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PLANNING FOR SPECIFIED COST AND PRECISION

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(Dedicated to Professor Jagdish N. Srivastava on his 65th Birthday)

An equational relationship between the information matrix and the precision matrix whose (i, j)th entry is the required variance of the elementary contrast $\alpha_i - \alpha_j$ is studied and used, particularly in the setting of block designs, for obtaining a direct relationship between required precision of estimates and available cost. Software pertinent to this problem is described.

I. Introduction

Our results are presented within the general setting of a linear model. The vector Y of observations is assumed to have expected value $E(Y) = X_1\alpha + X_2\beta$. Throughout the paper the entries of Y are understood to have covariance matrix $\text{cov}(Y) = I$. Matrices X_1 and X_2 are subject to selection by the experimenter. Each choice of X_1 and X_2 is called a *design*. Interest ies primarily in estimating linear functions in the v components of α, the $b \times 1$ vector β (associated usually with blocking variables in possibly several directions) consisting of nuisance parameters.

It is well known that the reduced normal equations for α, when least squares estimates are used, are $(QX_1)'(QX_1)\alpha = (QX_1)'Y$, where $Q = I - X_2(X_2'X_2)^- X_2'$ is the projection onto the space orthogonal to the column span of X_2. The coefficient matrix $C = (QX_1)'(QX_1)$ is known as the *information matrix* for variety effects. This work focusses attention on the case when the row sums of C are zero, a circumstance that arises in most discrete settings. The covariance matrix of a vector $\widehat{L'\alpha}$ of estimated linear functions of $\hat{\alpha}$ is

$$\operatorname{cov}(\widehat{L'\alpha}) = L'C^-L, \tag{1}$$

where A^- denotes a generalized inverse of the matrix A. Since the rows of L' are in the row span of X_1 the matrix $\operatorname{cov}(\widehat{L'\alpha})$ is independent of the choice of C^-.

Define a $v \times v$ matrix M whose (i,j)th entry is $m_{ij} = \operatorname{var}(\alpha_i \widehat{-} \alpha_j)$, for $i \neq j$, and $m_{ii} = 0$. Constantine (1992) gives an equational relationship between the matrix M and the information matrix C,

$$C = -2M^{-1} + \frac{2}{1'M^{-1}1} M^{-1}1\,1'M^{-1}, \tag{2}$$

where 1 is a column vector with all entries equal to 1. The object of this paper is to investigate the matrix M more closely and establish connections to other relevant measures of precision in the general linear model as well as more specialized settings, such as block designs.

In addition to having nonnegative entries, being symmetric and nonsingular, the matrix M has other properties worthy of note. Section 2 summarizes properties of M within the context of the general linear model. Special properties arise within the setting of block designs when the entries of M are shown to verify the "triangle inequality", making M a distance matrix. These are studied in Section 3. The property of being a distance matrix is a peculiarity of the additive block design setting and it does not generalize to models for elimination of heterogeneity in more than one direction.

The matrix M provides a natural starting point when questions of precision and planning are contemplated. In practical applications of design it is the matrix M that one attempts to specify in advance, if not in its entirety than at least some portions thereof. This amounts usually to either specifying the variances of all of the elementary contrasts or the covariances of a basis of such contrasts. A design is then sought that yields what the entries of M specify in terms of precision. Equation (2) provides a means by which such a design can be found. One can find the information matrix C from the given M by formula (2), and then find an actual design from the resulting C. Section 4 describes an algorithm that accomplishes this task in the setting of block designs.

2. THE PRECISION MATRIX

Assume that matrices X_1 and X_2 have constant row sums. This is common in discrete experimental settings. The information matrix C satisfies, therefore, $C1 = 0$, where 1 is a $v \times 1$ vector with all entries equal to one. Under such an assumption we summarize some properties of the matrix M.

