SOME RESULTS IN ESTIMATION AND TESTS OF LINEAR HYPOTHESES UNDER THE GAUSS-MARKOFF MODEL

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SUMMARY. A number of results, hitherto unrecorded in literature on the Cause-Markoff (G-M) model, are discussed.

Explicit expressions for BLU astimators of linear parametric functions, covariance matrix of BLUE's and test oritoria for tests of linear hypotheses are obtained in the case when the observations have a singular covariance matrix. These are obtained by first reducing a G-M model with a singular covariance matrix to one with a non-singular covariance matrix and with some restrictions on the parameters, and then applying the known theory in the latter case.

Some results in Linear Algebra which are of general interest and which are particularly useful in discussions on inference from linear models, are also given.

Finally some comments are made on the use of Householder transformation in the numerical computation of BLUE's and test criteria.

1. INTRODUCTION

A fairly extensive and general treatment of estimation of linear parametric functions and tests of linear hypotheses under the Gauss-Markoff model is contained in *The Linear Statistical Inference and its Applications* by Rao (1965). In the present paper we deal with some further results which are, hitherto, unrecorded in the literature on Gauss-Markoff theory, and which are of some interest in teaching the subject. The problem is considered in its wide generality without any of the restrictions used in earlier discussions.

The following notations are used. Matrices and vectors are denoted by bold face letters, such as $X, H, R, \beta, ...$

M(X) denotes the subspace generated by the columns of X

R(X) denotes the rank of X

X- denotes a generalised inverse of X (see Rao, 1967)

 $d(\mathcal{F})$, where \mathcal{F} is a linear space denotes the dimension of \mathcal{F}

 $\mathcal{M}(X) \cap \mathcal{M}(R)$ denotes the subspace of vectors common to $\mathcal{M}(X)$ and $\mathcal{M}(R)$

 X^2 denotes a matrix of maximum rank such that $X'X^2=0$, where X is a given matrix

 $P_X = X(X'X)^-X'$ denotes the projection operator which projects vectors onto $\mathcal{A}(X)$ (see Rao, 1967).

If $\Sigma = LD_{\lambda}L'$ be a positive definite matrix of order n, where $LL' = L'L = I_n$ and D_{λ} is diag $(\lambda_1, \lambda_2, ..., \lambda_n)$, $\Sigma^{1/2} = LD_{+,\lambda_1^2}L'$ is a square root of Σ .

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1.1. Statement of the problem. Let Y be a vector of observations with $E(Y) = X\beta$ and covariance matrix $\sigma^2 \Sigma$, where X and Σ are given matrices, β is a vector of unknown parameters and σ^2 is an unknown scalar. The model will be referred to as $(Y, X\beta, \sigma^2 \Sigma)$. The parameter β may be subject to a given set of (consistent) linear restrictions $R\beta = \xi$, in which case the problem will be referred to as $(Y, X\beta[R\beta = \xi], \sigma^2 \Sigma)$. No assumption is made on the ranks of Σ , X, and R.

The problems we consider are the estimation of unknown linear parametric functions and tests of hypotheses assigning certain values to given sets of parametric functions.

1.2. The reduced problem. Let N be an orthogonal complement of Σ , i.e. a matrix of maximum rank such that $N'\Sigma=0$. Since Σ is at least positive semi-definite, $\Sigma=CC'$, where $R(\Sigma)=R(C)=$ number of columns in C. Let F' be a left inverse of C, i.e., F'C=I. F' may be chosen to satisfy the additional condition F'N=0. Then make the transformation from Y to Y_1, Y_2 with the properties

$$Y_1 = F'Y, E(Y_1) = F'X\beta, D(Y_1) = \sigma^2 I$$
 ... (1.1)
 $Y_2 = N'Y, E(Y_2) = N'X\beta, D(Y_2) = 0.$

The vector Y_1 is non-stochastic and the equation $N'X\beta = Y_1$ is, therefore, in the nature of restrictions on β . Note that under a linear model, best linear estimates of estimable linear parametric functions remain invariant under nonsingular transformations of observations. Thus the problem associated with the model $(Y, X\beta[R\beta = \xi], \sigma^*\Sigma)$ is equivalent to the problem associated with

$$(Y_1, F'X\beta[R\beta = \xi, N'X\beta = Y_1], \sigma^2 I)$$
 ... (1.2)

in which the singularity of the covariance matrix is removed, but further restrictions on β are introduced.

