

Study of MINQUE and Simple estimator of Covariance Matrix in the multivariate linear Model

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Abstract:

Under the multivariate linear model $\{Y, X\beta, \Sigma \otimes V\}$, equality of MINQUE and so called "simple" estimator $(1/f)Y^TMY$, with $M = I - X(X'X)^+X^T$, $f = \text{rank}(X : V) - \text{rank}(X)$ for Σ is considered. It is revealed that this equality holds if and only if the quadratic form $\Sigma^{-1}Y'MY$ admits a Wishart-distribution under multivariate normality of Y . Also comparison of MINQUE and simple estimator of Σ in the multivariate normal linear model under the risk of entropy loss function criterion where the design matrix X need not have full rank and the dispersion matrix V can be singular A is considered . It is interested to prove that MINQUE is superior to simple estimator OLSE

Keywords: multivariate linear model, MINQUE, BLUE, OLSE, Wishart - distribution

Introduction:

We consider the multivariate linear model

$$Y = X\beta + \varepsilon, \quad E(\varepsilon) = 0, \quad \text{cov}(\varepsilon) = \Sigma \otimes V$$

where y is an $n \times p$ observable random matrix, an $n \times q$ matrix X and $n \times n$ nonnegative definite matrix V are known, while β is $q \times p$ matrix of

unknown parameter, the $p \times p$ positive definite matrix Σ is also unknown. The error matrix ε has the normal distribution $N(0, \Sigma \otimes V)$.

The matrices X and V are both allowed to be of arbitrary rank. But it is assumed, throughout this paper, that the model is consistent,

(Rao (1973), p. 297), i.e. $Y \in R(X:V)$, where $R(A)$ stands for the range of a matrix A and $(A:B)$ denotes the partitioned matrix with A and B placed next to each other. Suppose we wish to estimate the unknown positive definite Σ by using the competing estimators

$$(1/f)Y'M(MVM)^+MY \quad (1)$$

And

$$(1/f)Y'MY \quad (2)$$

Where $M = I - X(X'X)^+X'$, A^+ stands for the Moore-Penrose inverse of a matrix A , $f = \text{rank}(X:V) - \text{rank}(X)$. According to theorem 3.4 in Rao (1974), and A' denotes the transpose of A .

Formula (1) provides the MINQUE (Minimum Norm Quadrate Unbiased Estimator) for Σ , cf. Theorem 3.4(a) in Rao (1974). It can also be written as

$$(1/f)Y'(MVM)^+Y, \quad (3)$$

since we have $(MVM)^+ = M(MVM)^+$ in view of $R[(MVM)^+] \subseteq R(M)$, and then $(MVM)^+ = (MVM)^+M$ in view of the symmetry of $(MVM)^+$. According to Theorem 3.4 in Rao (1974), the MINQUE can be represented in further different forms. For example under the weakly

singular multivariate linear model, i.e. in case $R(X) \subseteq R(V)$, the estimator (2) can be written as

$$(1/f)Y^T (V^+ - V^+ X (X^T V^+ X)^+ X^T V^+) Y \quad (4)$$

Where $f = \text{rank}(V) - \text{rank}(X)$. This may also be derived from the results in Baksalary et al. (1990).

Formula (2) will be called "simple" estimator and of course coincides with (1) when $V=I$. However, in the general case the simple estimator (2) need not even be unbiased since we do not necessarily have $\text{trace}(MV)=f$. On the other hand, we always have $\text{trace}[(MVM)^+V] = \text{rank}(MV) = f$, which ensures unbiasedness of (3). (see e.g. Theorem 5 in Marsaglia and Styan (1974) for $\text{rank}(MV)=f$, and note that $\text{trace}[(MVM)^+V] = \text{rank}[(MVM)^+V]$ since $[(MVM)^+V]$ is idempotent. Needless to say that the MINQUE is unbiased by definition.

In the first section we investigate equality of MINQUE and simple estimator when X and V can be deficient in rank. and in the second section. The object of the present note is to make comparison of these two estimators, the criterion we used in this comparison is the risk of the entropy loss function, in which entropy loss function defined by

$$L(\Sigma, G) = \text{tr}(G\Sigma^{-1}) - \log|\text{tr}G\Sigma^{-1}| - p \quad (5)$$

where G is a positive definite matrix.

