On estimating the matrix of mean

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1. Introduction

Assume that

$$\begin{aligned} & X:\ m \times p \sim N(B, I_m \otimes \Sigma) \\ (1.1) \qquad & S:\ p \times p \sim W_p(\Sigma, n) \\ & X \text{ and } S \text{ are independent} \\ & B \text{ and } \Sigma \text{ are unknown.} \end{aligned}$$

Based on (X, S) we consider the problem of estimating B with respect to the loss function

$$(1.2) \qquad L(\hat{B}, (B, \Sigma)) = \mathrm{tr}\, \Sigma^{-1}(\hat{B} - B)'(\hat{B} - B).$$

The case $\Sigma = I_p$ is considered by Stein(1973) where the use of unbiased risk estimate was introduced. For unknown covariance case, Zidek(1978) derived the unbiased risk estimators for the estimators in certain classed of equivariant estimators using generalization of the Pitman-Robins representation (which involves in zonal polynomials). More recently Bilodeau and Kariya(1989) obtained the Efron-Morris type estimator in the case $m > p+1$ using two integration by parts formulae, namely the Stein identity and Wishart identity, while Konno did in the case $p > m + 1$. In this paper a unified approach to search for alternative estimators systematically will be carried out for the case $|p-m| > 1$. Our basic approach due to Stein (1973) and Loh (1988) is described in the following;

1. Narrow the class of the estimators, for example, using equivariance in the problem and work out the form of the estimator.

2. Compute the unbiased estimate of the risk of the estimators under consideration using the integration by parts formula.

3. Determine promising alternative estimators from the unbiased estimate of risk.

Since the first introduction by Stein, numerous researchers have applied this technique to the problems in statistical decision theory such as Berger (1980), Dey and Srinivasan

(1985), Efron and Morris (1976), Haff (1978,1980, 1982, 1988), Muirhead and Verathaworn (1985), Loh (1988), Bilodeau and Kariya (1989), Konno (1990a,1990b,1990c, 1991), and Perron (1989), Bilodeau (1990).

In Section 2 of this paper a certain form of equivariant estimators under the group of natural transformations is derived so that the representation of the unbiased estimate of the risk is available in terms of the eigenvalues of the usual F-matrix $X'XS^{-1}$. In Section 3 the unbiased estimate of risk is obtain using the identity due to Bilodeau and Kariya (1989) and calculus on eigenstructure of F-matrix. In Section 4, following an approach by Haff (1982,1988), an alternative estimator as the solution of the Euler-Lagrange system of partial differential equations is obtained. Furthermore, several examples of minimax estimators are given.

2. Deriving the class of estimators

First let us recall the results by Stein (1973) concerned with the problem of estimating matrix of mean with identity covariance matrix. Let

$$\tilde{X}; m \times p \sim N(\tilde{B}, I_m \otimes I_p) \qquad (m > p+1), \tag{2.1}$$

and the loss be $\mathrm{tr}(\hat{\tilde{B}} - \tilde{B})'(\hat{\tilde{B}} - \tilde{B})$. He introduced the estimators of the form

$$\hat{\tilde{B}}(\tilde{X}) = \tilde{X} + \frac{1}{2}\nabla_{\tilde{X}} h(Y), \tag{2.2}$$

where $Y = (y_1, \dots, y_p)'$, $y_1 > \cdots > y_p$ are the ordered eigenvalues of $\tilde{X}'\tilde{X}$, and $\nabla_{\tilde{X}} h(Y) = (\partial h(Y)/\partial \tilde{x}_{ij})$ for $\tilde{X} = (\tilde{x}_{ij})$. Then using the Normal identity and calculus on eigenstructure the unbiased estimate of the risk of these estimators is obtained in terms of the eigenvalues of $\tilde{X}'\tilde{X}$ and the first and second derivatives of $h(Y)$ with respect to Y. Next consider transformations $\tilde{X} \to \tilde{X}C$ for a $p \times p$ nonsingular matrix C. Then it is readily seen from Lemma 1.1 in Kariya and Sinha(1989) that the model (2.1) is transformed into

$$\tilde{\tilde{X}} \sim N(\tilde{B}C, I_m \otimes (C'C))$$

and the estimator of the form (2.2) is changed into

$$\begin{aligned} \hat{\tilde{B}}C &= \tilde{X}C + \frac{1}{2}\nabla_{\tilde{X}} h(Y) \cdot C \\ &= \tilde{\tilde{X}} + \frac{1}{2}\nabla_{\tilde{\tilde{X}}} h(\tilde{Y}) \cdot C'C \end{aligned}$$

where $\tilde{\tilde{X}} = \tilde{X}C$ and $\tilde{Y} = (\tilde{y}_1, \ldots, \tilde{y}_p)'$, $\tilde{y}_1 > \cdots > \tilde{y}_p > 0$ are the ordered eigenvalues of $\tilde{\tilde{X}}'\tilde{\tilde{X}}(C'C)^{-1}$. The last equality above holds since $\nabla_{\tilde{X}} = \nabla_{\tilde{\tilde{X}}} C'$.

