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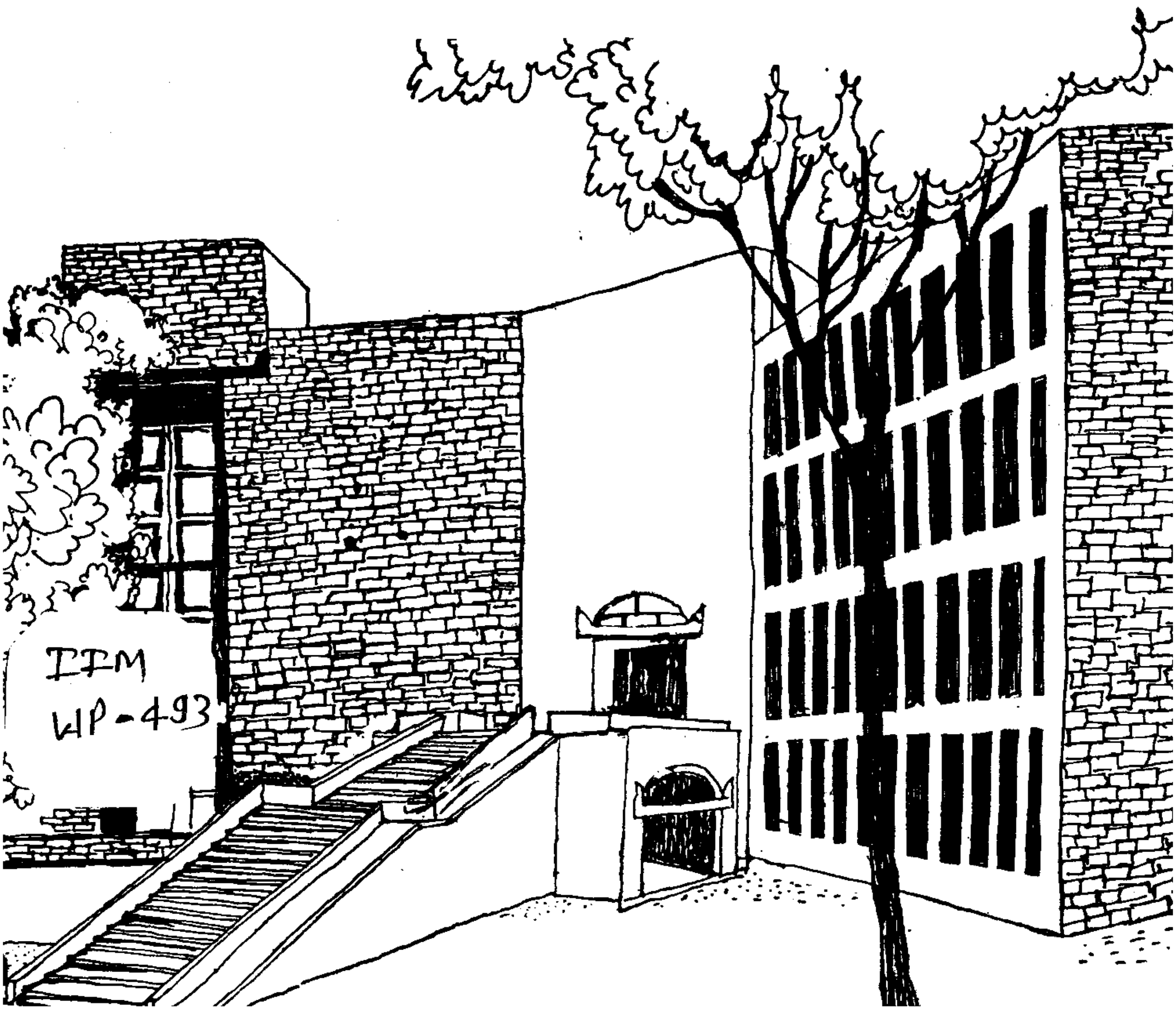

A NOTE ON TWO-PHASE METHOD FOR A CLASS OF METRIC MODELS IN INDIVIDUAL SCALING

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A NOTE ON TWO-PHASE METHOD FOR A CLASS OF METRIC MODELS IN INDIVIDUAL SCALING

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1. Introduction

In this note, we discuss the typical problem in individual scaling viz., finding a common configuration and weights attached to dimensions for each individual from the given interpoint distances or scalar products. Tucker and Messick [1963], Horan [1969] and others have developed procedures for solving the problem. Carroll and Chang [1970] defined a minimization criterion (STRAIN) in terms of product moments computed from raw data. They use an alternative least square (ALS) method for estimating the configuration and weights. Within the STRAIN frame work, Schonemann [1972] presented an algebraic solution in the case of exact data. Takane, Young and De Leeuw [1977] proposed a procedure called, ALSCAL in which the criterion function (SSTRESS) is in terms of distances obtained from raw data. The configuration and weights are obtained by solving certain normal equations in the least square method alternately.

