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EMPIRICAL BAYES ESTIMATORS OF NORMAL COVARIANCE MATRIX

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SUMMARY. Let \mathbf{S} follow a Wishart distribution, with n degrees of freedom and parameter $\mathbf{\Sigma}$. Haff (1979b, 1980) has proposed estimators of $\mathbf{\Sigma}$ which dominate the best multiples of \mathbf{S} under certain loss functions. We consider some other loss functions, show that these estimators are empirical Bayes and compare one of them with the best multiples of \mathbf{S} .

1. INTRODUCTION

Let \mathbf{S} be a $p \times p$ random matrix following a Wishart distribution with its probability density proportional to

$$|\mathbf{S}|^{\frac{n-p-1}{2}} e^{-\frac{1}{2} \text{tr} \mathbf{\Sigma}^{-1} \mathbf{S}} \quad \dots \quad (1.1)$$

We are interested in the estimation of $\mathbf{\Sigma}$ under the loss functions

$$L_1(\mathbf{\Sigma}, \hat{\mathbf{\Sigma}}) = \text{tr}(\hat{\mathbf{\Sigma}} \mathbf{\Sigma}^{-1} - \mathbf{I})^2,$$

$$L_2(\mathbf{\Sigma}, \hat{\mathbf{\Sigma}}) = \frac{\text{tr}(\hat{\mathbf{\Sigma}} - \mathbf{\Sigma})^2 \mathbf{S}^{-1}}{\text{tr} \mathbf{\Sigma}},$$

and

$$L_3(\mathbf{\Sigma}, \hat{\mathbf{\Sigma}}) = \frac{\text{tr}(\hat{\mathbf{\Sigma}} - \mathbf{\Sigma})^2 \mathbf{\Sigma}^{-1}}{\text{tr} \mathbf{\Sigma}}.$$

The loss function L_1 was first used by Selliah (1964) and is essentially “squared error”, L_2 is analogous to one considered by Efron and Morris (1976) for estimating $\mathbf{\Sigma}^{-1}$ and L_3 is similar to the loss function in Haff (1979a, 1981). Whereas following Selliah (1964), loss function L_1 has received the attention of many authors, for example Haff (1980), Sharma (1980), Sugiura and Fujimoto (1982), L_2 and L_3 have probably not appeared in the literature earlier. It is well known that $\mathbf{S}/(n+p+1)$ is the best multiple of \mathbf{S} under L_1 . Various better estimators have been obtained; Selliah (1964) showed that the best lower triangular equivariant estimator is such an estimator while Haff (1980) proved this property for an estimator of the form

$$a\mathbf{S} + b(\text{tr} \mathbf{S}^{-1})^{-1} \mathbf{I} \quad \dots \quad (1.2)$$

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In fact, Haff proved that the estimator (1.2) is better than the best multiple aS also under Stein's loss function

$$L_4(\mathbf{\Sigma}, \hat{\mathbf{\Sigma}}) = \text{tr } \hat{\mathbf{\Sigma}} \mathbf{\Sigma}^{-1} - \log \det. \hat{\mathbf{\Sigma}} \mathbf{\Sigma}^{-1} - p$$

if $b \leq 2(p-1)/n^2$. Haff gave an empirical Bayes interpretation to the estimator. We point out in Section 2 that the estimator under the loss functions L_2 and L_3 also could be viewed as empirical Bayes and compare it with the best multiples of S in Section 3. In Section 2, we also show that Haff's (1979b) estimator $a\mathbf{S} + b|\mathbf{S}|^{1/p} \mathbf{I}$, which dominates the best multiple aS under the loss function $\sum_{i \leq j} (\hat{\sigma}_{ij} - \sigma_{ij})^2 q_{ij}$, where $\hat{\mathbf{\Sigma}} = (\hat{\sigma}_{ij})$ and $q_{ij} > 0$, is empirical Bayes under the loss functions L_1, L_2 and L_3 .

