA allows the detection of spatial and temporal factors of influence and the classification of the parameters considered according to these factors.

INTRODUCTION

Principal components analysis (PCA) has become one of the main tools for structural investigations of multivariate data sets. There have been a lot of applications in chemometrics which consider classical, multivariate data tables, i.e. two-dimensional data arrays which are built up by measurements of p variables characterizing a set of n objects. In the last few years a tendency has been observed towards dealing with even higher dimensional data arrays (think, for instance, of a

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constant set of n objects being determined by p variables measured on q different occasions). Such investigations have been instigated due to the increasing complexity of experimental design and the improving performance of analytical instruments. As a consequence, attempts are being made to generalize classical methods from multivariate statistics. One of these generalizations is multi-way principal components analysis (MPCA) which was first introduced by Tucker in 1964 [1]. Essential practical and theoretical progress was achieved by Kroonenberg and De Leeuw in 1980 [2]. The first authors to mention this topic in the chemometric literature, to our knowledge, were Wold et al. in 1987 [3]. Since then an increasing number of reviews [4–7], applications [8,9], and theoretical developments [10] concerning MPCA have been published.

In the present work MPCA will be used to display the essential structures in a three-way data array. The data originated from a complex investigation of regional and seasonal variation of physicochemical parameters in a specific area of the Niger delta. Of course, for instrumental applications, even higher dimensional data arrays may be considered (compare ref. 3 for a list of instrumental setups in analytical chemistry yielding up to six-way arrays). The abstract basis for MPCA, however, remains unchanged. We therefore prefer to formulate the general n-way algorithm in a separate section, rather than the Kroonenberg algorithm for three-way data, which is properly contained within the general algorithm as a special case. Before doing so we shall mention some simplifying versions of the analysis.

UNFOLDING TECHNIQUES AND DATA REDUCTION

A naïve approach to the investigation of multiway arrays would be to reduce the analysis to situations where classical tools, like conventional PCA, may be applied. In the simplest case, for instance, a three-way array could be cut out along one of the three ways. One then obtains as many two-way data tables as there are elements in the third way. Each of these tables can be subjected to PCA. The number of such PCAs, however, rapidly increases with the number of modes and the number of elements per mode. Furthermore, the results of such separate PCAs frequently happen to contradict each other to a certain degree. Summarizing, this naïve approach is not appropriate for efficient data reduction; similarly, it is not very efficient to replace the analysis of a data table by separate univariate analyses. A somewhat more advanced approach is the so-called unfolding (in ref. 3 this is called a 'quick and dirty way'). The idea behind this is quite simple: define two of the three ways so that they form one single way. If one takes, for instance, twenty variables consistently measured on ten occasions, then one would arrive at 200 (new) variables (each variable on each occasion). So the three-way array is unfolded to a conventional data table. At least, one obtains one single PCA model, rather than several separate ones. This idea of unfolding may be generalized in a straightforward manner to n-way data arrays (compare Wold et al. [3]) and a slightly more general decomposition is even possible by identifying k ways on the one hand and the remaining $n-k$ ways on the other hand, yielding two new artificial ways (compare Geladi [4]). Nevertheless, such unfolding still does not meet the requirement of efficient data reduction. It would obviously be much easier to consider a display of twenty variables and another display of ten occasions rather than a display of 200 variables which, apart from this, are hard to interpret since they are artificially interconnected. Next one arrives at Tucker's original method, which is based on unfolding: first, identify variables and occasions to obtain scores for objects by conventional PCA. Next, identify objects and occasions to obtain loadings for variables by another conventional PCA. Finally, compute loadings for occasions after identifying objects and variables. By so doing, one achieves a decomposition of the three-way array into three separate representations. The task of data reduction is thus fulfilled. But now the computed constellations fail to be least squares solutions (compare ref. 2). This means that when decomposing an n-way array into n separate component models, then the Tucker solution does not, in general, give the best reproduction of the original array in terms of the

component models. This last obstacle, however, may be circumvented by using the Kroonenberg algorithm, which is described below. We emphasize that the abovementioned simplified versions of n-way analysis are useful only if standard software is available, but one should be aware of the fact that, to a certain degree, either data reduction is not performed efficiently, or that the least squares fit is not optimal.

