

INVERTING COVARIANCE MATRICES

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Abstract

Some useful tools in modelling linear experiments with general multi-way classification of the random effects and some convenient forms of the covariance matrix and its inverse are presented. Moreover, the Sherman-Morrison-Woodbury formula is applied for inverting the covariance matrix in such experiments.

Keywords: multi-way classification, cross, hierarchical, balanced, unbalanced, covariance matrix, inverting.

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1. INTRODUCTION AND SUMMARY

Any linear statistical experiment involves some varieties called factors or effects. One can distinguish two kinds of the effects: fixed and random. The allocation of the fixed effects determines the expectation of the observation vector, while the allocation of the random ones determines the variance-covariance matrix.

Many statistical operations, such as linear estimation, quadratic estimation, and testing, require inverting the covariance matrix (see, e.g., Rao, 1973, Kleffe and Seifert, 1986, or Jiang, 2004). From mathematical

point of view, the last problem reduces to inversion of a "patterned" matrix (cf. Graybill, 1983). In spite of the great progress in the subject, the attention of statistical literature focus on so called *balanced* models, being expressible in terms of the Kronecker product (among others Searle *et al.*, 1992, and Jiang, 2004). Similar results, for inverting matrices in a quadratic subspace, were obtained by Zmyślony and Drygas (1992). This technique is very elegant but it is not applicable in the *unbalanced* models. In the last case some explicit results have been presented for the *hierarchical* classification only (see Stepniak, 1974, 1991, Stepniak and Niezgoda, 1995) in quite different terms.

This paper is a further step in this direction. The initial technique, introduced in Section 2, is illustrated by the balanced hierarchical and cross classification. In fact the results presented in Section 3 are very close to these by Jiang (2004), but they are more direct in use and proof. Section 4 deals with inverting covariance matrices in the unbalanced classification. Some explicit results for 2-way case are derived by Sherman-Morrison-Woodbury formula of matrix analysis.

2. MULTI-WAY CLASSIFICATION

Formal definition of the multi-way classification (cf. Stepniak, 1983) will be preceded by example.

Suppose 24 experimental units are submitted to three independent classifications with 2, 3 and 2 subclasses, respectively. Denote by S_{ij} the set of experimental units belonging to the j -th subclass in the i -th classification. For example

$$S_{11} = \{1, 2, 5, 8, 10, 13, 18, 20, 21, 22, 23\},$$

$$S_{12} = \{3, 4, 6, 7, 9, 11, 12, 14, 15, 16, 17, 19, 24\},$$

$$S_{21} = \{4, 6, 8, 15, 16, 17, 18\},$$

$$S_{22} = \{10, 11, 12, 13, 14, 20\},$$

$$S_{23} = \{1, 2, 3, 5, 7, 9, 19, 21, 22, 23, 24\},$$

$$S_{31} = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14\},$$

$$S_{32} = \{15, 16, 17, 18, 19, 20, 21, 22, 23, 24\}.$$

To each S_{ij} corresponds a column vector $N_{ij} = (n_1, \dots, n_{24})^T$ of zeros and ones, where

$$n_k = \begin{cases} 1 & \text{if } k \in S_{ij} \\ 0 & \text{otherwise,} \end{cases}$$

for $k = 1, \dots, 24$. In our example

$$N_{11} = (1, 1, 0, 0, 1, 0, 0, 1, 0, 1, 0, 0, 1, 0, 0, 0, 0, 1, 0, 1, 1, 1, 0)^T,$$

$$N_{12} = (0, 0, 1, 1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 1, 1, 1, 0, 1, 0, 0, 0, 0, 1)^T,$$

$$N_{21} = (0, 0, 0, 1, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 0, 0, 0, 0, 0)^T,$$

$$N_{22} = (0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0)^T,$$

$$N_{23} = (1, 1, 1, 0, 1, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 1, 1, 1)^T,$$

$$N_{31} = (1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^T,$$

$$N_{32} = (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1)^T.$$

Then the observation vector $X = (X_1, \dots, X_{24})^T$, corresponding to the experimental units, may be presented in the form

$$X = \mu + \sum_{j=1}^2 N_{1j} a_{1j} + \sum_{j=1}^3 N_{2j} a_{2j} + \sum_{j=1}^2 N_{3j} a_{3j} + e,$$

where $\mu = (\mu_1, \dots, \mu_{24})^T$ is the expectation of X , a_{ij} is the effect of the j -th subclass in the i -th classification, while $e = (e_1, \dots, e_{24})^T$ is the vector of the experimental errors.