In this note, we consider the problem within the STRAIN framework and propose a two-phase method. In the first phase, the problem of determining the optimal weights (W_i) for a given configuration (X) is posed as a standard quadratic programming problem for which efficient finitely convergent algorithms are available. In the second phase, for a given set of weights (W_i), a system of equations is developed for obtaining the configuration X. The relation to the quadratic programming problem to obtain W_i and the approach to obtain X appear to be new. An explicit solution to the problem is obtained for one dimensional case and an approach is described for the two dimensional problem. Numerical examples are given for one and two dimensions cases. The solution obtained by the proposed method is also compared with the solution obtained by Schonemann [1972] for the two-dimensional problem.

2. Problem Formulation

Given P_i : n x n, (i = 1, ... N) symmetric and positive semi-definite matrices for N individuals, the mathematical problem is to find a n x t matrix X and t x t diagonal matrices

$$W_i = \text{diag}\ (w_{i1}, \ldots w_{it}),\quad i = 1, \ldots N$$

such that

$$\text{STRAIN} = \sum_{i=1}^{N} \text{tr}\ (P_i - XW_iX')^2 \tag{2.1}$$

is minimum subject to the condition

$$\frac{1}{N}\sum_{i=1}^{N} W_i = I_t \tag{2.2}$$

$$w_{ir} \geq 0, \quad i = 1, \ldots, N, \quad r = 1, \ldots t.$$

I_t is the identity matrix of order t and tr(A) denotes the trace of matrix A. When the optimal value of STRAIN is zero, we have

$$P_i = XW_iX' \qquad i = 1, \ldots N \tag{2.3}$$

We call this as the Exact Case and in this case, P_i s are exactly decomposed into XW_iX'. When the optimal value of the objective function in the problem given by (2.1) and (2.2) is strictly positive, we are in the fallible case and we cannot find exactly X and W_i such that (2.3) holds.

3. Proposed Procedure and its Relation to others

We propose a procedure with two phases for solving the above problem given by (2.1) and (2.2).

Phase A: To find optimal W_i for any given X:

For any given X, the STRAIN is function of W_i only and (2.1) can be written as

$$\text{STRAIN} = \sum_{i=1}^{N} \operatorname{tr}(XW_iX')^2 - 2\sum_{i=1}^{N} \operatorname{tr}(P_iXW_iX') + \sum_{i=1}^{N} \operatorname{tr}(P_i^2) \qquad (3.1)$$

From (3.1), it can be seen that the objective function (2.1) is quadratic and convex in w_{ir}, $i = 1, \ldots N$, $r = 1, \ldots t$. Note that $\sum_{i=1}^{N} \operatorname{tr}(P_i^2)$ is a given quantity which does not depend upon w_{ir}. Thus for a given X, the determination of optimal $W_i = \operatorname{diag}(w_{i1}, \ldots w_{it})$, $i = 1, \ldots N$ is a convex quadratic programming problem with linear constraints (2.2). To solve this problem, efficient finitely convergent algorithms are available. See for example, Wolfe [1959], Cottle and Dantzig [1968] and Ravindran [1972]. Thus exact optimum w_{ir} s are obtained directly for a given X.

Phase B: To obtain X for given W_i

In this phase, using the values of W_i, $i = 1, \ldots N$ obtained in Phase A, configuration X is estimated so that STRAIN as a function of X only is minimum.

Let X be an optimum solution to (2.1) for given W_i satisfying (2.2). Then a necessary condition satisfied by optimal X is clearly $\frac{\partial}{\partial X}$ (STRAIN) = 0 or from (3.1),

$$\sum_{i=1}^{N} (XW_iX' - P_i)\, XW_i = 0 \tag{3.2}$$

Let $y_r (r = 1, \ldots t)$ be a column vector of X. Then $X = (y_1 \ldots y_t)$. With this notation, (3.2) can be written as

$$\begin{array}{lllll} z_{11}y_1y_1'\,y_1 + \ldots\ldots + z_{1t}y_ty_t'\,y_1 & = & Q_1y_1 \\ \ldots\ldots\ldots\ldots & \ldots\ldots\ldots\ldots & \ldots\ldots \\ \ldots\ldots\ldots\ldots & \ldots\ldots\ldots\ldots & \ldots\ldots \\ z_{t1}y_1y_1'\,y_t + \ldots\ldots + z_{tt}y_ty_t'\,y_t & = & Q_ty_t \end{array} \tag{3.3}$$