MULTI-WAY PRINCIPAL COMPONENTS ANALYSIS

Consider an N-dimensional data array $\mathbf{Z}$ with general element $z_{i_1,i_2,\ldots,i_N}$ $(1 \leqslant i_1 \leqslant n_1, \ldots, 1 \leqslant i_N \leqslant n_N)$. As an illustration for the case $N = 3$, think, for instance, of the analytical supervision of a chemical process with z_{i_1,i_2,i_3} denoting the concentration of element No. i_2 in sample No. i_1 at time i_3. The aim of MPCA is to extract the informative part of the variance within $\mathbf{Z}$ and to separate it from noise. More exactly, one searches for small numbers $s_1 \leqslant n_1, \ldots, s_N \leqslant n_N$ of components which are able to explain a maximum amount of the variation in $\mathbf{Z}$. Components within each of the N ways are required to be orthogonal. A very popular application of MPCA is the graphical description of the essential data structure which may be obtained by restriction to the case $s_1 = s_2 = \cdots = s_N = 2$ where, for each of the N ways, a display can be established by using the two components as axes. Before formulating the theoretical background of MPCA one needs some introductory concepts for the manipulation of N-way arrays:

- Denote by $M^{n_1,\ldots,n_N}$ the linear space of N-way arrays of order $(n_1, \ldots, n_N)$.
- Define the transposition operator $\mathrm{T}: M^{n_1,\ldots,n_N} \to M^{n_N,\ldots,n_1}$ by assigning to the array $\mathbf{P} \in M^{n_1,\ldots,n_N}$ the array $\mathbf{P}^{\mathrm{T}} \in M^{n_N,\ldots,n_1}$ with general element $p^{\mathrm{T}}_{i_1,\ldots,i_N} := p_{i_N,\ldots,i_1}$.
- Define the Kronecker product $\otimes : M^{n_1,n_2} \times M^{n_3,n_4} \to M^{n_1 \cdot n_3, n_2 \cdot n_4}$ by assigning to each pair of two-dimensional matrices $(\mathbf{Q}, \mathbf{R}) \in M^{n_1,n_2} \times M^{n_3,n_4}$ the two-dimensional matrix $\mathbf{P} := \mathbf{Q} \otimes \mathbf{R} \in M^{n_1 \cdot n_3, n_2 \cdot n_4}$ with general element $p_{ij} := q_{\alpha\beta} \cdot r_{\gamma\delta}$, where $\alpha := [(i-1)/n_3] + 1$, $\beta := [(j-1)/n_4] + 1$, $\gamma := i - n_3 \cdot (\alpha - 1)$, $\delta := j - n_4 \cdot (\beta - 1)$ and $[\ ]$ denotes the integer fraction.
- Define the cutting operator $\mathrm{cut}^j_k : M^{n_1,\ldots,n_N} \to M^{n_1,\ldots,n_{k-1},n_{k+1},\ldots,n_N}$ $(1 \leqslant j \leqslant n_k)$ by assigning to the N-way array $\mathbf{P}$ the $(N-1)$-way array $\mathbf{P}^* := \mathrm{cut}^j_k(\mathbf{P})$ with general element $p^*_{i_1,\ldots,i_{N-1}} := p_{i_1,\ldots,i_{k-1},j,i_{k+1},\ldots,i_N}$.
- Define the vectorization operator vec: $M^{n_1,\ldots,n_N} \to M^{n_1 \cdots n_N}$ inductively in the following way:
  - For two-dimensional matrices one defines vec: $M^{n_1,n_2} \to M^{n_1 \cdot n_2}$ by assigning to each matrix $\mathbf{P}$ the vector $\boldsymbol{q} := \mathrm{vec}(\mathbf{P})$ with general component $q_k := p_{ij}$ where $j := [(k-1)/n_1] + 1$, $i := k - n_1 \cdot (j-1)$ ('stacking of columns of $\mathbf{P}$').
  - In the N-dimensional case, to the N-way array $\mathbf{P}$ there is assigned the vector $\boldsymbol{q} := \mathrm{vec}(\mathbf{P})$ which is explained by $\boldsymbol{q} := \mathrm{vec}(\mathbf{R})$ where $\mathbf{R} \in M^{n_2 \cdots n_N, n_1}$ is a two-dimensional matrix the jth column of which is fixed to be $\mathrm{vec}(\mathrm{cut}^j_1(\mathbf{P}))$. Note that this last expression is defined since $\mathrm{cut}^j_1(\mathbf{P})$ is a $(N-1)$-way array.

