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Estimation of the inverse scatter matrix of an elliptically symmetric distribution

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ABSTRACT

We consider estimation of the inverse scatter matrices Σ^{-1} for high-dimensional elliptically symmetric distributions. In high-dimensional settings the sample covariance matrix S may be singular. Depending on the singularity of S, natural estimators of Σ^{-1} are of the form $a\,S^{-1}$ or $a\,S^{+}$ where a is a positive constant and S^{-1} and S^{+} are, respectively, the inverse and the Moore–Penrose inverse of S. We propose a unified estimation approach for these two cases and provide improved estimators under the quadratic loss $\mathrm{tr}(\hat{\Sigma}^{-1}-\Sigma^{-1})^2$. To this end, a new and general Stein–Haff identity is derived for the high-dimensional elliptically symmetric distribution setting.

1. Introduction

The estimation of covariance and inverse covariance matrices in a high-dimensional framework has seen a surge of interest in the past years. Of these, estimates of the inverse covariance matrix are required in many multivariate inference procedures including the Fisher linear discriminant analysis, confidence intervals based on the Mahalanobis distance, optimal portfolio selection, graphical models, and weighted least squares estimator in multivariate linear regression models. Estimation of the precision matrix in the classical multivariate setting has been studied by Efron and Morris [12], Haff [21], Dey [9], Krishnamoorthy and Gupta [24], Dey et al. [10], Zhou et al. [43], and Tsukuma and Konno [42].

The natural estimator of the inverse covariance matrix, based on the sample covariance matrix, is well known to be inadequate in the high-dimensional context. When the dimension is of the same order of the sample size the sample covariance matrix becomes unstable and has large estimation error. It is also well known that the eigenvalues of sample covariance matrix are over-dispersed, that is, the eigenvalues of sample covariance matrix are not good estimators of their population counterpart Marčenko and Pastur [33]. Additionally, in the setting where the dimension of the sample covariance matrix is larger than the sample size, the inverse of the sample covariance matrix does not exist. An estimator of the precision

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matrix for the multivariate normal distribution based on the Moore–Penrose generalized inverse of the sample covariance matrix was developed in Kubokawa and Srivastava [27]. Kubokawa and Inoue [25] consider general types of ridge estimators for covariance and precision matrices, and derive asymptotic expansions of their risk functions. More generally, the idea to correct (shrink) the eigenvalues of the sample covariance matrix is also found in previous work by Ledoit and Wolf [29], El Karoui [14], Ledoit and Wolf [30] and Donoho [11]. The problem has been examined under many sparsity scenarios, for example, zero elements of the matrix [2,13,38,6] or its inverse [34,20,37,28,7,36], bandedness [3,4] among others.

Most of the results for improved estimation for covariance and inverse covariance matrices have been developed in the context of the multivariate normal distribution. In this article we consider a large subclass of the elliptically contoured distributions. Let $(X, U) = (X, U_1, \dots, U_n)$ be $n + 1$ p-dimensional random vectors having an elliptically symmetric distribution with joint density of the form

$$\begin{aligned}(x, u) \mapsto\ & |\Sigma|^{-(n+1)/2} f\left((x-\theta)^\top \Sigma^{-1}(x-\theta) + \sum_{i=1}^n u_i^\top \Sigma^{-1} u_i\right) \\ =\ & |\Sigma|^{-(n+1)/2} f\left(\mathrm{tr}\left[\Sigma^{-1}(x-\theta)(x-\theta)^\top + \Sigma^{-1} s\right]\right), \end{aligned} \tag{1.1}$$

where X and the U_i's are $p \times 1$ vectors, θ is a $p \times 1$ unknown location vector, $S = UU^\top$ is a $p \times p$ matrix and Σ is a $p \times p$ unknown scatter matrix proportional to the covariance matrix. In the following, $E_{\theta,\Sigma}$ will denote the expectation with respect to the density in (1.1) and $E^*_{\theta,\Sigma}$ the expectation with respect to the density

$$(x, u) \mapsto \frac{1}{K} |\Sigma|^{-(n+1)/2} F\left(\mathrm{tr}\left[\Sigma^{-1}(x-\theta)(x-\theta)^\top + \Sigma^{-1} s\right]\right), \tag{1.2}$$

where

$$F(t) = \frac{1}{2}\int_t^\infty f(u)du \tag{1.3}$$

and

$$K = \int_{\mathbb{R}^{p+k}} |\Sigma|^{-(n+1)/2} F\left(\mathrm{tr}\left[\Sigma^{-1}(x-\theta)(x-\theta)^\top + \Sigma^{-1} s\right]\right) dx\, du \tag{1.4}$$

is the normalizing constant which is assumed to be finite. Note that these two expectations are related since, for any integrable function $H(X, U)$, we have

$$K\, E^*_{\theta,\Sigma}[H(X,U)] = E_{\theta,\Sigma}[\varphi_{\theta,\Sigma}(X,U)\, H(X,U)] \tag{1.5}$$

where

$$\varphi_{\theta,\Sigma}(X,U) = \frac{F\left((X-\theta)^\top \Sigma^{-1}(X-\theta) + \sum_{i=1}^n U_i^\top \Sigma^{-1} U_i\right)}{f\left((X-\theta)^\top \Sigma^{-1}(X-\theta) + \sum_{i=1}^n U_i^\top \Sigma^{-1} U_i\right)}.$$

The general model in (1.1) has been considered by various authors, for more details, see Fourdrinier, Strawderman and Wells [19] where the model is viewed as the canonical form of the general linear model. For more on elliptically symmetric distributions and the various choices of $f(\cdot)$ in (1.1) see Bilodeau and Brenner [5] and Fang, Kotz, and Ng [15]. The class in (1.1) contains models such as the multivariate normal, t-, and Kotz-type distributions. In the setting of the multivariate normal distribution, since $F = f$, we have $E_{\theta,\Sigma} = E^*_{\theta,\Sigma}$. Improved estimation of the scatter matrix for elliptical distribution models, from a decision theoretic point of view, has been considered by Fang and Li [16], Fang and Li [32], Leung and Ng [31], and Tsukuma [41].