THEOREM 2.1. (1) *Let* $G = \operatorname{cov}(\alpha \widehat{-} \alpha_1 1)$ *and denote its* (i,j)*th entry by* g_{ij}. *Then*

$$m_{ij} = g_{ii} + g_{jj} - 2g_{ij},$$

and

$$g_{ij} = \frac{1}{2}(m_{1i} + m_{1j} - m_{ij}).$$

(2) *An arbitrary covariance of elementary contrasts is expressible in terms of variances of such contrasts as follows:* $\operatorname{cov}(\widehat{\alpha_i - \alpha_j}, \widehat{\alpha_k - \alpha_l}) = \frac{1}{2}(m_{il} + m_{jk} - m_{ik} - m_{jl})$.

(3) *The matrix M is invertible if and only if the information matrix C has* rank $v - 1$.

Proof. (1) The relationship between matrices M and G is proved as follows:

$$\begin{aligned} m_{ij} &= \operatorname{var}(\widehat{\alpha_i - \alpha_j}) = \operatorname{var}((\widehat{\alpha_i - \alpha_1}) - (\widehat{\alpha_j - \alpha_1})) \\ &= \operatorname{var}(\widehat{\alpha_i - \alpha_1}) + \operatorname{var}(\widehat{\alpha_j - \alpha_1}) - 2\operatorname{cov}(\widehat{\alpha_i - \alpha_1}, \alpha_j - \alpha_1) \\ &= g_{ii} + g_{jj} - 2g_{ij}. \end{aligned}$$

Note that since $g_{ii} = m_{1i}$ and $g_{jj} = m_{1j}$, we have

$$g_{ij} = \frac{1}{2}(m_{1i} + m_{1j} - m_{ij}). \tag{3}$$

(2) We have the following chain of equalities:

$$\begin{aligned} \operatorname{cov}(\widehat{\alpha_i - \alpha_j}, \widehat{\alpha_k - \alpha_l}) &= \operatorname{cov}((\widehat{\alpha_i - \alpha_1}) - (\widehat{\alpha_j - \alpha_1}), (\widehat{\alpha_k - \alpha_1}) - (\widehat{\alpha_l - \alpha_1})) \\ &= g_{ik} + g_{jl} - g_{jk} - g_{il} \\ &= (m_{il} + m_{jk} - m_{ik} - m_{jl})/2. \end{aligned}$$

(3) For the "if" part, see Constantine (1992).

The "only if" part is proved by contradiction. Suppose that the information matrix C has rank r less than $v - 1$. Without loss we assume

$$C = \begin{pmatrix} C_r & A \\ A' & C_{v-r} \end{pmatrix},$$

where C_r is a r by r nonsingular matrix. Then

$$C^- = \begin{pmatrix} C_r^{-1} & 0 \\ 0 & 0 \end{pmatrix}$$

is a generalized inverse of C. Hence

$$m_{v-1,j} = c^-_{v-1,v-1} + c^-_{jj} - 2c^-_{v-1,j} = c^-_{jj} \qquad j = 1, 2, \ldots, v$$

and

$$m_{v,j} = c^-_{vv} + c^-_{jj} - 2c^-_{v,j} = c^-_{jj} \qquad j = 1, 2, \ldots, v$$

since the entry c^-_{ij} is zero for $i = v - 1, v$. Therefore the $(v-1)$th row and the vth row of M are the same. This implies that the matrix M is singular. Hence the information matrix C must have rank $v - 1$ if the matrix M is nonsingular.

3. The M-Matrix in the Case of Block Designs

The entries of the matrix M could exhibit additional structure. An interesting instance is the block design case which involves the notion of distance. A matrix $D = (d_{ij})$ is called a *distance matrix* if it is symmetric, has nonnegative entries, the diagonal entries are 0, and the off-diagonal entries verify the triangle inequality $d_{ij} \le d_{ik} + d_{kj}$. For an M-matrix to be a distance matrix means that the variances of contrasts verify certain (triangle) inequalities. It turns out that these inequalities have an intuitive statistical meaning. The next Remark elucidates this point.

Remark. M is a distance matrix if and only if $\operatorname{cov}(\widehat{\alpha_i - \alpha_k}, \widehat{\alpha_j - \alpha_k})$ is nonnegative, for all triples with distinct entries i, j, k.

