

IMPROVED MULTIVARIATE NORMAL MEAN ESTIMATION WITH UNKNOWN COVARIANCE WHEN p IS GREATER THAN n

BY DIDIER CHÉTELAT AND MARTIN T. WELLS¹

Cornell University

We consider the problem of estimating the mean vector of a p -variate normal (θ, Σ) distribution under invariant quadratic loss, $(\delta - \theta)' \Sigma^{-1} (\delta - \theta)$, when the covariance is unknown. We propose a new class of estimators that dominate the usual estimator $\delta^0(X) = X$. The proposed estimators of θ depend upon X and an independent Wishart matrix S with n degrees of freedom, however, S is singular almost surely when $p > n$. The proof of domination involves the development of some new unbiased estimators of risk for the $p > n$ setting. We also find some relationships between the amount of domination and the magnitudes of n and p .

1. Introduction. Suppose a p -dimensional random vector X is observed which is normally distributed, with mean vector θ and unknown positive definite covariance matrix Σ , and we wish to estimate θ under the invariant quadratic loss

$$(1.1) \quad L(\theta, \delta) = (\delta - \theta)' \Sigma^{-1} (\delta - \theta).$$

Since the covariance matrix Σ is unknown, a random matrix S is observed along with X , which is assumed to be independent of X , and has a Wishart distribution with n degrees of freedom, where $p > n$. In high-dimensional estimation problems, where p , the number of features, is nearly as large as or larger than n , the number of observations, the ordinary least squares estimator does not typically provide a satisfactory estimate of θ .

Modern data sets are increasingly becoming characterized by a number of features that are much larger than the number of sample units (large- p , small- n) in contrast to classical data sets where the number of sample units is often much larger than the number of random variables (small- p , large- n). Modern applications in the $p > n$ setting include examples from microarrays, association mapping, proteomics, radiology, biomedical imaging, signal processing, climate modeling and finance. For instance, in the case of microarray data, the dimensionality is frequently in the thousands or beyond, while the sample size is typically in

Received January 2012; revised November 2012.

¹Supported in part by NSF Grant DMS-12-08488.

MSC2010 subject classifications. Primary 62F10; secondary 62C20, 62H12.

Key words and phrases. Covariance estimation, James–Stein estimation, invariant quadratic loss, large- p –small- n problems, location parameter, minimax estimation, Moore–Penrose inverse, risk function, singular Wishart distribution.

the order of tens. The large- p , small- n scenario poses challenges in most inferential settings. We are considering a canonical setting. For the usual multivariate location-scale estimation problem let $W = (W_1, \dots, W_p)$ denote an $N \times p$ matrix of data (N is the number of observations and p the number of features), where W_i are taken from a p -dimensional normal distribution with mean vector θ and covariance matrix Ξ . In this article we let the X and S be the sample mean and covariance of the features, respectively. In the context of this notation, $\Sigma = N^{-1}\Xi$ and $n = N - 1$.

The usual estimator under invariant quadratic loss is $\delta_0(X) = X$. It is minimax and admissible when $p \leq 2$ and $p \leq n$. However, when $p \geq 3$ and $p \leq n$, $\delta_0(X)$ remains minimax but is no longer admissible. Explicit improvements are known in the multivariate normal case [Berger and Bock (1976), Berger and Haff (1983), Berger et al. (1977), Gleser (1979, 1986), James and Stein (1961)] and in the case of elliptically symmetric distribution [Fourdrinier, Strawderman and Wells (2003), Srivastava and Bilodeau (1989)].

In this article we primarily concentrate on the case $p > n$ and construct a class of estimators, depending on the sufficient statistics (X, S) , of the form

$$(1.2) \quad \delta(X, S) = X + g(X, S),$$

which dominate $\delta_0(X)$ under invariant quadratic loss. Note that, although the loss in (1.1) is invariant, the estimate in (1.2) may not be [except for $\delta_0(X)$]. This class generalizes several estimators studied previously for the multivariate normal distribution to the $p \leq n$ setting [Berger and Bock (1976), Berger and Haff (1983), Berger et al. (1977), Gleser (1979, 1986), James and Stein (1961)]. Examples of estimators we study here in this setting extend the class of so-called Baranchik estimators and includes a new high-dimensional James–Stein estimator

$$\delta_a^{\text{JS}}(X, S) = \left(I - \frac{aS S^+}{X' S^+ X} \right) X,$$

where $0 \leq a \leq \frac{2(n-2)}{p-n+3}$ and S^+ is the Moore–Penrose inverse of S .

The estimation of the inverse covariance matrix, namely, the precision matrix Σ^{-1} , of a multivariate normal distribution has been an important problem in practical situations as well as from a theoretical perspective. But, when $p > n$, the Wishart-distributed sample covariance matrix is singular; in this case, one is tempted to construct estimators using the Moore–Penrose generalized inverse S^+ . Recently there has been an increased interest in the problem of estimating the covariance matrix of large dimension given variables of dimension larger than the number of observations [Bickel and Levina (2008), d'Aspremont, Banerjee and El Ghaoui (2008), Konno (2009), Ledoit and Wolf (2004), Levina, Rothman and Zhu (2008), Rothman et al. (2008)].

Our method of proof relies on an unbiased estimator of risk difference, say, $\rho(X, S)$. Specifically, we show that, for $g(X, S)$ of the form $-\frac{r(X' S^+ X) S S^+}{X' S^+ X} X$, the

estimator $\delta(X, S) = X + g(X, S)$ dominates X provided $\rho(X, S) \leq 0$. In the next section we present the main results and their proofs are given in Section 3. We need Stein's integration-by-parts identity [Stein (1981)] and the so-called Stein–Haff identity for the singular Wishart distribution. The Stein–Haff identity was derived by Haff (1979) and Stein (1977) for the full rank Wishart distribution. A similar identity for the elliptically contoured model has been given by Fourdrinier, Strawderman and Wells (2003). We make some concluding comments in Section 4.

For a matrix M , let M' denote its transpose, M^+ its Moore–Penrose pseudo-inverse and $\frac{\partial M}{\partial t}$ its componentwise derivative matrix, that is, the matrix such that $(\frac{\partial M}{\partial t})_{ij} = \frac{\partial M_{ij}}{\partial t}$. Moreover, let δ_{ij} denote the Kronecker delta.

2. Main results. Let X be a random vector distributed as $N_p(\theta, \Sigma)$ with unknown θ and Σ . Suppose an estimator of Σ is available, say, $S \sim \text{Wishart}_p(n, \Sigma)$, with S independent of X . By definition of the Wishart distribution, we can write $S = Y'Y$ for some matrix normal $Y \sim N_{n \times p}(0, I \otimes \Sigma)$. An elementary property of this distribution is that S is (almost surely) invertible if $p \leq n$, and (almost surely) singular if $p > n$ [cf. Srivastava and Khatri (1979)].

An usual estimator of θ is $\delta^0(X, S) = X$; however, it turns out that this estimator is inadmissible under quadratic loss. If some estimator $S \sim \text{Wishart}_p(n, \Sigma)$ is available, with $n \geq p \geq 3$, δ^0 is dominated by the so-called James–Stein estimator

$$\delta^{\text{JS}}(X, S) = \left(1 - \frac{(p-2)/(n-p+3)}{X'S^{-1}X}\right)X.$$

The main contribution of this article is to extend this type of result to a more general class of estimators in the $p > n$ setting.

For some positive, bounded and differentiable function $r: \mathbb{R} \rightarrow \mathbb{R}$, define the Baranchik-type estimator

$$\begin{aligned} \delta_r(X, S) &= \left(I - \frac{r(X'S^+X)SS^+}{X'S^+X}\right)X \\ (2.1) \qquad &= X + g(X, S), \end{aligned}$$

where I is the identity matrix and S^+ denotes the Moore–Penrose inverse of S . This estimator generalizes the usual Baranchik (1970) estimator to the unknown covariance setting for $p > n$.

THEOREM 1. *Let $\min(p, n) \geq 3$. Suppose that:*

- (i) *r satisfies $0 \leq r \leq \frac{2(\min(n, p)-2)}{n+p-2\min(n, p)+3}$;*
- (ii) *r is nondecreasing; and*
- (iii) *r' is bounded.*

Then under invariant quadratic loss, δ_r dominates δ^0 .

Throughout the article we will use the expression $\text{tr}(SS^+)$, which of course equals $\min(n, p)$. This notation allows us to simultaneously handle both the $p > n$ and $n \geq p$ cases. The condition $\min(p, n) \geq 3$ merely guarantees that condition (i) of Theorem 1 holds for some r and is reminiscent of the dimension cutoff in classical Stein estimation.