In this article, we consider estimation of the inverse scatter matrix Σ^{-1} in (1.1) under the quadratic loss

$$L(\hat{\Sigma}^{-1}, \Sigma^{-1}) = \mathrm{tr}\big((\hat{\Sigma}^{-1} - \Sigma^{-1})^2\big), \tag{1.6}$$

where $\hat{\Sigma}^{-1}$ estimates Σ^{-1} and $\mathrm{tr}(M)$ denotes the trace of a matrix M. By definition, the risk of $\hat{\Sigma}^{-1}$ is

$$R(\hat{\Sigma}^{-1}, \Sigma^{-1}) = E_{\theta,\Sigma}[L(\hat{\Sigma}^{-1}, \Sigma^{-1})]. \tag{1.7}$$

When S is invertible ($p \le n$), the "usual" estimators are of the form $a S^{-1}$ for some positive constant a. Tsukuma [41] showed that there exists a_* such that, $a_* S^{-1}$ is unbiased where

$$a_* = a_0 \left(\frac{2\,\pi^{p/2}}{\Gamma(p/2)} \int_0^\infty r^{p-1}\,(-2 f'(r^2))\, dr\right)^{-1}, \tag{1.8}$$

where $a_0 = n - p - 1$ and $S = UU^\top$. Note that for the normal distribution, $a_* = a_0$.

When S is singular (that is, when $p > n$) the estimation of Σ^{-1} is more delicate. The reference estimators parallel the case where S is invertible, however S^{-1} is replaced by S^{+} the Moore–Penrose inverse of S. Consequently, the usual estimators are of the form $a\,S^{+}$ for some positive constant a. Note that the choice of the constant a differs from the invertible case. Indeed, for instance, Kubokawa and Srivastava [27] used $a = p - n - 3$ when S is not invertible while, in the normal case, the choice of $a = n - p - 1$ corresponds to an unbiased estimator of Σ^{-1}, when S is invertible. In the setting of estimating Σ under invariant loss, the results in Konno [23] suggest using $a = 1/(n + p + 1)$.

In this article, we provide a unified approach of the settings where S is invertible and S is not invertible. To this end, we use the common notation S^{+} for both inverses since the Moore–Penrose inverse of S equals the regular inverse in the nonsingular setting. For a fixed positive constant a, we consider competitive inverse scatter matrix estimators to $a\,S^{+}$ of the form

$$\hat{\Sigma}_G^{-1} = a\,S^{+} + S\,G(X, S), \tag{1.9}$$

where $G(X, S)$ is some $p \times p$ matrix function. We develop conditions on the function G in order that $\hat{\Sigma}_G^{-1}$ improves on $a\,S^{+}$ under the loss (1.6) and risk (1.7). In particular, we find sufficient conditions on $G(X, S)$ so that the risk difference between $a\,S^{+} + S\,G(X, S)$ and $a\,S^{+}$,

$$\begin{aligned}\Delta(G) &= R(a\,S^{+} + S\,G(X, S),\, \Sigma^{-1}) - R(a\,S^{+},\, \Sigma^{-1}) \\ &= E_{\theta,\Sigma}\left[\operatorname{tr}\left(\{S\,G(X, S)\}^2 + 2\,a\,S^{+}\,S\,G(X, S)\right)\right] - 2\,E_{\theta,\Sigma}\left[\operatorname{tr}(\Sigma^{-1} S\,G(X, S))\right]\end{aligned} \tag{1.10}$$

is non-positive.

For estimation of the inverse scatter matrix relative to the quadratic loss in (1.6), we can address the construction of improved estimators for both the invertible and noninvertible cases in the unified framework. The paper is organized as follows. Section 2 develops a novel general Stein–Haff type identity for elliptically symmetric distributions and gives various forms of the unbiased estimate of the risk difference between $a\,S^{+}$ and orthogonally invariant estimators of the form of (1.9). Section 3 gives examples of the function $G(X, S)$ in (1.9) related to Efron and Morris [12] type estimators that lead to improved estimator of the inverse scatter matrix. Section 4 gives a number of examples of elliptically symmetric distributions that extend the classical normal theory. Concluding remarks are given in Section 5. The principal technical tools and proofs are given in the Appendix.

The following notation will be used throughout. The real p-dimensional orthogonal group of real $p \times p$ matrices is denoted $\mathcal{O}_p(\mathbb{R})$. The p-dimensional Wishart distribution with n degrees of freedom and covariance matrix Σ is written $W_p(n, \Sigma)$. For any matrix M, $\operatorname{vec}(M)$ denotes the vectorization of M and ∇_M is interpreted as the matrix with components $(\nabla_M)_{ij} = \partial/\partial M_{ij}$. The differential operator for a symmetric matrix S is $\mathcal{D}_S = \left(\frac{1}{2}\,(1 + \delta_{ij})\,(\nabla_S)_{ij}\right)$ and Haff differential operator is defined, for any $p \times p$ matrix function of a symmetric matrix S, $H(S)$, to be $D^{*}_{1/2}(H(S)) = \operatorname{tr}\big(\mathcal{D}_S\,H(S)\big)$.

2. Orthogonally invariant estimators

To develop analytical dominance properties of the proposed estimators, we need to derive the so-called Stein–Haff identity for the singular elliptically contoured distributions in (1.1). The Stein–Haff identity was derived by Stein [40] and Haff [22] for the full rank Wishart distribution and Kubokawa and Srivastava [27], Konno [23], and Chételat and Wells [8] for the singular Wishart distribution, respectively. A similar identity for the full rank elliptically symmetric distributions was developed by Kubokawa and Srivastava [26]. The following Stein–Haff type identity, which is proved in Appendix A.2, is an extension of a result in Konno [23] and Chételat and Wells [8] to the case of elliptical distributions of the form of (1.1). Note that a similar lemma has been provided in the elliptical case by Fourdrinier, Strawderman and Wells [18] through the Haff differential operator, however they only considered the case where the matrix S is nonsingular.

