Estimation of a high-dimensional covariance matrix with the Stein loss

Hisayuki Tsukuma*

June 3, 2015

Abstract

The problem of estimating a normal covariance matrix is considered from a decision-theoretic point of view, where the dimension of the covariance matrix is larger than the sample size. This paper addresses not only the nonsingular case but also the singular case in terms of the covariance matrix. Based on James and Stein’s minimax estimator and on an orthogonally invariant estimator, some classes of estimators are unifiedly defined for any possible ordering on the dimension, the sample size and the rank of the covariance matrix. Unified dominance results on such classes are provided under a Stein-type entropy loss. The unified dominance results are applied to improving on an empirical Bayes estimator of a high-dimensional covariance matrix.

AMS 2010 subject classifications: Primary 62H12; secondary 62C12.

Key words and phrases: Empirical Bayes method, inadmissibility, Moore-Penrose pseudo-inverse, pseudo Wishart distribution, singular multivariate normal distribution, singular Wishart distribution, statistical decision theory.

*Faculty of Medicine, Toho University, 5-21-16 Omori-nishi, Ota-ku, Tokyo 143-8540, Japan, E-Mail: tsukuma@med.toho-u.ac.jp
1 Introduction

This paper addresses the problem of a normal covariance matrix relative to the Stein loss, where the dimension of the covariance is larger than the sample size. This problem is precisely formulated as follows: Let \( \mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_n \) be independently and identically distributed as \( \mathcal{N}_p(0_p, \Sigma) \). Assume that \( p > n \) and \( \Sigma \) is a \( p \times p \) positive definite matrix of unknown parameters. Denote \( S = \sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i^t \). Then \( S \) is distributed as

\[ S \sim \mathcal{W}_p(n, \Sigma). \quad (1.1) \]

In the \( p > n \) case, Srivastava and Khatri (1979, page 72) and Díaz-García et al. (1997) called \( \mathcal{W}_p(n, \Sigma) \) the pseudo Wishart distribution with \( n \) degrees of freedom and mean \( n \Sigma \). We here consider the problem of estimating \( \Sigma \) relative to the Stein loss

\[ L_p(\delta, \Sigma) = \text{tr} \Sigma^{-1} \delta - \log \det(\Sigma^{-1} \delta) - p, \quad (1.2) \]

where \( \delta \) stands for an estimator of \( \Sigma \). Assume that, with probability one, \( \delta \) is an positive definite matrix based on \( S \). The accuracy of estimators is measured by the risk function \( R_p(\delta, \Sigma) = E[L_p(\delta, \Sigma)] \), where the expectation is taken with respect to the model (1.1).

If \( n \geq p \), then the Wishart matrix \( S \) has the same rank \( p \) as the covariance matrix \( \Sigma \) with probability one. In such case, many decision-theoretic studies have been done for the problem of estimating \( \Sigma \) in the literature. James and Stein (1961) first discussed decision-theoretic estimation of \( \Sigma \). They considered the LU decomposition of \( S \) and succeeded to derive a minimax estimator of \( \Sigma \) relative to the Stein loss (1.2). The James and Stein (1961) minimax estimator, however, depends on the coordinate system. The dependence results in inadmissibility of their minimax estimator. Typical improved estimators on James and Stein’s minimax estimator are orthogonally invariant estimators, which are not influenced by the coordinate system. The orthogonally invariant estimators have been proposed by Stein (1975, 1977). See also Dey and Srinivasan (1985), who gave other dominance results via orthogonally invariant estimators.

In the \( p > n \) case, Kubokawa and Srivastava (2008) and Konno (2009) studied decision-theoretic covariance estimation relative to quadratic losses.
However, an analytical dominance result in the $p > n$ case with the Stein loss \((1.2)\) has not been obtained as yet.

This paper gives some dominance results relative to the Stein loss \((1.2)\) in the $p > n$ case and extends the dominance results to the case where $\Sigma$ is singular. To this end, Section 2 starts with uniformly considering the estimation problem for any possible ordering on $n$, $p$ and the rank of $\Sigma$. The singular case does not allow us to use the Stein loss \((1.2)\) because the inverse of the singular $\Sigma$ does not exist. Therefore Section 2 defines a Stein-like loss function for estimation of the singular $\Sigma$. We give a unified expression of the James and Stein type estimator for all possible orderings on $n$, $p$ and the rank of $\Sigma$. Section 2 also provides a unified expression of orthogonally invariant estimators improving on the James and Stein type estimator relative to the Stein-like loss.

Section 3 mainly discusses the $p > n$ case for estimation of a nonsingular $\Sigma$ relative to the usual Stein loss \((1.2)\). An empirical Bayes estimator is derived from an inverse Wishart prior. Some improving methods on the empirical Bayes estimator are established by using the dominance results obtained in Section 2. The Monte Carlo simulations show that an improved estimator performs well when $p$ is much larger than $n$. Moreover alternative estimators are uniformly constructed for both nonsingular and singular cases in terms of $\Sigma$. In Section 4 we give some remarks on our results of this paper and related topics.

## 2 Unified dominance results on covariance estimation

### 2.1 Preliminaries

First, we describe the problem of estimating a covariance matrix uniformly in the nonsingular and the singular cases.

Assume that the $p \times n$ observation matrix $X$ has the form

$$X = BZ,$$

where $B$ is a $p \times r$ matrix of unknown parameters with $p \geq r$ and $Z$ is an $r \times n$ random matrix. Assume that $B$ is of full column rank, namely $r$, \(3\).
and $r$ is known. Let all the columns of $Z$ be independently and identically distributed as $N_r(0_r, I_r)$. Then the columns of $X$ are i.i.d. sample from $N_p(0_p, \Sigma)$, where $\Sigma = BB^t$ is a positive semi-definite matrix of rank $r$. Denote

$$S = XX^t,$$

which follows $W_p(n, \Sigma)$. In the case where $r < p$, $N_p(0_p, \Sigma)$ and $W_p(n, \Sigma)$ represent, respectively, the singular multivariate normal and the singular Wishart distributions. For the definition of the singular distributions, see Srivastava and Khatri (1979, pages 43 and 72) and also Díaz-García et al. (1997). Note also that $\Sigma$ is of rank $r$, while $S$ is of rank $\min(n, r)$ with probability one.

In this section, we handle only estimators which are positive semi-definite matrices of rank

$$q = \min(n, r)$$

with probability one. Write such estimators as $\delta_q$. Moreover, $\delta_q$ are also assumed to satisfy the condition that the rank of $\Sigma^+\delta_q$ is $q$ with probability one, where $\Sigma^+$ is the Moore-Penrose pseudo-inverse of $\Sigma$. Since $\delta_q$ and $\Sigma^+$ are positive semi-definite, the $q$ nonzero eigenvalues of $\Sigma^+\delta_q$ are positive. Note that $\text{tr} \, \Sigma^+\delta_q$ is equal to a sum of all the positive eigenvalues of $\Sigma^+\delta_q$. Both nonsingular and singular cases of the Stein loss $L_q(\delta_q, \Sigma)$ are uniformly defined as

$$L_q(\delta_q, \Sigma) = \text{tr} \, \Sigma^+\delta_q - \log \pi(\Sigma^+\delta_q) - q,$$

(2.2)

where $\pi(\Sigma^+\delta_q)$ stands for a product of all the positive eigenvalues of $\Sigma^+\delta_q$. Then we consider the problem of estimating $\Sigma$ relative to the Stein loss $(2.2)$. The corresponding risk function is denoted by

$$R_q(\delta_q, \Sigma) = E[L_q(\delta_q, \Sigma)],$$

(2.3)

where the expectation is taken with respect to the model $(2.1)$.

Next, we define some notation. Let $O(r)$ be the group of orthogonal matrices of order $r$. For $p \geq r$, the Stiefel manifold is denoted by $V_{p,r} = \{A \in \mathbb{R}^{p \times r} : A^tA = I_r\}$. It is noted that $V_{r,r} = O(r)$. Let $D_r$ be a set of $r \times r$ diagonal matrices whose diagonal elements $d_1, \ldots, d_r$ satisfy $d_1 > \cdots > d_r > 0$. Denote by $T^+_q$ the group of lower triangular matrices with positive diagonal elements.
The Stein loss (2.2) depends on the Moore-Penrose pseudo-inverse of $\Sigma$. Here some properties are listed for the Moore-Penrose pseudo-inverse. The proof of the following lemma is given in Harville (1997, Chapter 20).

**Lemma 2.1** Let $B$ be a $p \times r$ matrix of full column rank. Then the Moore-Penrose pseudo-inverse $B^+$ of $B$ uniquely exists and has the following properties:

1. $B^+ = (B^t B)^{-1} B^t$;
2. $H^+ = H^t$ for $H \in V_{p,r}$;
3. $B^+ = B^{-1}$ for a nonsingular matrix $B$;
4. $(B^+)^t = (B^t)^+$;
5. $(BC^t)^+ = (C^t)^+ B^+$ for a $q \times r$ matrix $C$ of full column rank.