Algebraically, the task of MPCA is formulated as the following minimization problem (we adopt the notation of Magnus and Neudecker [11]):

minimize $\boldsymbol{e}^{\mathrm{T}}\boldsymbol{e}$ with

$$\boldsymbol{e} := \mathrm{vec}(\mathbf{Z}^{\mathrm{T}}) - \bigotimes_{i=1}^{N} \mathbf{A}_i \cdot \mathrm{vec}(\mathbf{C}^{\mathrm{T}}) \qquad (1)$$

subject to $\mathbf{A}_i^{\mathrm{T}}\mathbf{A}_i = \mathbf{I}_{s_i}$

Here, $\mathbf{I}_{s_i}$ denotes the identity matrix of order s_i and the vector $\boldsymbol{e}$ is referred to as the residual vector and expresses that part of the data array $\mathbf{Z}$ that is not modeled by the component matrices $\mathbf{A}_i$. In the graphical application mentioned above the two columns of $\mathbf{A}_i$ would contain the display coordinates for each of the n_i items of the ith way. The core matrix $\mathbf{C}$ is of order $(s_1, s_2, \ldots, s_N)$ and describes how the components of the different ways relate each to another. To obtain a solution of Eqn. 1 one may use the alternating least squares algorithm proposed by Kroonenberg [12] in its generalization from the three-way PCA to n ways (according to ref. 11) which runs as follows:

Step 0. Choose starting matrices $\mathbf{A}_i^{(0)}$ of order

(n_i, s_i) whose columns are orthonormal (e.g. the first standard unit vectors).

Step 1. Put $\hat{\mathbf{A}}_1 := \mathbf{A}_2^{(0)} \otimes \mathbf{A}_3^{(0)} \otimes \cdots \otimes \mathbf{A}_N^{(0)}$. Define the (n_1, n_1)-matrix $\mathbf{P}$ with general element $p_{ij} := a_i^T a_j$, where $a_i := \hat{\mathbf{A}}_1^T \mathrm{vec}(\mathrm{cut}_1^i(\mathbf{Z}))$. Let $\mathbf{A}_1^{(1)}$ be the (n_1, s_1)-matrix whose columns are built up from (normalized) eigenvectors belonging to the s_1 largest eigenvalues of $\mathbf{P}$. Repeat this procedure with subsequent indices. For instance, now put $\hat{\mathbf{A}}_2 := \mathbf{A}_1^{(1)} \otimes \mathbf{A}_3^{(0)} \otimes \cdots \otimes \mathbf{A}_N^{(0)}$ and in the last run put $\hat{\mathbf{A}}_N := \mathbf{A}_1^{(1)} \otimes \mathbf{A}_2^{(1)} \otimes \cdots \otimes \mathbf{A}_{N-1}^{(1)}$. In the kth run, define the (n_k, n_k)-matrix $\mathbf{P}$ as above, with $a_i := \hat{\mathbf{A}}_k^T \mathrm{vec}(\mathrm{cut}_k^i(\mathbf{Z}))$. By doing so, one obtains matrices $\mathbf{A}_1^{(1)}, \ldots, \mathbf{A}_N^{(1)}$.

Step 2. Repeat the whole step 1 as long as the matrices $\mathbf{A}_i^{(m)}$ differ significantly from the matrices $\mathbf{A}_i^{(m-1)}$.

Step 3. If convergence is obtained, compute the core matrix $\mathbf{C}$ according to

$$\mathrm{vec}(\mathbf{C}^T) := \left(\bigotimes_{i=1}^{N} \mathbf{A}_i \right)^T \mathrm{vec}(\mathbf{Z}^T).$$

When passing from classical PCA to MPCA one has to take several essential differences into account:

– It is not possible to reduce the method to the solution of an eigenvalue problem.