Now let us return to the original model (1.1). If $\Sigma = C'C$ is unknown and the estimate of Σ, that is S, is available, it is natural to consider the estimator of the form

$$\hat{B}(X,S) = X + \frac{1}{2}\nabla_X h(F) \cdot S, \tag{2.3}$$

where $F = (f_1, \ldots, f_{min(m,p)})'$ and $f_1 > \cdots > f_{min(m,p)} > 0$ are the ordered eigenvalues of $X'XS^{-1}$. It is readily checked that these are invariant under the group of transformations

$$(X,S) \to (OXC, C'SC),$$

where O is an $m \times m$ orthogonal matrix and C is a $p \times p$ nonsingular matrix.

The following representation of the second term on the right hand side of (2.3) gives better understanding of our estimators. For $m > p$, (2.3) can be rewritten as

$$\hat{B}(X,S) = X[I_p + AH(F)A^{-1}], \tag{2.4}$$

where $H(F) = diag(h_1(F), h_2(F), \ldots, h_p(F))$, $h_k(F) = \partial h(F)/\partial f_k$, $k = 1, 2, \ldots, p$, A is a $p \times p$ nonsingular matrix such that $A'SA = I_P$ and $diag(F) = A'X'XA$. This can be seen from Lemma A1 in Appendix and straightforward calculation. Similarly, for $m \le p$ we can see, from Lemma A2, that (2.3) is expressed as

$$\hat{B}(X,S) = [I_m + RH(F)R']X, \tag{2.5}$$

where $H(F) = diag(h_1(F), \ldots, h_m(F))$, $diag(F) = R'XS^{-1}X'R$.

It is worth noting that (2.3) becomes

$$\hat{B}(X,S) = \begin{cases} X[I_p + c_1(X'X)^{-1}S + c_2 I_p/\mathrm{tr}\,(X'X)S^{-1}], & \textit{for } m \ge p+2; \\ [I_m + c_1(XS^{-1}X')^{-1} + c_2 I_m/\mathrm{tr}\,(X'X)S^{-1}]X & \textit{for } p \ge m+2, \end{cases}$$

if we put $f(F) = c_1 \log(\prod_k f_k) + c_2 \log(\sum_k f_k)$. This shows that the estimator of the form (2.3) includes the natural estimators.

3. Unbiased estimate of risk

In this section we shall compute the unbiased estimate of the risk of an almost arbitrary equivariant estimator of B. First we start with a notation.

Let

$$T(n,m,p;h) = \sum_{k=1}^{p}\Big\{2(m-p+1)h_k + 4f_k h_{kk} + 4\sum_{l>k}\frac{f_k h_k - f_l h_l}{f_k - f_l} + (n+p-3)f_k h_k^2 - 4f_k^2 h_{kk} h_k - 2\sum_{l>k}\frac{f_k^2 h_k^2 - f_l^2 h_l^2}{f_k - f_l}\Big\},$$

where $h_k = \partial h(F)/\partial l_k$ and $h_{kk} = \partial^2 h(F)/\partial l_k^2$, $k = 1, 2, \ldots, p$.

Now we have the following

Theorem 3.1. *Assume that* $h(F)$ *satisfies the regularity conditions of* Theorem 2.1 *in* Bilodeau and Kariya (1989). *Then the unbiased estimate of the risk of the estimator of the form* (2.3) *is given by*

(i) $$\hat{R}(\hat{B}(X,S); B, \Sigma) = pm + T(n,m,p;h) \qquad \textit{for } m > p+1,$$

and

(ii) $$\hat{R}(\hat{B}(X,S); B, \Sigma) = pm + T(n+m-p,p,m;h) \qquad \textit{for } p > m+1.$$