2. HAFF'S ESTIMATORS AS EMPIRICAL BAYES ESTIMATORS

We need the following result due to Eaton (1970) to exhibit the empirical Bayes nature of Haff's (1979b, 1980) estimators.

Let $(\mathcal{X}, \mathcal{B}, \mathcal{P})$ be a probability space with $P \in \mathcal{P} = \{P_\theta : \theta \in \Theta\}$, a family of probability distributions. Consider a mapping $g : \Theta \rightarrow (\mathcal{A}, (\cdot, \cdot))$, where $(\mathcal{A}, (\cdot, \cdot))$ is a finite dimensional inner product space with (\cdot, \cdot) the inner product. Let π be a prior distribution on Θ and the problem be one of estimating $g(\theta)$ with a loss function

$$L(\theta, a) = (g(\theta) - a, \tau(\theta)(g(\theta) - a))$$

where $a \in \mathcal{A}$ is the action and $\tau(\theta)$ is a positive definite linear transformation, for each $\theta \in \Theta$, from \mathcal{A} into \mathcal{A} . Then the Bayes estimator and the Bayes risk are given by

Lemma 2.1 (Eaton, 1970) : *The Bayes estimator $\hat{a}(X)$ of $g(\theta)$ is*

$$[E_{\theta|X} \tau(\theta)]^{-1} E_{\theta|X} (\tau(\theta)g(\theta))$$

with its Bayes risk equal to

$$E_\theta(g(\theta), \tau(\theta)g(\theta)) - E_X(E_{\theta|X} \tau(\theta)g(\theta), \hat{a}(X)),$$

where E_X, E_θ , and $E_{\theta|X}$ denote the expectations with respect to the marginal distribution of X , the prior distribution of θ and the posterior distribution of θ respectively.

Designate the distribution assumption (1.1) by $\mathbf{S} \sim W_p(\mathbf{\Sigma}, n)$. Assume that $\mathbf{\Sigma}^{-1} = \mathbf{A}$ (say) $\sim W_p(\mathbf{I}/c, k)$. Then $\mathbf{A} | S \sim W_p((\mathbf{S} + c\mathbf{I})^{-1}, m)$, where

$m = n + k$. Define an inner product on the vector space of all the $p \times p$ matrices as $(C, D) = \text{tr } CD'$ then, L_1 can be written as

$$L_1(\Sigma, \hat{\Sigma}) = (\hat{\Sigma} - \Sigma, \tau(\Sigma)(\hat{\Sigma} - \Sigma)),$$

where $\tau(\Sigma) = \Sigma^{-1} \otimes \Sigma^{-1}$. Here \otimes stands for the Kronecker product, that is, for $p \times p$ matrices C, D and H ,

$$(C \otimes D)H = CHD'. \tag{2.2}$$

The definition (2.2) is equivalent to

$$C \otimes D = \begin{pmatrix} d_{11}C & \dots & d_{1p}C \\ \vdots & & \vdots \\ d_{p1}C & \dots & d_{pp}C \end{pmatrix} \tag{2.3}$$

with the understanding that in carrying out the operation $(C \otimes D)H$ when $C \otimes D$ is defined by (2.3), the $p \times p$ matrix H is rearranged as a p^2 -dimensional column vector with the original $(i + 1)$ -th column of H put below its i -th column.

Clearly, $\tau(\Sigma)$ is linear and is positive definite with respect to the inner product (2.1). Thus, for the loss L_1 , from Lemma 2.1, the Bayes estimator is

$$[E_{A|S} A \otimes A]^{-1} E_{A|S} (A \otimes A)A^{-1} = [E_{A|S} A \otimes A]^{-1} E_{A|S} A. \tag{2.4}$$