Where z_{rs}, s = 1, ... t are the diagonal elements of

$$\Delta_r = \sum_{i=1}^{N} W_i\, w_{ir}, \quad r = 1, \ldots t ;$$

and

$$Q_r = \sum_{i=1}^{N} P_i\, w_{ir}, \quad r = 1, \ldots t$$

Solving for X in (3.2) is equivalent to solving equations in (3.3) for $y_1, y_2, \ldots y_t$. (3.3) is a system of non-linear homogeneous equations of third degree. We are looking for a non-trivial solution. The equations in (3.3) can be solved, for example, by Newton-Raphson method or some other appropriate numerical analysis method. Phase A and phase B are iterated till a satisfactory level of STRAIN is attained. Initially to start phase A, we can take X to be a gram factor of $\overline{P} = \frac{1}{N} \sum_{i=1}^{N} P_i$.

As mentioned before, Schonemann [1972] presented a solution for exact data and indicated a heuristic method for non-exact data. In the ALSCAL method proposed by Takane, Young and De Leeuw [1977], W_i $(i = 1, \ldots N)$ are obtained by solving normal equations in the least squares method which may entail the violation of non-negativity constraint (2.2) and further adjustment has to be made to make them non-negative. As pointed out in this note, the determination of W_i satisfying (2.1) and (2.2) for a given X, poses no problem since optimal W_i are obtained directly solving a quadratic programming problem. It can be seen that the minimization criterion defined in ALSCAL in terms of distances is also a convex quadratic function of W_i $(i = 1, \ldots N)$. This implies the validity of the quadratic programming formulation in this situation as well. Thus the proposed method is superior and direct for determining W_i for any given X over ALSCAL or any other method. Thus the main problem in Individual Scaling is the problem of determining the configuration X for given W_i $(i = 1, \ldots N)$. The equations in (3.3) can be solved by numerical analysis methods. We discuss below the special cases for t = 1 and t = 2, since in most applications one is interested in lower dimensions only.

4. Specialization to t = 1 and t = 2

Since phase A can be implemented exactly for a given X, we discuss the specialization for t = 1 and t = 2 only for phase B. For t = 1 and t = 2 the algebra in phase B is simplified and we give below a few results for these cases. We obtain a closed form solution X for given W_1 for the case t = 1.

Case (i) : t = 1:

In this case (3.3) reduces to

$$\left(\sum_{i=1}^{N} w_{i1}^{2}\right) \left(\sum_{j=1}^{n} x_{j1}^{2}\right) X = Q_1 X \tag{4.1}$$

where X is a n x 1 column vector. From (4.1), we have

$$\left[Q_1 - z_{11} \left(\sum_{j=1}^{n} x_{j1}^{2}\right) I_n\right] X = 0 \tag{4.2}$$

where

$$z_{11} = \sum_{i=1}^{N} w_{i1}^{2}$$

(4.2) implies that X is an eigen vector of Q_1 corresponding to the eigen value $z_{11} \sum_{j=1}^{n} x_{j1}^2$.

We find the eigen values and corresponding eigen vectors of Q_1. We select the eigen vector corresponding the eigen value for which

$$\left(\sum_{j=1}^{n} x_{j1}^2 \right) = \left(\frac{\text{Eigen value}}{z_{11}} \right)$$

Thus a closed form solution to (3.3) for t = 1 is obtained.

Case (ii): t = 2:

In this case, from (3.3), we have

$$\begin{aligned} z_{11}\, y_1 y_1' y_1 \;+\; z_{12}\, y_2 y_2' y_1 &= Q_1 y_1 \\ z_{21}\, y_1 y_1' y_2 \;+\; z_{22}\, y_2 y_2' y_2 &= Q_2 y_2 \end{aligned} \qquad (4.3)$$

A closed form solution to (4.3) seems difficult to obtain. As mentioned before we could obtain y_1, y_2 by numerical analysis approach. We however, give a remark in the spirit of the method used for t = 1 case, and relate the solution to the eigen vectors of some matrix.