Assuming all these effects are independent random variables with the expectation zero and the variances

$$\text{Var}(e_j) = \sigma_0 \quad \text{for } j = 1, \dots, 24, \text{ and,}$$

$$\text{Var}(a_{ij}) = \sigma_i \quad \text{for } i = 1, 2, 3 \text{ and possible } j,$$

one can write the variance-covariance matrix of X in the form

$$V = \sigma_0 I_{24} + \sum_{i=1}^3 \sigma_i V_i,$$

where

$$V_1 = \sum_{j=1}^2 N_{1j} N_{1j}^T,$$

$$V_2 = \sum_{j=1}^3 N_{2j} N_{2j}^T,$$

$$V_3 = \sum_{j=1}^2 N_{3j} N_{3j}^T.$$

Now we are ready to introduce a formal definition of multi-way classification.

Let n, q and k_1, \dots, k_q be positive integers such that $q \leq n$ and $k_i \leq n$, $i = 1, \dots, q$. Moreover, let N_{ij} , $i = 1, \dots, q$; $j = 1, \dots, k_i$, be n -dimensional columns of zeros and ones satisfying

$$(1) \quad \sum_{j=1}^{k_i} N_{ij} = 1_n, \quad i = 1, \dots, q,$$

and

$$(2) \quad N_{ij}^T N_{ij'} = 0, \quad i = 1, \dots, q; \quad j \neq j',$$

where 1_n means the column of n ones.

Definition 1. Any choice of such columns is said to be an *allocation* of n experimental units in q -way classification with k_1, \dots, k_q subclasses and is denoted by $\mathcal{A}(n, q; k_1, \dots, k_q / N_{ij}, i = 1, \dots, q; j = 1, \dots, k_i)$.

To each allocation corresponds the covariance matrix of the form

$$(3) \quad V = \sigma_0 I_n + \sum_{i=1}^q \sigma_i V_i,$$

where

$$(4) \quad V_i = \sum_{j=1}^{k_i} N_{ij} N_{ij}^T, \quad i = 1, \dots, q.$$

We shall assume that $\sigma_0 > 0$ and $\sigma_i \geq 0$ for $i = 1, \dots, q$.

It is worth to note that the notion of the allocation does not specify any relationship between the individual classifications. Some specifications of this kind lead to the well known terms such as cross and hierarchical (or nested) classification (cf. VanLeeuwen *et al.*, 1999). Let us mention that an allocation $\mathcal{A}(n, q; k_1, \dots, k_q / N_{ij}, i = 1, \dots, q; j = 1, \dots, k_i)$ is hierarchical if the matrices

$$(5) \quad V_i - V_{i+1} \quad \text{for } i = 1, \dots, q-1$$

have nonnegative entries. General definition of cross classification is more complex.

The structure of the covariance matrix simplifies in so called balanced case (cf. Searle *et al.*, 1992, and Jiang, 2004). We shall illustrate our notion by examples with balanced hierarchical and cross classification.

Suppose n and k_1, \dots, k_q satisfy the condition $n = r \prod_{i=1}^q k_i$ for some integer r . Then one can set

$$(6) \quad \begin{aligned} N_{1j} &= E_{1j} \otimes 1_{k_1} \otimes \dots \otimes 1_{k_q} \otimes 1_r, & j = 1, \dots, k_1, \\ N_{2j} &= 1_{k_1} \otimes E_{2j} \otimes \dots \otimes 1_{k_q} \otimes 1_r, & j = 1, \dots, k_2, \\ &\dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \\ N_{qj} &= 1_{k_1} \otimes 1_{k_2} \otimes \dots \otimes E_{qj} \otimes 1_r, & j = 1, \dots, k_q, \end{aligned}$$

where \otimes denotes the Kronecker product and E_{ij} means the k_i -dimensional column with one on the j -th place and zeros besides.