Proof. (i) From Cor. 2.1 in Bilodeau and Kariya (1989) the unbiased risk estimate for (2.3), equivalently (2.4), can be written as

$$(3.1) \qquad 2\mathrm{tr}\, \nabla_X' X A H(F) A^{-1} + 2\mathrm{tr}\, D_s A'^{-1} F H^2(F) A^{-1} + (n-p-1)\mathrm{tr}\, F H^2(F) + pm,$$

where $D_s = (d_s^{ij})$ is a $p \times p$ differential operator whose element is given by $(1/2)(1+\delta_{ij})\partial/\partial s_{ij}$ for $S = (s_{ij})$ and Kronecker's delta δ_{ij}. We shall compute (3.1) term by term. Noting that $\mathrm{tr}\, \nabla_X' X Q = m\mathrm{tr}\, Q + \mathrm{tr}\, X' \nabla_X Q'$ for a $p \times p$ matrx Q (see Konno (1990)) it can be seen that the first term of (3.1) yields

$$(3.2) \qquad 2m\mathrm{tr}\, H(F) + 2\mathrm{tr}\, X' \nabla_X (A H(F) A^{-1})'.$$

Furthermore, from Lemma A.1 in Appendix, we get that

$$(3.3) \qquad \begin{aligned} \mathrm{tr}\, X' \nabla_X (A H(F) A^{-1})' &= 2\mathrm{tr}\, W D_w (A H(F) A^{-1})' \\ &= 2\mathrm{tr}\, D_w W A H(F) A^{-1} - (p+1)\mathrm{tr}\, H(F), \end{aligned}$$

where $D_w = (d_w^{ij})$ and $d_w^{ij} = (1/2)(1+\delta_{ij})\partial/\partial w_{ij}$ for $W = (w_{ij})$ and a Kronecker's delta δ_{ij}. The last equality of (3.3) holds since $\mathrm{tr}\, D_w Q_1 Q_2 = \mathrm{tr}\,(Q_2 D_w Q_1 + Q_1 D_w Q_2')$ for $p \times p$

matrices Q_1 and Q_2 and $D_W W = ((p+1)/2)I_p$. Combining (3.2) with (3.3) and noting that $W = A'^{-1} diag(F) A^{-1}$ lead to

$$(3.4) \qquad 2\mathrm{tr}\, \nabla_X' AH(F)A^{-1} = 2(m-p-1)\mathrm{tr}\, H(F) + 4\mathrm{tr}\, D_W A'^{-1} diag(F)H(F)A^{-1}.$$

Applying Lemma A.3 in Appendix to the second term of (3.4) gives

$$(3.5) \qquad trD_W A'^{-1} diag(F)H(F)A^{-1} = \sum_{k=1}^{p}\left\{ f_k h_{kk} + h_k + \sum_{l>k} \frac{f_k h_k - f_l h_l}{f_k - f_l} \right\},$$

and similarly we can see that the second term of (3.1) provides

$$(3.6)\ \mathrm{tr}\, D_s A'^{-1} diag(F)H^2(F)A^{-1} = \sum_{k=1}^{p}\left\{ -2f_k h_k h_{kk} + (p-1)f_k h_k^2 - \sum_{l>k} \frac{f_k^2 h_k^2 - f_l^2 h_l^2}{f_k - f_l} \right\}.$$

From (3.4)through (3.5) we obtain the desired result.

(ii) This can be seen from Theorem 2.2 in Konno(1990a).

Remark 3.2. Stein (1973) showed that the unbiased estimate of the risk of the estimator (2.2) is

$$\hat{R} = \sum_{k=1}^{p}\left\{ 2(m-p+1)h_k + 4y_k h_{kk} + 4\sum_{l>k} \frac{y_k h_k - y_l h_l}{y_k - y_l} + y_k h_k^2 \right\} + pm,$$

in the case $\Sigma = I_p$. The notations above are defined similarly in Theorem 3.1.

Now let us compare the distribution of the eigenvalues of $X'XS^{-1}$ in the cases $m > p+1$ and $p > m+1$. Assume that $B = 0$ for simplicity. Then, from Muirhead (1982), it can be seen that the joint density of the ordered eigenvalues of $X'XS^{-1}$ is , apart from normalizing constants,

$$\prod_{k=1}^{p} \frac{f_k^{(m-p-1)/2}}{(1+f_k)^{(n+m)/2}} \prod_{l>k}^{p} (f_k - f_l) \prod_{k=1}^{p} df_k$$

in the case $m > p+1$ while it is

$$\prod_{k=1}^{m} \frac{f_k^{(p-m-1)/2}}{(1+f_k)^{(n+m)/2}} \prod_{l>k}^{m} (f_k - f_l) \prod_{k=1}^{m} df_k$$

in the case $p > m+1$. It is easily checked that the second distribution can be obtained from the first one by making the substitutions

$$(3.7) \qquad m \to p, \qquad p \to m, \qquad n \to n+m-p.$$

Theorem 3.1 tells us that the substitution rule (3.7) is available to the unbiased estimate of risk and the estimator of the form (2.3) so that the estimator better than the usual estimator X in the case $m > p+1$ results in that in the case $p > m+1$ by using substitution rule (3.7).