– In PCA the core matrix $\mathbf{C}$ is automatically diagonal and hence frequently suppressed by including it into $\mathbf{A}_1$ or $\mathbf{A}_2$. This is not the case for more than two ways.

– In contrast to PCA the solutions of MPCA need not be nested, e.g. if in the situation described above one finds an optimal $(n_1, 2)$-matrix $\mathbf{A}_1$ (after choosing $s_1 = 2$) then the first column of $\mathbf{A}_1$ need not constitute an optimal $(n_1, 1)$-matrix $\mathbf{A}_1^*$ (after choosing $s_1 = 1$).

– There are many more ways of data scaling in MPCA compared to PCA. The specific choice of scaling (e.g. scaling of variables or scaling of variables along occasions, etc.) should be in accordance with prior information on the data set and has to be respected in the interpretation of results.

– Due to the increased complexity in MCPA the variance percentages covered by a given number of components are generally much lower.

– In classical PCA it is possible to superpose object and variable displays and to interpret mutual influences. Due to the non-diagonality of the core matrix such simple superposition does not make sense in MPCA.

Concerning the last item, various attempts have been made to obtain joint representations of all ways allowing an interpretation of mutual dependencies. We shall follow here the approach of simplifying the core matrix structure. We restrict ourselves to the case $N = 3$ and $s_1 = s_2 = s_3 = 2$ (two-dimensional displays) which will be considered in the application below. In this case the core matrix is a $2 \times 2 \times 2$ data array with general entry c_{ijk}. This number c_{ijk} indicates how the components i, j, k of the three ways relate to one another. The larger c_{ijk} the more one has to take account of the corresponding components. If, in the given situation, all eight entries of $\mathbf{C}$ have equal magnitude, then it will become a tedious operation to interpret all these relevant combinations of components. Instead of this, one should try to simplify the structure of $\mathbf{C}$ by using rotations of the set of component scores obtained (note that, upon orthogonal transformation of $\mathbf{A}_i$, the degree of fit in Eqn. 1 remains unchanged). In ref. 12 a procedure is proposed which produces an 'optimal diagonal structure' of $\mathbf{C}$ by keeping $\mathbf{A}_3$ (representation of occasions) fixed and rotating $\mathbf{A}_1$ and $\mathbf{A}_2$ (representations of objects and variables). In general one can only expect to obtain 'almost diagonal' frontal planes of $\mathbf{C}$ (i.e. $\mathrm{cut}_3^1(\mathbf{C})$ and $\mathrm{cut}_3^2(\mathbf{C})$). Nevertheless this can substantially reduce the effort of interpretation.

With regard to the computational aspects of MPCA, one has to note first that the amount of time required is essentially higher than in conventional PCA due to the fact that no eigenvalue formulation of the problem is available. Although the Kroonenberg algorithm (as described above) looks quite simple in tensorial notation, one should realize that even in the case $N = 3$ the computation of one single element p_{ij} of the matrix $\mathbf{P}$ in step 1 (for one single way in one single iteration) requires the calculation of a sixfold sum over certain index-dependent products. Roughly speaking, the computational effort (number of multiplications) in three-way PCA is

proportional to $n_1^2 \cdot n_2^2 \cdot n_3^2 \cdot it$ (n_1, n_2, n_3 = number of objects, variables and occasions, it = number of iterations). The constant of proportionality may be reduced by a factor of ca. twenty if symmetries in the formal description of the algorithm are exploited. This, however, does not change the computational complexity. In all our applications a number $it = 3$ of iterations (each including three sub-iterations for the three ways) was absolutely sufficient. Before starting the Kroonenberg algorithm ref. 12 recommends that one first applies some iterations (e.g. five) of Tucker's original algorithm (which is much faster but does not yield optimal solutions).

In our computations we implemented the Kroonenberg algorithm in Turbo Pascal source code which was run on a PC 386-AT (32 MHz, numerical co-processor).