It is seen that when Σ is non-singular, F can be chosen as $\Sigma^{-1}I^{2}$, i.e., the reciprocal of a square root of Σ . The problem then reduces to

$$(\Sigma^{-1/2}Y, \Sigma^{-1/2}X\beta[R\beta = \xi], \sigma^2I).$$
 ... (1.3)

Thus, we can apply the well-known results of the least square theory in the special case, $(Y, X\beta[R\beta = \xi], \sigma^2 I)$, to deduce the corresponding expressions for the other cases (i.e., when instead of I we have a matrix Σ which may be singular or non-singular),

2. Some algebraic lemmas

We derive some results in Linear Algebra, which are needed in the discussion of the problems considered in the rest of the section.

Lemma 1: Let $\mathscr S$ be the subspace spanned by vectors of the form $X\beta$ where X is a fixed $n \times m$ matrix and β varies over the solutions of $II\beta = 0$, where II is another fixed matrix. Further let G be a matrix such that $\mathscr M(G') = \mathscr M(X') \bigcap \mathscr M(II')$. Then

(i)
$$\mathcal{F} = \mathcal{M}[X(H')^1]$$

(ii)
$$d(\mathfrak{F}) = R(X') - R(G') = R(X' : H') - R(H')$$
,

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Proof: The results of the lemma are easy to establish. (Result (ii) of the lemma is posed as an exercise in Rao, 1905, p. 172).

Lemma 2: Let A and B be two matrices with the same number of rows and C be a matrix such that $\mathcal{N}(C) = \mathcal{N}(A) \bigcap \mathcal{N}(B)$. Then C has the representation C = AF where $F = W^1$, $W = A'B^1$, and R(C) = R(A) + R(B) - R(A : B).

Proof: The result follows from those of Lemma 1.

Note 1: There is a lot of flexibility in the choice of B^1 and W. For example $B^1 = (I - BB^-)'$, $W^1 = (I - WW^-)'$ where B^- and W^- are any g-inverses of B and W respectively. If symmetry is desired, $B^1 = I - P_{B^1} W^1 = I - P_{B^2}$.

Note 2: It is of special interest to obtain a representation of $\mathcal{M}(A) \cap \mathcal{M}(B^4)$. The matrix C in such a case has the form

$$C = A(A'B)^{2}$$
.

Lemma 3: Let P be an operator which projects vectors onto a subspace of a vector space in which the inner product of two vectors α and β is defined by $\alpha' \Lambda \beta$, where Λ is a p.d. matrix. Then it is necessary and sufficient that (α) P is idempotent, and (b) ΛP is symmetrical.

If P projects vectors onto M(X), then

- (i) $P = X(X'\Lambda X)^{-}X'\Lambda$, which is unique for any choice of $(X'\Lambda X)^{-}$,
- (ii) R(P) = R(X), and
- P belongs to the subalgebra generated by XΥΛ.

Proof: (i) and (ii) are well-known when $\Lambda = I$ (see, Rao, 1965, p. 23) and the same method of proof goes through for a general Λ . (iii) for the special case $\Lambda = I$ was proved by Mann (1960, p. 2). To prove (iii) for a general Λ let us observe that $R(X'\Lambda X) = R(X'\Lambda X)^3$. Hence using Theorem 5.4 of Mitra (1968b), $X'\Lambda X$ has a ginverse which can be expressed as a polynomial of finite degree in $X'\Lambda X$. The result (iii) follows by multiplying this polynomial by X from the left and by $X'\Lambda$ from the right.

Lemma 4: Let P v project vectors onto M(X) and P vn onto M(XB). Then

- (i) $P_{XB}P_X = P_{XB}$, and
- (ii) $\mathcal{M}[X'(I-P_{XB})] = \mathcal{M}(B') \cap \mathcal{M}(X').$

Proof: Result (i) is obvious and result (ii) follows from Lemma 2.

