Construction of a Vector Equivalent to a Given Vector from the Point of View of the Analysis of Principal Components

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I. INTRODUCTION - All random vectors considered in this paper are assumed to be centered, with elements belonging to the set $L_2(\Omega,\alpha,\beta)$ of random variables with finite variances on (Ω,α,β) .

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Let \underline{X}_1 and \underline{X}_2 be two such vectors; let \underline{Z}_1 and \underline{Z}_2 be the random vectors of their principal components, respectively. In section III we study the problem of attaching weights to the elements of \underline{X}_2 in such a way that the vector of principal components Z_2^* of this weighted vector be as closed as possible to \underline{Z}_1 . In section IV we study ways of choosing a subvector \underline{X}_2^* of \underline{X}_2 , simultaneously attaching weights to the selected elements, so that the vector \underline{Z}_2^* of principal components of the resulting weighted \underline{X}_2^* will best approximate \underline{Z}_1 , over all choices of \underline{X}_2^* and all weighting rules.

When conducting a study based on principal components of a vector difficult or costly to observe, one would welcome a theoritically sound method of substituting to it a vector easier to measure and having approximately the same principal components. At this time not much is available. On the one hand, it is known that the simplest non-singular transformation of the original vector may perturb deeply the principal components; on the other hand, the results to be presented here indicate that the currently proposed techniques ([BEALE et alt 1967], [JOLIFFE 1973]) may suffer from insufficient theoritical foundations.

In section II we recall essential results obtained by ESCOUFIER ([1970], [1973-a], [1973-b]) which are the basis of the solutions to the problems investigated in this paper. To comply with printing space regulations, proofs are omitted (see quoted references).

II. METHEMATICAL BASES - Let X be a pxl random vector and $k \le p$ be the rank of E(XX'). It is known that there exists a pxp orthogonal matrix H^* such that

$$\underbrace{H^*' E(\underline{X}\underline{X}') \ \underline{H}^*} = \begin{bmatrix} \underline{D} & 0 \\ ---- & 0 \end{bmatrix}$$

where \underline{D} is a kxk diagonal matrix with positive diagonal elements. Let \underline{H} be the pxk submatrix of $\underline{\underline{H}}^*$ such that $\underline{\underline{H}}'$ $\underline{E}(\underline{X}\underline{X}')$ $\underline{\underline{H}}$ = $\underline{\underline{D}}$. <u>Definition 1</u>. The kxl random vector $\underline{Z} = \underline{H}^{\top}\underline{X}$ is called the vector of principal components of \underline{X} .

Definition 2. The pxl random vector X_1 , with the vector of principal components Z_1 , and the gxl random vector X_2 , with the vector of principal components Z_2 , are said to be equivalent if there exist a positive integer $k \leq \min{(p,g)}$, a constant α and a kxk matrix C such that :

i) $\underline{CC'} = \underline{C'C} = \alpha \underline{I}_k$, ii) $\underline{Z}_1 = \underline{C'Z}_2$. $(\underline{I}_k \text{ is the kxk identity matrix})$.

It is easily verified that the relation established in Definition 2 is an equivalence relation. Its value, in our context, stems from the following properties [ESCOUFIER, 1973-b]:

<u>Proposition 1</u>. If X_1 and X_2 are equivalent vectors, then

- i) for each diagonal element $\delta^{(1)}_{i}$ of $E(Z_1Z_1')$ there is a diagonal element $\delta^{(2)}_{j}$ of $E(Z_2Z_2')$ such that $\delta^{(2)}_{j} = \alpha \delta^{(1)}_{i}$;
 - ii) there exist permutation matrices P and Q such that

$$Q \subseteq P = \begin{bmatrix} A_1 & 0 & 0 & 0 \\ 0 & A_2 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & A_r \end{bmatrix}$$

where r is the number of distinct diagonal elements of $E(Z_2Z_2')$;

iii) if all the diagonal elements of $E(Z_2Z_2')$ are distinct, there is a permutation of of the indices $1, 2, \ldots, k$ for which $Z_{1i} = \sqrt[+]{\alpha} Z_2$, G'(i).