### 2.2 Constant multiple estimators

Consider a simple class of estimators whose forms are a constant multiple of $S$. The simple class is represented by

$$\delta_C^q(a) = aS,$$  \hspace{1cm} (2.4)

where $a$ is a positive constant and $q = \min(n,r)$. This class includes the unbiased estimator of $\Sigma$,

$$\delta_{UB}^q = \frac{1}{n}S.$$

However $\delta_{UB}^q$ is not the best estimator among the class (2.4) relative to the Stein loss (2.2). Note by Lemma 2.1 that $\Sigma^+ = (BB^t)^+ = (B^t)^+B^+$ and

$$\Sigma^+ S = (B^t)^+B^+B Z Z^t B^t = (B^t)^+Z Z^t B^t,$$

which implies that $\Sigma^+ \delta_C^q(a)$ has the same rank as $Z Z^t$.

**Proposition 2.1** Define $m = \max(n,r)$ and

$$a_m = \frac{1}{m}.$$

Then $\delta_{BC}^q = \delta_C^q(a_m)$ is the best estimator among the class (2.4) relative to the Stein loss (2.2). Hence for $r > n$, $\delta_{BC}^q$ dominates $\delta_{UB}^q$ relative to the Stein loss 2.2.
Proof. The nonzero eigenvalues of $\Sigma^+ S$ are identical to those of $B^+ S (B^t)^+$, so that the nonzero eigenvalues of $\Sigma^+ S$ are identical to those of the full-rank matrix
\[
\begin{cases} 
ZZ^t & \text{for } n \geq r, \\
Z^t Z & \text{for } n < r.
\end{cases}
\]
Since the number of nonzero eigenvalues of $\Sigma^+ S$ is $q = \min(n, r)$ with probability one, we obtain $\pi(a\Sigma^+ S) = a^q \pi(ZZ^t)$, so that the risk of $\delta_C^q(a)$ with respect to the Stein loss (2.2) is expressed as
\[
R_q(\delta_C^q(a), \Sigma) = n a \text{tr} \Sigma^+ \Sigma - q \log a - E[\log \pi(ZZ^t)] - q
\]
\[
= nr a - q \log a - E[\log \pi(ZZ^t)] - q.
\]
The risk of $\delta_C^q(a)$ is minimized by $\delta_C^q(a_m)$ with
\[
a_m = \frac{q}{nr} = \frac{1}{m}.
\]
Thus the proof is complete. ■

It follows from equation (82) of James and Stein (1961) that
\[
E[\log \pi(ZZ^t)] = \sum_{i=1}^q E[\log s_i],
\]  
(2.5)
where $s_i \sim \chi_{m-i+1}^2$. Hence $\delta_B^C$ has the constant risk
\[
R_q(\delta_B^C, \Sigma) = q \log m - \sum_{i=1}^q E[\log s_i].
\]  
(2.6)

2.3 The James and Stein type estimator

We next construct a James and Stein (1961) like estimator of $\Sigma$ for any possible ordering on $n$, $p$ and $r$.

Using the same arguments as in Srivastava (2003, equation (2.2)), we can write the $p \times n$ random matrix $X$ as a block matrix
\[
\begin{pmatrix} X_{11} & X_{12} \\
X_{21} & X_{22} \end{pmatrix},
\]
where \( X_{11} \) is a \( q \times q \) nonsingular matrix. Recall that \( X = BZ \). Partition \( B \) and \( Z \) into block matrices as, respectively,

\[
B = \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}, \quad Z = (Z_1, Z_2),
\]

where \( B_1 \) and \( Z_1 \) are, respectively, \( q \times r \) and \( r \times q \) matrices. Note that \( X_{11} = B_1 Z_1 \). Since \( X_{11} \) is nonsingular, \( B_1 \) has a full row rank. Thus, there exist unique elements \( \Theta \in T_q^+ \) and \( \Gamma_1 \in V_{r,q} \) such that \( B_1 = \Theta \Gamma_1^t \). The decomposition \( B_1 = \Theta \Gamma_1^t \) represents the QR decomposition of \( B_1 \). For the uniqueness of the QR decomposition, see Harville (1997, page 67).

Take \( \Gamma_2 \in V_{r,r-q} \) such that \( \Gamma = (\Gamma_1, \Gamma_2) \in O(r) \). For \( r \leq n \), the LQ decomposition of \( \Gamma^t Z \) can be written as \( YV^t \), where \( Y \in T_r^+ \) and \( V \in V_{n,r} \). For \( r > n \), \( \Gamma^t Z \) is denoted by the block matrix

\[
\Gamma^t Z = \begin{pmatrix} Z_1 \\ Z_2 \end{pmatrix},
\]

where \( Z_1 \) and \( Z_2 \) are, respectively, \( n \times n \) and \( (r - n) \times n \) matrices. The LQ decomposition of \( Z_1 \) can be written as \( Y_1 V^t \) for \( Y_1 \in T_n^+ \) and \( V \in O(n) \), which gives that

\[
\Gamma^t Z = \begin{pmatrix} Y_1 \\ Z_2 V \end{pmatrix} V^t = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix} V^t,
\]

where \( Y_2 = Z_2 V \). Hence \( \Gamma^t Z \) can uniquely and unifiedly be expressed as

\[
\Gamma^t Z = Y V^t \quad \text{for} \quad V \in V_{n,q} \quad \text{and} \quad Y = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}, \quad (2.7)
\]

where \( Y_1 \in T_q^+ \) and \( Y_2 \) is a \( (r - q) \times q \) matrix.

Let \( C = B \Gamma \), which is written as

\[
C = \begin{pmatrix} \Theta \Gamma_1^t \\ B_2 \end{pmatrix} (\Gamma_1, \Gamma_2) = \begin{pmatrix} \Theta & 0_{q \times (r-q)} \\ B_2 \Gamma_1 & B_2 \Gamma_2 \end{pmatrix}. \quad (2.8)
\]

Combining (2.7) and (2.8), we can uniquely decompose \( X \) as

\[
X = B \Gamma \Gamma^t Z = TV^t, \quad (2.9)
\]
where

\[ T = CY = \begin{pmatrix} \Theta Y_1 \\ B_2 \Gamma_1 Y_1 + B_2 \Gamma_2 Y_2 \end{pmatrix}. \]

It is then noted that \( \Theta Y_1 \in T_q^+ \).

The probability distributions of nonzero elements of \( Y \) are given as follows.

**Lemma 2.2** For \( i = 1, \ldots, q \) and \( j = i, \ldots, r \), denote by \( y_{j,i} \) the \((j,i)\)-th element of \( Y \). Then all the elements \( y_{j,i} \)’s are mutually independent and

\[ y_{i,i}^2 \sim \chi^2_{n-r+1}, \quad y_{j,i} \sim N(0,1) \quad (i = 1, \ldots, q, j = i + 1, \ldots, r). \]

**Proof.** It is noted that \( \Gamma^t Z \sim N_{r \times n}(0_{r \times n}, I_r \otimes I_n) \). For the \( n \geq r \) and \( n < r \) cases, see Lemma 3.2.1 of Srivastava and Khatri (1979) and Corollary 3.1 of Srivastava (2003), respectively. \( \square \)

Applying (2.9) to the Wishart matrix \( S = XX^t \) gives that

\[ XX^t = TT^t = \begin{pmatrix} T_1^t \\ T_2^t \end{pmatrix}, \]

where \( T = (T_1^t, T_2^t)^t \) is \( p \times q \) matrix such that \( T_1 = \Theta Y_1 \in T_q^+ \) and \( T_2 \) is a \((p-q) \times q\) matrix. Then we consider the class of estimators, which has the form

\[ \delta_q^T = TD_q T^t, \tag{2.10} \]

where \( D_q = \text{diag}(d_1, \ldots, d_q) \) and the \( d_i \)’s are positive constants.

**Proposition 2.2** Let \( D_q^{JS} = \text{diag}(d_1^{JS}, \ldots, d_q^{JS}) \), where \( d_i^{JS} = (n + r - 2i + 1)^{-1} \) for \( i = 1, \ldots, q \). Then the best estimator among the class (2.10) relative to the loss (2.2) is given by \( \delta_q^{JS} = TD_q^{JS} T^t \), which dominates \( \delta_q^{BC} \).