Lemma 5: Let G and X be matrices such that $\mathcal{A}(G') \subset \mathcal{A}(X')$ and D = G(X'X) - G'. Then G'D - G is independent of the choice of g-inverse of D.

Proof: Since D = G(X'X) - G' = G(X'X) - X'X(X'X) - G', R(D) = R(X(X'X) - G')= R(G) = R(G'). Then using Corollary 1a.3 of Mitra (1908a), $(X'X) - G'D_1^-$ and $D_1^-G(X'X) -$ are g-inverses of G and G' respectively where D_1^- and D_2^- are any two alternative choices of D^- . Hence

$$G'D_{\overline{i}}G(X'X)^{\perp}G'D_{\overline{i}}G = G'D_{\overline{i}}G = G'D_{\overline{i}}G$$

which proves the desired result.

Lemma 6: Let $\mathcal{M}(G') = \mathcal{M}(X') \cap \mathcal{M}(H')$ so that G = AH for some A. Then

$$\min_{H\beta=\xi} (Y-X\beta)'(Y-X\beta) = \min_{G\beta=A\xi} (Y-X\beta)'(Y-X\beta).$$

Proof: A solution β_0 of $H\beta = \xi$ is also a solution of $G\beta = A\xi$. Writing $Y - X\beta_0 = U$, the problem reduces to showing

$$\min_{H\beta=0} (U-X\beta)'(U-X\beta) = \min_{G\beta=0} (U-X\beta)'(U-X\beta).$$

Since the minimum in each case is the square of the length of the projection of U on an appropriate subspace, it is enough to show that the subspaces generated by $X\beta$ when β is subject to $H\beta=0$ or $C\beta=0$ are the same. Since the latter space trivially includes the other, the lemma is proved if the dimensions are the same, which is true by Lemma 1.

The following Lemma 7 provides a number of alternative closed expressions for the difference between least sum of squares with and without constraints on parameters. These are useful in the theory and applications of least squares. Some alternative expressions for the unconstrained least sum of squares are well-known (Rao. 1905. p. 185).

Lemma 7: Let β be any solution of $X'X\beta = X'Y'$, and (β^*, λ^*) be any solution of

$$X'X\beta + II'\lambda = X'Y$$

$$II\beta = \xi$$

and G is such that $\mathcal{M}(G') = \mathcal{M}(X') \cap \mathcal{M}(H')$. Then

$$\min_{N\beta=\xi} (Y-X\beta)'(Y-X\beta) - \min_{\beta} (Y-X\beta)'(Y-X\beta)$$

- (i) = $(\beta \beta^{\circ})'X'X(\beta \beta^{\circ})$
- (ii) = $-(\beta \beta^{\bullet})'II'\lambda^{\bullet} = -(II\beta \xi)'\lambda^{\bullet}$
- (iii) = $(G\beta \Lambda\xi)'[G(X'X) G'] (G\beta \Lambda\xi)$.

Proof: The result (i) is obvious. (ii) follows from (i) and the definition of λ^* .

To prove (iii), consider operators P_1 and P_2 which project vectors onto $\mathcal{M}(X)$ and $\mathcal{M}(X(G')^2)$ respectively. Then

$$\begin{split} X(\beta - \beta^*) &= P_1(Y - X\beta^*) = (P_1 - P_1)(Y - X\beta^*) \\ &= (I - P_1)(P_1 - P_1)(Y - X\beta^*) = (I - P_1)X(\beta - \beta^*) \\ &= DG(\beta - \beta^*) \text{ for some } D \end{split}$$

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using (ii) of Lemma 4. The result is proved if it is shown that

$$D'D = (G(X'X)^-G')^-,$$

for which observe that

$$G(X'X) \cap G'D'DG(X'X) \cap G' = G(X'X) \cap X'(I-P_*)X(X'X) \cap G' = G(X'X) \cap G'$$

віпсе

$$G(X'X)^{-}X'P_{4} = G(X'X)^{-}X'X(G')^{*}E = G(G')^{*}E = 0,$$

noting that P_1 is of the form X(G')'E.

The choice of the g-inverses in (ii) is immaterial in view of the result of Lemma 5.