Indeed,

$$\begin{aligned}\operatorname{var}(\widehat{\alpha_i - \alpha_j}) &= \operatorname{var}(\widehat{\alpha_i - \alpha_k} + \widehat{\alpha_k - \alpha_j})\\ &= \operatorname{var}(\widehat{\alpha_i - \alpha_k}) + \operatorname{var}(\widehat{\alpha_j - \alpha_k}) - 2\operatorname{cov}(\widehat{\alpha_i - \alpha_k}, \widehat{\alpha_j - \alpha_k}).\end{aligned}$$

The main result of this section asserts that the M-matrix in the case of block designs is in fact a distance matrix. Being a distance matrix proves helpful when one attempts to understand the permissible variation in the entries of the matrix M. Clearly, if entries (1, 2) and (1, 3) of M are specified, then entry (2, 3) can only vary over a much restricted interval; the permissible range is much more accurately assessed when one knows that M is a distance matrix.

We first introduce a preliminary result.

Lemma 3.1. *If A is a $v \times v$ positive definite matrix with nonpositive off-diagonal entries, and diagonal entries $a_{ii} \ge \sum_{j \ne i} |a_{ij}|$ for all i, then the inverse of A has nonnegative entries.*

Proof. Let the off-diagonal entries of A be $-a_{ij}$ and the diagonal entries be a_{ii}, where $a_{ij} \ge 0$, for all i, j. We will show that the inverse of A has nonnegative entries by using induction on v.

For $v = 2$, the Lemma is true.

Suppose that the result holds for matrices of dimension $v - 1$. Consider $v \times v$ a positive definite matrix A. Let P be a $v \times v$ matrix with diagonal entries $p_{ii} = 1$, $i = 1, \ldots, v$; $p_{1j} = \dfrac{a_{1j}}{a_{11}}$, $j = 2, \ldots, v$; and $p_{ij} = 0$ otherwise. Then

$$P'AP = \begin{pmatrix} a_{11} & 0 \\ 0 & B \end{pmatrix} \tag{4}$$

where B is a $(v-1) \times (v-1)$ matrix with diagonal entries $B_{ii} = a_{i+1,i+1} - a_{1,i+1}^2 a_{11}^{-1}$ and the off-diagonal entries $B_{ij} = -a_{i+1,j+1} - a_{1,i+1}a_{1,j+1}a_{11}^{-1}$.

Since $A>0$, it follows that $P'AP>0$, and therefore also that $B>0$. Furthermore, $b_{ij}\le 0$ for $i\ne j$ since $a_{kl}\ge 0$ for all k,l. Also for all $2\le i\le v$,

$$\begin{aligned}
b_{i-1,i-1} &= a_{ii}-a_{1i}^2a_{11}^{-1}\ge \sum_{j\ne i} a_{ij}-a_{1i}^2a_{11}^{-1}\\
&= \sum_{j\ne 1,i} a_{ij}+a_{1i}-a_{1i}^2a_{11}^{-1}=\sum_{j\ne 1,i} a_{ij}+a_{1i}a_{11}^{-1}(a_{11}-a_{1i})\\
&\ge \sum_{j\ne 1,i} a_{ij}+a_{1i}a_{11}^{-1}\sum_{j\ne 1,i} a_{1j}=\sum_{j\ne 1,i}(a_{ij}+a_{1i}a_{1j}a_{11}^{-1})\\
&= \sum_{j-1\ne i-1} |b_{i-1,j-1}|.
\end{aligned}$$

This shows that B satisfies the assumptions of the Lemma. Therefore, by the induction hypothesis, the inverse of B has non-negative entries. By (4) we have

$$P^{-1}A^{-1}P'^{-1}=\begin{pmatrix} a_{11}^{-1} & \\ & B^{-1}\end{pmatrix}.$$

Therefore

$$A^{-1}=P\begin{pmatrix} a_{11}^{-1} & \\ & B^{-1}\end{pmatrix}P'.$$

This shows that A^{-1} has non-negative entries since P, P' and B^{-1} have non-negative entries. This completes the proof of the Lemma.