**Proof.** Noting from Lemma 2.1 that

\[ C^t \Sigma^+ C = \Gamma^t B^t (BB^t)^+ B \Gamma = \Gamma^t B^t B^+ B \Gamma = I_r, \]

we observe

\[ E[\text{tr} \Sigma^+ \delta_q^T] = E[\text{tr} D_q T^t \Sigma^+ T] = E[\text{tr} D_q Y^t C^t \Sigma^+ CY] = E[\text{tr} D_q Y^t Y]. \tag{2.11} \]
In the $p \geq r > n$ case, we partition $Y$ as $Y = (Y_1^t, Y_2^t)^t$, where $Y_1 \in T_n^+$. From Lemma 2.2, it follows that $E[Y_2^t Y_2] = (r - n)I_n$ and $E[Y_1^t Y_1]$ is the diagonal matrix of order $n$ with the $i$-th diagonal element

$$E[y_{j,i}^2] = (n - i + 1) + (n - i) = 2n - 2i + 1.$$ 

Thus we obtain

$$E[tr D_n Y^t Y] = E[tr D_n Y_1^t Y_1 + tr D_n Y_2^t Y_2] = \sum_{i=1}^{n} (n + r - 2i + 1)d_i. \quad (2.12)$$

When $n \geq r$, it follows that

$$E[tr D_r Y^t Y] = \sum_{i=1}^{r} \sum_{j=i}^{r} E[d_i y_{j,i}^2] = \sum_{i=1}^{r} (n + r - 2i + 1)d_i. \quad (2.13)$$

Combining (2.11), (2.12) and (2.13) gives that

$$E[tr \Sigma^+ \delta_q^T] = \sum_{i=1}^{q} (n + r - 2i + 1)d_i. \quad (2.14)$$

It is seen that $\Sigma^+ \delta_q^T$ has the same nonzero eigenvalues as $D_q T^t \Sigma^+ T$, which implies that

$$\pi(\Sigma^+ \delta_q^T) = \pi(D_q T^t \Sigma^+ T) = \pi(D_q Y^t Y)$$

Since $Y^t Y$ is a $q \times q$ square matrix of full rank, it follows that

$$\pi(\Sigma^+ \delta_q^T) = det(D_q Y^t Y) = det(D_q) det(Y^t Y) = det(D_q) \pi(ZZ^t). \quad (2.15)$$

Using (2.14) and (2.15), we can write the risk of $\delta_q^T$ under the loss (2.2) as

$$R_q(\delta_q^T, \Sigma) = \sum_{i=1}^{q} \{(n + r - 2i + 1)d_i - \log d_i\} - E[\log \pi(ZZ^t)] - q.$$

Hence the $d_i$'s minimizing the risk are given by $d_i^{JS} = (n + r - 2i + 1)^{-1}$ for $i = 1, \ldots, q$. 

9
Since $\delta_{q}^{BC}$ belongs to the class $\{2.10\}$, $\delta_{q}^{JS}$ dominates $\delta_{q}^{BC}$ relative to the Stein loss $\{2.2\}$. In fact, $\delta_{q}^{JS}$ has the constant risk

$$R_{q}(\delta_{q}^{JS}, \Sigma) = \sum_{i=1}^{q} \log(n + r - 2i + 1) - E[\log(\pi(ZZ^t))],$$

(2.16)

which implies by (2.5) and (2.6) that

$$R_{q}(\delta_{q}^{JS}, \Sigma) - R_{q}(\delta_{q}^{BC}, \Sigma) = \sum_{i=1}^{q} \log(n + r - 2i + 1) - q \log m < 0,$$

where the inequality follows from concavity of the logarithmic function. Thus the proof is complete.

The probability density function of $T$ can be derived explicitly. The $n \geq p = r$ case is obtained from, for example, Srivastava and Khatri (1979, Lemma 3.2.2). For the $p > r$ case, see Srivastava (2003, Theorem 5.2) and Díaz-García and González-Farías (2005, Corollary 4).

### 2.4 Orthogonally invariant estimators

Make the QR decomposition of $B$ into $\Upsilon B_{0}^{t}$, where $\Upsilon \in V_{p,r}$ and $B_{0} \in \mathcal{T}_{r}$. We can uniquely express $S$ as $S = \Upsilon B_{0}^{t}ZZ^{t}B_{0}^{t}\Upsilon^{t}$. Define $W = B_{0}^{t}ZZ^{t}B_{0}$, which is distributed as $\mathcal{W}_{q}(n, \Omega)$ with $\Omega = B_{0}^{t}B_{0}$, where $\Omega$ is positive definite. The eigenvalue decomposition of $W$ is written as $RLR^{t}$, where $L \in \mathbb{D}_{q}, R \in V_{r,q}$ and $q = \min(n, r)$. Hence we can decompose $S$ as

$$S = HLH^{t},$$

where $L \in \mathbb{D}_{q}$ and $H = \Upsilon R \in V_{p,q}$.

Consider the class of estimators

$$\delta_{q}^{O} = \delta_{q}^{O}(S) = H\Phi(L)H^{t},$$

where $\Phi(L) = \text{diag}(\phi_{1}(L), \ldots, \phi_{q}(L))$ and the $\phi_{i}(L)$’s are absolutely continuous functions of $L$. The class $\delta_{q}^{O}$ is orthogonally invariant in the sense that it satisfies $\delta_{q}^{O}(S)O^{t} = \delta_{q}^{O}(OSO^{t})$ for any $O \in \mathcal{O}(p)$.

To evaluate the risk of $\delta_{q}^{O}$, we require the following lemma.
Lemma 2.3  Abbreviate $\phi_i(L)$ by $\phi_i$. Denote $L = \text{diag}(\ell_1, \ldots, \ell_q)$. Then we have

$$E[\text{tr} \Sigma^+ H \Phi(L) H^t] = E\left[\sum_{i=1}^{q} \left\{ (|n-r|-1) \frac{\phi_i}{\ell_i} + 2 \frac{\partial \phi_i}{\partial \ell_i} + 2 \sum_{j>i}^{q} \frac{\phi_i - \phi_j}{\ell_i - \ell_j} \right\} \right].$$

Proof. It follows from Lemma 2.1 that

$$\Sigma^+ = (\Upsilon \Omega \Upsilon^t)^+ = (\Omega \Upsilon^t)^+ \Omega^+ \Upsilon^t = \Upsilon \Omega^{-1} \Upsilon^t,$$

so that

$$E[\text{tr} \Sigma^+ H \Phi(L) H^t] = E[\text{tr} \Omega^{-1} R \Phi(L) R^t]. \quad (2.17)$$

Recall that $W \sim \mathcal{W}_r(n, \Omega)$ and the eigenvalue decomposition of $W$ is denoted by $RLR^t$. The remainder of the proof for $n \geq r$ is based on the same arguments as in Sheena (1995, Section 2) and, for $n < r$, on those as in Kubokawa and Srivastava (2008, Lemma A.1). Their results are applied to the r.h.s. of (2.17), so we get this lemma.

Lemma 2.4  The risk of $\delta_q^O$ under the loss (2.2) is written as

$$R(\delta_q^O, \Sigma) = E\left[\sum_{i=1}^{q} \left\{ (|n-r|-1) \frac{\phi_i}{\ell_i} + 2 \frac{\partial \phi_i}{\partial \ell_i} + 2 \sum_{j>i}^{q} \frac{\phi_i - \phi_j}{\ell_i - \ell_j} - \log \frac{\phi_i}{\ell_i} \right\} \right] - E[\log (Z^t)] - q.$$

Proof. Note that

$$\pi(\Sigma^+ \delta_q^O) = \pi(Z^t) \det(L^{-1} \Phi(L)). \quad (2.18)$$

Using (2.18) and Lemma 2.3 gives the risk expression of this lemma.

The following proposition results from Lemma 2.4.

Proposition 2.3  Define

$$\delta_q^{ST} = HLD_q H^t.$$  

Then $\delta_q^{ST}$ dominates $\delta_q^{JS}$ relative to the Stein loss (2.2).
Proof. We can prove this proposition in the same way as in Dey and Srinivasan (1985, Theorem 3.1). Using Lemma 2.4 and (2.16), we can write the difference in risk of $\delta^{ST}_q$ and $\delta^{JS}_q$ as

$$R_q(\delta^{ST}_q, \Sigma) - R_q(\delta^{JS}_q, \Sigma) = E[\hat{\Delta}^{ST}]$$

where

$$\hat{\Delta}^{ST} = \sum_{i=1}^{q} \left\{ (|n-r|+1)d^IS_i + 2 \sum_{j>i}^{q} \frac{d^IS_i \ell_i - d^JS_j \ell_j}{\ell_i - \ell_j} \right\} - q.$$

Hence if $\hat{\Delta}^{ST} \leq 0$, then $\delta^{ST}_q$ dominates $\delta^{JS}_q$. It is observed that

$$\sum_{i=1}^{q} \sum_{j>i}^{q} \frac{d^IS_i \ell_i - d^JS_j \ell_j}{\ell_i - \ell_j} = \sum_{i=1}^{q} \sum_{j>i}^{q} \frac{d^IS_i (\ell_i - \ell_j) + (d^IS_i - d^JS_j) \ell_j}{\ell_i - \ell_j}$$

$$< \sum_{i=1}^{q} \sum_{j>i}^{q} d^JS_i = \sum_{i=1}^{q} (q-i)d^JS_i,$$

where the inequality is verified by the ordering properties $\ell_1 > \cdots > \ell_q$ and $d^IS_1 < \cdots < d^JS_q$. Thus we obtain

$$\hat{\Delta}^{ST} < \sum_{i=1}^{q} (|n-r|+1+2q-2i)d^IS_i - q = \sum_{i=1}^{q} (n+r-2i+1)d^IS_i - q = 0,$$

which completes the proof. \[\square\]

Besides $\delta^{ST}_q$ given above, many types of orthogonally invariant estimators are proposed for the $n \geq p = r$ case. See, for example, Stein (1977), Dey and Srinivasan (1985), Haff (1991), Perron (1992), Sheena and Takehara (1992) and Yang and Berger (1994). Their results would be applicable to the cases when $\min(n,p) \geq r$ and $p \geq r > n$.