PROOF OF THEOREM 1. The hypotheses of the theorem imply that r is differentiable almost everywhere. Under invariant quadratic loss, the difference in risk between δ_r and δ^0 is given by

$$\begin{aligned}
 \Delta_\theta &= E_\theta[(X + g(X, S) - \theta)' \Sigma^{-1}(X + g(X, S) - \theta)] \\
 (2.2) \quad &\quad - E_\theta[(X - \theta)' \Sigma^{-1}(X - \theta)] \\
 &= 2E_\theta[g(X, S)' \Sigma^{-1}(X - \theta)] + E_\theta[g(X, S)' \Sigma^{-1}g(X, S)].
 \end{aligned}$$

In order to show the domination result, we need to show that under the sufficient conditions on r , (2.2) is nonpositive for all θ . First, for the leftmost term of (2.2) it can be shown that

$$2E_\theta[g(X, S)' \Sigma^{-1}(X - \theta)] = 2E_\theta[\text{div}_X g(X, S)].$$

Fourdrinier, Strawderman and Wells (2003) give a more general form of this result in their Lemma 1(i); it is essentially an extension of Stein’s classical integration by parts identity. By using Lemma 2 in Section 3, we have that

$$\begin{aligned}
 (2.3) \quad 2E_\theta[\text{div}_X g(X, S)] &= -2E_\theta \left[\text{div}_X \frac{r(X' S^+ X) S S^+ X}{X' S^+ X} \right] \\
 &= -2E_\theta \left[2r'(X' S^+ X) + r(X' S^+ X) \frac{\text{tr}(S S^+) - 2}{X' S^+ X} \right].
 \end{aligned}$$

For the right term of (2.2), we find, through Lemma 3 in Section 3,

$$\begin{aligned}
 &E_\theta[g(X, S)' \Sigma^{-1}g(X, S)] \\
 &= E_\theta \left[\text{tr} \left(\Sigma^{-1} S r^2(X' S^+ X) \frac{S^+ X X' S^+ S}{(X' S^+ X)^2} \right) \right] \\
 &= E_\theta \left[n \text{tr} \left(r^2(X' S^+ X) \frac{S^+ X X' S^+ S}{(X' S^+ X)^2} \right) \right. \\
 &\quad \left. + \text{tr} \left(Y' \nabla_Y \left\{ r^2(X' S^+ X) \frac{S S^+ X X' S^+}{(X' S^+ X)^2} \right\} \right) \right].
 \end{aligned}$$

The finiteness of the risk of δ_r is guaranteed to hold by Theorem 2 in Section 3 for all p and n .

Now applying Lemma 1 in Section 3, we find

$$\begin{aligned}
 & E_\theta \left[n \operatorname{tr} \left(r^2(X'S^+X) \frac{S^+X X'S^+S}{(X'S^+X)^2} \right) \right. \\
 & \quad \left. + \operatorname{tr} \left(Y' \nabla_Y \left\{ r^2(X'S^+X) \frac{S S^+ X X'S^+}{(X'S^+X)^2} \right\} \right) \right] \\
 (2.4) \quad & = E_\theta \left[n \frac{r^2(X'S^+X)}{X'S^+X} - 4r(X'S^+X)r'(X'S^+X) \right. \\
 & \quad \left. + r^2(X'S^+X) \frac{p - 2 \operatorname{tr}(SS^+) + 3}{X'S^+X} \right] \\
 & = E_\theta \left[r^2(X'S^+X) \frac{n + p - 2 \operatorname{tr}(SS^+) + 3}{X'S^+X} - 4r(X'S^+X)r'(X'S^+X) \right].
 \end{aligned}$$

Replacing (2.3) and (2.4) back into (2.2), we obtain

$$\begin{aligned}
 \Delta_\theta & = E_\theta \left[r^2(X'S^+X) \frac{n + p - 2 \operatorname{tr}(SS^+) + 3}{X'S^+X} \right. \\
 & \quad \left. - 2r(X'S^+X) \frac{\operatorname{tr}(SS^+) - 2}{X'S^+X} \right. \\
 & \quad \left. - 4r'(X'S^+X) \{1 + r(X'S^+X)\} \right].
 \end{aligned}$$

Since r is nonnegative and nondecreasing, it follows that $-4r'(X'S^+X)\{1 + r(X'S^+X)\} \leq 0$. Finally, for the X and S such that $r(X'S^+X) \neq 0$,

$$\begin{aligned}
 & r^2(X'S^+X) \frac{n + p - 2 \operatorname{tr}(SS^+) + 3}{X'S^+X} - 2r(X'S^+X) \frac{\operatorname{tr}(SS^+) - 2}{X'S^+X} \leq 0 \\
 \Leftrightarrow & \quad r(X'S^+X) \leq \frac{2(\operatorname{tr}(SS^+) - 2)}{n + p - 2 \operatorname{tr}(SS^+) + 3} = \frac{2(\min(n, p) - 2)}{n + p - 2 \min(n, p) + 3}.
 \end{aligned}$$

Therefore, under the three sufficient conditions on r , it follows that $\Delta_\theta \leq 0$ for any θ , that is, the domination result holds. \square

In the $p > n$ setting, we obtain the following two corollaries.

COROLLARY 1. *For $p > n \geq 3$, δ_r dominates δ^0 under invariant quadratic loss for all r nondecreasing, differentiable and satisfying*

$$(2.5) \quad 0 \leq r \leq \frac{2(n - 2)}{p - n + 3}.$$

COROLLARY 2 (James–Stein estimator with large p and small n). For $p > n \geq 3$ and $a \in \mathbb{R}$, the James–Stein-like estimator

$$(2.6) \quad \delta_a^{\text{JS}}(X, S) = \left(I - \frac{aS S^+}{X' S^+ X} \right) X$$

dominates δ^0 under invariant quadratic loss for all

$$0 \leq a \leq \frac{2(n - 2)}{p - n + 3}.$$

Note that if p is only moderately larger than n , Corollary 1 implies that one can construct an estimator with substantial improvement over δ^0 . However, in the ultra-high-dimensional setting the denominator in (2.5) could be quite large and, consequently, the amount of improvement over δ^0 could be quite small. The estimator in (2.6) generalizes the classical James–Stein with unknown covariance matrix,

$$\delta_a^{\text{JS}}(X, S) = \left(1 - \frac{a}{X' S^{-1} X} \right) X,$$

which is, of course, restricted to the case $p \leq n$, for $a \in \mathbb{R}_+$. In this setting, this result is consistent with previous bounds in Fourdrinier, Strawderman and Wells (2003) (where $n - 1$ is used instead of our n).

3. Technical results and proofs. It remains to clarify several of the somewhat technical computations used in the proof of Theorem 1. We provide them in this section; these computations are likely to be of independent interest and showcase several technical maneuvers that the reader could find useful in dealing with singular Wishart matrices.

PROPOSITION 1. Let Y be an $n \times p$ matrix, $S = Y'Y$, X a p vector and $F = X' S^+ X$. It then follows that

- (i) $\left\{ \frac{\partial S}{\partial Y_{\alpha\beta}} \right\}_{kl} = \delta_{\beta k} Y_{\alpha l} + \delta_{\beta l} Y_{\alpha k};$
- (ii) $\frac{\partial F}{\partial Y_{\alpha\beta}} = -2(X' S^+ Y')_{\alpha} (S^+ X)_{\beta} + 2(X' S^+ S^+ Y')_{\alpha} ((I - S S^+) X)_{\beta};$
- (iii) $\frac{\partial \{S^+ X X' S S^+\}_{kl}}{\partial Y_{\alpha\beta}}$
 $= (S^+ S^+ Y')_{k\alpha} ((I - S S^+) X X' S S^+)_{\beta l}$
 $- S_{k\beta}^+ (Y S^+ X X' S S^+)_{\alpha l} - (S^+ Y')_{k\alpha} (S^+ X X' S S^+)_{\beta l}$
 $+ (I - S S^+)_{k\beta} (Y S^+ S^+ X X' S S^+)_{\alpha l}$

$$\begin{aligned}
 &+ (S^+ X X')_{k\beta} (Y S^+)_{\alpha l} + (S^+ X X' Y')_{k\alpha} (S^+)_{\beta l} \\
 &+ (S^+ X X' S^+ Y')_{k\alpha} (I - S S^+)_{\beta l} \\
 &- (S^+ X X' S S^+)_{k\beta} (Y S^+)_{\alpha l} - (S^+ X X' S S^+ Y')_{k\alpha} (S^+)_{\beta l}.
 \end{aligned}$$

PROOF. First, notice that from the usual chain-rule that

$$\left\{ \frac{\partial S}{\partial Y_{\alpha\beta}} \right\}_{kl} = \frac{\partial}{\partial Y_{\alpha\beta}} S_{kl} = \frac{\partial}{\partial Y_{\alpha\beta}} \sum_q Y_{qk} Y_{ql} = \delta_{\beta k} Y_{\alpha l} + \delta_{\beta l} Y_{\alpha k}.$$

This shows (i).

Let A be a symmetric matrix and $t \in \mathbb{R}$, then

$$\begin{aligned}
 \frac{\partial A^+}{\partial t} &= -A^+ \frac{\partial A}{\partial t} A^+ + (I - A A^+) \frac{\partial A}{\partial t} A^+ A^+ \\
 &\quad + A^+ A^+ \frac{\partial A}{\partial t} (I - A A^+).
 \end{aligned}$$

This result was, it seems, first proved in Golub and Pereyra (1973), as their Theorem 4.3, but can be found in standard textbooks on elementary linear algebra. Also, again for A symmetric, we have $AA^+ = A^+A$ and $A(I - AA^+) = (I - AA^+)A = A^+(I - AA^+) = (I - AA^+)A^+ = 0$. This easily follows from elementary properties of the Moore–Penrose pseudoinverse.