1. Equality of the estimators:

By using the above mentioned identity

$$(MVM)^+ = M (MVM)^+ = (MVM)^+ M,$$

it is easy to see that (1), which equals (3), and (2) coincide for all values $Y \in R(X : V)$ if and only if

$$Z^T V (MVM)^+ V Z = Z^T VMVZ \quad (6)$$

for all $n \times 1$ vectors z . This is known to be satisfied if and only if the matrix $V(MVM)^+ V - VMV$ is skew-symmetric. But since the matrix is also symmetric it must be zero. Hence (6) is equivalent to

$$V (MVM)^+ V = VMV, \quad (7)$$

Let L denote the unique non-negative definite square root of V . Then (7) can be written as

$$LZZ^+L = LZZ^+L, \quad (8)$$

with $Z = LM$, by using $Z^+ = (Z^T Z)^+ Z^T$ and $LZ = VM$. Since $L^+L = LL^+$, $L^+LZZ^+ = ZZ^+ = ZZ^+LL^+$ and $L^+LZZ^T = ZZ^T = ZZ^TLL^+$, it is easily seen that (9) is equivalent to

$$ZZ^+ = ZZ^T \quad (9)$$

Obviously (9) is satisfied if and only if ZZ^T is idempotent, which reads

$$LMVML = LML,$$

or equivalently

$$VMVMV = VMV \quad (10)$$

Further, in the special case $\text{rank}(X:V)=n$ we obtain $\text{rank}(MV)=n-\text{rank}(X)$, cf. Theorem 5 in Marsaglia and Styan (1974). Since always $n-\text{rank}(X)=\text{rank}(M)$ we have $\text{rank}(MV)=\text{rank}(M)$, which means $R(MV)=R(M)$. with $K=VM$, Eq. (10) reads

$$KMVMK^T = KMK^T \quad (11)$$

Since we have $K^+KMV = MV$ and $K^+KM = M$ when $R(K^T) = R(M)$, (11) is

equivalent to $MVM=M$ (12)

when $\text{rank}(X:V) = n$. Observe that (13) may also be obtained directly from the equality of (4) and (3), which holds for all $n \times 1$ vectors if and only if $(MVM)^+ = M$. But since $M = M^+$, this gives (12). Observe on the other hand that (12) implies $\text{rank}(X:V) = n$ in view of $\text{rank}(X:V) = \text{rank}(X) + \text{rank}(MVM)$. Hence $VMVMV = VMV$, $\text{rank}(X:V) = n \Leftrightarrow MVM = M$.

Our derivations may be comprised in the following

Proposition(1)

Under the general multivariate linear model $\{Y, X\beta, \Sigma \otimes V\}$, MINQUE for Σ coincides with simple estimator for Σ for all $Y \in R(X:V)$ if and only if $VMVMV = VMV$, where $M = I - X(X'X)^+X'$. Moreover $R(X:V)$ is the whole space together with the above coincidence if and only if $MVM = M$. Note that when Y in the multivariate linear model is multivariate normally distributed, then the condition $VMVMV = VMV$ is necessary and sufficient for $\Sigma^{-1}Y'MY$ to have a Wishart-distribution i.e $W(k, \delta)$ -distribution, cf. Theorem 9.2.1 in Rao and Mitra (1971), in which case $k = \text{trace}(MV) = f$ and $\delta = 0$. Hence the question of equality of MINQUE and simple estimator for Σ in the multivariate linear model is equivalent to the question of $\Sigma^{-1}Y'MY$ having a Wishart distribution, $W(k, \delta)$, in the multivariate linear model with normally distributed Y . Observe that in general we do not have $k = \text{trace}(MV) = \text{rank}(MV) = f$. However, since (11) is equivalent to $Z^+ = Z'$, i.e. $LMVM = LM$, we see that the condition $VMVMV = VMV$ is equivalent to $VMVM = VM$, which means that VM and hence MV is idempotent. But for idempotent matrices rank and trace coincide. The former equivalence has also been observed by Bhimasankaram and Majumdar (1980) who trace it back to Mitra (1968).