To evaluate (2.4), let $M = (S + cI)^{-1}$, $M^{1/2}$ a symmetric matrix satisfying $(M^{1/2})^2 = M$; and $B = M^{-1/2}AM^{-1/2}$. Then $B|S \sim W_p(I, m)$ and

$$\begin{aligned} E_{A|S} (A \otimes A) &= E_{B|S} [(M^{1/2}BM^{1/2}) \otimes (M^{1/2}BM^{1/2})] \\ &= E_{B|S} [(M^{1/2} \otimes M^{1/2})(B \otimes B)(M^{1/2} \otimes M^{1/2})] \\ &= (M^{1/2} \otimes M^{1/2}) E_{B|S} (B \otimes B) (M^{1/2} \otimes M^{1/2}). \end{aligned}$$

Now, for any orthogonal R ;

$$\begin{aligned} E_{B|S} (B \otimes B) &= E_{B|S} [(RBR') \otimes (RBR')] \\ &= (R \otimes R) [E_{B|S} (B \otimes B)] (R' \otimes R')I. \end{aligned}$$

Hence,

$$\begin{aligned} [E_{B|S} (B \otimes B)]^{-1} I &= N \text{ (say)} \\ &= (R \otimes R) [E_{B|S} (B \otimes B)]^{-1} (R' \otimes R')I \\ &= RNR'. \end{aligned}$$

Choosing R to be a diagonal matrix with the diagonal elements 1 or -1 , it can be easily seen that $N = \alpha_m I$ for some real α_m . Thus,

$$[E_{B|S} (B \otimes B)]^{-1} I = \alpha_m I. \tag{2.5}$$

To calculate α_m , we use the (2.3) definition of \otimes , let \mathbf{I} in (2.5) be a p^2 -dimensional vector and rewrite (2.5) as

$$\alpha_m [E_{\mathbf{B}|\mathbf{S}}(\mathbf{B} \otimes \mathbf{B})] = \mathbf{I}. \quad \dots (2.6)$$

Equating the first components of the p^2 -dimensional vectors on the two sides of the relation (2.6), we get

$$\alpha_m(m^2 + 2m) + \alpha_m(p-1)m = 1$$

so that $\alpha_m = (m^2 + m(p+1))^{-1}$. Hence the Bayes estimator is

$$(\mathbf{S} + c\mathbf{I}) / (m + p + 1).$$

Similarly, L_3 can be written as

$$L_3(\mathbf{\Sigma}, \hat{\mathbf{\Sigma}}) = \left(\hat{\mathbf{\Sigma}} - \mathbf{\Sigma}, \frac{1}{\text{tr } \mathbf{\Sigma}} \mathbf{\Sigma}^{-1} (\hat{\mathbf{\Sigma}} - \mathbf{\Sigma}) \right)$$

so that $\tau(\mathbf{\Sigma}) = \mathbf{\Sigma}^{-1} / \text{tr } \mathbf{\Sigma}$ is positive definite and linear. Now, for large n , $\tau(\mathbf{\Sigma})$ is close to $n\mathbf{\Sigma}^{-1} / \text{tr } S$ and so using Lemma 2.1, the Bayes estimator is approximated by

$$\left[E_{\mathbf{\Sigma}|\mathbf{S}} \frac{\mathbf{\Sigma}^{-1}}{\text{tr } S} \right]^{-1} E_{\mathbf{\Sigma}|\mathbf{S}} \left(\frac{\mathbf{\Sigma}^{-1}}{\text{tr } S} \mathbf{\Sigma} \right) = [E_{\mathbf{\Sigma}|\mathbf{S}} \mathbf{\Sigma}^{-1}]^{-1} = \frac{\mathbf{S} + c\mathbf{I}}{m}. \quad \dots (2.7)$$

As $L_2(\mathbf{\Sigma}, \hat{\mathbf{\Sigma}}) / n$, for large n , is close to $L_3(\mathbf{\Sigma}, \hat{\mathbf{\Sigma}})$, an approximate Bayes estimator for L_2 also is $(S + cI) / m$.

Whether we consider the Bayes estimator $(\mathbf{S} + c\mathbf{I}) / (m + p + 1)$ under L_1 , or the approximate Bayes estimator $(\mathbf{S} + c\mathbf{I}) / m$ under L_2 and L_3 , the main idea is to estimate c and arrive at an estimator of $\mathbf{\Sigma}$ which is better than the best multiple of S in the frequency sense.