REMARK. The converse of Lemma 3.1 is not true in general. For example, let

$$A=\begin{pmatrix} 6 & -4 & 1.5 & -3.5\\ -4 & 3 & -1.5 & 2.5\\ 1.5 & -1.5 & 1.5 & -1.5\\ -3.5 & 2.5 & -1.5 & 3.5\end{pmatrix}.$$

It is easy to check that the matrix A is positive definite with some positive off-diagonal entries. Yet, the inverse of A has all entries positive.

THEOREM 3.1. *If the information matrix C has nonpositive off-diagonal entries and its rank is $v-1$, then M is a distance matrix.*

Proof. Let $C^-=(c_{ij}^-)$ be a generalized inverse of C. Then by (1) we have $m_{ij}=c_{ii}^-+c_{jj}^--2c_{ij}^-$. Hence

$$m_{ij}\le m_{ik}+m_{kj}\Leftrightarrow c_{kk}^-+c_{ij}^--c_{ik}^--c_{jk}^-\ge 0. \tag{5}$$

Note that (5) is trivial (both sides are 0) if $i=j$, or $i=k$, or $k=j$. As we mentioned in Section 1, the entry m_{ij} is independent of the choice of C^-. For fixed i,j,k, erase the kth row and the kth column of C; then find the inverse of the resulting $(v-1)\times(v-1)$ matrix; call it C^{*-1}. Make C^{*-1} into a $v\times v$ matrix by inserting a kth row and kth column of zeroes. This yields a generalized inverse C^- of C. This generalized inverse $C^-=(c_{ij}^-)$ has the property $c_{st}^-=0$ if $s=k$ or $t=k$. Hence $c_{kk}^-+c_{ij}^--c_{ik}^--c_{jk}^-=c_{ij}^-$. And therefore the left side of (5) will be satisfied if we can show that $c_{ij}^{-} \geq 0$. Indeed, since C is a rank $v-1$ positive semidefinite matrix with nonpositive offdiagonal entries and row sums 0, C^* satisfies the conditions of Lemma 3.1. Hence the inverse of C^* has non-negative entries. Therefore the generalized inverse C^- of C obtained from C^* has non-negative entries. Hence $c_{ij}^{-} \geq 0$. Since i, j, k are arbitrary, the left side of (5) holds for all i, j, k. This completes the proof of Theorem 3.1.

It is tempting to think that the nonpositivity of the off-diagonal entries of C is also a necessary condition for M to be a distance matrix. However, this is not true. Furthermore, a distance matrix M can yield a symmetric C with row sums zero and rank $v-1$, but not a positive semidefinite matrix. Such examples can easily be constructed.

COROLLARY 3.1. *Under the additive block design model the matrix M is a distance matrix.*

Proof. It is well known that the off-diagonal entries of the information matrix under this model are nonpositive. The proof is now completed with the help of Theorem 3.1.

REMARK. It is tempting to think that the matrix M is also a distance matrix in the two-way elimination of heterogeneity. However, this is not true. Consider the following design, with rows and columns as blocks:

1	1	1	2	1
2	1	1	3	3
3	2	1	4	3
4	2	3	4	4

The information matrix C for both columns and rows, cf. Cheng (1978), is:

$$C = \begin{pmatrix} 1.5 & -1.25 & -0.95 & 0.7 \\ -1.25 & 2.5 & -0.5 & -0.75 \\ -0.95 & -0.5 & 2.7 & -1.25 \\ 0.7 & -0.75 & -1.25 & 1.3 \end{pmatrix},$$

and the resulting matrix M is:

$$M = \begin{pmatrix} 0 & 0.9333 & 1.287 & 3.114 \\ 0.933 & 0 & 0.699 & 1.508 \\ 1.287 & 0.699 & 0 & 1.048 \\ 3.144 & 1.508 & 1.048 & 0 \end{pmatrix}.$$

It is easy to check that M is not a distance matrix. This explains why the algorithms that are described in the next section are restricted, at least for the time being, to the setting of additive block designs.