3 Estimation of a high-dimensional covariance matrix

3.1 An empirical Bayes estimator

We here deal with the problem of estimating $\Sigma$ in the model (1.1) relative to the usual Stein loss (1.2). Note that the covariance matrix $\Sigma$ is of rank $p$,
while the Wishart matrix $S$ is of rank $n$. Using an empirical Bayes method, we first provide a full-rank estimator as a target which should be improved.

Denote $X = (X_1, \ldots, X_n)$, where the $X_i$’s are i.i.d. sample from $\mathcal{N}_p(0_p, \Sigma)$. Note that $X$ is a $p \times n$ matrix and $S = XX^t$. Then the likelihood of $\Sigma$ is proportional to

$$L(\Sigma|X) \propto (\det \Sigma)^{-n/2} \exp \left( -\frac{1}{2} \text{tr} \Sigma^{-1}XX^t \right).$$

Assume that $\Sigma$ has a prior density $p(\Sigma|\lambda) \propto (\det \Sigma)^{-((k+p+1)/2)} \exp \left( -\frac{\lambda}{2} \text{tr} \Sigma^{-1} \right), \ \lambda > 0.$

The resulting Bayes estimator $\delta_{Bayes}^p$ is written as

$$\delta_{Bayes}^p = \frac{1}{n+k}(XX^t + \lambda I_p) = \frac{1}{n+k}(S + \lambda I_p). \quad (3.1)$$

Here we estimate $\lambda$ from the marginal density of $X$,

$$p(X|\lambda) = K\lambda^{kp/2}\{\det(XX^t + \lambda I_p)\}^{-(n+k)/2}$$

$$= K\lambda^{kp/2}\{\det(X^tX + \lambda I_n)\}^{-(n+k)/2},$$

where $K$ is a normalizing constant. Since $\det(XX^t + \lambda I_n) = \prod_{j=1}^n(\ell_j + \lambda)$, where the $\ell_j$’s are eigenvalues of $X^tX$, the logarithm of the marginal density $p(X|\lambda)$ is given by

$$\log p(X|\lambda) = \frac{kp}{2} \log \lambda - \frac{n+k}{2} \sum_{j=1}^n \log(\ell_j + \lambda) + \log K,$$

which is used to obtain

$$\frac{\partial}{\partial \lambda} \log p(X|\lambda) = \frac{kp}{2} \lambda^{-1} - \frac{n+k}{2} \sum_{j=1}^n \frac{1}{\ell_j + \lambda} = 0,$$

namely, the maximum likelihood estimator of $\lambda$ is a solution of

$$\sum_{j=1}^n \frac{\lambda}{\ell_j + \lambda} = \frac{kp}{n+k}.$$
Denote by \( \hat{\lambda}^{ML} \) the resulting maximum likelihood estimator of \( \lambda \). Substitute \( \hat{\lambda}^{ML} \) for \( \lambda \) in (3.1), we get the empirical Bayes estimator
\[
\delta_p^B = \frac{1}{n + k} (S + \hat{\lambda}^{ML} I_p).
\] (3.2)

Motivated by (3.2) and taking account of Proposition 2.1, we define the class of estimators as
\[
\delta_{EB}^B(b) = a_p(S + \hat{\lambda}_b I_p),
\] (3.3)
where \( a_p = p^{-1} \), \( b = b(S) \) is a differentiable bounded function of \( S \), and \( \hat{\lambda}_b (\geq 0) \) satisfies
\[
\sum_{j=1}^n \hat{\lambda}_b \ell_j \geq n \hat{\lambda}_b.
\] (3.4)

For existence of a unique solution \( \hat{\lambda}_b \), \( b \) requires at least that \( 0 \leq b < n \). Note also that \( \delta_p^{EB}(b) \) is of full-rank with probability one.

To compare risk functions, we need the lower and the upper bounds of \( \hat{\lambda}_b \). Note from Lemma 2.1 that
\[
\sum_{i=1}^n \ell_i^{-1} = \text{tr} (X^t X)^{-1} = \text{tr} (X X^t)^{-2} X^t = \text{tr} (XX^t)^+ = \text{tr} S^+.
\]

Also, note that \( \sum_{j=1}^n \ell_j = \text{tr} S \).

**Lemma 3.1** The lower and the upper bounds of \( \hat{\lambda}_b \) are given as follows.
\[
\frac{b}{n - b} \cdot \frac{n}{\text{tr} S^+} \leq \hat{\lambda}_b \leq \frac{b}{n - b} \cdot \frac{\text{tr} S}{n}.
\]

When \( b < 1 \), it particularly holds that \( \hat{\lambda}_b \leq b/\{(1 - b) \text{tr} S^+\} \).

**Proof.** Let \( f(x|c) = c/(x + c) \) for a positive constant \( c \). Since \( f(x|c) \) is convex in \( x \) for \( x \geq 0 \), it is observed that
\[
b = \sum_{j=1}^n f(\ell_j|\hat{\lambda}_b) \geq nf\left(\frac{1}{n} \sum_{j=1}^n \ell_j \bigg| \hat{\lambda}_b \right) = \frac{n^2 \hat{\lambda}_b}{\text{tr} S + n \hat{\lambda}_b},
\]
which gives the upper bound of $\hat{\lambda}_b$. Next, let $g(x) = x/(1 + x)$ for $x \geq 0$. The concavity of $g(x)$ leads to

$$b = \sum_{j=1}^{n} \frac{\hat{\lambda}_b \ell_j^{-1}}{1 + \hat{\lambda}_b \ell_j^{-1}} \leq \sum_{j=1}^{n} g(\hat{\lambda}_b \ell_j^{-1}) \leq n g\left(\frac{1}{n} \sum_{j=1}^{n} \hat{\lambda}_b \ell_j^{-1}\right) = \frac{n \hat{\lambda}_b \text{tr } S^+}{n + \hat{\lambda}_b \text{tr } S^+},$$

which gives the lower bound of $\hat{\lambda}_b$.

When $b < 1$, we can see that

$$b = \sum_{j=1}^{n} \frac{\hat{\lambda}_b \ell_j^{-1}}{1 + \hat{\lambda}_b \ell_j^{-1}} \geq \sum_{j=1}^{n} \frac{\hat{\lambda}_b \ell_j^{-1}}{1 + \hat{\lambda}_b \sum_{j=1}^{n} \ell_j^{-1}} = \frac{\hat{\lambda}_b \text{tr } S^+}{1 + \hat{\lambda}_b \text{tr } S^+},$$

which yields that $\hat{\lambda}_b \leq b/\{(1 - b) \text{tr } S^+\}$.

The finiteness of the risk of $\delta_{pEB}^B(b)$ is verified in the following lemma.

**Lemma 3.2** Assume that there exist positive constants $B_1$ and $B_2$ such that $B_1 \leq b \leq B_2 < n$. If $p - n - 1 > 0$, then the risk of $\delta_{pEB}^B(b)$ is finite.

**Proof.** A simple calculation yields that

$$R_p(\delta_{pEB}^B(b), \Sigma) = E\left[a_p \hat{\lambda}_b \text{tr } \Sigma^{-1} - \sum_{i=1}^{n} \log(\ell_i + \hat{\lambda}_b) - (p - n) \log \hat{\lambda}_b\right]$$

$$+ npa_p - p \log a_p + \log \det \Sigma - p.$$

From the given assumption, there exist positive constants $C_1$ and $C_2$ such that $C_1/n \leq b/(n - b) \leq n C_2$. Using Lemma 3.1 we observe that

$$\log C_1 - \log \text{tr } S^+ \leq \log \hat{\lambda}_b \leq \log C_2 + \log \text{tr } S.$$

The well-known inequalities $1 - x^{-1} \leq \log x \leq x - 1$ for $x > 0$ imply that $E[\log \hat{\lambda}_b]$ is finite if $E[\text{tr } S^+] < \infty$. Under the same condition, we can verify the finiteness of $E[\hat{\lambda}_b]$ and $E[\sum_{i=1}^{n} \log(\ell_i + \hat{\lambda}_b)]$.