Lemma 2.1. *Let $G(x, s)$ be a $p \times p$ matrix function such that, for any fixed x, $G(x, s)$ is weakly differentiable in s and such that $E_{\theta,\Sigma}\left[\left|\operatorname{tr}\left(\Sigma^{-1} S\,G(X, S)\right)\right|\right] < \infty$. We have*

$$E_{\theta,\Sigma}\left[\operatorname{tr}\left(\Sigma^{-1} S\,G(X, S)\right)\right] = K\,E^{*}_{\theta,\Sigma}\left[n\operatorname{tr}\left(G(X, S)\right) + \operatorname{tr}\left(U\,\nabla_{U^{\top}}\,G^{\top}(X, S)\right)\right]. \tag{2.1}$$

Remark 2.1. By noticing that $S = S\,S^{+}\,S$, an equivalent expression for (2.1) is

$$E_{\theta,\Sigma}\left[\operatorname{tr}\left(\Sigma^{-1} S\,G(X, S)\right)\right] = K\,E^{*}_{\theta,\Sigma}\left[n\operatorname{tr}\left(S^{+}\,S\,G(X, S)\right) + \operatorname{tr}\left(U\,\nabla_{U^{\top}}\left(G^{\top}(X, S)\,S^{+}\,S\right)\right)\right]. \tag{2.2}$$

An application of the extended Stein–Haff identity in Lemma 2.1, it is immediate to see that $\Delta(G)$ in (1.10) is given by the following proposition.

Proposition 2.1. *The risk difference in (1.10) is*

$$\Delta(G) = E_{\theta,\Sigma}\left[\operatorname{tr}\left(\{S\,G(X, S)\}^2 + 2\,a\,S^{+}\,S\,G(X, S)\right)\right] - 2\,K\,E^{*}_{\theta,\Sigma}\left[n\operatorname{tr}\left(G(X, S)\right) + \operatorname{tr}\left(U\,\nabla_{U^{\top}}\,G^{\top}(X, S)\right)\right]. \tag{2.3}$$

A drawback with the risk difference in (2.3) is its dependence with respect to both expectations $E_{\theta,\Sigma}$ and $E^*_{\theta,\Sigma}$. This is not an issue for the multivariate normal distribution since $E_{\theta,\Sigma} = E^*_{\theta,\Sigma}$. A remedy to this nonhomogeneity is to use (1.5) in order to deal with a quantity expressed through the only expectation $E_{\theta,\Sigma}$. Clearly, according to (1.5), we have

$$\begin{aligned}\Delta(G) = {} & E_{\theta,\Sigma}\left[\operatorname{tr}\left(\{S\,G(X,S)\}^2 + 2\,a\,S^+ S\,G(X,S)\right)\right] \\ & - 2\,E_{\theta,\Sigma}\left[\varphi_{\theta,\Sigma}(X,U)\,\left\{n\operatorname{tr}(G(X,S)) + \operatorname{tr}\left(U\,\nabla_{U^\top}\,G^\top(X,S)\right)\right\}\right].\end{aligned} \tag{2.4}$$

However the dependence of the integrand term in (2.4) on the unknown parameters θ and Σ through $\varphi_{\theta,\Sigma}(X,U)$ is still problematic. This dependence can be managed if the density in (1.1) is such that the ratio $F(t)/f(t)$ is bounded, in the sense that an upper bound for the risk difference $\Delta(G)$ can be found. Then, using this upper bound, sufficient conditions for improvement of $a\,S^+ + S\,G(X,S)$ over $a\,S^+$ can be derived.

In Theorem 2.1 we will require that there exists a positive constant b such that

$$\frac{F(t)}{f(t)} \le b. \tag{2.5}$$

The ratio f/F is refereed to as the reversed hazard rate. It is worth noticing that, when estimating a location parameter of a spherically symmetric distribution, a typical class of densities is the one introduced by Berger [1] who assumes that there exists a constant $c > 0$ such that

$$\frac{F(t)}{f(t)} \ge c. \tag{2.6}$$

Nevertheless, we will see in Section 3 that (2.6) is also an appropriate class of densities in the covariance and inverse scatter matrix context. In Section 4 we give some examples of densities satisfying (2.5) and (2.6). Note that, for these examples, the ratio $F(t)/f(t)$ is nonincreasing and hence $b = F(0)/f(0)$.

Here follows our first result of improvement of $a\,S^+ + S\,G(X,S)$ over $a\,S^+$.

Theorem 2.1. *Consider a density as in (1.1) satisfying (2.5) and assume that $|n-p| \ge 3$. Under the conditions*

$$\operatorname{tr}\left((n - |n-p| + 3)\,G(X,S) + U\,\nabla_{U^\top}\,G^\top(X,S)\right) \ge 0 \tag{2.7}$$

and

$$\operatorname{tr}(G(X,S)) \le 0 \tag{2.8}$$

the estimator $a\,S^+ + S\,G(X,S)$ improves over $a\,S^+$ if

$$\operatorname{tr}\left(\{S\,G(X,S)\}^2 + 2\,(a\,S^+ S - b\,(|n-p| - 3))\,G(X,S)\right) \le 0. \tag{2.9}$$