From the fact that the marginal density of \mathbf{S} is proportional to

$$|\mathbf{S}|^{n-p-1/2} c^{pk/2} / |\mathbf{S} + c\mathbf{I}|^{m/2}. \quad \dots (2.8)$$

Haff (1980) has proved that $g(\mathbf{S}) \propto (\text{tr } \mathbf{S}^{-1})^{-1}$ is a generalized maximum likelihood estimator of c and so the estimator (1.2) with an appropriate a can be described as empirical Bayes under L_i ($i = 1, 2, 3$).

From (2.8), we also notice that $E|\mathbf{S}|^{\beta/2} \propto c^{\beta p/2}$. Take $\beta = 2/p$, then $E|\mathbf{S}|^{1/p} \propto c$. Substituting the estimator of c in the Bayes or approximate Bayes estimator of $\mathbf{\Sigma}$ obtained above, Haff's (1979b) estimator $a\mathbf{S} + b|\mathbf{S}|^{1/p}\mathbf{I}$ also can be seen to be empirical Bayes under L_i ($i = 1, 2, 3$).

The results in the next section concern the estimator (1.2). We shall use the notation R_i for the risk under the loss function L_i .

3. THE ESTIMATORS $a\mathbf{S} + b(\text{tr } \mathbf{S}^{-1})^{-1}\mathbf{I}$

We first state Haff's (1979b) identity which we need for proving the dominance results in this section.

For any $p \times p$ matrix $\mathbf{M} = (m_{ij}(\mathbf{S}))$ of the $p \times p$ matrix \mathbf{S} , define $\mathbf{M}_{(c)} = (m'_{ij})$ where

$$m'_{ij} = \begin{cases} m_{ij} & \text{for } i = j \\ cm_{ij} & \text{for } i \neq j, \end{cases}$$

and $\mathbf{D}^*\mathbf{M} = \Sigma \Sigma \partial m_{ij} / \partial s_{ij}$. Suppose now $\mathbf{S} \sim W_p(\Sigma, n)$, $h(\mathbf{S})$ is real-valued and $\mathbf{T} = T(\mathbf{S})$ is a $p \times p$ matrix then

$$E[h(\mathbf{S}) \text{tr } \mathbf{T} \Sigma^{-1}] = 2Eh(\mathbf{S})\mathbf{D}^*\mathbf{T}_{(1/2)} + 2E \text{tr} \left[\frac{\partial h(\mathbf{S})}{\partial \mathbf{S}} \mathbf{T}_{(1/2)} \right] + (n-p-1)E[h(\mathbf{S}) \text{tr } \mathbf{S}^{-1}\mathbf{T}]. \quad \dots (3.1)$$

For the validity of (3.1), the reader is referred to Haff (1979b).

Next, we show that the best choice of a among estimators $a\mathbf{S}$ is n^{-1} under L_2 .

Theorem 3.1 : For the loss function L_2 , the best multiple of \mathbf{S} is \mathbf{S}/n . It is also the best unbiased estimator of Σ .

Proof : The risk of $a\mathbf{S}$ is

$$R_2(\Sigma, a\mathbf{S}) = E \text{tr}(a\mathbf{S} - \Sigma)^2 \mathbf{S}^{-1} / \text{tr } \Sigma = a^2n - 2a + (n-p-1)^{-1}$$

and it has minimum value $(p+1)n^{-1}(n-p-1)^{-1}$ at $a = n^{-1}$. The completeness of \mathbf{S} and the convexity of the loss function (see, for example, the proof for L_1 in Sharma (1980)) imply that \mathbf{S}/n is the best unbiased estimator of Σ .

The following theorem shows that it is possible to choose b such that $a\mathbf{S} + b(\text{tr } \mathbf{S}^{-1})^{-1}\mathbf{I}$ is better than $a\mathbf{S}$ under L_2 .