Since $S = Y'Y$, notice through a singular value decomposition argument that $SS^+Y' = Y'$ and, thus, $(I - SS^+)Y' = 0$. Using (i), we find that

$$\begin{aligned}
 \frac{\partial F}{\partial Y_{\alpha\beta}} &= X' \frac{\partial S^+}{\partial Y_{\alpha\beta}} X \\
 &= - \sum_{k,l} (X' S^+)_{k\beta} \{ \delta_{\beta k} Y_{\alpha l} + \delta_{\beta l} Y_{\alpha k} \} (S^+ X)_l \\
 &\quad + \sum_{k,l} (X' S^+ S^+)_{k\beta} \{ \delta_{\beta k} Y_{\alpha l} + \delta_{\beta l} Y_{\alpha k} \} ((I - S S^+) X)_l \\
 &\quad + \sum_{k,l} (X' (I - S S^+))_{k\beta} \{ \delta_{\beta k} Y_{\alpha l} + \delta_{\beta l} Y_{\alpha k} \} (S^+ S^+ X)_l \\
 &= - \sum_l (X' S^+)_{\beta} Y_{\alpha l} (S^+ X)_l - \sum_k (X' S^+)_{k\beta} Y_{\alpha k} (S^+ X)_\beta \\
 &\quad + \sum_l (X' S^+ S^+)_{\beta} Y_{\alpha l} ((I - S S^+) X)_l \\
 &\quad + \sum_k (X' S^+ S^+)_{k\beta} Y_{\alpha k} ((I - S S^+) X)_\beta \\
 &\quad + \sum_l (X' (I - S S^+))_{\beta} Y_{\alpha l} (S^+ S^+ X)_l
 \end{aligned}$$

$$\begin{aligned}
& + \sum_k (X'(I - SS^+))_k Y_{\alpha k} (S^+ S^+ X)_\beta \\
& = -2(X' S^+ Y')_\alpha (S^+ X)_\beta + 2(X' S^+ S^+ Y')_\alpha ((I - SS^+) X)_\beta,
\end{aligned}$$

which gives (ii).

Using (i), we have that for any conformable matrices A and B

$$\begin{aligned}
\left(A \frac{\partial S}{\partial Y_{\alpha\beta}} B \right)_{kl} & = \sum_{i,j} A_{ki} \left\{ \frac{\partial S}{\partial Y_{\alpha\beta}} \right\}_{ij} B_{jl} \\
& = \sum_{i,j} A_{ki} \{ \delta_{\beta i} Y_{\alpha j} + \delta_{\beta j} Y_{\alpha i} \} B_{jl} \\
& = \sum_j A_{k\beta} Y_{\alpha j} B_{jl} + \sum_i A_{ki} Y_{\alpha i} B_{\beta l} \\
& = A_{k\beta} (YB)_{\alpha l} + (AY')_{k\alpha} B_{\beta l}.
\end{aligned}$$

Therefore, using again $(I - SS^+)Y' = 0$,

$$\begin{aligned}
& \frac{\partial \{S^+ X X' S S^+\}_{kl}}{\partial Y_{\alpha\beta}} \\
& = \left\{ S^+ S^+ \frac{\partial S}{\partial Y_{\alpha\beta}} (I - SS^+) X X' S S^+ \right. \\
& \quad - S^+ \frac{\partial S}{\partial Y_{\alpha\beta}} S^+ X X' S S^+ + (I - SS^+) \frac{\partial S}{\partial Y_{\alpha\beta}} S^+ S^+ X X' S S^+ \\
& \quad + S^+ X X' \frac{\partial S}{\partial Y_{\alpha\beta}} S^+ + S^+ X X' S S^+ S^+ \frac{\partial S}{\partial Y_{\alpha\beta}} (I - SS^+) \\
& \quad \left. - S^+ X X' S S^+ \frac{\partial S}{\partial Y_{\alpha\beta}} S^+ + S^+ X X' S (I - SS^+) \frac{\partial S}{\partial Y_{\alpha\beta}} S^+ S^+ \right\}_{kl} \\
& = (S^+ S^+ Y')_{k\alpha} ((I - SS^+) X X' S S^+)_{\beta l} \\
& \quad - S_{k\beta}^+ (Y S^+ X X' S S^+)_{\alpha l} - (S^+ Y')_{k\alpha} (S^+ X X' S S^+)_{\beta l} \\
& \quad + (I - SS^+)_{k\beta} (Y S^+ S^+ X X' S S^+)_{\alpha l} \\
& \quad + (S^+ X X')_{k\beta} (Y S^+)_{\alpha l} + (S^+ X X' Y')_{k\alpha} (S^+)_{\beta l} \\
& \quad + (S^+ X X' S^+ Y')_{k\alpha} (I - SS^+)_{\beta l} \\
& \quad - (S^+ X X' S S^+)_{k\beta} (Y S^+)_{\alpha l} - (S^+ X X' S S^+ Y')_{k\alpha} (S^+)_{\beta l},
\end{aligned}$$

which gives (iii). \square

LEMMA 1. Under the hypotheses of Theorem 1, we have

$$\begin{aligned} & \text{tr}\left(Y'\nabla_Y\left\{r^2(X'S^+X)\frac{SS^+XX'S^+}{(X'S^+X)^2}\right\}\right) \\ &= -4r(X'S^+X)r'(X'S^+X) + r^2(X'S^+X)\frac{p - 2\text{tr}(SS^+) + 3}{X'S^+X}, \end{aligned}$$

where ∇_Y is interpreted as the matrix with components $(\nabla_Y)_{ij} = \frac{\partial}{\partial Y_{ij}}$.

PROOF. To simplify computations, in what will follow, we let $F \equiv X'S^+X$. We then have

$$\begin{aligned} & \left[Y'\nabla_Y\left\{r^2(F)\frac{SS^+XX'S^+}{F^2}\right\}\right]_{ij} \\ &= \sum_{\alpha,\beta} (Y')_{i\alpha} \frac{\partial}{\partial Y_{\alpha\beta}} \left\{ r^2(F) \frac{(SS^+XX'S^+)_{\beta j}}{F^2} \right\} \\ (3.1) \quad &= 2 \sum_{\alpha,\beta} (Y')_{i\alpha} r(F)r'(F) \frac{\partial F}{\partial Y_{\alpha\beta}} \cdot \frac{(SS^+XX'S^+)_{\beta j}}{F^2} \\ (3.2) \quad &+ \sum_{\alpha,\beta} (Y')_{i\alpha} r^2(F) \frac{(\partial/\partial Y_{\alpha\beta})\{(SS^+XX'S^+)_{\beta j}\}}{F^2} \\ (3.3) \quad &+ \sum_{\alpha,\beta} (Y')_{i\alpha} r^2(F) \frac{-2(\partial F/\partial Y_{\alpha\beta})(SS^+XX'S^+)_{\beta j}}{F^3}. \end{aligned}$$

To simplify (3.1) and (3.3), we apply Proposition 1(ii) to get

$$\begin{aligned} & \sum_{\alpha,\beta} (Y')_{i\alpha} \left\{ \frac{\partial F}{\partial Y_{\alpha\beta}} \right\} (SS^+XX'S^+)_{\beta j} \\ &= -2 \sum_{\alpha,\beta} (Y')_{i\alpha} (X'S^+Y')_{\alpha} (S^+X)_{\beta} (SS^+XX'S^+)_{\beta j} \\ &+ 2 \sum_{\alpha,\beta} (X'S^+S^+Y')_{\alpha} (Y)_{\alpha i} (S^+XX'SS^+)_{j\beta} ((I - SS^+)X)_{\beta} \\ &= -2X'S^+X(SS^+XX'S^+)_{ij}. \end{aligned}$$

Using this, we get for (3.1)

$$\begin{aligned} & 2 \sum_{\alpha,\beta} (Y')_{i\alpha} r(F)r'(F) \frac{\partial F}{\partial Y_{\alpha\beta}} \cdot \frac{(SS^+XX'S^+)_{\beta j}}{F^2} \\ (3.4) \quad &= -4r(F)r'(F) \frac{(SS^+XX'S^+)_{ij}}{F} \end{aligned}$$

and (3.3) becomes

$$\begin{aligned}
 (3.5) \quad & \sum_{\alpha, \beta} (Y')_{i\alpha} r^2(F) \frac{-2(\partial F / \partial Y_{\alpha\beta}) \cdot (SS^+ XX'S^+)_{\beta j}}{F^3} \\
 & = 4r^2(F) \frac{(SS^+ XX'S^+)_{ij}}{F^2}.
 \end{aligned}$$