Proof. Subtracting and adding the term $\left(|n-p| - 3\right)\operatorname{tr}(G(X,S))$, the risk difference in (2.4) can be written as

$$\begin{aligned}\Delta(G) = {} & E_{\theta,\Sigma}\left[\operatorname{tr}\left(\{S\,G(X,S)\}^2 + 2\,a\,S^+ S\,G(X,S)\right)\right] \\ & - 2\,E_{\theta,\Sigma}\left[\varphi_{\theta,\Sigma}(X,U)\,\left\{\left(n - |n-p| + 3\right)\operatorname{tr}(G(X,S)) + \operatorname{tr}\left(U\,\nabla_{U^\top}\,G^\top(X,S)\right)\right\}\right] \\ & - 2\,E_{\theta,\Sigma}\left[\varphi_{\theta,\Sigma}(X,U)\,\left\{\left(|n-p| - 3\right)\operatorname{tr}(G(X,S))\right\}\right].\end{aligned}$$

With this expression, successively using Condition (2.7) and Condition (2.5), Condition (2.8) and the fact that $|n-p|-3 \ge 0$, it is clear that $\Delta(G)$ is bounded from above by

$$E_{\theta,\Sigma}\left[\operatorname{tr}\left(\{S\,G(X,S)\}^2 + 2\,(a\,S^+ S - b\,(|n-p| - 3))\,G(X,S)\right)\right],$$

which is nonpositive if (2.9) holds. □

Note that the constant a in (2.9) is the factor multiplying the projector $S^+ S$. It may be convenient that $S^+ S$ appears homogeneously in the improvement conditions. This is specified in the remark below following the same lines in the proof of Theorem 2.1 and using Identity (2.2) of Remark 2.1. Also note that the conditions for domination depends on the underlying density in (1.1) through the constant b. Consequently, in the context of inverse scatter matrix estimation the improvement is not robust with respect to the class of elliptically symmetric distribution as in location parameter estimation (see Fourdrinier, Strawderman and Wells [18]). This is not surprising since the constant for unbiasedness, a_* in (1.8), also depends on f.

Remark 2.2. Under the conditions

$$\operatorname{tr}\left((n - |n-p| + 3)\,S^+ S\,G(X,S) + U\,\nabla_{U^\top}\left(G^\top(X,S)\,S^+ S\right)\right) \ge 0 \tag{2.10}$$

and

$$\mathrm{tr}\left(S^{+}\, S\, G(X,S)\right) \le 0 \tag{2.11}$$

the estimator $a\,S^{+} + S\,G(X,S)$ improves over $a\,S^{+}$ as soon as the inequality

$$\mathrm{tr}\left(\{S\,G(X,S)\}^2 + 2\,(a - b\,(|n-p|-3))\,S^{+}\,S\,G(X,S)\right) \le 0 \tag{2.12}$$

holds.

Theorem 2.1 is particularly appropriate to deal with orthogonally invariant estimators of the form

$$\hat{\Sigma}_{\phi}^{-1} = H_1\,\phi(L)\,H_1^{\top} \tag{2.13}$$

through the eigenvalue decomposition of S as

$$S = H_1\,L\,H_1^{\top} \tag{2.14}$$

where $L = \mathrm{diag}(l_1, \ldots, l_{n\wedge p})$ with

$$l_1 > l_2 > \cdots > l_{n\wedge p}, \tag{2.15}$$

and where H_1 is a matrix such that $H_1^{\top}\,H_1 = I_{n\wedge p}$. The dimensions of H_1 are specified as follows: when $p \le n$, H_1 is a $p \times p$ orthogonal matrix ($H_1^{\top}\,H_1 = I_p$) while, when $p > n$, H_1 is a $p \times n$ semi-orthogonal matrix ($H_1^{\top}\,H_1 = I_n$). In this last case, it will be convenient to complete H_1 by a $p \times (p-n)$ matrix H_2 such that $H = (H_1\ H_2)$ is $p \times p$ orthogonal matrix (see Appendix A.3). Note that, when $p \le n$, we will consider that $H = H_1$.

The diagonal matrix $\phi(L) = \mathrm{diag}(\phi_1(L), \ldots, \phi_{n\wedge p}(L))$ in (2.13) is more conveniently expressed as

$$\phi_k(L) = \frac{\delta_k(L)}{l_k} \quad \text{for } k = 1, \ldots, n \wedge p. \tag{2.16}$$

We will assume that

$$\delta_1(L) \ge \delta_2(L) \ge \cdots \ge \delta_{n\wedge p}(L) \tag{2.17}$$

and are differentiable with

$$\frac{\partial \delta_k(L)}{\partial l_k} \ge 0 \quad \text{for } k = 1, \ldots, n \wedge p. \tag{2.18}$$

Setting $S\,G(X,S) = \hat{\Sigma}_{\phi}^{-1} - a\,S^{+}$ (note that $L = H_1^{\top}\,S\,H_1$ and $L^{-1} = H_1^{\top}\,S^{+}\,H_1$), we have

$$S\,G(X,S) = H_1\,\Psi(L)\,H_1^{\top} \tag{2.19}$$

where $\Psi(L) = \mathrm{diag}(\psi_1(L), \ldots, \psi_{n\wedge p}(L))$ with

$$\psi_k(L) = \frac{\delta_k(L) - a}{l_k} \quad \text{for } k = 1, \ldots, n \wedge p. \tag{2.20}$$

Hence

$$G(X,S) = H_1\,L^{-1}\,\Psi(L)\,H_1^{\top} = H_1\,L^{-2}\,(\delta(L) - a\,I_{n\wedge p})\,H_1^{\top}. \tag{2.21}$$

In this context, we have the following result for the orthogonally invariant estimators $\hat{\Sigma}_{\phi}^{-1}$ in (2.13).