Theorem 3.2 : Let $\hat{\Sigma}_2$ be given by (1.2) with

$$a < (n-p+1)^{-1}, \quad 0 < b \leq 2p[(n-p+1)^{-1} - a]. \quad \dots (3.2)$$

Then $R_2(\Sigma, \hat{\Sigma}_2) < R_2(\Sigma, a\mathbf{S})$ for all Σ .

Proof : Let $R_2(\Sigma, \hat{\Sigma}_2) - R_2(\Sigma, a\mathbf{S}) = \alpha_2(\Sigma)$, where

$$\alpha_2(\Sigma) = \frac{b}{\text{tr } \Sigma} E \left[\frac{b \text{tr } \mathbf{S}^{-1}}{(\text{tr } \mathbf{S}^{-1})^2} + \frac{2ap}{\text{tr } \mathbf{S}^{-1}} - 2 \frac{\text{tr } \mathbf{S}^{-1}\Sigma}{\text{tr } \mathbf{S}^{-1}} \right].$$

Now $\alpha_2(\Sigma) < 0$ if

$$(b + 2ap)E(\text{tr } S^{-1})^{-1} - 2E(\text{tr } S^{-1}\Sigma/\text{tr } S^{-1}) < 0. \quad \dots \quad (3.3)$$

However, (3.3) is true as proved below.

Using Haff's identity (3.1),

$$\begin{aligned} E(\text{tr } S^{-1})^{-1} &= \frac{2}{p} E(\text{tr } S^{-1})^{-2} \text{tr}(S^{-2} \Sigma_{(1/2)}) + \frac{n-p-1}{p} E \frac{\text{tr } S^{-1}\Sigma}{\text{tr } S^{-1}} \\ &= \frac{2}{p} E \frac{\text{tr } S^{-2}\Sigma}{(\text{tr } S^{-1})^2} + \frac{n-p-1}{p} E \frac{\text{tr } S^{-1}\Sigma}{\text{tr } S^{-1}}. \quad \dots \quad (3.4) \end{aligned}$$

Hence, $\text{tr } S^{-2}\Sigma \leq \text{tr } S^{-1}\Sigma \text{tr } S^{-1}$ implies that

$$E(\text{tr } S^{-1})^{-1} < \frac{n-p+1}{p} E \frac{\text{tr } S^{-1}\Sigma}{\text{tr } S^{-1}}$$

so that $\alpha_2(\Sigma) < 0$ if

$$(b + 2ap)(n-p+1)/p - 2 \leq 0, \quad b > 0,$$

which is true from (3.2).

Under Stein's loss function L_4 also S/n is the best multiple of S . Haff (Theorem 4.3, 1980) has given estimators better than S/n under L_4 . His result can be combined with Theorem 3.1 to obtain estimators of Σ which are better than S/n both under L_2 and Stein's loss function.

Corollary 3.1: Let $\hat{\Sigma}_{2,4}$ be the estimator $S/n + b(\text{tr } S^{-1})^{-1}I$ with $0 < b \leq 2(p-1)/n^2$. Then, for all Σ , $R_2(\Sigma, \hat{\Sigma}_{2,4}) < R_2(\Sigma, S/n)$ and $R_4(\Sigma, \hat{\Sigma}_{2,4}) < R_4(\Sigma, S/n)$.

Theorems similar to 3.1 and 3.2, for the loss function L_3 are given below.

Theorem 3.3: For the loss function L_3 , the best multiple of S is $S/(n+p+1)$.

Proof: $R_3(\Sigma, aS) = a^2 E \text{tr } S^2 \Sigma^{-1} + \text{tr } \Sigma - 2a E \text{tr } S / \text{tr } \Sigma$. Since, from the identity (3.1) or otherwise, $ES^2 = n(n+1)\Sigma^2 + n\Sigma \text{tr } \Sigma$, we have $R_3(\Sigma, aS) = a^2 n(n+p+1) - 2an + 1$, which is minimized at $a = (n+p+1)^{-1}$.