Definition 2. Any allocation $\mathcal{A}(n, q; k_1, \dots, k_q / N_{ij}, i = 1, \dots, q; j = 1, \dots, k_i)$ satisfying the condition (6) for some r is said to be *balanced cross allocation*.

For such allocation the matrices V_i , defined by (4), reduce to

where J_k denotes $k \times k$ matrix of ones.

We note that the matrices V_1, \dots, V_q appearing in (7) satisfy the conditions

and

Thus we get the following corollaries

Corollary 3. *In the balanced cross allocation the matrices I_n, V_1, \dots, V_q and J_n belong to a commutative quadratic subspace.*

Corollary 4. *The inverse of the covariance matrix V in the balanced cross classification may be expressed as a linear combination of I_n, V_1, \dots, V_q and J_n .*

Now suppose $\frac{n}{k_q}$ and $\frac{k_{i+1}}{k_i}$ are integers for $i = 1, \dots, q-1$. Then one can set

where $s_i = \frac{k_{i+1}}{k_i}$, $i = 1, \dots, q-1$ and $s_q = \frac{n}{k_q}$.

This implies that

It is worth to note that the matrices V_1, \dots, V_q appearing in (11) satisfy the conditions

Thus we get the following corollaries.

Corollary 6. *In the balanced hierarchical allocation the matrices I_n, V_1, \dots, V_q belong to a commutative quadratic subspace.*

Corollary 7. *The inverse of the covariance matrix V in the balanced hierarchical allocation may be expressed as a linear combination of I_n, V_1, \dots, V_q .*

In the next section we derive some explicit forms for inverse of the covariance matrices in the balanced hierarchical and cross classification. Such a possibility comes from the fact that in a commutative quadratic subspace there exists a basis of mutually orthogonal projectors (cf. Seely, 1971).

3. INVERTING COVARIANCE MATRIX FOR BALANCED CLASSIFICATION

We shall start from the balanced *cross* classification.

Theorem 8. *Let $\mathcal{A}(n, q; k_1, \dots, k_q/N_{ij}, i = 1, \dots, q; j = 1, \dots, k_i)$ be balanced cross allocation i.e. allocation defined by (6)–(7) with the covariance matrix $V = \sigma_0 I_n + \sum_{i=1}^q \sigma_i V_i$. Then*

$$V^{-1}$$

$$(13) \quad = \frac{1}{\sigma_0} \left[I_n - \sum_{i=1}^q \frac{\rho_i}{1 + \rho_i \frac{n}{k_i}} V_i + \sum_{i=1}^q \frac{\rho_i}{k_i} \left(\frac{1}{1 + \rho_i \frac{n}{k_i}} - \frac{1}{1 + \sum_{j=1}^q \rho_j \frac{n}{k_j}} \right) J_n \right],$$

where $\rho_i = \frac{\sigma_i}{\sigma_0}$ for $i = 1, \dots, q$.

Proof. Define matrices

$$(14) \quad P_i = \begin{cases} \frac{1}{n} J_n & \text{for } i = 0, \\ \frac{k_i}{n} V_i - P_0 & \text{for } i = 1, \dots, q. \end{cases}$$

We note that $P_i^2 = P_i$ for $i = 0, \dots, q$ and $P_i P_j = 0$ for $i \neq j$. Thus P_0, P_1, \dots, P_q are orthogonal projectors on the corresponding orthogonal subspaces of R^n . In consequence, one can write

$$\begin{aligned} V &= \sigma_0 \left(I_n - \sum_{i=0}^q P_i \right) + \sigma_0 \sum_{i=0}^q P_i + \sum_{i=1}^q \sigma_i \frac{n}{k_i} (P_i + P_0) \\ &= \sigma_0 \left[\left(I_n - \sum_{i=0}^q P_i \right) + \sum_{i=1}^q \left(1 + \rho_i \frac{n}{k_i} \right) P_i + \left(1 + \sum_{i=1}^q \rho_i \frac{n}{k_i} \right) P_0 \right]. \end{aligned}$$