Note that $E[\text{tr } S^+] = E[\text{tr } (X^t X)^{-1}] = E[\text{tr } (Z^t \Sigma Z)^{-1}]$, where $Z \sim \mathcal{N}_{p \times n}(0_{p \times n}, I_p \otimes I_n)$, so that

$$0 < E[\text{tr } S^+] < E[\text{tr } (Z^t Z)^{-1}] \text{tr } \Sigma^{-1}.$$

Note also that $Z^t Z \sim \mathcal{W}_n(p, I_n)$. Thus for $p - n - 1 > 0$, it follows that $E[\text{tr } (Z^t Z)^{-1}] = n(p - n - 1)^{-1}$, which completes the proof. ■
3.2 Dominance results

In the case that \( p = r > n \), define the eigenvalue decomposition of \( S \) as \( S = H LH^t \) with \( H \in V_{p,n} \) and \( L = \text{diag}(\ell_1, \ldots, \ell_n) \in \mathbb{D}_n \). Take \( H_0 \) as a \( p \times (p - n) \) matrix such that \((H, H_0) \in O(p)\). Consider here the following shrinkage estimator

\[
\delta_p^{SH}(b) = \delta_p^{EB}(b) - a_p \hat{\lambda}_b H H^t = a_p (S + \hat{\lambda}_b H_0 H_0^t),
\]

where \( \hat{\lambda}_b \) and \( b \) are defined in (3.3). The rank of \( \delta_p^{SH}(b) \) is \( p \) with probability one. If \( p - n - 1 > 0 \), the risk of \( \delta_p^{SH}(b) \) is finite, which is verified in the same way as Lemma 3.2. The following proposition can be obtained for domination of \( \delta_p^{SH}(b) \) over \( \delta_p^{EB}(b) \).

**Proposition 3.1** In the model (1.1), we consider the problem of estimating \( \Sigma \) relative to the usual Stein loss (1.2). Assume that there exists a positive constant \( C \) such that \( b \leq C < n \). Let \( c_0 = 6(n + 1)/(3p - 4n - 4) \) for \( 3p - 4n - 4 > 0 \). If \( b \geq c_0 n / (1 + c_0) \) and \( \sum_{i=1}^{n} \partial b / \partial \ell_i \geq 0 \), then \( \delta_p^{SH}(b) \) dominates \( \delta_p^{EB}(b) \) relative to the usual Stein loss (1.2).

The proof of Proposition 3.1 requires suitable bounds of the logarithmic function \( \log(1 + x) \). Here we employ an upper and a lower bounds of \( \log(1 + x) \) based on the Padé approximants. For details of the Padé approximants, see Baker and Graves-Morris (1996). The approximants yield the following simple lemma, whose proof is omitted since it can easily be verified.

**Lemma 3.3** For \( x \geq 0 \), it follows that

\[
\frac{2x}{2 + x} \leq \log(1 + x) \leq \frac{x(6 + x)}{2(3 + 2x)}.
\]

The upper and the lower bounds given above are concave in \( x \).

**Proof of Proposition 3.1.** Note that

\[
\delta_p^{SH}(b) = a_p \{H LH^t + H_0(\hat{\lambda}_b I_{p-n})H_0^t\}
\]

and also

\[
\delta_p^{EB}(b) = a_p \{H (L + \hat{\lambda}_b I_n) H^t + H_0(\hat{\lambda}_b I_{p-n})H_0^t\}.
\]
The difference in risk of $\delta_p^{SH}(b)$ and $\delta_p^{EB}(b)$ is written by

$$
R_p(\delta_p^{SH}(b), \Sigma) - R_p(\delta_p^{EB}(b), \Sigma) = E[-a_p\hat{\lambda}_b \text{tr} \Sigma^{-1} HH^t - \log \det L + \log \det (L + \hat{\lambda}_b I_n)]
$$

$$
= E[-a_p\hat{\lambda}_b \text{tr} \Sigma^{-1} HH^t + \sum_{i=1}^{n} \log(1 + \hat{\lambda}_b \ell_i^{-1})]. \quad (3.5)
$$

Using Lemma 2.3 gives that $R_p(\delta_p^{SH}(b), \Sigma) - R_p(\delta_p^{EB}(b), \Sigma) = E[\hat{\Delta}^{SH}]$, where

$$
\hat{\Delta}^{SH} = \sum_{i=1}^{n} \{ -a_p(p - n - 1)\hat{\lambda}_b \ell_i^{-1} - 2a_p \frac{\partial \hat{\lambda}_b}{\partial \ell_i} + \log(1 + \hat{\lambda}_b \ell_i^{-1}) \}. \quad (3.6)
$$

Thus, if $\hat{\Delta}^{SH} \leq 0$, then $\delta_p^{SH}(b)$ dominates $\delta_p^{EB}(b)$.

Differentiating both sides of (3.4) with respect to $\ell_i$ yields that

$$
\left( \frac{\partial \hat{\lambda}_b}{\partial \ell_i} \right) \sum_{j=1}^{n} \frac{1}{\ell_j + \hat{\lambda}_b} - \frac{\hat{\lambda}_b}{(\ell_i + \hat{\lambda}_b)^2} - \left( \frac{\partial \hat{\lambda}_b}{\partial \ell_i} \right) \sum_{j=1}^{n} \frac{\hat{\lambda}_b}{(\ell_j + \hat{\lambda}_b)^2} = \frac{\partial b}{\partial \ell_i},
$$

so that

$$
\sum_{i=1}^{n} \frac{\partial \hat{\lambda}_b}{\partial \ell_i} = \frac{\sum_{i=1}^{n} \hat{\lambda}_b(\ell_i + \hat{\lambda}_b)^{-2} + \sum_{i=1}^{n} \frac{\partial b}{\partial \ell_i}}{\sum_{i=1}^{n} \ell_i(\ell_i + \hat{\lambda}_b)^{-2}} \geq 0. \quad (3.7)
$$

Let $f(x) = x(6 + x)/(6 + 4x)$. Using Lemma 3.3 we observe that

$$
\sum_{i=1}^{n} \log(1 + \hat{\lambda}_b \ell_i^{-1}) \leq \sum_{i=1}^{n} f(\hat{\lambda}_b \ell_i^{-1})
$$

$$
\leq nf\left( \frac{1}{n} \sum_{i=1}^{n} \hat{\lambda}_b \ell_i^{-1} \right) = \frac{\hat{\lambda}_b \text{tr} S^+ (6n + \hat{\lambda}_b \text{tr} S^+)}{6n + 4\hat{\lambda}_b \text{tr} S^+}, \quad (3.8)
$$

where the second inequality follows from concavity of $f(x)$. Combining (3.5), (3.6) and (3.8) gives that

$$
\hat{\Delta}^{SH} \leq -a_p(p - n - 1)\hat{\lambda}_b \text{tr} S^+ + \frac{\hat{\lambda}_b \text{tr} S^+ (6n + \hat{\lambda}_b \text{tr} S^+)}{6n + 4\hat{\lambda}_b \text{tr} S^+}
$$

$$
= a_p\hat{\lambda}_b \text{tr} S^+ \times \frac{6n(n+1) - (3p - 4n - 4)\hat{\lambda}_b \text{tr} S^+}{6n + 4\hat{\lambda}_b \text{tr} S^+}. \quad (3.9)
$$
Using the lower bound of $\hat{\lambda}_b$ given in Lemma 3.1, we can see that $\hat{\Delta}^SH \leq 0$ if $3p - 4n - 4 > 0$ and
\[
6n(n + 1) - (3p - 4n - 4)\frac{bn}{n - b} \leq 0,
\]
namely $b \geq c_0n/(1 + c_0)$. Hence the proof is complete.

We give two examples for $b$. First, $b$ is restricted to a positive constant. The estimator $\delta_p^{SH}(b)$ can be written as
\[
\delta_p^{SH}(b) = \delta_n^{BC} + a_p\hat{\lambda}_bH_0H'_0,
\]
where $\delta_n^{BC}$ is given by (2.4). The risk of $\delta_p^{SH}(b)$ can alternatively be expressed as
\[
R_p(\delta_p^{SH}(b), \Sigma) = R_n(\delta_n^{BC}, \Sigma) + R_{p-n}(a_p\hat{\lambda}_bH_0H'_0, \Sigma),
\]
where $R_n$ and $R_{p-n}$ are defined in (2.3). It is much hard to find out an optimal constant for $b$. Furthermore, the performance of $\delta_p^{SH}(b)$ would worsen if $b$ is too large. So we take
\[
b_0 = \frac{c_0n}{1 + c_0}. \tag{3.10}
\]
The resulting estimator $\delta_p^{SH}(b_0)$ dominates $\delta_p^{EB}(b_0)$ when $3p - 4n - 4 > 0$.

Next, consider
\[
b_1 = b_1(S) = (1 + \ell_n/\ell_1)b_0. \tag{3.11}
\]
Note that $\ell_1 \geq \ell_n$, so $b_1$ is bounded below and above as $b_0 \leq b_1 \leq 2b_0$. Also, it is observed that
\[
\sum_{i=1}^n \frac{\partial b_1}{\partial \ell_i} = b_0\ell_1^{-2}(\ell_1 - \ell_n) \geq 0.
\]
Hence it is seen from Proposition 3.1 that $\delta_p^{SH}(b_1)$ dominates $\delta_p^{EB}(b_1)$ relative to the usual Stein loss (1.2) for $3p - 4n - 4 > 0$.