3. LEAST SQUARES THEORY WHEN THE COVARIANCE MATRIX IS SINGULAR

It is shown in Section 1 that the problem (Y, X β , $\sigma^2\Sigma$) can be reduced to the problem

$$(Y_1 = F'Y, F'X\beta(N'X\beta = Y_1 = N'Y), \sigma^2I)$$
 ... (3.1)

so that we can apply the simple least square theory with restrictions on parameters, which is well-known (Rao, 1965, pp. 189, 199). It may be recalled that in (3.1) $N = \Sigma^4$ and F' is a left inverse of C (i.e., F'C=I) where $\Sigma = CC'$ with E(C) equal to the number of columns of C. We shall use the model (3.1) for an application of the known theory of inference on unknown parameters, but express the final results in terms of Y, X and Σ , and g-inverses of matrices depending on them. The theory of G-M model with a singular covariance matrix has been recently considered by Khatri (1968) in a somewhat different way.

Estimability: A parametric function $p'\beta$ is said to be estimable if there exists a linear function L'Y of Y such that $E(L'Y) \equiv p'\beta$, i.e., there exists a vector L such that L'X = p'. We shall consider problems of inference involving estimable functions only.

A characterization of linear functions of I' which have a constant expectation (i.e., independent of unknown parameters) is given by Rao (1968).

3.1. Normal equations and BLUE's. The normal equations in the case (3.1) are those obtained by minimising

$$(Y_1 - F'X\beta)'(Y_1 - F'X\beta) = (Y - X\beta)'F'F(Y - X\beta)$$
 ... (3.2)

subject to the condition $Y_1 = N'X\beta$. We observe that $\Sigma F'F\Sigma = \Sigma$, i.e., F'F is a g-inverse of Σ . Indeed in (3.2), we can choose instead of F'F any g-inverse Σ - of Σ . The restriction $Y_1 = N'X\beta$ may be written, if desired, as $Y_2 = R\beta$ where $Y_3 = (I - \Sigma \Sigma^-)X$ and $R = (I - \Sigma \Sigma^-)X$. Thus in terms of original expressions Y, X, Σ , the normal equations are obtained by minimising

$$(Y-X\beta)'\Sigma^-(Y-X\beta)$$
 ... (3.3)

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subject to the restriction $Y_0 = R\beta$, where Σ^- is any g-inverse of Σ . The minimising equations are

$$\begin{pmatrix} X'\Sigma^{-}X & R' \\ R & 0 \end{pmatrix} \begin{pmatrix} \beta \\ \lambda \end{pmatrix} = \begin{pmatrix} X'\Sigma^{-}Y \\ Y_3 \end{pmatrix} \dots (3.4)$$

where \(\lambda\) is a vector of Lagrangian multipliers. If

$$\begin{pmatrix} D_1 & D_2 \\ D_2 & D_2 \end{pmatrix} ... (3.5)$$

is a g-inverse of the matrix of normal equations, then a solution for β is

$$\beta^* = D_1(X'\Sigma^-Y) + D_2Y_2$$
 ... (3.6)

and the BLUE of an estimable parametric function $p'\beta$ is $p'\beta^{\bullet}$. The variance of the estimator is $\sigma^{z}p'D_{1}p$.

Special cases: If $\mathcal{M}(X) \subset \mathcal{M}(\Sigma)$, then $N'\Sigma = 0 \Longrightarrow N'X = 0$ and the restrictions on β become vacuous. The normal equations in such a case are simply obtained by minimising

$$(Y-X\beta)'\Sigma^{-}(Y-X\beta)$$
. ... (3.7)

The normal equation is

$$X'\Sigma^{-}X\beta = X'\Sigma^{-}Y \qquad ... (3.8)$$

which has a solution of the form

$$\hat{\beta} = (X'\Sigma^-X)^-X'\Sigma^-Y \qquad ... (3.9)$$

for any choices of the g-inverses in (3.9). If $p'\beta$ is an estimable parametric function, it is estimated by $p'\hat{\beta}$ and its variance is

$$\sigma^{t}p'(X'\Sigma^{-}X)^{-}p$$
 ... (3.10)

as in the case of a non-singular E.

If $\mathcal{M}(X) \subset \mathcal{M}(N)$, then the only estimable parametric functions are linear combinations of $N'X\beta$, which are, therefore, estimable with zero variance.