Corollary 2.1. *Consider a density as in* (1.1) *satisfying* (2.5) *with* $|n-p| \ge 3$. *Assume that Condition* (2.17) *and Condition* (2.18) *are satisfied. Then* $\hat{\Sigma}_{\phi}^{-1}$ *in* (2.13) *improves over* $a\,S^{+}$ *as soon as*

$$2\,b\,(|n-p|-3) - a \le \delta_k(L) \le a. \tag{2.22}$$

Proof. First note that Condition (2.8) holds since, we have

$$\mathrm{tr}\,(G(X,S)) = \sum_{i=k}^{n\wedge p} \frac{\delta_k(L) - a}{l_k^2} \le 0$$

by (2.21) and the second inequality in (2.22). Also Corollary A in Appendix A.3 guarantees that Condition (2.7) is satisfied under Conditions (2.17) and (2.18) and the second inequality in (2.22).

Now, as we have

$$\operatorname{tr}\left(\{S\,G(X,S)\}^2 + 2\,a\,S^+\,S\,G(X,S)\right) = \operatorname{tr}\left(\hat{\Sigma}_\phi^{-2} - a^2\,(S^+)^2\right) = \sum_{k=1}^p \frac{\delta_k^2(L) - a^2}{l_k^2},$$

the left hand-side of (2.9) is expressed as

$$\begin{aligned}\operatorname{tr}\left(\{S\,G(X,S)\}^2 + 2\,[a - b\,(|n-p|+3)]\,G(X,S)\right) &= \sum_{k=1}^p \left\{\frac{\delta_k^2(L) - a^2}{l_k^2} - 2\,b\,(|n-p|+3)\,\frac{\delta_k(L) - a}{l_k^2}\right\} \\ &= \sum_{k=1}^p \frac{1}{l_k^2}\,(\delta_k(L) - a)\,(\delta_k(L) + a - 2\,b\,(|n-p|+3)),\end{aligned}$$

which is nonpositive under Condition (2.22). □

As a first simple application of Corollary 2.1, consider $\hat{\Sigma}_\phi^{-1} = a_1\,S^+$, with $a_1 > 0$, as an alternative estimator to $a\,S^+$. Here, as $\Phi(L) = a_1\,L^{-1}$, we have $\delta(L) = a_1\,I_{n\wedge p}$ (so that $\psi(L) = (a_1 - a)L^{-1}$). Corollary 2.1 guarantees that improvement condition (2.22) of $a_1\,S^+$ over $a\,S^+$ is

$$2\,b\,(|n-p|-3) - a \le a_1 \le a.$$

In the normal case (i.e. $f(t) \propto \exp(t/2)$) and when S is invertible (i.e. $p \le n$), the reference estimator is the unbiased estimator $a\,S^+$ with $a = n - p - 1$. As, in this context, $F = f$, and then $E_{\theta,\Sigma} = E^*_{\theta,\Sigma}$, we can take $b = 1$ so that Condition (2.22) reduces to

$$n - p - 5 \le a_1 \le n - p - 1.$$

This is Condition (i) in Theorem 2.1 of Tsukuma and Konno [42].

Note that a natural choice of a is $a = b(|n-p|-3)$ so that (2.22) holds with $\delta(L) = b(|n-p|-3)I_{n\wedge p}$. In the normal setting with $b = 1$, this choice of a coincides with the one in Kubokawa and Srivastava [27].

Two additional examples that satisfy (2.22), which are generalizations of Remark 2.1 in Tsukuma and Konno [42], set $\delta_i^{AU}(L) = a - (2a - 2b(|n-p|-3))(i-1)/(n\wedge p - 1)$ and $\delta_i(L) = 2b(|n-p|-3) - a + (2a - 2b(|n-p|-3))l_i/l_{i+1}$.

3. Efron–Morris type estimators

Theorem 2.1 is not well adapted to some orthogonally invariant estimators, for instance to Efron and Morris [12] type estimators that are of the form $a\,S^+ + \beta(t)/t\,S\,S^+$, where $t = \operatorname{tr}(S)$ and β is a nonnegative function. These estimators correspond, in (2.16), to $\delta_k = a + l_k\,\beta(t)/t$, so that Condition (2.22) is not satisfied. Actually, Theorem 2.1 may not apply to estimators which are not orthogonally invariant such as the following estimators which extend the ones considered by Tsukuma and Konno [42]. Let Q be a $p \times q$ matrix of constants with rank $\operatorname{rk}(Q) = q$ and let $G(X,U) = \beta(t)/t\,S^+\,Q_0$ where β is a differentiable real valued function, $t = \operatorname{tr}(S)$ and $Q_0 = Q\,(Q^\top Q)^{-1}\,Q^\top$. We will consider conditions under which $a\,S^+ + \beta(t)/t\,S\,S^+\,Q_0$ improves over $a\,S^+$. In particular, we will assume that β is nonnegative and nondecreasing. Note that, in the Gaussian case and when $p \le n$, Tsukuma and Konno [42] give similar improvement conditions of estimators of the form $a\,S^{-1} + \beta(t)/t\,Q_0$ over $(n-p-1)\,S^{-1}$.

For such an example, it is more appropriate to use the Haff differential operator. Thanks to the identity in (2.2) of Remark 2.1 and Lemma A.1, the risk difference in (2.4) can be written as

$$\begin{aligned}\Delta(G) &= E_{\theta,\Sigma}\left[\operatorname{tr}\left(\{S\,G(X,S)\}^2 + 2\,a\,S^+\,S\,G(X,S)\right)\right] \\ &\quad - 2\,E_{\theta,\Sigma}\left[\varphi_{\theta,\Sigma}(X,U)\,\{a_0 \operatorname{tr}\left(S^+\,S\,G(X,S)\right) + 2\,D^*_{1/2}(S\,G(X,S))\}\right] \\ &= E_{\theta,\Sigma}\left[\operatorname{tr}\left(\{S\,G(X,S)\}^2 - 2\,(a_0\,\varphi_{\theta,\Sigma}(X,U) - a)\,S^+\,S\,G(X,S)\right)\right] \\ &\quad - 4\,E_{\theta,\Sigma}\left[\varphi_{\theta,\Sigma}(X,U)\,D^*_{1/2}(S\,G(X,S))\right]. \end{aligned} \tag{3.1}$$