By adapting a table from Rao and Mitra (1971,p.161) to the situation under model $\{Y, X\beta, \Sigma \otimes V\}$ with normally distributed Y , one may obtain a general representation of V being necessary and sufficient for $\Sigma^{-1}Y'MY$ to have $W(\text{trac}(M),0)$ -distribution . From this representation one immediately observes $MVM = M$, showing that $\text{rank}(X:V)=n$ is implicitly comprised therein. Complementing the table, for non- singular V however , Chikuse (1981)concludes that $W(\text{trace}(M),0)$ -ness of $\Sigma^{-1}Y'MY$ is equivalent to equality of $Y'MY$ and $Y'M(MVM)^+MY$. General characterizations of the class of all matrices satisfying the identity $VMVMV = VMV$ (or $VMVM = VM$) may be derived from theorem 4.4 in Bhimasankaram and Majumdar(1980) or theorem 2 in Baksalary et al. (1980). A general non- negative definite solution to $MVM = M$ with respect to V can also be obtained from Baksalary (1984), whose result is claimed to be advantageous over that derived by Khatri and Mitra(1976, Lemma 2.1).

1.2.Relationship with known results

It is well known that one representation of the BLUE(Best Linear Unbiased Estimator)for $X\beta$ is given by

$$X (X' T^{-1} X)^+ X' T^{-1} Y \quad (13)$$

with $T = V + XX'$, whereas the OLSE (Ordinary Least Square Estimator) for $X\beta$ reads

$$XX^+Y \quad (14)$$

Conditions for equality of (13) and (14) for all $Y \in R(X:V)$ are well known in the literature. one of them being $XX^+V = VXX^+$, c f. Puntanen and Styan (1989). Trivially the latter condition is equivalent to the symmetry of the matrix MV .

Now taking the results of the previous section into account, we can state that coincidence of MINQUE and simple estimator for Σ for all $Y \in R(X:V)$ holds together with coincidence of BLUE and OLSE for $X\beta$ for all $Y \in R(X:V)$ if and only if MV is idempotent and symmetric, or in other words, MV is an orthogonal projector.

As mentioned before we have $R(MV) = R(M)$ when $\text{rank}(X:V) = n$. This means that under $\text{rank}(X:V) = n$ the matrix MV is an orthogonal projector if and only $MV = M$. On the other hand, $MV = M$ entails $\text{rank}(X:V) = n$. Hence we may state

Proposition(2):

Under the multivariate linear model $\{Y, X\beta, \Sigma \otimes V\}$, coincidences of MINQUE and simple estimator for Σ for all $Y \in R(X:V)$ holds together with Coincidences of BLUE and OLSE for $X\beta$ for all $Y \in R(X:V)$ if and only if MV is an orthogonal projector, where $M = I - X(X'X)^+X'$.

Moreover $R(X:V)$ is the whole space together with the above coincidences if and only if $MV = M$.

As mentioned above, the condition $MV = M$ as well as the condition $MV = M$ entails $\text{rank}(X:V) = n$, which may equivalently be expressed as

$$\text{rank}(V) = n - \text{rank}(X) + \dim[R(X) \cap R(V)] \quad (15)$$

cf. Marsaglia and Styan (1974). Hence under each of these two conditions, V is non-singular if and only if $\text{rank}(X) = \dim[R(X) \cap R(V)]$, which in turn is equivalent to $R(X) \subseteq R(V)$.

Eventually note that when MV is symmetric, i.e. M and V commute, then M and V can be simultaneously diagonalized by some orthogonal matrix, cf. Rao (1973, p.41). Hence we have $V = M$ if and only if there exists an orthogonal matrix U such that

$$M = U \begin{bmatrix} I_s & 0 \\ 0 & 0 \end{bmatrix} U^T \text{ and } V = U \begin{bmatrix} I_s & 0 \\ 0 & D \end{bmatrix} U^T$$

where $s = n - \text{rank}(X)$ and D is a $(n - s) \times (n - s)$ non-negative definite diagonal matrix.

2. Comparison of estimators:

The following lemmas are necessary for a proof of our main theorem.