3.2. Estimation of σ^2 . We use the model (3.1) and estimate σ^3 in the usual way by considering

$$\begin{split} R_{\delta}^{2} &= \min_{Y_{1} = R\beta} (Y_{1} - F'X\beta)'(Y_{1} - F'X\beta) \\ &= \min_{Y_{1} = R\beta} (Y - X\beta)'\Sigma^{-}(Y - X\beta). \quad \dots \quad (3.11) \end{split}$$

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An unbiased estimate of σ^2 is R_0^2/f where f is the degrees of freedom of R_0^2 given by the expression (see Rao, 1965, p. 190)

$$f = R(\Sigma) - \left[R \begin{pmatrix} F'X \\ N'X \end{pmatrix} - R(N'X) \right]$$

$$= R(\Sigma) - R(X) + R(N'X)$$

$$= R(\Sigma : X) - R(X) \qquad \dots (3.12)$$

since $R(N'X) = R(\Sigma : X) - R(\Sigma)$ and $R(\Sigma)$ is equal to the number of variables in Y_1 .

If Y has a multivariate normal distribution, by applying the first fundamental theorem of least squares (Rao, 1965, p. 153), R_0^2/σ^2 has a χ^2 -distribution on f degrees of freedom.

3.3. An alternative approach to BLUE estimation. We choose L such that $L'\Sigma L$ is a minimum subject to L'X = p'. Consider the matrix

$$\begin{pmatrix} \Sigma & X \\ X' & 0 \end{pmatrix}$$
 ... (3.13)

and a g-inverse

$$\begin{pmatrix} D_1 & D_1 \\ D_2 & D_1 \end{pmatrix}. \qquad ... (3.14)$$

Then the optimum choice of L is D_1p . The BLUE of $p'\beta$ is $p'D_1'Y$ with variance $p'(D_*\Sigma D_1)p\sigma^2$. The estimate of σ^2 is $R_0^2|f$ where

$$R_0^2 = Y'(I - XD_2')'\Sigma^{-}(I - XD_2')Y$$
 ... (3.15)

and $f = R(\Sigma : X) - R(X)$.

3.4. Tests of linear hypotheses. Let $II\beta = d$ be a set of linear hypotheses consistent with the linear restrictions $R\beta = Y_2$. Then

$$R_1^2 = \min_{Y_0 = R_0, d = R_0} (Y - X\beta) \Sigma (Y - X\beta) \qquad ... (3.16)$$

and the d.f. for R; is

$$h = R(\Sigma) - R \begin{pmatrix} F'X \\ N'X \\ H \end{pmatrix} - R \begin{pmatrix} N'X \\ H \end{pmatrix}$$

$$= R(\Sigma) - R \begin{pmatrix} X \\ H \end{pmatrix} + R \begin{pmatrix} N'X \\ H \end{pmatrix}$$

$$= R(\Sigma) - R \begin{pmatrix} X \\ H \end{pmatrix} + R \begin{pmatrix} R \\ H \end{pmatrix}. \dots (3.17)$$

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For tests of significance $(R_1^*-R_2^*)/\sigma^2$ has a χ^2 distribution by an application of the second fundamental theorem of least squares (Rao, 1965, p. 155), central when the hypothesis is true, on (h-f) d.f. It is interesting to write

$$h-f = R \binom{N'X}{H} - R(N'X) - \left[R \binom{X}{H} - R(X) \right]. \quad ... \quad (3.18)$$

4. LEAST SQUARES SOLUTION BY HOUSEHOLDER TRANSFORMATIONS

Golub (1905), Businger and Golub (1905), and Björck and Golub (1908) considered a reduction of observational equations by Householder transformation (see Rao, 1905, p. 20) for obtaining numerical values of residual (least) sum squares and estimates of unknown parameters. In the problem $(X, X\beta, \sigma^2 I)$, where X'X is of full rank, the method consists in reducing the matrix $(X \equiv 1)$ to the form

$$\begin{pmatrix} T & Q_1 \\ \dots & Q_1 \end{pmatrix} \qquad \dots \tag{4.1}$$

by Householder transformation on matrix X, where T is a nonsingular upper triangular matrix, and Q_1 , Q_1 are column vectors. Then the least square estimator of β is

$$\hat{\beta} = T^{-1} Q_1$$
 ... (4.2)

and the residual sum of squares is

$$R_0^2 = Q_2' Q_2$$
 ... (4.3)

which are simple to calculate. We suggest a slight variation of the reduction process which is useful when the rank of X'X is not full, making T singular. Let X be $n \times m$ matrix with rank r < m. n.

