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ON GAUSSIAN ELIMINATION AND MINIMUM VIOLATOR ALGORITHM IN SIMPLE TREE ORDER

By

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1. Introduction

Let $Y_i (i=0, 1, \cdots, k)$ be mutually independent and normally distributed with mean θ_i and variance λ_i. Consider the M.L.E. of θ_i under the partial ordering of the type,

$$(1.1) \qquad \theta_i - \theta_0 \geqq 0,\ i=1, 2, \cdots, k.$$

The above problem is a special case of the isotonic regression, which was called "simple tree order" [1, p. 74]. This problem and its algorithm were discussed by Bartholomew [2]. Barlow, et al. [1] discussed this problem as minimum violator algorithm in a general manner and also presented some examples. We discussed an algorithm by means of the projection method in Kudô and Choi [5] assuming normal distribution. Although our algorithm is essentially the same as that of Bartholomew [2], it will shed some lights on the geometrical properties involved in the use of Gaussian elimination in the isotonic regression analysis [1], [3].

Let $Y'=(Y_0, \cdots, Y_k)$ and transform $\bar{x}=\bar{A}y$, where

$$(1.2) \qquad \bar{A}=\begin{bmatrix} 1 & 0' \\ L & I_k \end{bmatrix}=\begin{bmatrix} 1 & 0' \\ & A \end{bmatrix},\ L'=(-1, \cdots, -1),\ 0'=(0, \cdots, 0),$$

and I_k is $(k \times k)$ unit matrix, then $\bar{X}, \bar{X}'=(X_0, X_1, \cdots, X_k)=(X_0, X)$, is distributed as $N(\bar{\mu}, \bar{\Lambda})$, where $\bar{\mu}'=(\mu_0, \mu_1, \cdots, \mu_k)=(\mu_0, \mu)$, $\mu_0=\theta_0$, $\mu_i=\theta_i-\theta_0$ $(i=1, \cdots, k)$, and

$$(1.3) \qquad \bar{\Lambda}(k+1)=\bar{A}\bar{D}(k+1)\bar{A}'=\bar{D}(k+1)+\lambda_0\begin{bmatrix} 0 & L' \\ L & E \end{bmatrix}$$

$$=\begin{bmatrix} \lambda_0 & -\lambda_0 \cdots\cdots -\lambda_0 \\ -\lambda_0 & \\ \vdots & D(k)+\lambda_0 E \\ -\lambda_0 & \end{bmatrix}=\begin{bmatrix} \lambda_0 & \lambda_0 L' \\ \lambda_0 L & \Lambda(k) \end{bmatrix},$$

where $\bar{D}(k+1)$ and $D(k)$ are covariance matrices of $Y_i (i=0, \cdots, k)$ and $(i=1, \cdots, k)$, i.e., the diagonal matrices with $\lambda_i (i=0, \cdots, k)$ and $(i=1, \cdots, k)$ respectively and E

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is a $(k \times k)$ matrix with all elements equal to 1.

We can easily show that the underlying M.L.E. of θ or μ for a given sample y^1o r $\bar{x}^1 = \bar{A}y^1 = (x_0^1, x^1)$, equals to the solution of the following minimizing problem;

(1.4) $$\operatorname*{Min}_{Ay \geqq 0} (y - y^1)' \bar{D}^{-1} (y - y^1)$$

or

(1.5) $$\operatorname*{Min}_{x \geqq 0} (\bar{x} - \bar{x}^1)' \Lambda^{-1} (\bar{x} - \bar{x}^1)$$

respectively. (See Kudô and Choi [5])

(1.5) can be rewritten as

(1.6) $$\operatorname*{Min}_{x \geqq 0} \left[(x - x^1)' \Lambda^{-1} (x - x^1) + \frac{\{(x_0 - x_0^1) - \lambda_0 L' \Lambda^{-1} (x - x^1)\}^2}{\lambda_0 (1 - L' \Lambda^{-1} L)} \right].$$

As the second term is zero, the problem of finding $\bar{x}$ satisfying (1.6) is essentially reduced to that of x with

(1.7) $$\operatorname*{Min}_{x \geqq 0} (x - x^1)' \Lambda^{-1} (x - x^1).$$

2. Algorithm

In Kudô and Choi [5], we described an algorithm to obtain the solutions of (1.4) and (1.7) for an arbitrary positive definite matrix Λ. Following the notions of [5], we partition the vector $x' = (x'_{(1)}, x'_{(2)}) = (x_1, \cdots, x_m; x_{m+1}, \cdots, x_k)$, and the sweepout operation on the following matrix, taking the corresponding covariance matrix of $x_{(1)}$ as a pivotal matrix, yields the following,