Lemma(1): Let V be $n \times n$ nonnegative definite matrix with rank r and Σ be positive definite matrix. Random matrix $X \sim N_{n \times p}(\mu, \Sigma \otimes V)$ if and only if $X = \mu + AU$, where A is $n \times r$ matrix with rank r and $AA' = V$, $U \sim N_{r \times p}(0, \Sigma \otimes I_r)$

Proof: Obviously, $X \sim N_{n \times p}(\mu, \Sigma \otimes V)$ if and only if

$Y = (X - M)\Sigma^{-\frac{1}{2}} \sim N_{r \times p}(0, I_p \otimes V)$, that means, $Y_1, Y_2, \dots, Y_p \text{ iid} \sim N(0, V)$, where Y_1, Y_2, \dots, Y_p , are the column vectors of y , we know that for every $i=1, \dots, p$, $y_i \sim N(0, V)$ if and only if $Y_i = AW_i$, where A is $n \times r$ matrix with rank r and $AA' = V, W \sim N(0, I_r)$. A proof of this proposition can be found in Rao (1973), p.521. Let $W = (W_1, \dots, W_p)$. Then $W \sim N_{r \times p}(0, I_p \otimes I_r)$. Hence $Y \sim N_{n \times p}(0, I_p \otimes V)$ if and only if $Y = AW$, that implies $X \sim N_{n \times p}(\mu, \Sigma \otimes V)$ if and only if $X = \mu + AU$ where $U = W\Sigma^{-\frac{1}{2}} \sim N_{r \times p}(0, \Sigma \otimes I_r)$. The proof of lemma (2.1) is completed.

Lemma(2): let X be an $n \times p$ matrix and V $n \times n$ nonnegative definite matrix. Then $\text{rank}(VM) = \text{rank}(X:V) - \text{rank}(X)$ where $M = I - X(X'X)^+ X'$.

A proof can be found in Wang and Chow (1994)

Lemma(3):

$$\hat{\Sigma}_m = \frac{\sum_{i=1}^k U_i U_i'}{k} \quad (16)$$

$$\hat{\Sigma}_s = \frac{\sum_{i=1}^k \lambda_i U_i U_i'}{k}, \quad (17)$$

Where U_1, \dots, U_k are iid $\sim N(0, \Sigma)$ and $\lambda_1 \geq \dots \geq \lambda_k > 0$ are the positive eigenvalues of MV .

Proof: since $MV=0$, thus $\hat{\Sigma}_m$ and $\hat{\Sigma}_s$ can be written as

$$\hat{\Sigma}_m = \varepsilon' M (MVM)^+ M \varepsilon / k$$

$$\hat{\Sigma}_s = \varepsilon' M \varepsilon / k$$

In view of lemma 1 and $\varepsilon \sim N(0, \Sigma \otimes V)$, $r = \text{rank}(v)$ we note that there is an $n \times r$ matrix A with rank r such that

$$\varepsilon \sim A\delta, \quad \delta \sim N_{\text{rxp}}(0, \Sigma \otimes I), \quad AA' = V,$$

Thus

$$\hat{\Sigma}_m = \delta' Q_1 \delta / K \quad (18)$$

$$\hat{\Sigma}_s = \delta' Q_2 \delta / K \quad (19)$$

Where

$$Q_1 = A'M(MAA'M)^+ MA, \quad Q_2 = A'MA$$

It is easy to verify that $Q_1 Q_2 = Q_2 Q_1$, which implies (see for example , Rao (1973),p.41) that there is an $n \times r$ orthogonal matrix T such that both $T'Q_1T$ and $T'Q_2T$ are diagonal. By using lemma(2), it is can be show that

$$\begin{aligned} \text{rank}(Q_1) &= \text{rank}(A'MA) = \text{rank}(A'M) = \text{rank}(VM) \\ &= \text{rank}(V:X) - \text{rank}(X) = k \end{aligned} \quad (20)$$

We note that Q_1 is projection matrix, thus

$$T'Q_1T = \begin{pmatrix} I_k & o \\ o & o \end{pmatrix} \quad (21)$$

$$T'Q_2T = \begin{pmatrix} \Lambda_k & o \\ o & o \end{pmatrix} \quad (22)$$

Where $\Lambda_k = \text{diag}(\lambda_1, \dots, \lambda_k)$

Denote

$$U = T'\delta \quad (23)$$

Then

$$U \sim N_{\text{rxp}}(0, \Sigma \otimes I_r) \quad (24)$$

Let $U' = (U_1, \dots, U_r)$. Then U_1, \dots, U_r are iid $\sim N(0, \Sigma)$.