This leaves the term (3.2) to analyze. Using Proposition 1(iii),

$$\begin{aligned}
 & \sum_{\alpha, \beta} (Y')_{i\alpha} \frac{\partial}{\partial Y_{\alpha\beta}} \{ (SS^+ XX'S^+)_{\beta j} \} \\
 & = \sum_{\alpha, \beta} (Y')_{i\alpha} \frac{\partial \{ S^+ XX'SS^+ \}_{j\beta}}{\partial Y_{\alpha\beta}} \\
 & = \sum_{\alpha, \beta} \{ (S^+ S^+ Y')_{j\alpha} Y_{\alpha i} ((I - SS^+) XX'SS^+)_{\beta\beta} \\
 & \quad - S^+_{j\beta} (Y')_{i\alpha} (Y S^+ XX'SS^+)_{\alpha\beta} \\
 & \quad - (S^+ Y')_{j\alpha} Y_{\alpha i} (S^+ XX'SS^+)_{\beta\beta} \\
 & \quad + (I - SS^+)_{j\beta} (Y')_{i\alpha} (Y S^+ S^+ XX'SS^+)_{\alpha\beta} \\
 & \quad + (S^+ XX')_{j\beta} (Y')_{i\alpha} (Y S^+)_{\alpha\beta} \\
 & \quad + (S^+ XX'Y')_{j\alpha} Y_{\alpha i} (S^+)_{\beta\beta} \\
 & \quad + (S^+ XX'S^+ Y')_{j\alpha} Y_{\alpha i} (I - SS^+)_{\beta\beta} \\
 & \quad - (S^+ XX'SS^+)_{j\beta} (Y')_{i\alpha} (Y S^+)_{\alpha\beta} \\
 & \quad \quad - (S^+ XX'SS^+ Y')_{j\alpha} Y_{\alpha i} (S^+)_{\beta\beta} \} \\
 & = (S^+ XX'SS^+(I - SS^+))_{ij} \\
 & \quad - (SS^+ XX'S^+)_{ij} - \text{tr}(S^+ XX'SS^+)(SS^+)_{ij} \\
 & \quad + \text{tr}((I - SS^+) XX'SS^+)(S^+)_{ij} \\
 & \quad + (SS^+ XX'S^+)_{ij} + \text{tr}(S^+)(SXX'S^+)_{ij} \\
 & \quad + \text{tr}(I - SS^+)(SS^+ XX'S^+)_{ij} \\
 & \quad - (SS^+ XX'S^+)_{ij} - \text{tr}(S^+)(SXX'S^+)_{ij} \\
 & = (p - \text{tr}(SS^+) - 1) \{ SS^+ XX'S^+ \}_{ij} - (X'S^+X) \{ SS^+ \}_{ij}.
 \end{aligned}$$

Next, applying this computation in (3.2), we obtain

$$\begin{aligned}
 & \sum_{\alpha, \beta} (Y')_{i\alpha} r^2(F) \frac{(\partial/\partial Y_{\alpha\beta})\{(SS^+ X X' S^+)\}_{\beta j}}{F^2} \\
 (3.6) \quad & = (p - \text{tr}(SS^+) - 1)r^2(F) \frac{(SS^+ X X' S^+)_{ij}}{F^2} \\
 & \quad - r^2(F) \frac{(SS^+)_{ij}}{F}.
 \end{aligned}$$

Now we can combine (3.4), (3.6) and (3.5) together to complete the proof. That is, we have

$$\begin{aligned}
 & \text{tr}\left(Y' \nabla_Y \left\{ r^2(F) \frac{SS^+ X X' S^+}{F^2} \right\}\right) \\
 & = \sum_i \left\{ -4r(F)r'(F) \frac{(SS^+ X X' S^+)_{ii}}{F} \right. \\
 & \quad + 4r^2(F) \frac{(SS^+ X X' S^+)_{ii}}{F^2} \\
 & \quad + (p - \text{tr}(SS^+) - 1)r^2(F) \frac{(SS^+ X X' S^+)_{ii}}{F^2} \\
 & \quad \left. - r^2(F) \frac{(SS^+)_{ii}}{F} \right\} \\
 & = -4r(F)r'(F) + r^2(F) \frac{p - 2\text{tr}(SS^+) + 3}{F}
 \end{aligned}$$

as desired. \square

LEMMA 2. Under the hypotheses of Theorem 1 we have

$$\text{div}_X \frac{r(X' S^+ X) SS^+ X}{X' S^+ X} = 2r'(X' S^+ X) + r(X' S^+ X) \frac{\text{tr}(SS^+) - 2}{X' S^+ X}.$$

PROOF. Again, to simplify computations, let us denote $X' S^+ X$ by F . We find

$$\begin{aligned}
 & \text{div}_X \left\{ r(F) \frac{SS^+ X}{F} \right\} \\
 & = \sum_i \frac{\partial}{\partial X_i} \left\{ r(F) \frac{(SS^+ X)_i}{F} \right\} \\
 & = \sum_i r'(F) \frac{\partial F}{\partial X_i} \frac{(SS^+ X)_i}{F} + r(F) \frac{(\partial/\partial X_i)\{(SS^+ X)_i\}}{F}
 \end{aligned}$$

$$\begin{aligned}
 & -r(F) \frac{(\partial F / \partial X_i)(SS^+ X)_i}{F^2} \\
 = & \sum_i r'(F) \left\{ \frac{\partial}{\partial X_i} \sum_{k,l} X_k X_l S_{kl}^+ \right\} \frac{(SS^+ X)_i}{F} \\
 & + r(F) \frac{(\partial / \partial X_i) \sum_k (SS^+)_{ik} X_k}{F} \\
 & - r(F) \frac{\{(\partial / \partial X_i) \sum_{k,l} X_k X_l S_{kl}^+\} (SS^+ X)_i}{F^2} \\
 = & \sum_i r'(F) \{(X' S^+)_i + (X' S^+)_i\} \frac{(SS^+ X)_i}{F} \\
 & + r(F) \frac{(SS^+)_{ii}}{F} - r(F) \frac{\{(X' S^+)_i + (X' S^+)_i\} \cdot (SS^+ X)_i}{F^2} \\
 = & 2r'(F) + r(F) \frac{\text{tr}(SS^+) - 2}{F}
 \end{aligned}$$

as desired. \square

The following result is an extension of a result in [Konno \(2009\)](#). This type of result was first obtained by [Kubokawa and Srivastava \(2008\)](#) and then was extended by [Konno \(2009\)](#). In our generalization we make use of a divergence version of Stein’s lemma that comes with somewhat weaker moment conditions, rather than the element-by-element assumptions in [Konno \(2009\)](#). These weaker moment conditions allow us to cover the p equals n and $n + 1$ cases.

LEMMA 3. *Let $Y \sim N_{n \times p}(0, I_n \otimes \Sigma)$, let $S = Y'Y$ which has, by definition, a $\text{Wishart}_p(n, \Sigma)$ distribution, and let $G(S)$ be a $p \times p$ random matrix that depends on S . Let ∇_Y be interpreted as the matrix with components $(\nabla_Y)_{ij} = \frac{\partial}{\partial Y_{ij}}$, and for A the symmetric positive definite square root of Σ , define $\tilde{Y} = YA^{-1}$ and $H = AGA^{-1}$. Then*

$$E[\text{tr}(\Sigma^{-1}SG)] = E[n \text{tr}(G) + \text{tr}(Y'\nabla_Y G')]$$

under the conditions

$$(3.7) \quad E[|\text{div}_{\text{vec}(\tilde{Y})} \cdot \text{vec}(\tilde{Y}H)|] < \infty,$$

where $\text{vec}(M)$ denotes the vectorization of a matrix M .

PROOF. Define $\tilde{S} = \tilde{Y}'\tilde{Y} = A^{-1}SA^{-1}$. Notice that, by construction, $\tilde{Y} \sim N_{n \times p}(0, I_n \otimes I_p)$ —this means, by definition of the matrix normal distribution,

that $\text{vec}(\tilde{Y}) \sim N_{np}(0, I_{np})$. We can write

$$\begin{aligned} E[\text{tr}(\tilde{S}H)] &= E\left[\sum_{\alpha,i,j} \tilde{Y}_{\alpha i} \tilde{Y}_{\alpha j} H_{ji}\right] \\ &= E[\text{vec}(\tilde{Y}) \cdot \text{vec}(\tilde{Y}H)]. \end{aligned}$$

Using the divergence form of Stein’s lemma, which can be found in Lemma A.1 in [Fourdrinier and Strawderman \(2003\)](#), we obtain, under the moment conditions outlined in (3.7),

$$\begin{aligned} E[\text{vec}(\tilde{Y}) \cdot \text{vec}(\tilde{Y}H)] &= E[\text{div}_{\text{vec}(\tilde{Y})} \text{vec}(\tilde{Y}H)] \\ &= E\left[\sum_{\alpha,i,j} \frac{\partial}{\partial \tilde{Y}_{\alpha i}} \tilde{Y}_{\alpha j} H_{ji}\right] \\ &= E\left[\sum_{\alpha,i,j} \delta_{ij} H_{ji} + \tilde{Y}_{\alpha j} \frac{\partial H_{ji}}{\partial \tilde{Y}_{\alpha i}}\right] \\ &= E\left[n \sum_i H_{ii} + \sum_{\alpha,i,j} \tilde{Y}_{\alpha j} \frac{\partial}{\partial \tilde{Y}_{\alpha i}} H_{ji}\right]. \end{aligned}$$