PHYSICOCHEMICAL CHARACTERIZATION OF THE BONNY ESTUARY WATERS (NIGER DELTA)

The application to be described here had its origin in studies carried out at the University of Port Harcourt (Nigeria). The aim was to reveal spatiotemporal variations in certain physicochemical factors of water. In detail the following fifteen properties (concentrations in the chemical context) were measured as variables of the data set (the abbreviations used in the figures are given in parentheses): temperature of air and water, transparency (trp), pH, conductivity (cond), chloride (Cl-), hardness (hrd), total alkalinity (alk), dissolved oxygen (O2), biological oxygen demand (O2b), chemical oxygen demand (O2c), oil and grease (oil), ammonia-nitrogen (NH3-N), nitrate-nitrogen (NO3-N), nitrite-nitrogen (NO2-N). Measurements were taken at ten regular sampling stations (objects of the data set) distributed along the Bonny estuary of the Niger delta. Among these, the first five sampling stations were located around the effluent discharge point of the Port Harcourt oil refinery (downstream). The remaining five stations served as reference for waters that did not receive effluent, and were distributed along the University of Science and Technology area (upstream). Finally, this constellation was consistently recorded twice a month in the course of a whole year. Since January measurements were available for the downstream stations only, we excluded them from our computations. Thus, the third way of the data array is built up of $2 \times 11 = 22$ consecutive temporal occasions.

As a pre-treatment the data were subjected to so-called '*j* scaling', which means that centering and variance scaling of each variable was carried out along objects and occasions. In this way temporal variations may be detected which would be equalized in the case of so-called '*jk* scaling', where standardization is carried out for each variable at each occasion separately along objects. Fig. 1 shows the (separated) displays of objects, variables and occasions resulting from the corresponding matrices $\mathbf{A}_1$, $\mathbf{A}_2$ and $\mathbf{A}_3$. To make components within one way comparable they were scaled afterwards according to their contribution to the fit of Eqn. 1. In regard to the object display one can clearly recognize the two-class subdivision into effluent-receiving and non-effluent-receiving stations. Apart from this, there is a remarkable arrangement in Fig. 1a: stations 6–10, in their physicochemical characterization, exactly follow their geographical order towards the mouth of the Bonny river. Among variables, as was to be expected, the temperature of air and water built up an isolated group. Apart from these, one observes high loadings for nitrate-nitrogen and the (hardness, chloride, conductivity, alkalinity) group on the first axis, and for chemical oxygen demand on the second axis. The similarity of hardness, chloride, conductivity and alkalinity is not surprising, since all of them are related to salinity. The representation of occasions reveals a clear temporal factor (first axis) within the data. It seems reasonable to distinguish two major groups, one ranging from February to May and the other ranging from August to December. June and July occupy a medium position. It is interesting to note that, within the second half of the year, the range from August to October reaches an extreme position in terms of the physicochemical characterization of waters. These represent the actual flood months, when real, fresh inland water enters the river water.