Proposition 1 should make clear what is to be understood by the "equivalence" of X_1 and X_2 .

 $U_{\underline{X}}(Y) = \sum_{i=1}^{p} \left[E(X_{i}Y) \cdot X_{i} \right] \text{ for all } Y \in L_{2}(\Omega,Q,P).$

The following properties are then established:

a)- the set of operators U $_{\underline{X}}$ is a subset of the class of Hilbert+Schmidt operators on L $_2$ and so is a Hilbert space ;

b) - if
$$\sum = \begin{bmatrix} \sum_{11} & \sum_{12} \\ \sum_{21} & \sum_{22} \end{bmatrix}$$
 is the covariance

matrix of the vector $\underline{X} = \begin{bmatrix} \underline{X}_1 \\ \underline{Y}_1 \\ \underline{X}_2 \\ \underline{Y}_2 \end{bmatrix}$, the scalar product for the Hilbert

$$\langle U_{\underline{x}_1}, U_{\underline{x}_2} \rangle = Tr (\sum_{12} \sum_{21});$$

c)- if \boldsymbol{z}_k is a principal component of \boldsymbol{x} associated with the eigenvalue $\boldsymbol{\lambda}_k$, then

$$U_{\underline{X}}(z_k) = \lambda_k z_k$$

From the above, the following practical criterion can be deduced [ESCOUFIER, 1973-b]:

<u>Proposition 2</u>. The vectors \underline{x}_1 and \underline{x}_2 are equivalent in the sense of Definition 2 if and only if the coefficient

$$\mathbb{R}^{\mathbb{N}}(\underline{\mathbb{X}}_1,\underline{\mathbb{X}}_2) = \mathbb{T}^{\mathbb{N}}(\underline{\Sigma}_{12},\underline{\Sigma}_{21}) / \left[\mathbb{T}^{\mathbb{N}}(\underline{\Sigma}_{11}^2) \cdot \mathbb{T}^{\mathbb{N}}(\underline{\Sigma}_{22}^2) \right]^{1/2}$$

is equal to 1.

III. THE FIRST PROBLEM - From the last proposition it can be seen that the first problem can be restated as:

- Given vectors \underline{Y} and \underline{X} find a diagonal matrix $\underline{\Delta}$ so as to maximize RV $(\underline{Y}$, $\underline{\Delta}$, \underline{X}), where

 $RV(\underline{Y}, \underline{\Delta}\underline{X}) = Tr\left[\underline{\Delta}E(\underline{X}\underline{Y}')E(\underline{Y}\underline{X}')\underline{\Delta}\right] / \left\{ Tr\left[E(\underline{Y}\underline{Y}')\right]^2 . Tr\left[\underline{\Delta}E(\underline{X}\underline{X}')\underline{\Delta}\right]^2 \right\}^{1/2};$ Hence look for $\underline{\Delta}$ to maximize

$$\operatorname{Tr}\left[\underset{\sim}{\triangle} \operatorname{E}(\underline{X}\underline{Y}') \operatorname{E}(\underline{Y}\underline{X}') \underset{\sim}{\triangle} \right] / \left\{ \operatorname{Tr}\left[\underset{\sim}{\triangle} \operatorname{E}(\underline{X}\underline{X}') \underset{\sim}{\triangle} \right]^{2} \right\}^{1/2}.$$

Denote by m_j the j-th diagonal element of Δ , by v_{ij} the elements of E(XX'), by u_{ij} the elements of E(YX') and define the vectors V, M and the matrix A by

$$\widetilde{U} = (U_j) \text{ where } U_j = \sum_i u_{ij},$$

 $\widetilde{M} = (M_j) \text{ where } M_j = m_j^2,$

$$A = (A_{ij})$$
 where $A_{ij} = v_{ij}^2$.