We observe that the last row represents the canonical form of V . Therefore,

$$\begin{aligned} V^{-1} &= \frac{1}{\sigma_0} \left[\left(I_n - \sum_{i=0}^q P_i \right) + \sum_{i=1}^q \frac{1}{1 + \rho_i \frac{n}{k_i}} P_i + \frac{1}{1 + \sum_{i=1}^q \rho_i \frac{n}{k_i}} P_0 \right] \\ &= \frac{1}{\sigma_0} \left[I_n - \sum_{i=1}^q \frac{\rho_i \frac{n}{k_i}}{1 + \rho_i \frac{n}{k_i}} P_i - \frac{\sum_{i=1}^q \rho_i \frac{n}{k_i}}{1 + \sum_{i=1}^q \rho_i \frac{n}{k_i}} P_0 \right] \end{aligned}$$

$$\begin{aligned}
 &= \frac{1}{\sigma_0} \left[I_n - \sum_{i=1}^q \frac{\rho_i \frac{n}{k_i}}{1 + \rho_i \frac{n}{k_i}} (P_i + P_0) \right. \\
 &\quad \left. + \sum_{i=1}^q \rho_i \frac{n}{k_i} \left(\frac{1}{1 + \rho_i \frac{n}{k_i}} - \frac{1}{1 + \sum_{j=1}^q \rho_j \frac{n}{k_j}} \right) P_0 \right]
 \end{aligned}$$

and, by (14), the desired result is proved. ■

In particular, for $q = 1$ the formula (13) reduces to

$$(15) \quad V^{-1} = \frac{1}{\sigma_0} \left[\mathbf{I}_n - \frac{\rho_1}{1 + \rho_1 a} V_1 \right],$$

where $a = \frac{n}{k_1}$ (cf. Stepniak, 1974).

Now let us pass to the balanced *hierarchical* classification.

Theorem 9. *Let $\mathcal{A}(n, q; k_1, \dots, k_q / N_{ij}, i = 1, \dots, q; j = 1, \dots, k_i)$ be balanced hierarchical allocation i.e. allocation defined by (10)–(11) with the covariance matrix $V = \sigma_0 I_n + \sum_{i=1}^q \sigma_i V_i$. Then*

$$\begin{aligned}
 &V^{-1} \\
 (16) \quad &= \frac{1}{\sigma_0} \left[\mathbf{I}_n - \sum_{i=1}^{q-1} \frac{\rho_i}{(1 + n \sum_{j=i}^q \frac{\rho_j}{k_j})(1 + n \sum_{j=i+1}^q \frac{\rho_j}{k_j})} V_i - \frac{\rho_q}{1 + \frac{n}{k_q} \rho_q} V_q \right].
 \end{aligned}$$

Proof. Define matrices

$$(17) \quad Q_i = \begin{cases} \frac{k_1}{n} V_1 & \text{for } i = 1, \\ \frac{k_i}{n} V_i - \frac{k_{i-1}}{n} V_{i-1} & \text{for } i = 2, \dots, q. \end{cases}$$

We note that $Q_i^2 = Q_i$ for $i = 1, \dots, q$, $Q_i Q_{i'} = 0$ for $i \neq i'$ and $\sum_{j=1}^i Q_j = \frac{k_i}{n} V_i$. Thus one can write

$$\begin{aligned} V &= \sigma_0 \left(I_n - \sum_{i=1}^q Q_i \right) + \sigma_0 \sum_{i=1}^q Q_i + n \sum_{i=1}^q \frac{\sigma_i}{k_i} \sum_{j=1}^i Q_j \\ &= \sigma_0 \left[\left(I_n - \sum_{i=1}^q Q_i \right) + \sum_{i=1}^q Q_i + n \sum_{i=1}^q \frac{\rho_i}{k_i} \sum_{j=1}^i Q_j \right] \\ &= \sigma_0 \left[\left(I_n - \sum_{i=1}^q Q_i \right) + \sum_{i=1}^q \left(1 + n \sum_{j=i}^q \frac{\rho_j}{k_j} \right) Q_i \right]. \end{aligned}$$