4. Minimax estimators

First we derive the variational form of Bayes estimator following an approach due to Haff (1982, 1988). We then show minimax theorems of some estimators.

Here we concentrate on the case $m > p+1$. Let $\pi(\Lambda)$ be an orthogonally invariant prior distribution (i.e., $\pi(H\Lambda H') = \pi(\Lambda)$ for any orthogonal matrix H) where $\Lambda = (B'B)^{(1/2)}\Sigma^{-1}(B'B)^{(1/2)}$. Denote by $f(F|\lambda)$ the conditional density of $F = (f_1, \ldots, f_p)'$ given $\lambda = (\lambda_1, \ldots, \lambda_p)'$, λ_k $(k = 1, 2 \ldots, p)$, being the k-th largest eigenvalue of Λ. Finally the marginal density of F is denoted by

$$g_\pi(F) = \int f(F|\lambda)d\pi^*(\lambda),$$

where $\pi^*(\lambda) = \int_H \pi(H\Lambda H')dH$. Following argument in Haff(1982,1988) the Bayes risk of the estimator $\hat{B}(X,S) = X + \nabla_X h(F) \cdot S$ is given by

$$r(\tilde{h}, d\tilde{h}, \pi) = \int \{pm + T(n, m, p; h)\} g_\pi(F)dF,$$

where $\tilde{h} = (h_1, \ldots, h_p)'$, $d\tilde{h} = (h_{11}, \ldots, h_{pp})'$. Since the loss function is convex, the formal Bayes rule is then unique and is obtained by minimizing the functional $r(\tilde{h}, d\tilde{h}, \pi)$. Theorem 2.1 in Haff(1988) tells us that functional $\tilde{h}$ minimizing that functional must satisfy the Euler-Lagrange partial differential equations

$$\frac{\partial T}{\partial h_k} = \frac{\partial}{\partial f_k}\frac{\partial}{\partial h_{kk}}T + \left(\frac{\partial T}{\partial h_{kk}}\right)\left(\frac{\partial}{\partial f_k}\log g_\pi(F)\right), \qquad k = 1, 2, \ldots, p.$$

It is readily checked that the solution of this system is given by

$$h_k = -\left[(m-p-1) + 2\sum_{l \neq k}\frac{f_k}{f_k - f_l} - 2f_k\frac{\partial}{\partial f_k}\log g_\pi(F)\right]$$
$$\Big/\left[f_k\left\{(n+p+1) - 2\sum_{l \neq k}\frac{f_k}{f_k - f_l} + 2f_k\frac{\partial}{\partial f_k}\log g_\pi(F)\right\}\right], \qquad k = 1, 2, \ldots, p.$$

If $g_\pi(F)$ is constant, then the estimator of B becomes

$$\hat{B}(X,S) = X[I_p + AH(F)A^{-1}], \tag{4.1}$$

where A is a $p \times p$ nonsingular matrix such that $A'SA = I_p$ and $A'X'XA = diag(F)$, $H(F) = diag(h_1, \dots, h_p)$, and

$$h_k = -\left[(m-p-1) + 2\sum_{l \neq k} \frac{f_k}{f_k - f_l}\right] \Big/ \left[f_k \left\{n+p+1-2\sum_{l \neq k} \frac{f_k}{f_k - f_l}\right\}\right], \qquad k = 1, 2, \dots, p.$$

This result is parallel to that obtained by Stein (1973) for the case $\Sigma = I_p$. However the estimator derived here appears intractable for the risk computations, so it seems difficult to prove the minimax theorem for (4.1). Instead we shall consider an approximation to the term $\sum_{l \neq k} f_k/(f_k - f_l)$. Note that $\sum_{l \neq 1} f_1/(f_1 - f_l) > p-1$ and $\sum_{l \neq p} f_p/(f_p - f_l) < 0$, so we replace the term by $p-k$ simply. It turn out that $\sum_{k=1}^{p} \sum_{l \neq k} f_k/(f_k - f_l) = \sum_{k=1}^{p}(p-k)$. Furthermore we have the following theorem.