By simply expanding the traces it can be verified that

$$Tr \left[\triangle E(XY') E(YX') \triangle \right] = \underline{U}'\underline{M} ,$$

$$Tr \left[\triangle E(XX') \triangle \right]^2 = \underline{M}'\underline{A}\underline{M} .$$

Thus we are lead to the quadratic programming problem for $\ensuremath{\mathtt{M}}$:

Problem P1
$$\begin{cases} \text{Minimize } \underline{M}' \underline{A} \underline{M} \\ \text{Subject to } \underline{U}' \underline{M} = 1 \text{ and } \underline{M} \geqslant 0. \end{cases}$$

Note that if E(XX') is positive semi-definite, so is A [GOWER, 1971]. In such a case, the function (M'AM) is convex on the convex set (U'M = 1) and $M \ge 0$.

It was found convenient to substitute to Problem Pl on the unknown \underline{M} the following equivalent problem on the unknown vector \underline{N} :

Problem P2
$$\begin{cases} \text{Minimize } \underline{N}' & \underline{C} & \underline{N}, \\ \text{Subject to } \underline{e}' \underline{N} = 1 \text{ and } \underline{N} \ge 0, \end{cases}$$

where $\underline{e}' = (1 \ 1, \ldots, 1)$ and where \underline{N} and \underline{C} are defined by :

$$\widetilde{N} = (N_j) \text{ where } N_j = U_j M_j = U_j m_j^2,$$

$$\widetilde{C} = (C_{ij}) \text{ where } C_{ij} = \frac{A_{ij}}{U_i U_j} = \frac{v_{ij}^2}{U_i U_j}.$$

The authors have solved Problem P2 for many sets of statistical data. Numerical evidence on these test cases will not be given here but reported on elsewhere [CAMBON, 1974].

To be noted is the fact that the constraint $\underline{e'N} = 1$ will force most of the currently proposed quadratic programming algorithms into the difficulty of a degenerated case. For this reason the authors have developed a specific algorithm which will now be justified and summarized.

 $\underline{\mathbb{C}}$ being (nxn), denote by I a subset of $\left\{1,2,\ldots,n\right\}$ and by J the complement of I. Denote by $\underline{\mathbb{C}}_{I}$ the submatrix of $\underline{\mathbb{C}}$ formed by the $\underline{\mathbb{C}}_{ij}$'s with $i \in I$, $j \in I$; by $\underline{\mathbb{C}}_{J}$ the submatrix of $\underline{\mathbb{C}}$ formed by the $\underline{\mathbb{C}}_{ij}$'s with $i \in J$, $j \in I$. From the Kuhn-Tucker conditions for Problem P2, it can be proved that:

Proposition 3. Let
$$N_I = C_I^{-1} \in .$$
 If

 $N_{I} \geqslant 0$ and $C_{J}N_{I} \geqslant e$, then the vector $N = (N_{I})$:

$$N_{i} = \begin{cases} \frac{1}{e^{i}N_{I}} & N_{Ii} & \text{if } i \in I, \\ 0 & \text{if } i \in J, \end{cases}$$
(2)

is an optimal solution of Problem P2, and $N' \subseteq N = (e'N_T)^{-1}$

A technique to find an optimal solution would be to start computing $N_{I} = C_{I}^{-1}$ e for all subsets of indices I and to retain the first found to satisfy (1). The number of sets I to be considered can be greatly restricted in accordance with the following propositions. Jamele on he sendence som alod is heldelided a sedeng nor - h

Proposition 4. Let $\underline{P} = (P_i) = \frac{\underline{C}^{-1}\underline{e}}{\underline{e}^{\dagger}\underline{C}^{-1}\underline{e}}$, $\underline{I}^* = \{i:P_i \gg 0\}$,

 $J^*=\left\{\ i:P_i<0\right\}\ .\ \ \text{There is an optimal solution }N=(N_i)\ \ \text{of Problem P2}$ such that $N_j=0$ for at least one index $j\in J^*$

 \underline{Proof} . It is known that \underline{P} is an optimal solution of P2 without the positivity constraint. Considerany feasible vector $Q = (Q_i)$ for P2 such taht $Q_j > 0$ for all $j \in J^*$. Let $r \in J^*$ be such taht $Q_r/P_r > Q_j/P_j$ for all $j \in J^*$, $k = (Q_r/P_r)/(1-Q_r/P_r)^{-1}$, and $Q_r^k = (1-k)\underline{P} + kQ_r^k$. Since the function F to be minimized is convex and $0 \le k \le 1$, $F(Q^k) \le F(Q)$ But Q^k is feasible for P2 and $Q_r^k = 0$. The conclusion follows.