Now for the Efron–Morris type estimator we have

$$S\,G(X,S) = \frac{\beta(t)}{t}\,S\,S^+\,Q_0. \tag{3.2}$$

Note that, as $S\,S^+$ and Q_0 are projectors, their product $S\,S^+\,Q_0$ is a projector as well so that

$$\{S\,G(X,S)\}^2 = \frac{\beta^2(t)}{t^2}\,S\,S^+\,Q_0 \tag{3.3}$$

and

$$S^+\,S\,G(X,S) = \frac{\beta(t)}{t}\,S^+\,S\,S^+\,Q_0 = \frac{\beta(t)}{t}\,S^+\,Q_0. \tag{3.4}$$

To deal with the term $D^*_{1/2}(S\,G(X,S))$, it is convenient to recall that

$$D^*_{1/2}(S\,G(X,S)) = \mathrm{tr}\big(\mathcal{D}_S\,(S\,G(X,S))\big). \tag{3.5}$$

We have, according to (3.2) and using (A.2) in Appendix A.1,

$$\begin{aligned}
\mathcal{D}_S\,S\,G(X,S) &= \mathcal{D}_S\,\frac{\beta(t)}{t}\,S\,S^+\,Q_0 \\
&= \left\{\mathcal{D}_S\,\frac{\beta(t)}{t}\,I_p\right\}\,S\,S^+\,Q_0 + \left\{\frac{\beta(t)}{t}\,I_p\,\mathcal{D}_S\right\}^\top\,S\,S^+\,Q_0 \\
&= \left(\frac{\beta(t)}{t}\right)'\,S\,S^+\,Q_0 + \frac{\beta(t)}{t}\,\mathcal{D}_S\,S\,S^+\,Q_0 \\
&= \left(\frac{\beta(t)}{t}\right)'\,S\,S^+\,Q_0 + \frac{\beta(t)}{t}\,\left\{\mathcal{D}_S\,S\,S^+\right\}\,Q_0 + \left\{S\,S^+\,\mathcal{D}_S\right\}^\top\,Q_0 \\
&= \left(\frac{\beta(t)}{t}\right)'\,S\,S^+\,Q_0 + \frac{\beta(t)}{t}\,\left\{\mathcal{D}_S\,S\,S^+\right\}\,Q_0
\end{aligned} \tag{3.6}$$

since $\left\{S\,S^+\,\mathcal{D}_S\right\}^\top$ is a $p \times p$ matrix with elements which are linear combinations of $\partial/\partial S_{ij}$ and Q_0 does not depend on S. Hence, according to (3.5) and (3.6), it follows that

$$D^*_{1/2}(S\,G(X,S)) = \left(\frac{\beta'(t)}{t} - \frac{\beta(t)}{t^2}\right)\,\mathrm{tr}\left(Q_0\,S\,S^+\right) + \frac{\beta(t)}{t}\,\mathrm{tr}\left(Q_0\,\mathcal{D}_S\,S\,S^+\right), \tag{3.7}$$

upon expanding $(\beta(t)/t)'$. Now substituting in (3.1) the terms in (3.3), (3.4) and (3.7) give

$$\begin{aligned}
\Delta(G) = E_{\theta,\Sigma}\Bigg[&\frac{\beta^2(t)}{t^2}\,\mathrm{tr}\big(S\,S^+\,Q_0\big) - 2\left(a_0\,\varphi_{\theta,\Sigma}(X,U) - a\right)\,\frac{\beta(t)}{t}\,\mathrm{tr}\big(S^+\,Q_0\big) \\
&- 4\,\varphi_{\theta,\Sigma}(X,U)\left(\frac{\beta'(t)}{t} - \frac{\beta(t)}{t^2}\right)\mathrm{tr}\left(Q_0\,S\,S^+\right) - 4\,\varphi_{\theta,\Sigma}(X,U)\,\frac{\beta(t)}{t}\,\mathrm{tr}\left(Q_0\,\mathcal{D}_S\,S\,S^+\right)\Bigg].
\end{aligned} \tag{3.8}$$

At this stage, an upper bound of the left hand-side of (3.8) can be developed. Indeed note that

$$\begin{aligned}
\mathrm{tr}\left(\{S\,G(X,S)\}^2\right) &= \frac{\beta^2(t)}{t^2}\,\mathrm{tr}\left(S\,S^+\,Q_0\,S\,S^+\,Q_0\right) \\
&= \frac{\beta^2(t)}{t^2}\,\mathrm{tr}\left(S\,S^+\,Q_0\right) \\
&= \frac{\beta^2(t)}{t^2}\,\mathrm{rk}(S\,S^+\,Q_0) \\
&\le \frac{\beta^2(t)}{t^2}\,\min(\mathrm{rk}(S\,S^+), \mathrm{rk}(Q_0)) \\
&\le \frac{\beta^2(t)}{t^2}\,q,
\end{aligned} \tag{3.9}$$

since

$$\mathrm{rk}(Q_0) = \mathrm{tr}(Q_0) = \mathrm{tr}(Q^\top\,Q\,(Q^\top\,Q)^{-1}) = \mathrm{tr}(I_q) = q. \tag{3.10}$$

Hence, assuming that $\beta(t)$ is a nondecreasing function of t and using Conditions (2.5) and (3.9), it is clear from the expression in (3.8) that

$$\begin{aligned}
\Delta(G) \le E_{\theta,\Sigma}\Bigg[&\frac{\beta^2(t)}{t^2}\,q - 2\left(a_0\,\varphi_{\theta,\Sigma}(X,U) - a\right)\,\frac{\beta(t)}{t}\,\mathrm{tr}\big(S^+\,Q_0\big) \\
&+ 4\,b\,\frac{\beta(t)}{t^2}\,q - 4\,\varphi_{\theta,\Sigma}(X,U)\,\frac{\beta(t)}{t}\,\mathrm{tr}\left(Q_0\,\mathcal{D}_S\,S\,S^+\right)\Bigg].
\end{aligned} \tag{3.11}$$

In the following results, based on (3.11), we distinguish the cases where S is invertible and where S is noninvertible. If S is invertible then $p \le n$, $S^+ = S^{-1}$ and $\mathcal{D}_S\,S\,S^+ = \mathcal{D}_S\,S\,S^{-1} = \mathcal{D}_S\,I_p = 0$ so that the last term on the right hand-side of (3.11) vanishes. This is in contrast with the case where S is not invertible since, in that situation, $p > n$, $a_0 < 0$ and $\mathcal{D}_S\,S\,S^+ \neq 0$.