The risk expression (3.9) suggests further modified estimators
\[
\delta_p^{mJS}(b) = \delta_n^{JS} + a_p\hat{\lambda}_bH_0H'_0,
\]
and
\[
\delta_p^{mST}(b) = \delta_n^{ST} + a_p\hat{\lambda}_bH_0H'_0, \tag{3.12}
\]
where $\delta_n^{JS}$ and $\delta_n^{ST}$ are defined in Subsections 2.3 and 2.4, respectively. Then the following proposition can be proved in the same way as in Subsections 2.3 and 2.4.
Proposition 3.2 In the model (1.1), we consider the problem of estimating $\Sigma$ relative to the usual Stein loss (1.2). Under the assumptions of Proposition 3.1, $\delta_p^{SH}(b)$ is dominated by $\delta_p^{mJS}(b)$, and moreover $\delta_p^{mJS}(b)$ is dominated by $\delta_p^{mST}(b)$.

Proposition 3.1 suggests that $\delta_p^{SH}(b)$ dominates $\delta_p^{EB}(b)$ if they depend on a common large $b$. For a small $b$, it seems to hold the reverse dominance relation. In fact, we obtain the following proposition.

Proposition 3.3 In the model (1.1), we consider the problem of estimating $\Sigma$ relative to the usual Stein loss (1.2). Assume that $n \geq 2$ and $p - n - 1 > 0$. Let $c_* = 2(n - 1)/(p - n + 1)$ and

$$b_* = c_*/(1 + c_*). \quad (3.13)$$

If $C_0 \leq b \leq b_*$ for a positive constant $C_0$ and $\sum_{i=1}^{n} \partial b/\partial \ell_i \leq 0$, then $\delta_p^{EB}(b)$ dominates $\delta_p^{SH}(b)$ relative to the usual Stein loss (1.2).

Proof. In the similar way to (3.7), it is seen that

$$\sum_{i=1}^{n} \frac{\partial \hat{\lambda}_b}{\partial \ell_i} \leq \sum_{i=1}^{n} \frac{\hat{\lambda}_b (\ell_i + \hat{\lambda}_b)^{-2}}{\ell_i (\ell_i + \hat{\lambda}_b)^{-2}} = \sum_{i=1}^{n} \frac{\hat{\lambda}_b}{\ell_i} \times \frac{\ell_i (\ell_i + \hat{\lambda}_b)^{-2}}{\sum_{j=1}^{n} \ell_j (\ell_j + \hat{\lambda}_b)^{-2}} \leq \hat{\lambda}_b \text{tr} S^+. \quad (3.14)$$

It follows from Lemma 3.3 that

$$\sum_{i=1}^{n} \log(1 + \hat{\lambda}_b \ell_i^{-1}) \geq \sum_{i=1}^{n} \frac{2\hat{\lambda}_b \ell_i^{-1}}{2 + \hat{\lambda}_b \ell_i^{-1}} \geq \sum_{i=1}^{n} \frac{2\hat{\lambda}_b \ell_i^{-1}}{2 + \hat{\lambda}_b \sum_{j=1}^{n} \ell_j^{-1}} = \frac{2\hat{\lambda}_b \text{tr} S^+}{2 + \hat{\lambda}_b \text{tr} S^+}. \quad (3.15)$$

Combining (3.6), (3.14) and (3.15) gives that

$$\hat{\Delta}^{SH} \geq -a_p (p - n - 1) \hat{\lambda}_b \text{tr} S^+ - 2a_p \hat{\lambda}_b \text{tr} S^+ + \frac{2\hat{\lambda}_b \text{tr} S^+}{2 + \hat{\lambda}_b \text{tr} S^+} = a_p \hat{\lambda}_b \text{tr} S^+ \times \frac{2(n - 1) - (p - n + 1) \hat{\lambda}_b \text{tr} S^+}{2 + \hat{\lambda}_b \text{tr} S^+}.$$
If $b \leq b_*$ ($< 1$), using the upper bound of Lemma 3.1 for $b < 1$ leads to

$$2(n - 1) - (p - n + 1)\hat{\lambda}_b \text{tr} S^+ \geq 2(n - 1) - (p - n + 1)\frac{b}{1 - b} \geq 2(n - 1) - (p - n + 1)\frac{b_*}{1 - b_*} = 0,$$

which implies that $\hat{\Delta}^{SH} \geq 0$. Thus the proof is complete.

Assume that $b$ is a small constant satisfying $b \leq b_*$. The estimator $\delta_p^E(b)$ is expressed as

$$\delta_p^E(b) = a_p(S + \hat{\lambda}_b I_p) = a_p(H(L + \hat{\lambda}_b I_n)H^t + H_0(\hat{\lambda}_b I_{p-n})H_0^t),$$

so the $(p - n)$ eigenvalues among the $p$ nonzero eigenvalues of $\delta_p^E(b)$ are identically $a_p \hat{\lambda}_b = \hat{\lambda}_b / p$. It is seen from Lemma 3.1 that

$$\frac{b}{n - b} \cdot \frac{n}{\text{tr} S^+} \leq \hat{\lambda}_b \leq \frac{b}{1 - b} \cdot \frac{1}{\text{tr} S^+}.$$ 

Note that $nt_n^{-1} \geq \text{tr} S^+ \geq \ell_n^{-1}$, so that $\ell_n / n \leq (\text{tr} S^+)^{-1} \leq \ell_n$. Moreover in the large-$p$ and small-$n$ case, $c_*$ and $b_*$ probably is a very small value. Then $\hat{\lambda}_b / p$ may become extremely small, which implies that $\delta_p^E(b)$ may loss stability and deteriorate in performance. Therefore from Proposition 3.3, $b_*$ may be a better choice for $b$. See the next subsection, which gives some simulated values of the risk of $\delta_p^E(b_*)$.

We can treat the Haff (1980) type empirical Bayes estimator

$$\delta_p^{HF}(c) = a_p(S + cu I_p),$$

where $u = 1 / \text{tr} S^+$ and $c$ is a positive constant. Some dominance results on $\delta_p^{HF}(c)$ and $\delta_p^{mST}(c) = \delta_p^{HF} - cu HH^t$ can be derived, and the details are omitted.

### 3.3 Monte Carlo studies

The Monte Carlo experiments have been performed for comparing the risks of some estimators for some $p$ and $n$. Each experiment is based on 2,000 independent replications. We have investigated estimators $\delta_p^E(b)$ and $\delta_p^{mST}(b)$,
which are defined in (3.3) and (3.12), respectively. It has been assumed that 
\( b = b_0 \) and \( b_1 \), which are given in (3.10) and (3.11), respectively. Also the 
risk of \( \delta_p^{EB}(b_*) \) has been estimated in our experiments, where \( b_* \) is given by 
(3.13).

Note that \( b_0, b_1 \) and \( b_* \) satisfy \( b(S) = b(cS) \) for any positive number \( c \). 
Also, when \( S \) is transformed into \( cS \) for a positive number \( c \), \( \hat{\lambda}_b \)
satisfying \( b(S) = b(cS) \) becomes \( c\hat{\lambda}_b \). Hence the risks of \( \delta_p^{EB}(b) \) and \( \delta_p^{mST}(b) \) with \( b = b_0, b_1 \) and \( b_* \) are invariant under the scale transformation \( S \rightarrow cS \) and 
\( \Sigma \rightarrow c\Sigma \) for any positive number \( c \). Furthermore the risks of \( \delta_p^{EB}(b) \) and 
\( \delta_p^{mST}(b) \) are invariant under the orthogonal transformation \( S \rightarrow P\Sigma P^t \) and 
\( \Sigma \rightarrow P\Sigma P^t \) for any \( P \in O(p) \).

In our experiments, it has been assumed, without loss of generality, that 
\( \Sigma \) is a diagonal matrix whose diagonal elements (namely, eigenvalues) are 
larger than or equal to one. The following diagonal matrices were considered 
for an unknown covariance \( \Sigma \) which should be estimated:

1) \( I_p \);
2) \( \text{diag}(10, 10^{1-1/p}, 10^{1-2/p}, \ldots, 10^{1-(p-2)/p}, 10^{1-(p-1)/p}) \);
3) \( \text{diag}(100, 100^{1-1/p}, 100^{1-2/p}, \ldots, 100^{1-(p-2)/p}, 100^{1-(p-1)/p}) \).

In Case 1), all the eigenvalues of \( \Sigma \) are identical. In Case 2) and 3), the 
eigenvalues of \( \Sigma \) are widely scattered and the largest eigenvalue is about 
tenfold or hundredfold of the smallest eigenvalue.

Table 1 shows some simulated risk values. In the table, the value in 
parentheses stands for estimated standard error on risk. For reference, the 
exact risk of James and Stein’s (1961) minimax estimator are 37.096 \((p = n = 50)\), 72.0995 \((p = n = 100)\) and 106.959 \((p = n = 150)\), which can be 
computed from (2.16) and (2.5) of this paper.