Proposition 5. An optimal solution of Problem P2 can be found as the best of the optimal solutions of the $|J^*|$ (n-1)-di-mensional problems on N: $\begin{cases} \text{minimize } N' & C(n-j) & N \\ \text{subject to } e'N'=1 & N > 0 \end{cases}$ (3)

$$\begin{cases} \text{minimize } \overset{\mathbb{N}'}{\sim} \overset{\mathbb{C}}{\sim} (n - j) \overset{\mathbb{N}}{\sim} , \\ \text{subject to } \overset{\mathbb{C}'}{\sim} \overset{\mathbb{N}'}{=} 1 , \overset{\mathbb{N}}{\sim} \geqslant 0 , \end{cases}$$
 (3)

where $\mathcal{R} = \{1, 2, \ldots, n\}$ and where j spans J^* .

Proof. From Proposition 4, it is seen that one can find an optimal solution of P2 by looking at the solutions of each of the $\left| \mathsf{J}^* \right|$ problems:

ms: $\begin{cases} & \text{minimize } \underline{N}'\underline{C}\underline{N} \\ & \text{subject to } \underline{e}'\underline{N} = 1 \text{ , } \underline{N} \geqslant 0 \\ & \text{and the additional constaint } N_j = 0 \text{ ,} \end{cases}$

for je J. For each j, this last problem is equivalent to (3).

Clearly (3) is a problem of type P2 with dimensions reduced by 1. We may therefore repeatedly invoke the above proposition to justify the following algorithm. A queue Q is built which elements are sets of indices I for which $N_I = C_I^{-1}$ $\stackrel{.}{\approx}$ has to be calculated in accordance with Proposition 3. (We recall that in a "queue", elements are added "at the bottom" and removed "from the to

the second element moving up at the top).

- 1 Set the queue Q to the single element $\{1,2,\ldots,n\}$ and $\alpha = 0$;
- 2 If Q is empty, print error diagnostic and stop; otherwise, select and remove the first element I. Compute $N_I = C_I^{-1}$ \in ;
- 3 Let $K = \{k : N_{Ik} < 0\}$. If K is empty, go to Step 5; otherwise :
- 4 For each $k \in K$, if (I- $\{k\}$) is not a subset of an element of \mathbf{Q} , then ádd (I- $\{k\}$) to \mathbf{Q} . Go to Step 2;
- 5 If $\alpha \geqslant e' N_I$, go to Step 2; otherwise, set $\alpha = e' N_I$;
- 6 If $C_{i}N_{i} \ge C$ (see (1)), set N_{i} as per (2) and stop; otherwise

The numerical efficiency of the algorithm will depend greatly on the particular code used to compute $\mathbf{c}_{\mathrm{I}}^{-1}$ \mathbf{e}_{I} . It will be seen in Section IV that, by using the Choleski decomposition of $c_{
m I}^{-1}$, one can make the test $\mathbb{C}_{i}\mathbb{N}_{I}\geqslant\underline{e}$ of step 6 an immediate byproduct of

IV. THE SECOND PROBLEM - Let \underline{Y} and \underline{X} be two vectors, possibly equal. Assume X to be n-dimensional and for k \leqslant n denote by \mathscr{V}_k the set of all k-dimensional subvectors of X. If I is a set of k distinct indices, we shall denote by $X_{ extstyle I}$ the subvector of X retaining those elements of X with indices in I and by $\widehat{X}(X_I)$ the vector $(\triangle X_I)$ solution of the first problem studied in Section III. Thus this second problem can be stated as :

- Determine the vector $\mathbf{x}_{\mathbf{I}} = \mathbf{V}_{\mathbf{k}}$ which maximizes RV $\left[\begin{array}{c} \mathbf{x} \end{array}, \widehat{\mathbf{x}} \left(\mathbf{x}_{\mathbf{I}}\right)\right]$ over $\boldsymbol{\mathcal{V}}_{\mathbf{k}}$.