Theorem 3.4: Let $\hat{\Sigma}_3$ be the estimator (1.2) with

$$a < p/(np+2), \quad 0 < b \leq 2[p - a(np+2)]/(n-p+3). \quad \dots \quad (3.5)$$

Then $R_3(\Sigma, \hat{\Sigma}_3) < R_3(\Sigma, aS)$ for all Σ .

Proof: Let $R_3(\Sigma, \hat{\Sigma}_3) - R_3(\Sigma, aS) = \alpha_3(\Sigma)$,

where
$$\alpha_3(\Sigma) = \frac{b}{\text{tr } \Sigma} E \left[\frac{b \text{tr } \Sigma^{-1}}{(\text{tr } S^{-1})^2} + \frac{2a \text{tr } S \Sigma^{-1}}{\text{tr } S^{-1}} - \frac{2p}{\text{tr } S^{-1}} \right]$$

Now, from (3.1),

$$E \frac{\text{tr } \Sigma^{-1}}{(\text{tr } \mathbf{S}^{-1})^2} = \frac{4E \text{tr}(\mathbf{S}^{-2})_{(2)}}{(\text{tr } \mathbf{S}^{-1})^3} + (n-p-1)E \frac{\text{tr } \mathbf{S}^{-1}}{(\text{tr } \mathbf{S}^{-1})^2} \leq (n-p+3)E(\text{tr } \mathbf{S}^{-1})^{-1} \dots \quad (3.6)$$

and

$$E \frac{\text{tr } \mathbf{S} \Sigma^{-1}}{\text{tr } \mathbf{S}^{-1}} = p(p+1)E(\text{tr } \mathbf{S}^{-1})^{-1} + 2E \frac{\text{tr}(\mathbf{S}^{-2})_{(2)} \mathbf{S}_{(1/2)}}{(\text{tr } \mathbf{S}^{-1})^2} + (n-p-1)pE(\text{tr } \mathbf{S}^{-1})^{-1} = (np+2)E(\text{tr } \mathbf{S}^{-1})^{-1}. \dots \quad (3.7)$$

From (3.6) and (3.7), it can be seen that $\alpha_3(\Sigma) < 0$ if

$$b(n-p+3) + 2a(np+2) - 2p \leq 0, \quad b > 0,$$

which is true from (3.5).

Theorem 3.2 and 3.4 can be combined to get the following corollary.

Corollary 3.2 : Let $\hat{\Sigma}_{2,3}$ be the estimator (1.2) with

$$a \leq (n+1)^{-1}, \quad 0 < b \leq \min \left\{ \frac{2[p-a(np+2)]}{n-p+3}, \frac{2p[1-a(n-p+1)]}{n-p+1} \right\},$$

then, for all Σ ,

$$R_2(\Sigma, \hat{\Sigma}_{2,3}) < R_2(\Sigma, a\mathbf{S}) \quad \text{and} \quad R_3(\Sigma, \hat{\Sigma}_{2,3}) < R_3(\Sigma, a\mathbf{S}).$$

Recall that $\mathbf{S}/(n+p+1)$ is the best multiple of \mathbf{S} under Selliah's loss function L_1 also. Combining Theorem 3.4 and Haff's (1980) Theorem 4.5, we get estimators better than $\mathbf{S}/(n+p+1)$ both under L_3 and Selliah's loss function. This is stated as Corollary 3.3 below.

Corollary 3.3 : Let $\hat{\Sigma}_{1,3}$ be the estimator $\mathbf{S}/(n+p+1) + b(\text{tr } \mathbf{S}^{-1})^{-1}I$, with $0 < b \leq 2(p-1)(n-p+3)^{-1}(n+p+1)^{-1}$, then for all Σ ,

$$R_1(\Sigma, \hat{\Sigma}_{1,3}) < R_1(\Sigma, \mathbf{S}/(n+p+1)) \quad \text{and} \quad R_3(\Sigma, \hat{\Sigma}_{1,3}) < R_3(\Sigma, \mathbf{S}/(n+p+1)).$$

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