For large \( n \) \((= p/2)\), \( \delta_p^{mST}(b) \) provides substantial reduction in risk of 
\( \delta_p^{EB}(b) \), but almost not for small \( n \) \((= 5)\). In the large-\( n \) case, \( \delta_p^{mST}(b_0) \) is 
slightly better than \( \delta_p^{mST}(b_1) \) and, in the small-\( n \) case, \( \delta_p^{mST}(b_1) \) is the best 
estimator among estimators considered here.

The estimator \( \delta_p^{EB}(b_*) \) has an undesirable performance when \( n = 5 \), and 
however it enhances the performance as \( n \) increases for each \( p \). In Case 3) 
with large \( n \) \((= p/2)\), \( \delta_p^{EB}(b_*) \) has the smallest risk.
All the risks of estimators investigated here considerably varies with the change of $p$, $n$ and $\Sigma$. For example, the risks of $\delta_{p}^{EB}(b_0)$ and $\delta_{p}^{EB}(b_*)$ have very different behavior with increasing $n$. Our numerical results suggest that, although an optimal selection of $b$ would involve difficulty in practical application, we could recommend $\delta_{p}^{mST}(b_1)$ if $p$ is much larger than $n$.

3.4 A unified dominance result including both nonsingular and singular cases

In Subsection 3.2, we provided some dominance results for $p = r > n$. The dominance results can be extended to all possible cases of orderings on $n$, $p$ and $r$ in the model (2.1).

Note that the possible orderings on $n$, $p$ and $r$ are expressed by either $\min(n, p) \geq r$ or $p \geq r > n$. Let $q = \min(n, r)$ and $m = \max(n, r)$. The eigenvalue decomposition of $S$ is written as $HLH^t$, where $H \in \nu_{p,q}$ and $L = \text{diag}(\ell_1, \ldots, \ell_q) \in \mathbb{D}_q$. Take $H_0 \in \nu_{p,p-q}$ such that $(H, H_0) \in \mathcal{O}(p)$. Let $\hat{\lambda}_b$ be a unique solution of the equation

$$\sum_{i=1}^{q} \frac{\lambda}{\ell_i + \lambda} = b,$$

where $b$ is a differentiable function of $S$ and satisfies $0 \leq b < q$. The estimators $\delta_r^{EB}(b)$ and $\delta_r^{SH}(b)$ are defined by, respectively,

$$\delta_r^{EB}(b) = \begin{cases} a_n(S + \hat{\lambda}_bHH^t) & \text{for } \min(n, p) \geq r, \\ a_r(S + \hat{\lambda}_bI_p), & \text{for } p \geq r > n, \end{cases}$$

$$\delta_r^{SH}(b) = \delta_r^{EB}(b) - a_m\hat{\lambda}_bHH^t = \begin{cases} a_nS & \text{for } \min(n, p) \geq r, \\ a_r(S + \hat{\lambda}_bH_0H_0^t), & \text{for } p \geq r > n, \end{cases}$$

where $a_m = m^{-1}$.

In the $\min(n, p) \geq r$ and the $p = r > n$ cases, the definition (3.16) and (3.17) imply that $\delta_r^{EB}(b)$ and $\delta_r^{SH}(b)$ have the same rank as $\Sigma$. However, in the $p > r > n$ case, $\delta_r^{EB}(b)$ and $\delta_r^{SH}(b)$ are of rank $p$, while $\Sigma^+\delta_r^{EB}(b)$ and $\Sigma^+\delta_r^{SH}(b)$ are of rank $r$. This is verified as follows: When $p > r > n,$
recall that $H = \Upsilon R$ where $\Upsilon \in V_{p,r}$ and $R \in V_{r,n}$, which are defined in the beginning of Subsection 2.4. Take $\Upsilon_0 \in V_{p,p-r}$ and $R_0 \in V_{r,r-n}$ such that $(\Upsilon, \Upsilon_0) \in \mathcal{O}(p)$ and $(R, R_0) \in \mathcal{O}(r)$. Define $H_0H_0^t = \Upsilon R_0R_0^t \Upsilon^t + \Upsilon_0 \Upsilon_0^t$. Then it is seen that

$$HH^t + H_0H_0^t = \Upsilon RR^t + R_0R_0^t \Upsilon^t + \Upsilon_0 \Upsilon_0^t = \Upsilon \Upsilon^t + \Upsilon_0 \Upsilon_0^t = I_p$$

and

$$\Upsilon^t H_0H_0^t \Upsilon = R_0R_0^t.$$ Since $\Sigma^+ = \Upsilon \Omega^{-1} \Upsilon^t$, where $\Upsilon \in V_{p,r}$ and $\Omega$ is $r \times r$ positive definite, it is observed that

$$\Upsilon^t \delta_r^{EB}(b) \Upsilon = a_r(R(L + \hat{\lambda}_b I_n)R^t + \hat{\lambda}_b R_0 R_0^t),$$

$$\Upsilon^t \delta_r^{SH}(b) \Upsilon = a_r(RLR^t + \hat{\lambda}_b R_0 R_0^t),$$

so that $\delta_r^{EB}(b)$ and $\delta_r^{SH}(b)$ are of rank $p$, while $\Sigma^+ \delta_r^{EB}(b)$ and $\Sigma^+ \delta_r^{SH}(b)$ are of rank $r$. In such $p > r > n$ case, $\Upsilon R_0 R_0^t \Upsilon^t$ is not observable. Thus it is hard to find an estimator $\delta$ satisfying that both $\delta$ and $\Sigma^+ \delta$ are of rank $r$.

The difference in risk of $\delta_r^{SH}(b)$ and $\delta_r^{EB}(b)$ with respect to the Stein loss (2.2) can be written as

$$R_r(\delta_r^{SH}(b), \Sigma) - R_r(\delta_r^{EB}(b), \Sigma) = E[-a_m \hat{\lambda}_b \text{tr} \Sigma^+ HH^t + \log \det(I_q + \hat{\lambda}_b L^{-1})]$$

for both the $\min(n, p) \geq r$ and the $p \geq r > n$ cases. Hence the same arguments as in the proof of Proposition 3.1 lead to the following proposition.

**Proposition 3.4** In the model (2.1), we consider the problem of estimating $\Sigma$ relative to the Stein loss (2.2). Let $c_0 = 6(q + 1)/(3m - 4q - 4)$ for $3m - 4q - 4 > 0$. Assume that $c_0q/(1 + c_0) \leq b \leq C < q$ for a positive constant $C$ and $\sum_i \partial \phi_j / \partial \ell_i \geq 0$. Then $\delta_r^{SH}(b)$ dominates $\delta_r^{EB}(b)$ for any possible ordering on $n$, $p$ and $r$.

Further improvements on $\delta_r^{SH}(b)$ can be established in the same way as in Subsections 2.3 and 2.4. Also, we can derive the reverse dominance relation such that $\delta_r^{EB}(b)$ dominates $\delta_r^{SH}(b)$ as in Proposition 3.3.
4 Some remarks

This paper addresses the problem of estimating a high-dimensional covariance matrix of multivariate normal distribution and also discusses a unified extension to all possible cases of orderings on the dimension, the sample size and the rank of the covariance matrix. We conclude this paper with giving some remarks.

In this paper, it is assumed that \( \Sigma \) has a known rank \( r \) in the singular model (2.1). When \( \min(n, p) \geq r \) or \( p = r > n \), the observation matrix \( X \) is of rank \( r \) with probability one and inherits the rank from the singular covariance matrix \( \Sigma \). Thus, even if \( r \) is unknown, a value of \( r \) is evaluable from \( X \) as long as \( \min(n, p) \geq r \) or \( p = r > n \). However the \( p > r > n \) case with unknown \( r \) does not permit the evaluation of \( r \), which deeply affects the accuracy of estimators, particularly when \( r \) is much smaller than \( p \).

Instead of the Stein loss (1.2), we may employ the quadratic loss

\[
L_Q(\delta, \Sigma) = \text{tr} \, \Sigma^{-1}(\delta - \Sigma) \Sigma^{-1}(\delta - \Sigma). \tag{4.1}
\]

Selliah (1964) treated the \( n \geq p = r \) case of covariance estimation under (4.1) and obtained an improved estimator based on the LU decomposition of \( S \). For other approaches, see Haff (1979, 1980, 1991), Yang and Berger (1994) and Tsukuma (2014). See also Konno (2009), who discussed the \( p = r > n \) case under the quadratic loss (4.1). For the singular case, the quadratic loss (4.1) probably should be replaced by

\[
L_Q^* (\delta, \Sigma) = \text{tr} \, \Sigma^+(\delta - \Sigma) \Sigma^+(\delta - \Sigma).
\]

Indeed, we can easily obtain an improved estimator similar to Selliah (1964) via the same way as in Subsection 2.3, but the details are omitted here.