Let $\beta_1 = y_1' y_1$ and $\beta_2 = y_2' y_2$. We have from (4.3),

$$[(Q_2 - z_{22}\,\beta_2\, I_n)\,(Q_1 - z_{11}\,\beta_1\, I_n) - z_{12}^2 \mu^2 I_n]\, y_1 = 0 \qquad (4.4)$$

$$[(Q_1 - z_{11}\,\beta_1\, I_n)\,(Q_2 - z_{22}\,\beta_2\, I_n) - z_{12}^2 \mu^2 I_n]\, y_2 = 0 \qquad (4.5)$$

Where

$$\mu^2 = (y_1' y_2)^2 = (y_2' y_1)^2$$

Suppose β_1 and β_2 are known, We find the eigen values and corresponding eigen vectors of R and R$'$ where

$$R = Q_2 Q_1 - z_{22}\,\beta_2\, Q_1 - z_{11}\,\beta_1\, Q_2 \qquad (4.6)$$

(4.4) and (4.5) imply that there exists an eigen value E of R, such that

$$\mu^2 = \frac{E + z_{11}\,\beta_1\,\beta_2\, z_{22}}{z_{12}^2} \qquad (4.7)$$

The right side of (4.7) is calculated for each of the eigen values of R. We select those eigen vectors y_1 and y_2 from the set of eigen vectors R and R$'$ respectively for which $y_1' y_1 = \beta_1$, $y_2' y_2 = \beta_2$ and $(y_1' y_2)^2 = \mu^2$ obtained by (4.7). Thus a solution is obtained when β_1 and β_2 are known. A possibility is to try for several pairs of values (β_1, β_2) and obtain y_1 and y_2 satisfying $y_1' y_1 = \beta_1$, $y_2' y_2 = \beta_2$ and $(y_1' y_2)^2 = \mu^2$ with μ^2 given by (4.7).

5. Numerical Examples

Numerical examples for t = 1 and t = 2 cases, covering phase A and phase B methods are given below. We have taken the same example considered by Schonemann [1972] for fallible data. For this example, we obtain one-dimensional and two-dimensional configurations and the weights. For t = 2, results are compared with the results obtained by Schonemann [1972].

Example 1:

Here N = 3, n = 4, t = 1 and P_1, P_2, P_3 are as in Schonemann [1972]. Given P_1, P_2 and P_3 matrices for three individuals, we want to find a 4 x 1, configuration matrix X and weights w_{11}, w_{21} and w_{31} assigned by three individuals.

Initial value of X is obtained as gram factor of $\bar{P}$ which is given by $X' = (2.1, 3.2, 1.0, 1.07)$. For this X, we find w_{11}, w_{21} and w_{31} by solving a quadratic programming problem as $w_{11} = 1.3891$, $w_{21} = 0.4994$, $w_{31} = 1.1115$. Using these values, $Q_1 = \sum_{i=1}^{3} P_i w_{i1}$ is calculated. The eigen values and corresponding eigen vectors are found. We found that eigen vector $X' = (2.180, 3.456, 0.910, 1.190)$ with $\sum_{j=1}^{4} x_{j1}^2 = 18.94$ corresponding to the eigen value 64.84 satisfies (4.2). Repeating phase A and phase B, after a few iterations, the final solution is obtained as $X' = (2.197, 3.482, 0.911, 1202)$; $w_{11} = 1.33$, $w_{21} = 0.56$, $w_{36} = 1.11$ and STRAIN = 45.65.

<u>Example 2</u>:

Here we take the same data as in example 1 and final two - dimensional (t = 2) configuration. Thus P_1, P_2 and P_3 are as in Example 1. Here also we take for the initial (4 x 2) matrix X as a gram factor of $\overline{P}$ and initiate phase A to find W_1, W_2 and W_3. In phase B, we solve the equations (4.3) by Newton-Raphson method. Iterating phase A and phase B, after thirty iterations, it was found that the values of W_i and X remained the same upto two decimal places. The final X and W_i (i = 1, 2, 3) are given by

$$X = \begin{bmatrix} 0.90 & 2.03 \\ 1.81 & 2.98 \\ 2.04 & 1.03 \\ 2.08 & 0.10 \end{bmatrix} \qquad \begin{aligned} W_1 &= \text{diag}\ (0.97,\ 1.50) \\ W_2 &= \text{diag}\ (0.73,\ 0.49) \\ W_3 &= \text{diag}\ (1.30,\ 1.01) \\ \text{STRAIN} &= 0.9442 \end{aligned}$$

Schonemann [1972] proposed the solution developed for exact case as an approximation to the fallible case. For this problem, Schonemann [1972] obtained a solution for which STRAIN = 1.2194. The value of STRAIN obtained by the proposed method is smaller than the value given in Schonemann [1972].

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