This last expression can be expressed in a compact matrix form as

$$E[\text{tr}(\tilde{S}H)] = E[n \text{tr}(H) + \text{tr}((\tilde{Y}'\nabla_{\tilde{Y}})'H)].$$

Finally, we notice

$$\begin{aligned} E[\text{tr}(H)] &= E[\text{tr}(AGA^{-1})], \\ E[\text{tr}(\tilde{S}H)] &= E[\text{tr}(A^{-1}SGA^{-1})], \\ E[\text{tr}((\tilde{Y}'\nabla_{\tilde{Y}})'H)] &= E[\text{tr}(A(Y'\nabla_Y)'GA^{-1})], \end{aligned}$$

which concludes the proof. \square

THEOREM 2. *Let $Y \sim N_{n \times p}(0, I_n \otimes \Sigma)$ and for A the symmetric positive definite square root of Σ , let $\tilde{Y} = YA^{-1}$. Let r be any bounded differentiable nonnegative function $r : \mathbb{R} \rightarrow [0, C_1]$ with bounded derivative $|r'| \leq C_2$. Define*

$$G = r^2(X'S^+X) \frac{S^+XX'S^+S}{(X'S^+X)^2}$$

and $H = AGA^{-1}$. Then for all p and n

$$(3.8) \quad E[|\text{div}_{\text{vec}(\tilde{Y})} \text{vec}(\tilde{Y}H)|] < \infty.$$

PROOF. We first compute $\operatorname{div}_{\operatorname{vec}(\tilde{Y})} \operatorname{vec}(\tilde{Y}H)$. As always, to ease notation, we shall write $F = X'S^+X$. We have

$$\begin{aligned} & \operatorname{div}_{\operatorname{vec}(\tilde{Y})} \operatorname{vec}(\tilde{Y}H) \\ &= \sum_{\alpha,i,j} \frac{\partial}{\partial \tilde{Y}_{\alpha i}} \{ \tilde{Y}_{\alpha j} H_{ji} \} \\ &= n \sum_i H_{ii} + \sum_{\alpha,j} \tilde{Y}_{\alpha j} \frac{\partial H_{ji}}{\partial \tilde{Y}_{\alpha i}} \\ &= n \sum_i H_{ii} + \sum_{\alpha,\beta,i,j} \tilde{Y}_{\alpha j} A_{\beta i} \frac{\partial}{\partial Y_{\alpha\beta}} \left\{ r^2(F) \frac{\{AS^+XX'SS^+A^{-1}\}_{ji}}{F^2} \right\} \\ &= n \sum_i H_{ii} + \sum_{\alpha,\beta,i,j} \tilde{Y}_{\alpha j} A_{\beta i} \\ & \quad \times \left\{ 2r(F)r'(F) \frac{\partial F}{\partial Y_{\alpha\beta}} \frac{\{AS^+XX'SS^+A^{-1}\}_{ji}}{F^2} \right. \\ & \quad + \frac{r^2(F)}{F^2} \sum_{k,l} A_{jk} \frac{\partial \{S^+XX'SS^+\}_{kl}}{\partial Y_{\alpha\beta}} A_{li}^{-1} \\ & \quad \left. - r^2(F) \{AS^+XX'SS^+A^{-1}\}_{ji} \frac{2 \partial F / \partial Y_{\alpha\beta}}{F^3} \right\}. \end{aligned} \tag{3.9}$$

We simplify each part of the expression. For (3.9), using Proposition 1(ii), we find

$$\begin{aligned} & 2 \sum_{\alpha,\beta,i,j} \tilde{Y}_{\alpha j} A_{\beta i} r(F)r'(F) \frac{\partial F}{\partial Y_{\alpha\beta}} \frac{\{AS^+XX'SS^+A^{-1}\}_{ji}}{F^2} \\ &= 4 \frac{r(F)r'(F)}{F^2} \\ & \quad \times \sum_{\alpha,\beta,i,j} \{-(X'S^+Y')_{\alpha} \tilde{Y}_{\alpha j} \{AS^+XX'SS^+A^{-1}\}_{ji} A_{i\beta} (S^+X)_{\beta} \\ & \quad + (X'S^+S^+Y')_{\alpha} \tilde{Y}_{\alpha j} \{AS^+XX'SS^+A^{-1}\}_{ji} A_{i\beta} ((I - SS^+)X)_{\beta} \} \\ &= -4 \frac{r(F)r'(F)}{F^2} (X'S^+Y'YA^{-1}AS^+XX'SS^+A^{-1}AS^+X) \\ & \quad + 4 \frac{r(F)r'(F)}{F^2} (X'S^+S^+Y'YA^{-1}AS^+XX'SS^+A^{-1}A(I - SS^+)X) \\ &= -4r(F)r'(F). \end{aligned} \tag{3.12}$$

Similarly, for (3.11)

$$\begin{aligned}
 & \sum_{\alpha, \beta, i, j} \tilde{Y}_{\alpha j} A_{\beta i} r^2(F) \{AS^+ XX' SS^+ A^{-1}\}_{ji} \frac{2 \partial F / \partial Y_{\alpha \beta}}{F^3} \\
 &= 4 \frac{r^2(F)}{F^3} \sum_{\alpha, \beta, i, j} (X' S^+ Y')_{\alpha} \tilde{Y}_{\alpha j} \{AS^+ XX' SS^+ A^{-1}\}_{ji} A_{i \beta} (S^+ X)_{\beta} \\
 (3.13) \quad &= 4 \frac{r^2(F)}{F^3} (X' S^+ Y' Y A^{-1} AS^+ XX' SS^+ A^{-1} AS^+ X) \\
 &= 4 \frac{r^2(F)}{F}.
 \end{aligned}$$

This leaves us with (3.10). Using Proposition 1(iii), we obtain

$$\begin{aligned}
 & \sum_{\alpha, \beta, i, j} \tilde{Y}_{\alpha j} A_{\beta i} \frac{r^2(F)}{F^2} \sum_{k, l} A_{jk} \frac{\partial \{S^+ XX' SS^+\}_{kl}}{\partial Y_{\alpha \beta}} A_{li}^{-1} \\
 &= \frac{r^2(F)}{F^2} \sum_{\alpha, \beta, i, j, k, l} \tilde{Y}_{\alpha j} A_{\beta i} A_{jk} A_{li}^{-1} \\
 & \quad \times \{ (S^+ S^+ Y)_{k\alpha} ((I - SS^+) XX' SS^+)_{\beta l} \\
 & \quad - S_{k\beta}^+ (Y S^+ XX' SS^+)_{\alpha l} \\
 & \quad - (S^+ Y)_{k\alpha} (S^+ XX' SS^+)_{\beta l} \\
 & \quad + (I - SS^+)_{k\beta} (Y S^+ S^+ XX' SS^+)_{\alpha l} \\
 & \quad + (S^+ XX')_{k\beta} (Y S^+)_{\alpha l} \\
 & \quad + (S^+ XX' Y')_{k\alpha} (S^+)_{\beta l} \\
 & \quad + (S^+ XX' S^+ Y')_{k\alpha} (I - SS^+)_{\beta l} \\
 & \quad - (S^+ XX' SS^+)_{k\beta} (Y S^+)_{\alpha l} \\
 & \quad - (S^+ XX' SS^+ Y')_{k\alpha} (S^+)_{\beta l} \} \\
 &= \frac{r^2(F)}{F^2} \sum_{\alpha, \beta, i, j, k, l} \{ A_{jk} (S^+ S^+ Y)_{k\alpha} \tilde{Y}_{\alpha j} A_{i \beta} ((I - SS^+) XX' SS^+)_{\beta l} A_{li}^{-1} \\
 & \quad - \tilde{Y}'_{j\alpha} (Y S^+ XX' SS^+)_{\alpha l} A_{li}^{-1} A_{i \beta} S_{\beta k}^+ A_{kj} \\
 & \quad - A_{jk} (S^+ Y)_{k\alpha} \tilde{Y}_{\alpha j} A_{i \beta} (S^+ XX' SS^+)_{\beta l} A_{li}^{-1} \\
 (3.14) \quad & \quad + \tilde{Y}'_{j\alpha} (Y S^+ S^+ XX' SS^+)_{\alpha l} A_{li}^{-1} A_{i \beta} (I - SS^+)_{\beta k} A_{kj}
 \end{aligned}$$

