

## 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

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

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

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

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

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  $aS + b|S|^{1/p} \mathbf{I}$ , which dominates the best multiple  $aS$  under the loss function  $\sum_{i \leq j} (\hat{\sigma}_{ij} - \sigma_{ij})^2 q_{ij}$ , where  $\hat{\Sigma} = (\hat{\sigma}_{ij})$  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  $\pi$  be a prior distribution on  $\Theta$  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  $E_X$ ,  $E_\theta$ , and  $E_{\theta|X}$  denote the expectations with respect to the marginal distribution of  $X$ , the prior distribution of  $\theta$  and the posterior distribution of  $\theta$  respectively.

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

$$(C \otimes D)H = CHD'. \quad \dots (2.2)$$

The definition (2.2) is equivalent to

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

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

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

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  $\alpha_m$ . Thus,

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

To calculate  $\alpha_m$ , 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

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

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  $E|\mathbf{S}|^{1/2} \propto c$ . Substituting the estimator of  $c$  in the Bayes or approximate Bayes estimator of  $\mathbf{\Sigma}$  obtained above, Haff's (1979b) estimator  $a\mathbf{S} + b|\mathbf{S}|^{1/2}\mathbf{I}$  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  $\mathbf{D}^*\mathbf{M} = \sum \sum \partial m_{ij} / \partial s_{ij}$ . Suppose now  $\mathbf{S} \sim W_p(\boldsymbol{\Sigma}, n)$ ,  $h(\mathbf{S})$  is real-valued and  $\mathbf{T} = T(\mathbf{S})$  is a  $p \times p$  matrix then

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

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  $\boldsymbol{\Sigma}$ .

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

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

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  $\boldsymbol{\Sigma}$ .

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

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

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

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

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

However, (3.3) is true as proved below.

Using Haff's identity (3.1),

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

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  $\Sigma$  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  $\Sigma$ ,  $R_2(\Sigma, \hat{\Sigma}_{2,4}) < R_2(\Sigma, S/n)$  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,  $E S^2 = n(n+1)\Sigma^2 + n\Sigma \text{tr } \Sigma$ , 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

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

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

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),

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

and

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

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  $\Sigma$ ,

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

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  $\Sigma$ ,

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

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