The observation matrix \( X \) has the form \( X = BZ \), where \( B \) is an unknown matrix of parameters and \( Z \) is a random matrix. The dominance results of Section 2 can be extended to the estimation problem of a scale matrix in an elliptical distribution model, where the p.d.f. of \( Z \) has the form \( f(\text{tr} \, ZZ^t) \) for an integrable function \( f \). The \( n \geq p = r \) case with the usual Stein loss (1.2) has been studied by Kubokawa and Srivastava (1999). Their dominance results can be extended to our singular case.
Acknowledgments

The work is supported by Grant-in-Aid for Scientific Research (15K00055), Japan.

References

[1] Baker, G.A. Jr. and Graves-Morris, P. (1996). Padé Approximants (2nd ed.), Cambridge University Press, Cambridge.

[2] Díaz-García, J.A. and González-Farías, G. (2005). Singular random matrix decompositions: distributions, J. Multivariate Anal., 94, 109–122.

[3] Díaz-García, J.A., Gutierrez-Jáimez, R. and Mardia, K.V. (1997). Wishart and pseudo-Wishart distributions and some applications to shape theory, J. Multivariate Anal., 63, 73–87.

[4] Dey, D.K. and Srinivasan, C. (1985). Estimation of a covariance matrix under Stein’s loss, Ann. Statist., 13, 1581–1591.

[5] Haff, L.R. (1979). An identity for the Wishart distribution with applications, J. Multivariate Anal., 9, 531–544.

[6] Haff, L.R. (1980). Empirical Bayes estimation of the multivariate normal covariance matrix, Ann. Statist., 8, 586–597.

[7] Haff, L.R. (1991). The variational form of certain Bayes estimators, Ann. Statist., 19, 1163–1190.

[8] Harville, D.A. (1997). Matrix algebra from a statistician’s perspective, Springer, New York.

[9] James, W. and Stein, C. (1961). Estimation with quadratic loss, In Proc. Fourth Berkeley Symp. Math. Statist. Probab., 1, pp.361–379, University of California Press, Berkeley.

[10] Konno, Y. (2009). Shrinkage estimators for large covariance matrices in multivariate real and complex normal distributions under an invariant quadratic loss, J. Multivariate Anal., 100, 2237–2253.
[11] Kubokawa, T. and Srivastava, M.S. (1999). Robust improvement in estimation of a covariance matrix in an elliptically contoured distribution, *Ann. Statist.*, **27**, 600–609.

[12] Kubokawa, T. and Srivastava, M.S. (2008). Estimation of the precision matrix of a singular Wishart distribution and its application in high-dimensional data, *J. Multivariate Anal.*, **99**, 1906–1928.

[13] Perron, F. (1992). Minimax estimators of a covariance matrix, *J. Multivariate Anal.*, **43**, 16–28.

[14] Selliah, J.B. (1964). Estimation and testing problems in a Wishart distribution, Technical reports No.10, Department of Statistics, Stanford University.

[15] Sheena, Y. (1995). Unbiased estimator of risk for an orthogonally invariant estimator of a covariance matrix, *J. Japan Statist. Soc.*, **25**, 35–48.

[16] Sheena, Y. and Takemura, A. (1992). Inadmissibility of non-order-preserving orthogonally invariant estimators of the covariance matrix in the case of Stein’s loss, *J. Multivariate Anal.*, **41**, 117–131.

[17] Srivastava, M.S. (2003). Singular Wishart and multivariate beta distributions, *Ann. Statist.*, **31**, 1537–1560.

[18] Srivastava, M.S. and Khatri, C.G. (1979). *An Introduction to Multivariate Statistics*, North Holland, New York.

[19] Stein, C. (1975). Estimation of a covariance matrix, Rietz Lecture, 39th Annual Meeting IMS, Atlanta, GA.

[20] Stein, C. (1977). Lectures on the theory of estimation of many parameters. In *Studies in the Statistical Theory of Estimation, Part I* (I.A. Ibragimov and M.S. Nikulin, eds.). *Proceedings of Scientific Seminars of the Steklov Institute, Leningrad Division* **74**, 4–65. (In Russian)

[21] Tsukuma, H. (2014). Improvement on the best invariant estimators of the normal covariance and precision matrices via a lower triangular subgroup, *J. Japan Statist. Soc.*, **44**, 195–218.
[22] Yang, R. and Berger, J.O. (1994). Estimation of a covariance matrix using the reference prior, *Ann. Statist.*, **22**, 1195–1211.
Table 1: Simulated risk with respect to the usual Stein loss.

| $\Sigma$ | $p$ | $n$ | $\delta_p^{EB}(b_0)$ | $\delta_p^{mST}(b_0)$ | $\delta_p^{EB}(b_1)$ | $\delta_p^{mST}(b_1)$ | $\delta_p^{EB}(b_1)$ |
|---------|-----|-----|----------------------|----------------------|----------------------|----------------------|----------------------|
| 1) 50   | 5   |  28.6 (0.07) | 28.5 (0.08) | 18.4 (0.08) | 18.2 (0.09) | 113.4 (0.10) |
|        | 15  |  5.0 (0.01)  | 2.7 (0.02)  | 4.8 (0.01)  | 2.0 (0.02)  | 86.2 (0.06)  |
|        | 25  |  24.3 (0.08) | 8.7 (0.02)  | 26.5 (0.10) | 9.6 (0.03)  | 67.3 (0.06)  |
| 100    | 5   |  115.8 (0.13)| 115.8 (0.13)| 82.4 (0.16) | 82.3 (0.16) | 301.1 (0.14) |
|        | 15  |  13.3 (0.02) | 10.8 (0.03) | 10.4 (0.02) | 7.3 (0.03)  | 228.7 (0.07) |
|        | 25  |  41.2 (0.08) | 14.1 (0.02) | 44.3 (0.09) | 15.4 (0.02) | 165.3 (0.06) |
| 150    | 5   |  230.7 (0.16)| 230.7 (0.16)| 170.9 (0.22)| 170.9 (0.22)| 516.7 (0.18) |
|        | 40  |  18.0 (0.02) | 13.7 (0.03) | 14.9 (0.01) | 9.6 (0.03)  | 377.5 (0.06) |
|        | 75  |  59.0 (0.07) | 19.9 (0.02) | 63.1 (0.08) | 21.5 (0.02) | 276.1 (0.06) |
| 2) 50   | 5   |  26.0 (0.07) | 25.9 (0.08) | 19.1 (0.07) | 18.9 (0.08) | 105.6 (0.12) |
|        | 15  |  13.3 (0.02) | 11.0 (0.01) | 14.4 (0.03) | 11.6 (0.02) | 81.7 (0.07)  |
|        | 25  |  44.2 (0.13) | 27.6 (0.06) | 46.3 (0.14) | 28.9 (0.07) | 65.1 (0.06)  |
| 100    | 5   |  103.0 (0.14)| 102.9 (0.14)| 75.4 (0.17) | 75.3 (0.17) | 282.9 (0.17) |
|        | 25  |  23.7 (0.01) | 21.3 (0.01) | 23.7 (0.01) | 20.8 (0.01) | 217.6 (0.08) |
|        | 50  |  76.7 (0.12) | 48.2 (0.06) | 79.5 (0.13) | 49.9 (0.06) | 160.5 (0.06) |
| 150    | 5   |  207.4 (0.18)| 207.4 (0.18)| 155.4 (0.23)| 155.4 (0.23)| 488.0 (0.21) |
|        | 40  |  35.6 (0.01) | 31.3 (0.01) | 36.1 (0.01) | 31.1 (0.01) | 361.2 (0.08) |
|        | 75  |  110.7 (0.11)| 69.6 (0.06) | 114.5 (0.12)| 71.9 (0.06) | 268.6 (0.06) |
| 3) 50   | 5   |  35.7 (0.02) | 35.6 (0.02) | 38.4 (0.08) | 38.2 (0.07) | 87.1 (0.14)  |
|        | 15  |  61.9 (0.17) | 59.2 (0.16) | 65.1 (0.20) | 62.2 (0.18) | 70.8 (0.09)  |
|        | 25  |  125.6 (0.33)| 105.7 (0.27)| 127.5 (0.34)| 107.2 (0.28)| 59.8 (0.07)  |
| 100    | 5   |  87.4 (0.11) | 87.4 (0.11) | 77.2 (0.08) | 77.2 (0.08) | 237.3 (0.21) |
|        | 25  |  99.4 (0.12) | 96.7 (0.12) | 104.7 (0.15)| 101.8 (0.14)| 188.8 (0.10) |
|        | 50  |  219.5 (0.31)| 186.2 (0.25)| 221.8 (0.32)| 188.1 (0.26)| 148.2 (0.07) |
| 150    | 5   |  165.1 (0.18)| 165.1 (0.18)| 135.9 (0.17)| 135.9 (0.17)| 415.0 (0.26) |
|        | 40  |  154.4 (0.13)| 149.7 (0.12)| 161.3 (0.16)| 156.1 (0.14)| 318.2 (0.10) |
|        | 75  |  317.2 (0.31)| 269.7 (0.25)| 320.3 (0.31)| 272.2 (0.26)| 249.2 (0.07) |