Theorem 4.1. *In the case* $m > p+1$ *the estimator*

$$\hat{B}^{(1)}(X,S) = X[I_p - AH^{(1)}(F)A^{-1}], \tag{4.2}$$

where $H^{(1)}(F) = diag(d_1/f_1, \dots, d_p/f_p)$ *and* $d_1 \geq \cdots \geq d_p$ *are nonnegative constants, is minimax with respect to the loss function* (1.2) *if* $d_k = (m+p-2k-1)/(n-p+2k+1)$, $k = 1, 2, \dots, p$.

Remark 4.2. The estimator (4.2) is better than the crude Efron-Morris estimator $X[I_p - \{(m-p-1)/(n+p+1)\}(X'X)^{-1}S]$.

The next theorem is a generalization of Lin and Tsai's result (1973).

Theorem 4.3. *Assume that* $m > p+1$ *and that* $\gamma_k(t)$ $(k = 1, 2, \dots, p)$ *be functions satisfying*

(i) $$0 \leq \gamma_k(t) \leq 2(m-p-1)/(n+p+1),$$

(ii) $$\gamma_k(t) \text{ is nondecreasing, } k = 1, \cdots p,$$

(iii) $$\gamma_1(t) \geq \gamma_2(t) \geq \cdots \geq \gamma_p(t) \text{ for } \forall t \geq 0.$$

Then the estimator $\hat{B}^{(\gamma)}(X,S) = X[I_p - AH^{(\gamma)}(F)A^{-1}]$, *where* $\gamma = (\gamma_1, \dots, \gamma_p)'$ *and*

$$H^{(\gamma)}(F) = diag(\gamma_1/f_1, \dots, \gamma_p/f_p),$$

is minimax.

Remark 4.4. Using the substitution rule (3.7) and replacing the form of estimator by that of (2.5) in the estimator (4.1) and the theorems 4.1 and 4.3, we can obtain the minimax estimators in the case $p > m + 1$.

Appendix

Here we record the calculus on eigenstructure.

Lemma A.1. *Assume that* $m > p$. *Let* $W = (w_{ij}) = X'X$ *and* $D_W = (d_W^{ij})$ *where* $d_W^{ij} = (1/2)(1 + \delta_{ij})\partial/\partial w_{ij}$ *for a Kronecker's delta* δ_{ij}. *Then*

(i) $$\nabla_X h(F) = 2XD_w h(F),$$

(ii) $$d_W^{ij} f_k = a_{ki} a_{kj},$$

where $A = (a_{ij})$ *is a* $p \times p$ *nonsingular matrix such that* $A'SA = I_p$ *and* $A'X'XA = diag(F)$.

Proof. (i) can be seen from Konno(1990). (ii) can be seen by minor modification of the proof of Prop. 3.1 in Loh(1988).

Lemma A.2. *Assume that* $m \leq p$. *Let* $\tilde{F} = (\tilde{f}_{ij}) = XS^{-1}X'$ *and* $D_{\tilde{F}} = (d_{\tilde{F}}^{ij})$ *where* $d_{\tilde{F}}^{ij} = (1/2)(1 + \delta_{ij})\partial/\partial \tilde{f}_{ij}$. *Then*

(i) $$\nabla_X h(F) = 2(D_{\tilde{F}} h(F))XS^{-1},$$

(ii) $$d_{\tilde{F}}^{ij} f_k = R_k R_k',$$

where R_k *is the eigenvector corresponding to the eigenvalue* f_k *such that* $R = (R_1, \ldots, R_m)$ *and* $XS^{-1}X' = Rdiag(F)R'$.

Proof. See Konno (1990).

Lemma A.3. *Assume that* $\varphi(F) = diag(\varphi_1(F), \varphi_2(F), \ldots, \varphi_p(F))$ *is differentiable on* $\{f_1 > f_2 > \cdots > f_p\}$. *Then we have*

(i) $$\operatorname{tr} D_w A'^{-1} \varphi(F) A^{-1} = \sum_{k=1}^{p} \left\{ \varphi_{kk} + \sum_{l>k} \frac{\varphi_k - \varphi_l}{f_k - f_l} \right\},$$

and

(ii) $$\operatorname{tr} D_s A'^{-1}\varphi(F)A^{-1} = \sum_{k=1}^{p}\left\{p\varphi_k - f_k\varphi_{kk} - \sum_{l>k}\frac{f_k\varphi_k - f_l\varphi_l}{f_k - f_l}\right\},$$

where $\varphi_{kk} = \partial\varphi_k(F)/\partial f_k$, $k = 1, 2, \ldots, p$.

Proof. It follows from trivial modification of the proof of Lemma 3.1 (p. 59) in Loh (1988).

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