4. ALGORITHMS

In practical experiments researchers usually wish to control both the cost of the experiment and the precision of the parameters to be estimated. When the average cost per observation is known, the overall cost becomes proportional to the number of observations. This section offers algorithms that take these experimental concerns as input data and yield as output the actual design which conforms (as much as can be expected) to the specified requirements. This accomplishment is restricted to the additive model of block designs.

We thus assume that the expected value of observation y_{ij} can be written as $\alpha_i + \beta_j$, with α_i being the effect of variety i and β_j being the effect of block j. The observations are independently distributed each having the same variance. There are v varieties, the unknown effects of which are to be estimated.

Specifically, we provide two main programs. The first does not address considerations of cost. It uses as input only the matrix M. The $v \times v$ input matrix M must be symmetric and nonsingular with positive off-diagonal entries. These properties alone are far from insuring that a design exists with variances of elementary contrasts close to the entries of M. The user must cautiously select the entries of M in accordance with the results established in Sections 2 and 3. The program prompts and asks whether the user wants to enter all the entries of M, or just a selected few in which the user takes specific interest. In the latter case the program completes the matrix M. Provided that M is acceptable, the program produces a variety-block incidence matrix N, by way of which the design is specified. It then computes the matrix $M(N)$ whose diagonal entries are zero and whose (i, j)th off-diagonal is the actual variance of the estimate of $\alpha_i - \beta_j$ under the design N. It subsequently calculates a measure of compatibility between what was given (matrix M) and what was achieved (matrix $M(N)$) in the form of a percentage error between the corresponding entries of the two matrices. The user is expected to peruse the results and, if satisfied, eventually adopt the design for actual experimentation.

The second version of the program incorporates cost by having the user specify an upper and lower bound on the number of observations, along with the matrix M. Since an interval for the number of observations is given, the matrix M is regarded as specified up to a positive scalar multiple only. The multiple is then automatically adjusted by the program to make the precisions specified by M compatible with the aforementioned interval. Note that the ratio of variances in M is unaffected by such rescaling. The option of entering all entries of M or just a selected few remains available. Output and percentage error similar to those given in the first case are then offered to the user.

Much simplification is attained by using the exact equational relationship betwen matrix M and the information matrix of the design denoted by C, as it appears in (2). The algorithm serves a purpose similar to those of Jones (1976) and

Jones and Eccleston (1980) who aim to attain certain ratios on precisions of variances by essentially using the same ratios on the replication numbers. Considering the exact relationshp between M and C mentioned above, our approach achieves virtually complete control between precision requirements and design.

PROGRAMMING METHOD

The algorithm computes the matrix C from the given matrix M by using equation (1), and then finds a matrix N from the resulting matrix C such that the sum of squares of the entries of matrix $M - M(N)$ is small.

The following properties are used in the algorithm.

1. $g(\Sigma N_i) = \Sigma g(N_i)$.

2. $C = g(N)$ has diagonal entries C_{ii} larger than or equal to 0.5 and the off-diagonal entries C_{ij} are nonpositive.

By property 1, matrix C is the sum of C_j's, where C_j is the information matrix for block j only. We can thus build the matrix N block by block. At each step the program first tests the entries of what is left in the matrix C. If some C_{ii} is too small, say $C_{ii} < 0.2$, then we will not build a block which involves variety i. Likewise, if some C_{ij} is too large, say $C_{ij} > -0.1$, then we will not build a block which involves both variety i and variety j. These two numbers, 0.2 and -0.1, generally vary with M. For convenience, we call these two numbers the test number for C_{ii} and the test number for C_{ij}, respectively. By considering the case of a block of size 2, the test number for C_{ii} should be between 0 and 0.25. We make the test number for C_{ii} vary from 0 to 0.2 and the test number for C_{ij} vary from -0.1 to 0.1 with increments of 0.01. For each choice of the test numbers the program computes the matrix $C(N)$ from the matrix N by using equation (2), upon generating N, and then computes the matrix $M(N)$ from the matrix $C(N)$ by the formula.

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