When n and k are large, it becomes unpractical to try all k-dimensional subvectors of X and for this reason we propose a sequential algorithm analogous to the one used in step-wise re-

From the analysis carried in Section III, it is easily seen that for a given set I the vector $\mathbf{x}_{\mathbf{I}}$ is feasible for the present problems if and only if the vector $N_I = C_I^{-1}$ e is non negative and that the coefficient RV $[X, \widehat{X}(X_I)]^2$ is then proportional to $\alpha_{I} = e'C_{I}^{-1}$ e. Thus our problem becomes that of maximizing.

 $\alpha_{I} = e'C_{I}^{-1}$ e subject to $C_{I}^{-1} \approx 90$, over all subsets I of k distinct indices. Suppose now that I is a subset of only (k-1) indices which is known to be feasible (i.e. $N_I = C_I^{-1} \in \mathbb{R} > 0$). The step-wise technique consists in the determination of that index $j \neq I$ such that, with $(I,j) = I - \{j\}$, N(I,j) will be feasible and $\alpha(I,j)$ will be maximized (over all choices of j).

The technicalities will now be described, assuming for simplicity that the set I contains the first (k-1) indices : I = $\{1,2,\ldots,k-1\}$.

Consider the matrix

$$\underline{\mathbf{c}}^{+} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ \underline{\mathbf{c}} \end{bmatrix}$$

where C is given by (3), and let $C^+ = R R'$ be the Choleski decomposition [FORSYTHE, MOLER, 1967] of C^+ (which is positive semi-definite), i.e R is upper-triangular. We assume that the choice of the elements of the set I has been made sequentially by this same algorithm and that the first (k-1) steps of the Choleski decomposition of C^+ have been carried, column-wise, leading to the (n+1)x(k-1) matrix

where $r'_{j\bullet} = (r_{j1} r_{j2} \cdot i \cdot r_{j(k-1)})$ for $j \geqslant k$ and $C_{I} = R_{I} R'_{I},$ $R_{I} r_{(n+1)\bullet} = e.$

For j # I (j # n+1), define

$$w_{j} = c_{jj} - \sum_{i=1}^{k-1} r_{ji}^{2}$$

$$s_{i} = 1 - \sum_{i=1}^{k-1} r_{i} r_{i}$$

 $(s_j = 1 - r'_{j \cdot e} R_I^{-1}_{j \cdot e})$. If the index j is to be added to the set I

with the feasible vector $X_{(1,i)}$, we must have the corresponding matrix $C_{(I,j)}$ non-singular, hence $w_i > 0$. The Choleski decomposition C(I,j) = R(I,j) R'(I,j) would then give :

$$\mathbb{E}_{(\mathbf{I},\mathbf{j})}^{-1} = \begin{bmatrix} \mathbb{E}_{\mathbf{I}}^{-1} & \vdots & 0 \\ \frac{\mathbb{E}_{\mathbf{I}}^{-1}}{\sqrt{\mathbf{w}_{\mathbf{j}}}} & \mathbb{E}_{\mathbf{I}}^{-1} & \vdots & \frac{1}{\sqrt{\mathbf{w}_{\mathbf{j}}}} \end{bmatrix}, \ \mathbb{E}_{(\mathbf{I},\mathbf{j})}^{-1} \stackrel{\mathbf{e}}{=} \begin{bmatrix} \mathbb{E}_{\mathbf{I}}^{-1} & \mathbb{e} \\ \mathbb{E}_{\mathbf{I}}^{-1} & \mathbb{e} \\ \frac{\mathbb{E}_{\mathbf{I}}^{-1}}{\sqrt{\mathbf{w}_{\mathbf{j}}}} & \mathbb{E}_{\mathbf{J}}^{-1} & \vdots & \mathbb{E}_{\mathbf{J}}^{-1} \end{bmatrix}$$