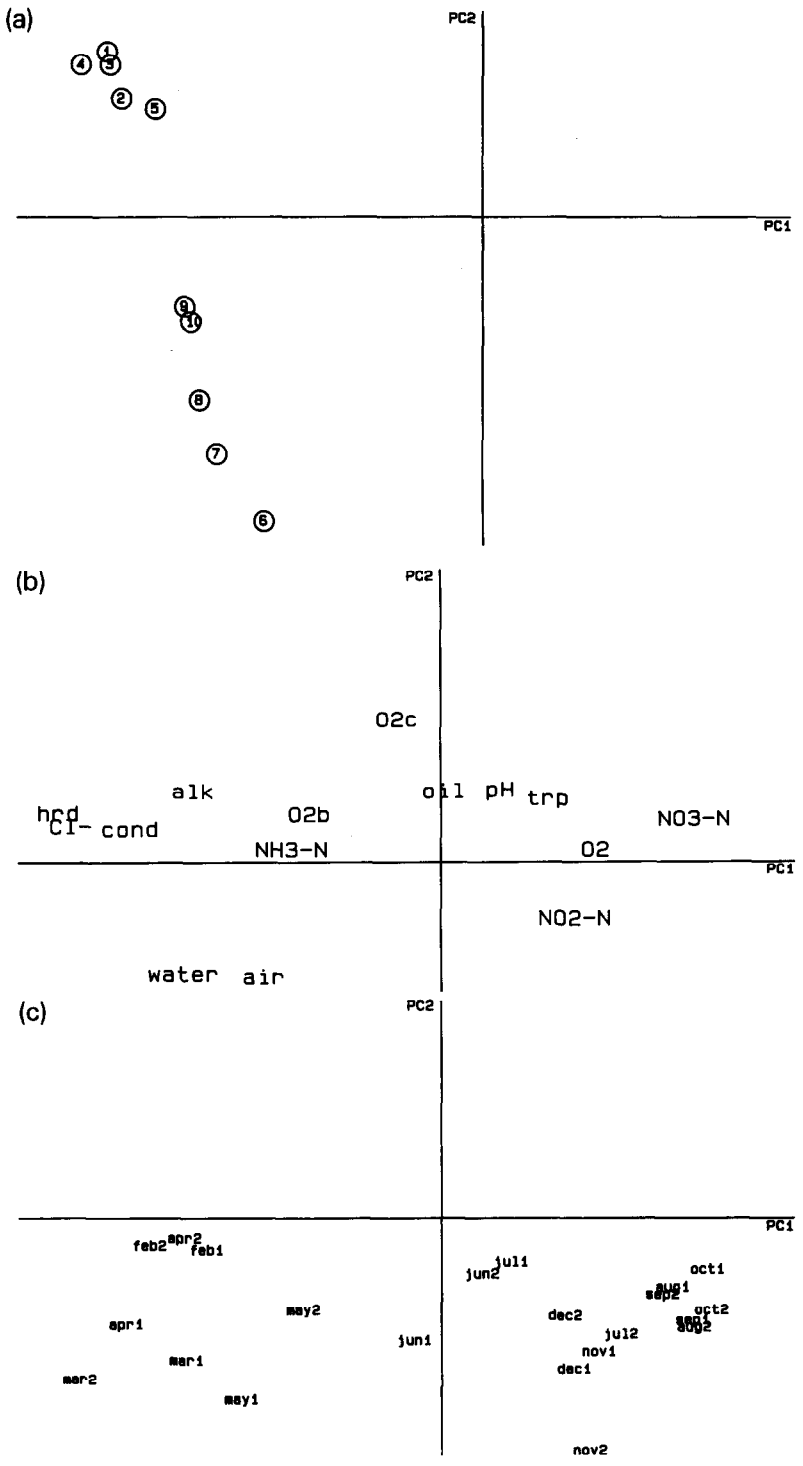

Fig. 1. Display of objects (a), variables (b) and occasions (c) for the multi-way principal components analysis of a three-dimensional data array (for abbreviations see text).

Until now we have only presented a separate analysis of variables, objects and occasions, without knowing how certain identified factors among these link together. This link is determined by the abovementioned $2 \times 2 \times 2$ core matrix, the two frontal planes of which are

$$\begin{pmatrix} -24.5 & -2.5 \\ -2.4 & -0.6 \end{pmatrix} \quad \begin{pmatrix} -1.8 & 3.0 \\ 12.9 & -13.3 \end{pmatrix}$$

Here, the columns refer to components of variables, rows represent components of objects, the first matrix relates to the first component of occasions and the second matrix relates to the second component of occasions. The corresponding squared elements c_{ijk}^2 measure the contribution of components i, j, k for the three ways in the total fit of Eqn. 1. Hence, in the present situation one would have first of all to consider the following three combinations of components: $i = 1$, $j = 1$, $k = 1$ ($c_{111} = -24.5$), $i = 2$, $j = 1$, $k = 2$ ($c_{212} = 12.9$) and $i = 2$, $j = 2$, $k = 2$ ($c_{222} = -13.3$). Furthermore one has to take account of the signs of the core elements before superposing the relevant components. We do not intend to give a joint interpretation of the three ways using the original core matrix. Rather, the procedure of rotation described above will be applied to give this matrix a 'more diagonal shape'. Doing so, one finds that, after appropriate rotation of objects and variables in the plane (keeping occasions fixed), the new core matrix is:

$$\begin{pmatrix} 25.0 & -4.4 \\ 3.6 & -0.7 \end{pmatrix} \quad \begin{pmatrix} 0.5 & -4.3 \\ -5.6 & 17.5 \end{pmatrix}$$