Theorem 3.1. *Consider a density as in (1.1) satisfying (2.5) and (2.6), that is,* $0 < c \leq F(t)/f(t) \leq b$. *Assume that S is invertible and $p < n - 3$. Assume also that $\beta(t)$ is a differentiable nondecreasing function of $t = \mathrm{tr}(S)$ and $a_0 = n - p - 1$. Then $a\,S^+ + \beta(t)/t\, S\, S^+\, Q_0$ improves over $a\,S^+$ provided that*

$$0 < a < a_0\, c - 2\, b \tag{3.12}$$

and

$$0 < \beta(t) < 2\,(a_0\, c - 2\, b). \tag{3.13}$$

Proof. By the assumption, $a_0 > 0$, it follows from (3.11) that, according to (2.6),

$$\Delta(G) \leq E_{\theta,\Sigma}\left[\frac{\beta^2(t)}{t^2}\, q - 2\left(a_0\, c - a\right)\frac{\beta(t)}{t}\,\mathrm{tr}\left(S^{-1}\, Q_0\right) + 4\, b\, \frac{\beta(t)}{t^2}\, q\right]. \tag{3.14}$$

Now Inequality (A.74) states here that

$$\mathrm{tr}(S^{-1}\, Q_0) \geq \frac{\mathrm{tr}(\,Q_0)}{\mathrm{tr}(S)} = \frac{q}{t},$$

since H_1 is a semi-orthogonal matrix. Therefore, as $a < a_0\, c$ according to (3.12), we have

$$-2\left(a_0\, c - a\right)\frac{\beta(t)}{t}\,\mathrm{tr}\left(S^{-1}\, Q_0\right) \leq -2\left(a_0\, c - a\right) q\, \frac{\beta(t)}{t^2}$$

and hence it follows from (3.14) that

$$\Delta(G) \leq E_{\theta,\Sigma}\left[\frac{\beta(t)}{t^2}\, q\left\{\beta(t) - 2\left(a_0\, c - a - 2\, b\right)\right\}\right]. \tag{3.15}$$

Consequently, according to (3.13), $\Delta(G) \leq 0$. □

Theorem 3.2. *Consider the density in (1.1) satisfying (2.5) and (2.6). Assume that S is noninvertible and that*

$$p \geq 3\, n\, \frac{n}{n-2} \quad \text{with } n \geq 3, \tag{3.16}$$

$$\frac{b}{c} < \frac{2\, p - 4\, n + 1}{p\,(1 + 2/n) - (n-1)} \tag{3.17}$$

and

$$q > \frac{3\, n + (b/c - 1)(p - n - 1)}{1 - (2/n)\,(b/c)}. \tag{3.18}$$

Assume also that $\beta(t)$ is a differentiable nondecreasing function of t. Then the estimator $a\,S^+ + \beta(t)/t\, S\, S^+\, Q_0$ improves over $a\,S^+$ provided that

$$0 < a \leq \left[(b - c)\,(n - p - 1) + c\,(q - 3\, n)\right]\frac{n}{q} - 2\, b \tag{3.19}$$

and

$$0 < \beta(t) < \left[(b - c)\,(n - p - 1) + c\,(q - 3\, n)\right]\frac{n}{q} - 2\, b - a. \tag{3.20}$$

Proof. First note that Condition (3.18) is equivalent to the positivity of the upper bound of a in (3.19). As we have $p \geq q$, note also that Condition (3.17) is equivalent to the fact that p is greater than the lower bound for q in (3.18). Finally, as $b/c \geq 1$, note that Condition (3.16) is equivalent to the fact that the upper bound for b/c in (3.17) is greater than or equal to 1.

Since it can be checked from (3.18) that $2\, n - q < 0$, it results from Lemma A.2 that $\mathrm{tr}\left(Q_0\, \mathcal{D}_S\, S\, S^+\right) \geq 0$ for $p \geq 2\, n - 1$, which is guaranteed by (3.16). Hence, from (3.11), a first new upper bound for $\Delta(G)$ is given by

$$\Delta(G) \leq E_{\theta,\Sigma}\left[\tfrac{\beta^2(t)}{t^2}\, q - 2\left(a_0\, b - a\right)\tfrac{\beta(t)}{t}\,\mathrm{tr}\left(S^+\, Q_0\right) + 4\, b\, \tfrac{\beta(t)}{t^2}\, q - 4\, c\, \tfrac{\beta(t)}{t}\,\mathrm{tr}\left(Q_0\, \mathcal{D}_S\, S\, S^+\right)\right]. \tag{3.21}$$