$$\begin{aligned}
 & + \tilde{Y}'_{j\alpha}(YS^+)_{\alpha l} A_{li}^{-1} A_{i\beta}(XX'S^+)_{\beta k} A_{kj} \\
 & + A_{jk}(S^+XX'Y')_{k\alpha} \tilde{Y}_{\alpha j} A_{i\beta}(S^+)_{\beta l} A_{li}^{-1} \\
 & + A_{jk}(S^+XX'S^+Y')_{k\alpha} \tilde{Y}_{\alpha j} A_{i\beta}(I - SS^+)_{\beta l} A_{li}^{-1} \\
 & - \tilde{Y}'_{j\alpha}(YS^+)_{\alpha l} A_{li}^{-1} A_{i\beta}(SS^+XX'S^+)_{\beta k} A_{kj} \\
 & \quad - A_{jk}(S^+XX'SS^+Y')_{k\alpha} \tilde{Y}_{\alpha j} A_{i\beta}(S^+)_{\beta l} A_{li}^{-1} \} \\
 = & \frac{r^2(F)}{F^2} \{ \text{tr}(AS^+S^+Y'YA^{-1}) \cdot \text{tr}(A(I - SS^+)XX'SS^+A^{-1}) \\
 & - \text{tr}(A^{-1}Y'YS^+XX'SS^+A^{-1}AS^+A) \\
 & - \text{tr}(AS^+Y'YA^{-1}) \text{tr}(AS^+XX'SS^+A^{-1}) \\
 & + \text{tr}(A^{-1}Y'YS^+S^+XX'SS^+A^{-1}A(I - SS^+)A) \\
 & + \text{tr}(A^{-1}Y'YS^+A^{-1}AXX'S^+A) \\
 & + \text{tr}(AS^+XX'Y'YA^{-1}) \cdot \text{tr}(AS^+A^{-1}) \\
 & + \text{tr}(AS^+XX'S^+Y'YA^{-1}) \text{tr}(A(I - SS^+)A^{-1}) \\
 & - \text{tr}(A^{-1}Y'YS^+A^{-1}ASS^+XX'S^+A) \\
 & \quad - \text{tr}(AS^+XX'SS^+Y'YA^{-1}) \text{tr}(AS^+A^{-1}) \} \\
 = & \frac{r^2(F)}{F^2} \cdot \{ -X'S^+X - \text{tr}(SS^+) \cdot X'S^+X \\
 & \quad + X'S^+X + X'SS^+X \cdot \text{tr}(S^+) + X'S^+X \cdot (p - \text{tr}(SS^+)) \\
 & \quad \quad - X'S^+X - X'SS^+X \cdot \text{tr}(S^+) \} \\
 = & \frac{r^2(F)}{F} (p - \text{tr}(SS^+) - 1).
 \end{aligned}$$

Having re-expressed $\text{div}_{\text{vec}(\tilde{Y})} \text{vec}(\tilde{Y}H)$, we now need to bound it above. By virtue of (3.12), (3.13) and (3.14), we have

$$\begin{aligned}
 & E[|\text{div}_{\text{vec}(\tilde{Y})} \text{vec}(\tilde{Y}H)|] \\
 (3.15) \quad & = E \left[\left| n \text{tr}(H) + 4 \frac{r^2(F)}{F} \right. \right. \\
 & \quad \left. \left. + (p - \text{tr}(SS^+) - 1) \frac{r^2(F)}{F} - 4r(F)r'(F) \right| \right] \\
 & \leq C_1^2 |3 + p - \text{tr}(SS^+) + n| E \left[\frac{1}{F} \right] + 4C_1 C_2.
 \end{aligned}$$

It only remains to show that $E[\frac{1}{F}]$ is finite. By definition of the Wishart matrix distribution, we can define a $T \sim \text{Wishart}_p(n, I_n)$ such that $S = ATA$. Let $T = H'DH$ be the spectral decomposition of T , with $D = \text{diag}(\lambda_i)$. Write the eigenvalues of T^+ as λ_i^+ , so that $D^{-1} = \text{diag}(\lambda_i^+)$, and let λ_{\min}^+ be the smallest nonzero eigenvalue of T^+ . The following two identities follow from [Tian and Cheng \(2004\)](#) [Theorem 1.1, equations (1.2) and (1.4)] and symmetry of T :

$$\begin{aligned} (ATA)^+ &= (T^+TA)^+T^+(AT^+T)^+, \\ (T^+TA)^+(T^+T) &= (T^+TA)^+. \end{aligned}$$

Using these identities, we have

$$\begin{aligned} X'S^+X &= X'(ATA)^+X = X'(T^+TA)^+T^+(AT^+T)^+X \\ &= \sum_k \{X'(T^+TA)^+H'\}_k^2 \lambda_k^+ \\ &\geq \lambda_{\min}^+ \cdot X'(T^+TA)^+H'H(AT^+T)^+X \\ &= \lambda_{\min}^+ \cdot X'(T^+TA)^+(T^+T)(AT^+T)^+X \\ &= \lambda_{\min}^+ \cdot X'(T^+TA)^+(AT^+T)^+X. \end{aligned}$$

Applying Cauchy–Schwarz provides us with the bound

$$X'(T^+TA)^+(T^+TA)X \leq X'(T^+TA)^+(AT^+T)^+XX'(AT^+T)(T^+TA)X$$

so that we then have

$$\begin{aligned} \frac{1}{F} &= \frac{1}{X'S^+X} \leq \frac{1}{\lambda_{\min}^+} \frac{1}{X'(T^+TA)^+(AT^+T)^+X} \\ &\leq \frac{1}{\lambda_{\min}^+} \frac{X'AT^+TAX}{X'(T^+TA)^+(T^+TA)X}. \end{aligned}$$

To ease notation, let us write $Q = AT^+TA$ and $R = (T^+TA)^+(T^+TA)$. Collecting the results together, we bound (3.15) by

$$(3.16) \quad \leq C_1^2|3 + p - 2\text{tr}(SS^+)| + n|E\left[\frac{1}{\lambda_{\min}^+} \frac{X'QX}{X'RX}\right]| + 4C_1C_2.$$

We now use some independence results. We can write the singular value decomposition of T as $T = H'DH$, but we can also write it as $T = H_1'D_1H_1$, where H_1 is semi-orthogonal ($H_1H_1' = I$) and D_1 is the matrix of the positive eigenvalues of T . If T has full rank (i.e., $n \geq p$), then this coincides with the singular value decomposition of T . In the full rank case, [Srivastava and Khatri \(1979\)](#) [Section 3.4,

equation (3.4.3)] provide the joint density of H and $D = \text{diag}(d_i)$ in the standard Wishart case (which applies to T) as

$$(3.17) \quad \begin{aligned} f_{H,D}(H, D) &= C(p, n) |D|^{(n-p-1)/2} \left[\text{etr} \left(-\frac{1}{2} D \right) \right] \left[\prod_{i < j} (d_i - d_j) \right] g_p(H) \end{aligned}$$

for constants $C(p, n)$ and functions g_p . Therefore, H and D are independent. In the rank-deficient case ($p > n$), [Srivastava \(2003\)](#) (Section 3) provides an equivalent expression which, in the singular Wishart case, gives

$$(3.18) \quad \begin{aligned} f_{H_1, D_1}(H_1, D_1) &= K(p, n) |D_1|^{(p-n-1)/2} \left[\text{etr} \left(-\frac{1}{2} D_1 \right) \right] \left[\prod_{i < j} (d_i - d_j) \right] g_{n,p}(H_1) \end{aligned}$$

for constants $K(p, n)$ and functions $g_{n,p}$, so, again, we find H_1 and D_1 independent by factorization. Now, λ_{\min}^+ is a function, in the full rank case (resp., rank-deficient case), of only D^{-1} (resp., D_1^{-1}), and we can write $T^+T = H'H$ (resp., $T^+T = H_1'H_1$), so λ_{\min}^+ and T^+T are independent. Being functions of S , they are also both independent of X . Now, the nonzero eigenvalues of T^+ are the inverses of the nonzero eigenvalues of T , a general fact about Moore–Penrose pseudo-inverses. Therefore, denoting the largest eigenvalue of T as λ_{\max} , we can split up the expectations in (3.16) and get the bound

$$(3.19) \quad \leq C_1^2 |3 + p - 2 \text{tr}(SS^+) + n| E[\lambda_{\max}] E \left[\frac{X'QX}{X'RX} \right] + 4C_1C_2.$$

Now, it follows from positive semi-definiteness of T that $E[\lambda_{\max}] \leq E[\text{tr}(T)]$. If $n \geq p$, $\text{tr}(T) \sim \chi_{pn}^2$ [cf. [Muirhead \(1982\)](#), Theorem 3.2.20] and so $E[\text{tr}(T)] = pn < \infty$. If $p > n$, recall we can write $T = Z'Z$ for $Z \sim N_{n \times p}(0, I_n \otimes I_p)$ by definition of the Wishart distribution; and $ZZ' \sim \text{Wishart}_n(p, I_n)$ so that $\text{tr}(T) = \text{tr}(ZZ') \sim \chi_{pn}^2$; so, again, $E[\text{tr}(T)] = pn < \infty$. Therefore, in either case, $E[\lambda_{\max}] \leq pn < \infty$.