Therefore

$$\begin{aligned} V^{-1} &= \frac{1}{\sigma_0} \left[\left(I_n - \sum_{i=1}^q Q_i \right) + \sum_{i=1}^q \frac{1}{1 + n \sum_{j=i}^q \frac{\rho_j}{k_j}} Q_i \right] \\ &= \frac{1}{\sigma_0} \left[I_n - \sum_{i=1}^q \frac{n \sum_{j=i}^q \frac{\rho_j}{k_j}}{1 + n \sum_{j=i}^q \frac{\rho_j}{k_j}} Q_i \right] \end{aligned}$$

and, by (17), the desired result is proved. ■

Remark 10. For $q = 1$ the formula (16) reduces to (15).

Remark 11. For $q = 2$ the form (16) coincides with Stępnia (1991, formula (3)) and with Stępnia and Niezgoda (1995, formula (7)).

An alternative way for inverting the covariance matrix in the balanced hierarchical classification is indicated by Corollary 7. Namely, the inverse V^{-1} may be obtained by solving the equation

$$\left(I_n + \sum_{i=1}^q \rho_i V_i \right) \left(I_n + \sum_{i=1}^q x_i V_i \right) = I_n$$

with respect to x_1, \dots, x_q . This can be rewritten as a system of equations

$$\rho_q + x_q + n \frac{\rho_q}{k_q} x_q = 0,$$

$$\rho_i + x_i + n \sum_{j=i}^q \frac{\rho_j}{k_j} x_i + n \rho_i \sum_{j=i+1}^q \frac{x_j}{k_j} = 0 \quad \text{for } i = q-1, \dots, 1.$$

From the first one we get immediately

$$x_q = -\frac{\rho_q}{1 + \frac{n}{k_q} \rho_q}$$

and, by substitution to the second one,

$$x_{q-1} = -\frac{\rho_{q-1}}{\left(1 + n \sum_{j=q-1}^q \frac{\rho_j}{k_j}\right) \left(1 + n \frac{\rho_q}{k_q}\right)}.$$

Next, by successive substitutions,

$$x_i = -\frac{\rho_i}{\left(1 + n \sum_{j=i}^q \frac{\rho_j}{k_j}\right) \left(1 + n \sum_{j=i+1}^q \frac{\rho_j}{k_j}\right)} \quad \text{for } i = q-2, \dots, 1.$$

The final result coincides with (16).

4. INVERTING COVARIANCE MATRIX FOR UNBALANCED CLASSIFICATION

The method of inverting based on the orthogonal decomposition does not extend for the unbalanced case. On the other way, solving linear equations, used in Stepniak and Niezgoda (1995) for the unbalanced *hierarchical* classification is not easy. LaMotte (1972) suggests for this case a step-by-step procedure which is, however, rather far from the explicitness.

In the unbalanced *cross* classification the problem of inverting appears even more complex and, as far, it has not been undertaken in statistical literature, at least in the analytic form. We are just taking an effort in this area.

The following result (cf. Horn and Johnson, 1985, p. 19, or Golub and Van Loan, 1989, p. 51) plays a key role in our consideration.

Lemma 12 (Sherman-Morrison-Woodbury formula). *Suppose a nonsingular matrix A of $n \times n$ has a known inverse A^{-1} and consider a matrix*

$$B = A + FGH,$$

where F is $n \times r$, H is $r \times n$, and G is $r \times r$ and nonsingular. If, moreover, B is nonsingular, then

$$B^{-1} = A^{-1} - A^{-1}F(G^{-1} + HA^{-1}F)^{-1}HA^{-1}.$$

By using this lemma one can obtain a recurrent formula for inverting the covariance matrix in the unbalanced q -way classification. An explicit result will be provided for $q = 2$.