Consider the first column of X. If it has a non-zero element, then apply Householder transformation to have a non-zero value in the first position and sweep out the rest of the elements in the column. If all the elements of the first column are zeros, move to the next nearest column which has at least one non-zero value, say the i-th, and apply Householder transformation to have a non-zero value in the first position (and not in the i-th position) and sweep out the rest of the elements in the i-th column. Now omit the first row and repeat the process stated on the reduced matrix, and so on till all the columns of X are covered. Then by a rearrangement of columns (i.e., by renaming the parameters) if necessary the reduced matrix is of the form

$$\begin{pmatrix} T & U & Q_1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & Q_2 \end{pmatrix} \qquad \dots \tag{4.4}$$

where T is a nonsingular upper triangular $(r \times r)$ matrix, Q_1 is $r \times 1$ vector and Q_3 is $(n-r) \times 1$ vector. A solution to normal equations is

$$(\beta_1, ..., \beta_r)' = T^{-1}Q_1, \beta_{r+1} = 0, ..., \beta_m = 0$$
 ... (4.5)

and the residual sum of squares is

$$R_{*}^{2} = O'_{*} O_{*}, \qquad ... (4.6)$$

The estimable parametric functions are linear functions of $(T \in U)\beta$.

In actual practice, where approximations have to be made in numerical computations, it may be difficult to decide whether a particular value at any stage of reduction is a real deviation from zero or is due to rounding off errors. Some investigations made in this connection will be published elsewhere.

Now we make a brief comment on the case of constraints on parameters considered by Björck and Golub (1968). Let $H\beta=\xi$ represent the constraints. Then we consider the matrix

$$\begin{pmatrix} H & \xi \\ \dots & Y \end{pmatrix} \qquad \dots \qquad (4.7)$$

Björck and Golub suggest a sweep-out of the columns of the matrix $\binom{II}{X'}$ by Householder transformation. But it seems to be more advantageous to proceed in a slightly different way. Choose a non-zero element in the first row of II, say in the i-th column, and sweep out the other elements in the i-th column of the matrix (4.7). Omitting the first row and the swept-out column the same procedure is applied on the remaining matrix by choosing a non-zero element in the first row of the reduced II matrix. If a row consists of all zeros at any stage, the next row is considered. Such a process of sweep out is continued till no row with a non-zero element is left in any reduced II matrix. For further operations which start with the first row of a reduced X matrix, apply Householder transformation. The resulting matrix will be of the type, after a rearrangement of columns, if necessary, and after omitting zero rows in the reduced form of II.

$$\begin{pmatrix} U_1 & U_2 & U_3 & Q_0 \\ 0 & T_1 & T_1 & Q_1 \\ 0 & 0 & 0 & Q_1 \end{pmatrix} ... (4.8)$$

where U, and T, are upper triangular and non-singular matrices. Let the order of

$$\begin{pmatrix} U_1 & U_1 \\ 0 & T_1 \end{pmatrix} ... (4.9)$$

be $h \times h$. Then a solution to normal equations is

$$(\beta_1, ..., \beta_h)' = \begin{pmatrix} U_1 & U_1 \\ 0 & T_1 \end{pmatrix}^{-1} \begin{pmatrix} Q_0 \\ Q_1 \end{pmatrix}$$
 ... (4.10)

$$\beta_{h+1} = 0, ..., \beta_m = 0$$

and the residual sum of squares is

$$R_0^* = Q_1^*Q_1^*$$
 ... (4.11)

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The estimable parametric functions are linear combinations of

$$\begin{pmatrix} U_1 & U_2 & U_3 \\ 0 & T_1 & T_2 \end{pmatrix} \qquad ... \quad (4.12)$$

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