Note that the degree of fit in Eqn. 1 remains unchanged after such a rotation, i.e. the sum of c_{ijk}^2 is the same in both cases. Nevertheless, the percentage of the sum of squared non-diagonal elements decreased from 23% to 8%. Actually, only two combinations of relevance remain: all first components of the three ways and all second components. This fact allows the superposition of all three representations to yield a single one, and the interpretation of factors by projection of all points onto either of the two component axes. The superposed display is shown in Fig. 2. As has already been mentioned, the configuration of occasions is still the same, but objects and variables are moved in contrast to Fig. 1. Projection of all points onto the horizontal axis (main contribution in the core matrix) motivates the identification of the first axis as a temporal factor, differentiating

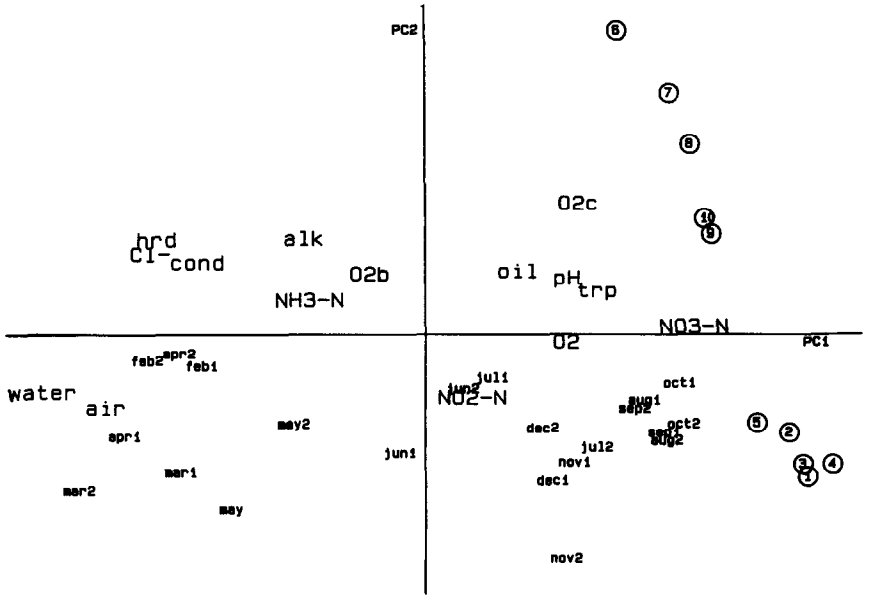

Fig. 2. Superposed display of objects, variables, and occasions after a rotation procedure with simplification of core matrix structure.

between the two halves of a year and determined mainly by air and water temperature, hardness, chloride, conductivity and (negatively correlated) nitrate-nitrogen. One recognizes especially that projection of the (hardness, chloride, conductivity) and of the (aug1, aug2, sep1, sep2, oct1, oct2) group onto the first axis yields opposite positions. This confirms the abovementioned relation between rainfalls from August to October — bringing fresh water — and (low) salinity. In regard to nitrate-nitrogen one observes higher values in the second half of the year (positions on the right-hand side of the first axis) compared to the first half. All other physicochemical parameters have minor importance with respect to temporal variations. Furthermore these facts are consistently valid for all ten sampling stations since these are nearly projected onto a single point of the first axis.

Turning to projections onto the vertical axis, one can clearly identify this factor as a spatial one since it distinguishes between the effluent-receiving and non-effluent-receiving regions. This distinction is first of all determined by values of chemical oxygen demand, minor contributions come from 'salinity' and temperature variables. This spatial factor is again quite stable over time (occasions are not projected onto different ends of the vertical axis).

CONCLUDING REMARKS

Summarizing, one may conclude that multi-way principal components analysis allows one to determine that, in the example considered, the greatest part of the variation in the data is explained by a dominant temporal factor (governed by salinity, temperature and nitrate-nitrogen) and, independently, by a spatial factor (governed by chemical oxygen demand). While salinity is closely related to rainfall, another relation seems to exist between effluents near the pipeline discharge point and chemical oxygen demand. The impact of this effluent on phytoplankton productivity and its relations to physicochemical parameters will be discussed in a future paper [13].

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