The coefficient RV $\left[\frac{y}{2}, \frac{\hat{y}}{2} \left(\frac{x}{2(1.i)}\right)\right]^2$ will be proportional to

$$\alpha_{(I,j)} = \underline{e} \underline{R}^{-1} \underline{R}^{-1} \underline{R}^{-1} \underline{e} + (s_j^2/w_j) = \alpha_I + (s_j^2/w_j)$$
 (6)

The feasibility condition of non-negativity of = $C_{(1,j)}^{-1}$ must be respected. It can be verified by substitution of the above relations that

N(I,j) =
$$\mathbb{R}^{-1}$$
 (I,j) \mathbb{R}^{-1} (I,j) \mathbb{R}^{-1} \mathbb{R}^{-

where Z_i is the solution of the triangular system $R'_{i}Z_{j} = r_{j}$.

We can now summarize one basic cycle of the algorithm assuming that k is given, that I is a set of indices with less than k elements and that the corresponding matrix (4) is available, as s; and w; for all j . I:

1 - Define J = { j : j ≠ I, w_j > 0 and s_j > 0 };
2 - If J is empty, stop. Otherwise select j₀ ∈ J which maximizes (s_i^2/w_i) (see (6));

3 - Solve for Z_{j_0} the triangular system $R_1 Z_{j_0} = r_{j_0}$;

4 - If $N_{(I,j)} = N_{I}^{-(s_{j}/w_{j})} Z_{j}$ is non-negative, then accept j set I : = $I \circ \{j_0\}$, N_I : = $N(I,j_0)$ and go to Step 5. Otherwise set $J := J-\{j\}$ and repeat Step 2;

5 - Carry one more step of the Choleski decomposition of C^+ , computing the column corresponding to column "j " of \mathcal{L}^+ (to obtain $\mathbb{R}_{(I,j_0)}^{(I,j_0)}$ and, for $j \in J$, set ((5)): $s_j := s_j^{-r}(n+1)j_0^{-r}jj_0^{-r}, w_j := w_j^{-r}jj_0^2$

$$s_{j} := s_{j}^{-r}(n+1)j_{0}^{r}j_{0}^{j}, w_{j} := w_{j}^{-r}j_{0}^{2};$$

6 - If $k_0 < k$, set k_0 : = k_0 +1 and repeat a complete cycle from Step 1. Otherwise, stop.

Note that a "stop" a Step 2 implies that the set of indices already chosen connot be enlarged by addition of a single element so as to increase the RV coefficient.

To initiate the algorithm one may choose any one element X_i of X and set $I=\{i\}$. The square of the RV coefficient is then proportional to C_i^{-1} ; this suggests initiation with that index for which the diagonal element of \underline{C} is minimum.

It must be made clear that this algorithm does not necessarily produce the optimal solution. As in the step-wise regression technique, it produces the best solution of order k knowing which solution has been selected to the order (k-1).

Subject to this conditionality restriction upon convergence to the optimal solution, a count of the number of operations for a k-th cycle shows the algorithm to be quite efficient.

We conclude the study of this second problem by pointing out that the first problem (Section III) can be interpreted as a special case of the second: the case where k = n. Thus the algorithm of this section could be used in an attempt to solve Problem P2. The following proposition, deduced from the Kuhn-Tucker conditions for Problem P2 and the above analysis, provides a criterion to detect the optimal solution:

Proposition 6. A solution produced by the algorithm of this Section is optimal for Problem P2 of Section III if and only if, at stop,

s; < 0 for all j c J

or all n variables have been accepted (The proof is omitted).

CONCLUSION. - The theory summarized in Section II has shed new lights on two practical problems of interest to the applied statistician. Arguments on convexity and a factorization of the matrices involved have led to algorithms to solve those problems. A deeper numerical analysis of the problems, particularly the first one, should lead to more efficient algorithms and computer programs.

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