Substituting (21),(23) in (18) yields (16)

i.e.

from (21) we get $T'Q_1T = I_s \rightarrow Q_1 = (T^{-1})'T^{-1}$

from (23) we get $\delta = UT'^{-1}$

equation (18) becomes:

$$\begin{aligned}
\hat{\Sigma}_m &= (UT'^{-1}(T'^{-1}T^{-1})(UT')^{-1} / K \\
&= (T'^{-1})'U'(T'^{-1}T^{-1})U(T^{-1})' / K \\
&= U'(T'^{-1})'(T'^{-1})T^{-1}(T^{-1})'U / K \\
&= U'I.U / K \\
&= U'U / K
\end{aligned}$$

Then

$$\hat{\Sigma}_m = \sum_{i=1}^k \frac{U_i'U_i}{k}$$

Also substituting (22),(24) in (19) yields (17)

From (22) we get

$$\begin{aligned}
T'Q_2T &= \Lambda_s \rightarrow T'Q_2T = \lambda_k \\
\Rightarrow Q_2 &= (T')^{-1} \lambda_k T^{-1}
\end{aligned}$$

From equation (19) we get

$$\begin{aligned}
\hat{\Sigma}_s &= (UT'^{-1})[(T')^{-1} \lambda_k T^{-1}](UT'^{-1}) / K \\
&= (T'^{-1})'U'(T')^{-1} \lambda_k T^{-1}U(T^{-1})' / K \\
&= (T'^{-1})'(T'^{-1})U' \lambda_k UT^{-1}(T^{-1})' / K \\
&= IU' \lambda_k UI / K \\
&= U' \lambda_k U / K \\
&= \lambda_k U'U / K
\end{aligned}$$

Then

$$\hat{\Sigma}_s = \sum_{i=1}^k \frac{\lambda_i U_i'U_i}{k}$$

Theorem: under entropy loss function

- (a) $R(\hat{\Sigma}_m) = R(\hat{\Sigma}_s)$, if $\lambda_1 = \dots = \lambda_k = 1$,
(b) $R(\hat{\Sigma}_m) < R(\hat{\Sigma}_s)$, otherwise.

Where $R(\hat{\Sigma}_m)$, $R(\hat{\Sigma}_s)$ are the risk of $\hat{\Sigma}_m$, $\hat{\Sigma}_s$ respectively.

Proof:

From (5) we have

$$\begin{aligned}
L(\Sigma, \hat{\Sigma}_s) &= tr(\hat{\Sigma}_s \Sigma^{-1}) - \log \left| \hat{\Sigma}_s \Sigma^{-1} \right| - p \\
&= tr(\Sigma^{-\frac{1}{2}} \hat{\Sigma}_s \Sigma^{-\frac{1}{2}}) - \log \left| \Sigma^{-\frac{1}{2}} \hat{\Sigma}_s \Sigma^{-\frac{1}{2}} \right| - p
\end{aligned}$$

also

$$L(\Sigma, \hat{\Sigma}_m) = tr(\Sigma^{-\frac{1}{2}} \hat{\Sigma}_m \Sigma^{-\frac{1}{2}}) - \log \left| \Sigma^{-\frac{1}{2}} \hat{\Sigma}_m \Sigma^{-\frac{1}{2}} \right| - p$$

It follows from (17) that

$$\begin{aligned}
L(\Sigma, \hat{\Sigma}_s) &= tr \left(\frac{\sum \lambda_i \Sigma^{-\frac{1}{2}} U_i U_i' \Sigma^{-\frac{1}{2}}}{k} \right) - \log \left| \frac{\sum \lambda_i \Sigma^{-\frac{1}{2}} U_i U_i' \Sigma^{-\frac{1}{2}}}{k} \right| - p \\
&= tr \left(\frac{\sum \lambda_i V_i V_i'}{k} \right) \log \left| \frac{\sum \lambda_i V_i V_i'}{k} \right| - p,
\end{aligned}$$

Where

$$V_i = \Sigma^{-\frac{1}{2}} U_i \quad V_1, \dots, V_k \text{ i.i.d } N_p(0, I)$$