We still have to check that the expectation involving X , Q and R in (3.19) is finite. Let $r = \text{rk}(R) = \text{rk}(Q) = \text{rk}(S)$ and write the spectral decomposition of (T^+TA) as $U\Lambda U'$, with $\Lambda = \text{diag}(L, 0_{(p-r)})$ where L is the vector of the r nonzero eigenvalues of (T^+TA) . Then $R = (T^+TA)^+(T^+TA) = U \text{diag}(I_r, 0_{(p-r)})U'$; let us define the $p \times (p-r)$ matrix $E = U[0_{(p-r) \times r} I_{(p-r)}]'$, that is, so that $RE = 0$ and E has full column rank $p-r$. Notice that $QE = AT^+TAU[0_{(p-r) \times r} I_{(p-r)}]' = AU\Lambda U'U[0_{(p-r) \times r} I_{(p-r)}]' = 0$. Since Q and R are symmetric positive semidefinite, we can use results in [Magnus \(1990\)](#) [Theorem 1(i) with $A = Q$ and $B = R$] to conclude that

$$E \left[\frac{X'QX}{X'RX} \right] < \infty.$$

This concludes the proof of the theorem. \square

4. Numerical study. This section provides some numerical results to showcase the improvement in risk of the minimax estimator over the usual estimator. More precisely, we compared the James–Stein estimator in (2.6) given by

$$\delta^{JS} = \left(I - \frac{(n - 2)SS^+}{(p - n + 3)X'S^+X} \right) X$$

and the usual estimator $\delta^0 = X$ under invariant loss. (In addition, we considered the positive James–Stein estimator to be discussed in Section 5.) The empirical approximations of the invariant risk of these estimators were plotted for $p = 10, 20, 50$ and $n = \frac{p}{2}, p - 1$. Three covariance matrix structures were considered:

Spiked: A diagonal matrix with the first $p/2$ diagonal elements equal to 1, and the last $p/2$ equal to 10.

Autoregressive: Autoregressive covariance matrices of the form

$$\Sigma = \begin{pmatrix} 1 & \rho & \rho^2 & & \\ \rho & 1 & \rho & & \\ \rho^2 & \rho & 1 & & \\ & & & \ddots & \\ & & & & \ddots \end{pmatrix}$$

for $\rho = 0.5$.

Block diagonal: Block diagonal matrices with $p/2$ blocks of the form $\begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$ for $\rho = 0.5$.

In all cases, the true mean was chosen as $\theta \propto (1, \dots, 1)$.

We remind the reader that the risk of the trivial estimator is always p , regardless of θ or Σ . With this in mind, we see from Figure 1 that in all six scenarios the pattern of domination of the new estimator is similar to one of the usual James–Stein estimators. Also note that, as predicted by the theoretical results, the domination decreases as the smaller n tends to p .

5. Comments. An interesting property of the Moore–Penrose inverse is that for any A , AA^+ is the matrix that projects onto the subspace spanned by A (its column space). It follows that the proposed generalized Baranchik estimator can be expressed as

$$\begin{aligned} \delta_r(X, S) &= (I - SS^+)X + \left(1 - \frac{r(X'S^+X)}{X'S^+X} \right) SS^+X \\ (5.1) \qquad &= P_{S^\perp}X + \left(1 - \frac{r(X'S^+X)}{X'S^+X} \right) P_SX, \end{aligned}$$

where $P_S = SS^+$ and $P_{S^\perp} = I - SS^+$ are the projection matrices onto the column space of S and its orthogonal complement, respectively. In terms of the kernel and

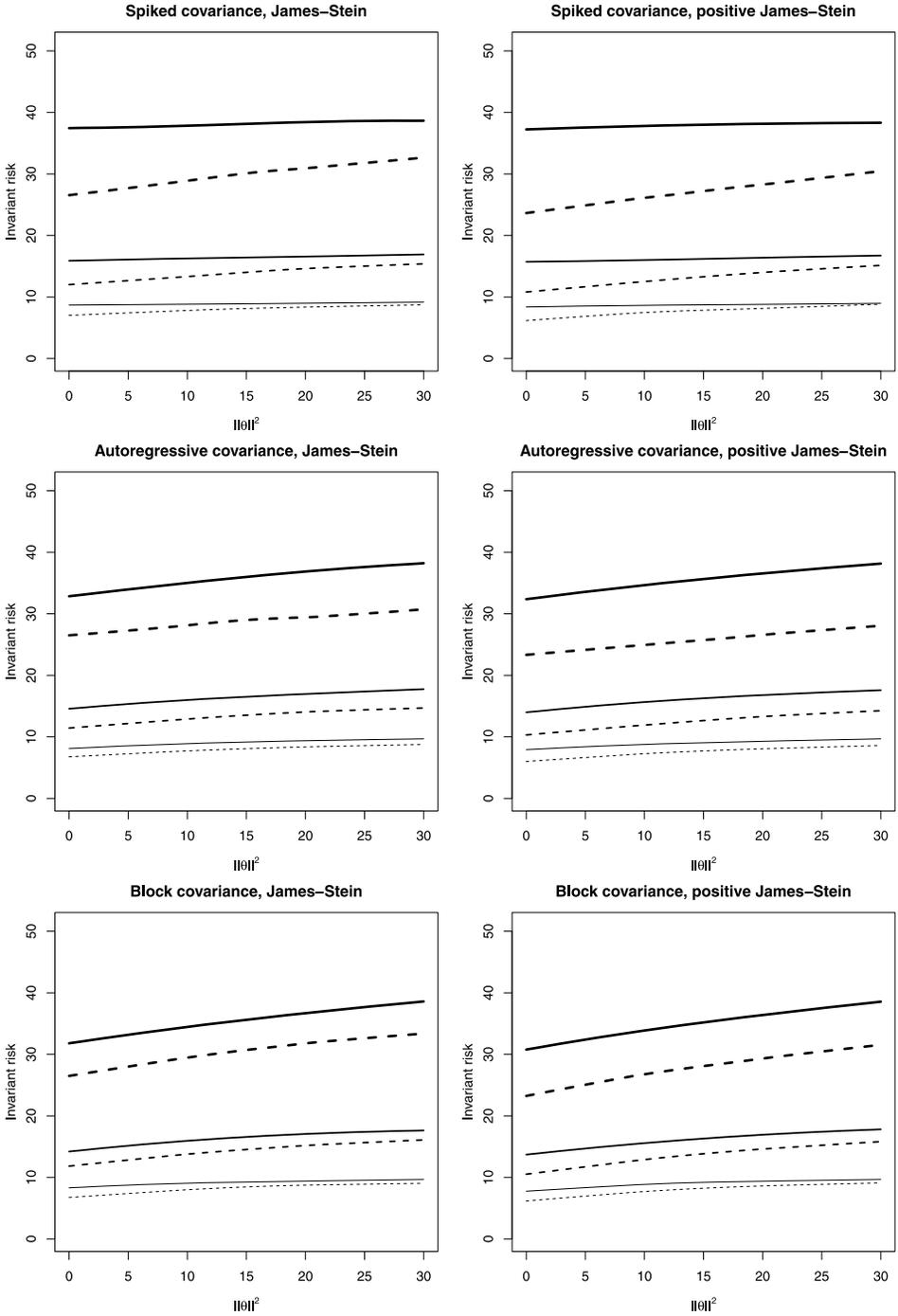


FIG. 1. The risk function plots of δ_a^{JS} and δ_a^{JS+} for $a = (n - 2)/(p - n + 3)$ are in the left and right columns, respectively. The lines, from thinnest to thickest, are for $p = 10, 20$ and 50 . The solid and dashed lines are, respectively, for $n = p/2$ and $n = p - 1$.

image of the symmetric matrix S , $\text{Ker}(P_{S^\perp}) = \text{Im}(S)$ and $\text{Im}(P_{S^\perp}) = \text{Ker}(S^+)$. When $p > n$, this means we can interpret our estimator as applying shrinkage only on the component of X in the subspace spanned by our covariance matrix estimator S . In particular, note that the estimator $P_S \delta_r(X, S) = (1 - \frac{r(X'S^+X)}{X'S^+X})P_S X$ dominates $P_S X$ under invariant loss function (1.1), since $R(P_S \delta_r, \theta) - R(P_S X, \theta) = R(\delta_r, \theta) - R(X, \theta) \geq 0$ if r satisfies the conditions of Theorem 1. This suggests there might be an easier, more abstract proof of Theorem 1, one not relying on brute computations but on the already known full rank S case, although we have not been able to obtain such a result.

A natural extension of the James–Stein estimator, δ_a^{JS} in (2.6), is a positive-part-type James–Stein estimator. The form of the estimator in (5.1) suggests

$$(5.2) \quad \delta_a^{\text{JS}^+} = (I - SS^+)X + \left(1 - \frac{a}{X'S^+X}\right)_+ SS^+X,$$

where $b_+ = \max(b, 0)$. Simulation evidence from Figure 1 suggests that for $a = (n - 2)/(p - n + 3)$, $\delta_a^{\text{JS}^+}$ dominates δ_a^{JS} under invariant loss.

One of the interesting differences between the $n > p$ and $p > n$ cases is the reversal of the roles of p and n . This is essentially due to the distribution of the singular values of S . Recall that for $S = ATA$, $T \sim W_p(n, I_n)$. We can write the singular value decomposition of T as $T = H'DH$, but we can also write it as $T = H_1'D_1H_1$, where H_1 is semi-orthogonal ($H_1H_1' = I$) and D_1 is the matrix of the positive eigenvalues of T . If T has full rank (i.e., $n \geq p$), this coincides with the singular value decomposition of T . In the full rank case the joint density of H and D is given in (3.17), whereas in the rank-deficient case ($p > n$) joint density is given by (3.18), from which stems the reversal of the roles of p and n .