(2.1) $$\begin{bmatrix} \Lambda_{11}^{-1} & 0 & 0 \\ -\Lambda_{21}\Lambda_{11}^{-1} & I & 0 \\ -B_1'\Lambda_{11}^{-1} & 0 & I \end{bmatrix} \begin{bmatrix} \Lambda_{11} & \Lambda_{12} & x_{(1)} \\ \Lambda_{21} & \Lambda_{22} & x_{(2)} \\ B_1' & B_2' & V^{-1/2}y \end{bmatrix} = \begin{bmatrix} I & * & \Lambda_{11}^{-1}x_{(1)} \\ 0 & * & x_{(2)} - \Lambda_{21}\Lambda_{11}^{-1}x_{(1)} \\ 0 & * & V^{-1/2}y - B_1'\Lambda_{11}^{-1}x_{(1)} \end{bmatrix},$$

where $V = \bar{D}(k+1)$, $B = AV^{1/2}$ and B is also partitioned correspondingly. The optimal solutions $\hat{y}$ and $\hat{x}$ of (1.4) and (1.7) are respectively of the forms;

(2.2) $$\begin{aligned} \hat{y} &= V^{1/2}(V^{-1/2}y - B_1'\Lambda_{11}^{-1}x_{(1)}) \\ &= y - VA_1'(A_1VA_1')^{-1}A_1y \end{aligned}$$

and

(2.3) $$\hat{x} = \begin{bmatrix} 0 \\ x_{(2)} - \Lambda_{21}\Lambda_{11}^{-1}x_{(1)} \end{bmatrix},$$

if and only if

(2.4) $$\Lambda_{11}^{-1}x_{(1)} = (B_1B_1')^{-1}A_1y \leqq 0$$

and

(2.5) $$x_{(2)} - \Lambda_{21}\Lambda_{11}^{-1}x_{(1)} = B_2(V^{-1/2}y - B_1'\Lambda_{11}^{-1}A_1y) > 0.$$

We can arrive at the solution while all of the successive steps of the Gaussian eliminations taking every possible subset of variables as the pivotal matrix are exhausted. In this note we show that the number of Gaussian eliminations is reduced to the minimum in the case when Λ is of the form (1.3).

For preparation we calculate the inverse of Λ of (1.3).

LEMMA. *For a matrix Λ $(k\times k)$ of the form* (1.3), *the matrix $G=(g_{ij})$ satisfying the relation,*

$$\Lambda\Lambda^{-1}=(D+\lambda_0 E)(D^{-1}+G)=I\,, \tag{2.6}$$

is given by

$$g_{ij}=-\frac{\lambda_0}{1+\lambda_0\sum_{\nu=1}^{k}\lambda_\nu^{-1}}(\lambda_i\lambda_j)^{-1}\,. \tag{2.7}$$

PROOF. From (2.6),

$$\lambda_0 ED^{-1}+DG+\lambda_0 EG=0\,, \text{ that is,}$$

$$\lambda_0 E\begin{bmatrix}\lambda_1^{-1} & & 0\\ & \ddots & \\ 0 & & \lambda_k^{-1}\end{bmatrix}+\begin{bmatrix}\lambda_1 & & 0\\ & \ddots & \\ 0 & & \lambda_k\end{bmatrix}\cdot(g_{ij})+\lambda_0 E\cdot(g_{ij})=0\,. \tag{2.8}$$

For convenience in notation, consider the first column of (2.8), which is

$$\lambda_0\lambda_1^{-1}\begin{bmatrix}1\\ \vdots\\ 1\end{bmatrix}+\begin{bmatrix}\lambda_1 g_{11}\\ \vdots\\ \lambda_k g_{k1}\end{bmatrix}+\lambda_0\Big(\sum_{i=1}^{k}g_{i1}\Big)\begin{bmatrix}1\\ \vdots\\ 1\end{bmatrix}=\begin{bmatrix}0\\ \vdots\\ 0\end{bmatrix}. \tag{2.9}$$