From (16) we have

$$L(\Sigma, \hat{\Sigma}_m) = \left[tr \left(\frac{\sum V_i V_i'}{k} \right) - \log \left| \frac{\sum V_i V_i'}{k} \right| - p \right]$$

Now :

$$\begin{aligned}
R(\hat{\Sigma}_s) &= E \left[L(\Sigma, \hat{\Sigma}_s) \right] \\
&= E \left[tr \left(\frac{\sum_{i=1}^k \lambda_i V_i V_i'}{k} \right) - \log \left| \frac{\sum_{i=1}^k \lambda_i V_i V_i'}{k} \right| - p \right],
\end{aligned}$$

$$\begin{aligned}
R(\hat{\Sigma}_m) &= E \left[L(\Sigma, \hat{\Sigma}_m) \right] \\
&= E \left[\operatorname{tr} \left(\frac{\sum_{i=1}^k V_i V_i'}{k} \right) - \log \left| \frac{\sum_{i=1}^k V_i V_i'}{k} \right| - p \right],
\end{aligned}$$

Obviously,

$$R(\hat{\Sigma}_s) = R(\hat{\Sigma}_m) \quad , \lambda_1 = \dots = \lambda_k = 1.$$

$$\text{Let } L(\lambda_1, \dots, \lambda_k) = E \left\{ \operatorname{tr} \left(\frac{\sum_{i=1}^k \lambda_i V_i V_i'}{k} \right) - \log \left| \frac{\sum_{i=1}^k \lambda_i V_i V_i'}{k} \right| - p \right\}$$

Because $L(\lambda_1, \dots, \lambda_k)$ is a symmetric and convex function, $L(\lambda_1, \dots, \lambda_k)$ has minimum value, and when $\lambda_1 = \dots = \lambda_k = \lambda$, $L(\lambda_1, \dots, \lambda_k)$ takes minimum value.

Now , Let

$$\begin{aligned}
h(\lambda) &= E \left\{ \operatorname{tr} \left(\frac{\lambda \sum_{i=1}^k V_i V_i'}{k} \right) - \log \left| \frac{\lambda \sum_{i=1}^k V_i V_i'}{k} \right| - p \right\} \\
&= E \left\{ \operatorname{tr} \left(\frac{\lambda \sum_{i=1}^k V_i V_i'}{k} \right) - \log \left(\frac{\lambda^p}{k} \left| \frac{\sum_{i=1}^k V_i V_i'}{k} \right| \right) - p \right\}
\end{aligned}$$

$$= E \left\{ \operatorname{tr} \left(\frac{\lambda \sum_{i=1}^k V_i V_i'}{k} \right) - \log(\lambda^p) - \log \left| \frac{\sum_{i=1}^k V_i V_i'}{k} \right| - p \right\}$$

Then

$$h'(\lambda) = E \left\{ \operatorname{tr} \left(\frac{\sum_{i=1}^k V_i V_i'}{k} \right) - \frac{p \lambda^{p-1}}{\lambda^p} \right\}$$

So

$$h'(\lambda) = 0 \quad \Rightarrow \quad E \left\{ \operatorname{tr} \left(\frac{\sum_{i=1}^k V_i V_i'}{k} \right) \right\} - \frac{p}{\lambda} = 0.$$

Since $V_j \sim N_p(0, I)$ then $V_j = (V_{j1}, \dots, V_{jp})'$,

$V_{j1}, \dots, V_{jp} \text{ i.i.d. } \sim N(0, 1)$ so that

$$V_j V_j' = \begin{bmatrix} V_{j1} \\ \cdot \\ \cdot \\ \cdot \\ V_{jp} \end{bmatrix} (V_{j1} \quad \cdot \quad \cdot \quad \cdot \quad V_{jp})$$

So

$$E \operatorname{tr}(V_j V_j') = \sum E V_{jk}^2 = p$$

Thus

$$\begin{aligned}
h'(\lambda) &= \text{tr}E \left\{ \text{tr} \sum_{i=1}^k V_i V_i' - \frac{P \lambda^{p-1}}{\lambda^p} \right\} = 0 \\
&= \left[P - \frac{P}{\lambda} \right] = 0 \\
\rightarrow P &= \frac{P}{\lambda} \\
\rightarrow P &= \lambda P \\
\therefore \lambda &= 1
\end{aligned}$$

The proof of theorem is completed.

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