In the heteroscedastic normal mean estimation problem, James and Stein (1961) used the loss function that was weighted by the inverse of the variances and, consequently, the problem is essentially transformed to the homoscedastic case under ordinary squared error loss. Similarly, in this article, we used the invariant loss function in (1.1), therefore skirting a somewhat subtle issue. In the heteroscedastic setting where there are differing coordinate variances, minimax estimation and Bayes (or empirical Bayes) estimates can be qualitatively different. It turns out that minimax estimators in general shrink most on the coordinates with smaller variances, while Bayes estimators shrink most on large variance coordinates. Brown (1975) shows that the James–Stein shrinkage estimator does not dominate the X when the largest variance is larger than the sum of the rest. Moreover, Casella (1980) points out that the James–Stein shrinkage estimator may not be a desirable shrinkage estimator under heteroscedasticity even when it is minimax. Morris and Lysy (2012) and Brown, Nie and Xie (2013) give an excellent perspective on minimaxity of the shrinkage estimator from Bayes and empirical Bayes points of view. Consequently, it would be of interest to examine the shrinkage patterns of the proposed estimates in the case of a noninvariant loss function and assess how well the invariant loss works for $p > n$ applications.

One can imagine an extension of the results of this article beyond the normal distribution setting. Consider a model with the joint density for (X, S) the form

$$(5.3) \quad f(\text{tr } \Sigma^{-1}[(X - \theta)(X - \theta)' + S]),$$

where the $p \times 1$ location vector θ and the $p \times p$ scale matrix Σ are unknown. In the setting of $p \leq n$, Fourdrinier, Strawderman and Wells (2003) and Kubokawa and Srivastava (2001) give some results on improved location estimation for elliptically symmetric distributions. For more on elliptical symmetry and the various choices of $f(\cdot)$ in (5.3), see Fang, Kotz and Ng (1990); the class in (5.3) contains models such as the multivariate normal, t - and Kotz-type distributions.

Finally, simulation study reveals that, when p is much larger than n , the estimate of Σ and Σ^{-1} are quite poor. This observation agrees with Kubokawa and Srivastava (2008), where Haff (1979)-type improved estimates of Σ are proposed. It would be of interest to use an improved estimator of Σ in $\delta_r(X, S)$ in (2.1). As pointed out in the testing context by Srivastava and Fujikoshi (2006) and Srivastava (2007), a shortcoming of S^+ is that the associated estimator is only orthogonally invariant, while the sample mean vector is invariant.

Acknowledgments. The authors are grateful to the Associate Editor and referees for helpful comments that strengthened the exposition and scope of this paper.

REFERENCES

- BARANCHIK, A. J. (1970). A family of minimax estimators of the mean of a multivariate normal distribution. *Ann. Math. Statist.* **41** 642–645. [MR0253461](#)
- BERGER, J. O. and BOCK, M. E. (1976). Combining independent normal mean estimation problems with unknown variances. *Ann. Statist.* **4** 642–648. [MR0403085](#)
- BERGER, J. and HAFF, L. R. (1983). A class of minimax estimators of a normal mean vector for arbitrary quadratic loss and unknown covariance matrix. *Statist. Decisions* **1** 105–129. [MR0694363](#)
- BERGER, J., BOCK, M. E., BROWN, L. D., CASELLA, G. and GLESER, L. (1977). Minimax estimation of a normal mean vector for arbitrary quadratic loss and unknown covariance matrix. *Ann. Statist.* **5** 763–771. [MR0443156](#)
- BICKEL, P. J. and LEVINA, E. (2008). Regularized estimation of large covariance matrices. *Ann. Statist.* **36** 199–227. [MR2387969](#)
- BROWN, L. D. (1975). Estimation with incompletely specified loss functions (the case of several location parameters). *J. Amer. Statist. Assoc.* **70** 417–427. [MR0373082](#)
- BROWN, L. D., NIE, H. and XIE, X. (2013). Ensemble minimax estimation for multivariate normal means. *Ann. Statist.* To appear.
- CASELLA, G. (1980). Minimax ridge regression estimation. *Ann. Statist.* **8** 1036–1056. [MR0585702](#)
- D’ASPROMONT, A., BANERJEE, O. and EL GHAOU, L. (2008). First-order methods for sparse covariance selection. *SIAM J. Matrix Anal. Appl.* **30** 56–66. [MR2399568](#)
- FANG, K. T., KOTZ, S. and NG, K. W. (1990). *Symmetric Multivariate and Related Distributions. Monographs on Statistics and Applied Probability* **36**. Chapman & Hall, London. [MR1071174](#)
- FOURDRINIER, D. and STRAWDERMAN, W. E. (2003). On Bayes and unbiased estimators of loss. *Ann. Inst. Statist. Math.* **55** 803–816. [MR2028618](#)

- FOURDRINIER, D., STRAWDERMAN, W. E. and WELLS, M. T. (2003). Robust shrinkage estimation for elliptically symmetric distributions with unknown covariance matrix. *J. Multivariate Anal.* **85** 24–39. [MR1978175](#)
- GLESER, L. J. (1979). Minimax estimation of a normal mean vector when the covariance matrix is unknown. *Ann. Statist.* **7** 838–846. [MR0532247](#)
- GLESER, L. J. (1986). Minimax estimators of a normal mean vector for arbitrary quadratic loss and unknown covariance matrix. *Ann. Statist.* **14** 1625–1633. [MR0868326](#)
- GOLUB, G. H. and PEREYRA, V. (1973). The differentiation of pseudo-inverses and nonlinear least squares problems whose variables separate. *SIAM J. Numer. Anal.* **10** 413–432. [MR0336980](#)
- HAFF, L. R. (1979). An identity for the Wishart distribution with applications. *J. Multivariate Anal.* **9** 531–544. [MR0556910](#)
- JAMES, W. and STEIN, C. (1961). Estimation with quadratic loss. In *Proc. 4th Berkeley Sympos. Math. Statist. and Prob., Vol. 1* 361–379. Univ. California Press, Berkeley, CA. [MR0133191](#)
- 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. [MR2560366](#)
- KUBOKAWA, T. and SRIVASTAVA, M. S. (2001). Robust improvement in estimation of a mean matrix in an elliptically contoured distribution. *J. Multivariate Anal.* **76** 138–152. [MR1811829](#)
- 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. [MR2466543](#)
- LEDOIT, O. and WOLF, M. (2004). A well-conditioned estimator for large-dimensional covariance matrices. *J. Multivariate Anal.* **88** 365–411. [MR2026339](#)
- LEVINA, E., ROTHMAN, A. and ZHU, J. (2008). Sparse estimation of large covariance matrices via a nested Lasso penalty. *Ann. Appl. Stat.* **2** 245–263. [MR2415602](#)
- MAGNUS, J. R. (1990). On certain moments relating to ratios of quadratic forms in normal variables: Further results. *Sankhyā Ser. B* **52** 1–13. [MR1178889](#)
- MORRIS, C. and LYSY, M. (2012). Shrinkage estimation in multi-level normal models. *Statist. Sci.* **27** 115–134. [MR2953499](#)
- MUIRHEAD, R. J. (1982). *Aspects of Multivariate Statistical Theory*. Wiley, New York. [MR0652932](#)
- ROTHMAN, A. J., BICKEL, P. J., LEVINA, E. and ZHU, J. (2008). Sparse permutation invariant covariance estimation. *Electron. J. Stat.* **2** 494–515. [MR2417391](#)
- SRIVASTAVA, M. S. (2003). Singular Wishart and multivariate beta distributions. *Ann. Statist.* **31** 1537–1560. [MR2012825](#)
- SRIVASTAVA, M. S. (2007). Multivariate theory for analyzing high dimensional data. *J. Japan Statist. Soc.* **37** 53–86. [MR2392485](#)
- SRIVASTAVA, M. S. and BILODEAU, M. (1989). Stein estimation under elliptical distributions. *J. Multivariate Anal.* **28** 247–259. [MR0991949](#)
- SRIVASTAVA, M. S. and FUJIKOSHI, Y. (2006). Multivariate analysis of variance with fewer observations than the dimension. *J. Multivariate Anal.* **97** 1927–1940. [MR2301265](#)
- SRIVASTAVA, M. S. and KHATRI, C. G. (1979). *An Introduction to Multivariate Statistics*. North-Holland, New York. [MR0544670](#)
- STEIN, C. M. (1981). Estimation of the mean of a multivariate normal distribution. *Ann. Statist.* **9** 1135–1151. [MR0630098](#)
- STEIN, C. (1977). Lectures on the theory of estimation of many parameters. In *Studies in the Statistical Theory of Estimation, Part 1* 74–65. Proc. Scientific Seminars Steklov Institute, Leningrad Division. (In Russian.) [MR0501548](#)

TIAN, Y. and CHENG, S. (2004). Some identities for Moore–Penrose inverses of matrix products.
Linear Multilinear Algebra **52** 405–420. [MR2102196](#)

DEPARTMENT OF STATISTICAL SCIENCE
COMSTOCK HALL
CORNELL UNIVERSITY
ITHACA, NEW YORK 14853
USA
E-MAIL: dc623@cornell.edu
mtw1@cornell.edu