Writing $\sum_{i=1}^{k}g_{i1}=G_1$, (2.9) yields

$$g_{i1}=(-\lambda_0 G_1-\lambda_0\lambda_1^{-1})\lambda_i^{-1}\,,\ i=1,\cdots,k\,, \tag{2.10}$$

therefore

$$G_1=(-\lambda_0 G_1-\lambda_0\lambda_1^{-1})\Big(\sum_{\nu=1}^{k}\lambda_\nu^{-1}\Big)\,,$$

and then

$$G_1=(-\lambda_0\lambda_1^{-1})\Big(\sum_{\nu=1}^{k}\lambda_\nu^{-1}\Big)/\Big(1+\lambda_0\sum_{\nu=1}^{k}\lambda_\nu^{-1}\Big)\,. \tag{2.11}$$

Putting (2.11) into (2.10), we have

$$g_{i1}=-\frac{\lambda_0}{1+\lambda_0\sum_{\nu=1}^{k}\lambda_\nu^{-1}}(\lambda_i\lambda_1)^{-1} \qquad \text{Q.E.D.}$$

Now we state the final proposition.

PROPOSITION 2.1. *Suppose the components of a sample vector x; $x_1,\cdots,x_k$, or equivalently $y_1,\cdots,y_k$, are in the ascending order; $x_i\leqq x_{i+1}(i=1,\cdots,k-1)$, then there exists m such that the last column in the result of sweepout of* (2.1), *taking the first m as the pivot,*

$$
\begin{bmatrix} \Lambda_{11}^{-1}x_{(1)} \\ \\ x_{(2)}-\Lambda_{21}\Lambda_{11}^{-1}x_{(1)} \end{bmatrix} = \begin{bmatrix} z_1 \\ \vdots \\ z_m \\ z_{m+1} \\ \vdots \\ z_k \end{bmatrix} \tag{2.12}
$$

satisfies the following

$$
z_i \leqq 0\,, \quad i \leqq m \tag{2.13}
$$

and

$$
0 < z_{m+1} \leqq \cdots\cdots \leqq z_k\,. \tag{2.14}
$$

PROOF. According to the lemma, we can write

$$
\Lambda_{11}^{-1}x_{(1)} = (D^{-1}+G)\,x_{(1)} = \begin{bmatrix} \lambda_1^{-1} & & 0 \\ & \ddots & \\ 0 & & \lambda_m^{-1} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix} - c\cdot \begin{bmatrix} (\lambda_1\lambda_1)^{-1} \cdots (\lambda_1\lambda_m)^{-1} \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ (\lambda_m\lambda_1)^{-1} \cdots (\lambda_m\lambda_m)^{-1} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix},
$$

where $c=-\lambda_0/(1+\lambda_0 \sum_{\nu=1}^{m} \lambda_\nu^{-1})$. Then we have

$$
\begin{bmatrix} z_1 \\ \vdots \\ z_m \end{bmatrix} = \begin{bmatrix} \lambda_1^{-1}(x_1+K) \\ \vdots \\ \lambda_m^{-1}(x_m+K) \end{bmatrix}, \tag{2.15}
$$

where $K=c\cdot(\sum_{\nu=1}^{m} x_\nu/\lambda_\nu)$.

(2.15) implies (2.13), and (2.14) is easily shown from the fact that $\Lambda_{21}=\lambda_0 E$.

Q.E.D.

The above proposition enables us to state the rule for computing the solution: (1) Examine the observation if there is an violator to the hypotheses (1.1), or an observation y_i with $y_i<y_0$, (2) if there is none, the values in the sample themselves are the estimates and the step terminates here, otherwise arrange the observation in the ascending order, (3) transform y to x by (1.2), (4) perform Gausian eliminations successively either until when the conditions (2.13) and (2.14) are satisfied (case (a)) or until all the steps of k sweepouts are made (case (b)), (5) x_0 in (2.5) is the solution to (1.7) and solution to (1.4) is obtained by letting θ_i=(weighted mean of $y_0, y_1, \cdots, y_m$)$=\left(\sum_{\nu=0}^{m} \lambda_\nu^{-1}y_\nu\right)/\left(\sum_{\nu=0}^{m} \lambda_\nu^{-1}\right)$, $i=0, 1, \cdots, m$ and $\theta_i=y_i\,(i=m+1, \cdots, k)$ in case of (a) and $\hat{\theta}_i=\left(\sum_{\nu=0}^{k} \lambda_\nu^{-1}y_\nu\right)/\left(\sum_{\nu=0}^{k} \lambda_\nu^{-1}\right)$, $i=0, 1, \cdots, k$ in case of (b). and then (6) the observations are rearranged back to the original.

The above algorithm is previously derived by Eeden [4] and also mentioned in page 243 of [2].

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