Given 2-way allocation $\mathcal{A}(n, 2; k_1, k_2/N_{ij}, i = 1, 2; j = 1, \dots, k_i)$ define scalars

$$n_{i\cdot} = N_{1i}^T N_{1i}, \quad i = 1, \dots, k_1,$$

$$n_{\cdot j} = N_{2j}^T N_{2j}, \quad j = 1, \dots, k_2,$$

$$n_{ij} = N_{1i}^T N_{2j}, \quad i = 1, \dots, k_1; j = 1, \dots, k_2,$$

$$\rho = \frac{\sigma_1}{\sigma_0}, \quad \text{and} \quad \lambda = \frac{\sigma_2}{\sigma_0},$$

and matrices

$$N_{n \times k_1} = [N_1, \dots, N_{k_1}], \quad \text{where } N_i = N_{1i} \text{ for } i = 1, \dots, k_1,$$

$$M_{n \times k_2} = [M_1, \dots, M_{k_2}], \quad \text{where } M_j = M_j(\rho) = N_{2j} - \rho \sum_{i=1}^{k_1} \frac{n_{ij}}{1 + \rho n_{i\cdot}} N_{1i}$$

$$\text{for } j = 1, \dots, k_2,$$

$$D_{k_1 \times k_1} = D(\rho) = \rho \text{diag} \left[\frac{1}{1 + \rho n_{1\cdot}}, \dots, \frac{1}{1 + \rho n_{k_1\cdot}} \right],$$

and

$$C_{k_2 \times k_2} = C(\rho, \lambda) = \begin{bmatrix} \frac{1}{\lambda} + n_{\cdot 1} - \rho \sum_{i=1}^{k_1} \frac{n_{i1}^2}{1 + \rho n_{i\cdot}} & -\rho \sum_{i=1}^{k_1} \frac{n_{i1}n_{i2}}{1 + \rho n_{i\cdot}} & \cdots & -\rho \sum_{i=1}^{k_1} \frac{n_{i1}n_{ik_2}}{1 + \rho n_{i\cdot}} \\ -\rho \sum_{i=1}^{k_1} \frac{n_{i2}n_{i1}}{1 + \rho n_{i\cdot}} & \frac{1}{\lambda} + n_{\cdot 2} - \rho \sum_{i=1}^{k_1} \frac{n_{i2}^2}{1 + \rho n_{i\cdot}} & \cdots & -\rho \sum_{i=1}^{k_1} \frac{n_{i2}n_{ik_2}}{1 + \rho n_{i\cdot}} \\ \vdots & \vdots & \ddots & \vdots \\ -\rho \sum_{i=1}^{k_1} \frac{n_{ik_2}n_{i1}}{1 + \rho n_{i\cdot}} & -\rho \sum_{i=1}^{k_1} \frac{n_{ik_2}n_{i2}}{1 + \rho n_{i\cdot}} & \cdots & \frac{1}{\lambda} + n_{\cdot k_2} - \rho \sum_{i=1}^{k_1} \frac{n_{ik_2}^2}{1 + \rho n_{i\cdot}} \end{bmatrix}^{-1}.$$

Now we are ready to state the main result in this paper.

Theorem 13. *The inverse of the covariance matrix in 2-way allocation $\mathcal{A}(n, 2; k_1, k_2/N_{ij}, i = 1, 2; j = 1, \dots, k_i)$ may be presented in the form*

$$(18) \quad V^{-1} = \frac{1}{\sigma_0} [I_n - NDN^T - MCM^T],$$

where N, M, D and C are defined above.

Proof. In this situation one can write

$$V = \sigma_0 \left(I_n + \rho \sum_{i=1}^{k_1} N_{1i} N_{1i}^T + \lambda \sum_{j=1}^{k_2} N_{2j} N_{2j}^T \right).$$

Let us set in Lemma 12 $A = I_n + \rho \sum_{i=1}^{k_1} N_{1i} N_{1i}^T$, $G = \lambda I_{k_2}$ and $F = H^T = [N_{21}, \dots, N_{2k_2}]$. It is well known (cf. Stępniać, 1974) that $A^{-1} = I_n - NDN^T$. Now the desired result follows by a routine algebra. ■

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