Then, from the first inequality in (A.19), it follows from (3.21) that another upper bound for $\Delta(G)$ is

$$\Delta(G) \leq E_{\theta,\Sigma}\left[\frac{\beta^2(t)}{t^2}\, q + 4\, b\, \frac{\beta(t)}{t^2}\, q - 2\, A\, \frac{\beta(t)}{t}\,\mathrm{tr}\left(S^+\, Q_0\right) - 2\, B\, \frac{\beta(t)}{t}\,\mathrm{tr}\left(S^+\right)\right], \tag{3.22}$$

where $A = a_0\, b - a + c\,(p + 1 - 2\,n) = (b - c)\,(n - p - 1) - c\,n - a$ and $B = q - 2\,n$. As $A < 0$ and $\operatorname{tr}\big(S^+\,Q_0\big) \le \operatorname{tr}\big(S^+\big)$, (3.22) implies that

$$\Delta(G) \le E_{\theta,\Sigma}\left[\frac{\beta^2(t)}{t^2}\,q + 4\,b\,\frac{\beta(t)}{t^2}\,q - 2\,(A + c\,B)\,\frac{\beta(t)}{t}\,\operatorname{tr}\big(S^+\big)\right]. \tag{3.23}$$

Now, through straightforward calculations, we have

$$A + c\,B = (b - c)\,(n - p - 1) + c\,(q - 3\,n) \ge 0 \tag{3.24}$$

as soon as Condition (3.19) is satisfied. Then, since (A.73) in Lemma A.4 guarantees that $\operatorname{tr}\big(S^+\big) \ge n/t$, we can derive from (3.23) and (3.24) the following upper bound for $\Delta(G)$:

$$\Delta(G) \le E_{\theta,\Sigma}\left[\frac{\beta^2(t)}{t^2}\,q + 4\,b\,\frac{\beta(t)}{t^2}\,q - 2\,(A + c\,B)\,n\,\frac{\beta(t)}{t^2}\right]. \tag{3.25}$$

According to (3.24), the integrand in (3.25) can be written as

$$\frac{\beta(t)}{t^2}\,q\left\{\beta(t) - 2\,[(b - c)\,(n - p - 1) + c\,(q - 3\,n)]\,\frac{n}{q} - 2\,b - a\right\},$$

which is negative if Conditions (3.19) and (3.20) are satisfied. Then the risk difference in (3.25) is nonpositive, so that the estimator $a\,S^+ + \beta(t)/t\,S\,S^+\,Q_0$ improves over $a\,S^+$. □

4. Elliptically symmetric distribution examples

In Fourdrinier, Mezoued and Strawderman [17], several examples of density in the Berger class (Condition (2.6)) are provided. Note that Condition (2.5) may be satisfied or not. Note also that, for these examples, $F(t)/f(t)$ is monotone in t, either nondecreasing or nonincreasing. This ratio is typically nondecreasing when the density in (1.1) is a variance mixture of normals (in which case $c = F(0)/f(0)$ and $b = \lim_{t\to\infty} F(t)/f(t)$).

For each of the estimators discussed above, conditions on a and $\beta(t)$ need to be satisfied in order to attain improvement. The optimal a can be derived for a particular elliptically symmetric distribution as in Tsukuma [41], however, it requires numerical work to calculate since there is no closed form expression. The choice of $\beta(t)$ is more complicated and can be taken to be a constant as in the examples considered in Efron and Morris [12] and Tsukuma and Konno [42].

Example 4.1. Let the density in (1.1) be a variance mixture of normal distributions where the mixing variable V has density g with respect to the Lebesgue measure, that is, for any $t \ge 0$,

$$f(t) \propto \int_0^\infty v^{-p/2}\,\exp\left(\frac{-t}{2\,v}\right) g(v)\,dv.$$

We have

$$\frac{F(t)}{f(t)} = \frac{\int_0^\infty v^{-p/2+1}\,\exp\left(\frac{-t}{2\,v}\right)\,g(v)\,dv}{\int_0^\infty v^{-p/2}\,\exp\left(\frac{-t}{2\,v}\right)\,g(v)\,dv} = E_t[V] \tag{4.1}$$

where E_t denotes the expectation with respect to a density proportional to $v \mapsto v^{-p/2}\,\exp(-t/2v)\,g(v)$. As this density has increasing monotone likelihood ratio in t, $E_t[V]$ is nondecreasing in t. Then, denoting by E the expectation with respect to g,

$$c = \frac{F(0)}{f(0)} = \frac{\int_0^\infty v^{-p/2+1}\,g(v)\,dv}{\int_0^\infty v^{-p/2}\,g(v)\,dv} = \frac{E[V^{-p/2+1}]}{E[V^{-p/2}]} > 0,$$

provided that $E[V^{-p/2}] < \infty$.

A typical example of variance mixture of normals is a multivariate t-distribution with k degrees of freedom for which $g(v) \propto v^{-k/2-1}\,\exp(-k/2v)$. Through the change of variable $v = t/u$ in the integrals in (4.1), it is easily checked that

$$\frac{F(t)}{f(t)} = t\,\frac{\int_0^\infty u^{(p+k)/2-2}\,\exp\left(-\frac{u}{2}\left(1 + \frac{k}{t}\right)\right)\,du}{\int_0^\infty u^{(p+k)/2-1}\,\exp\left(-\frac{u}{2}\left(1 + \frac{k}{t}\right)\right)\,du},$$

so that $b = \lim_{t\to\infty} F(t)/f(t) = \infty$. Hence Theorems 2.1, 3.1 and 3.2 cannot apply to the t-distributions. However, for a truncated mixing density $g\,\mathbb{1}_{[0,A]}$ with $A > 0$ (normalized by $\int_0^A g(v)\,dv$ so that it is a real pdf), it is clear from (4.1) that $b = A$ and is finite. Hence the above theorems apply for such truncated versions and, in particular, for the truncated t.

Note that the well known Kotz' density corresponding to $f(t) \propto t^q\,\exp(-t/2)$ is a mixture of normals when the parameter q is negative (but it is not when $q > 0$) with mixing density having a compact support, since it is a beta distribution with parameter $p/2 + q$ and $-q$, provided $q > -p/2$.

We give below a few examples where $F(t)/f(t)$ is nonincreasing, and hence for which $b = F(0)/f(0)$ and $c = \lim_{t\to\infty} F(t)/f(t)$.

Example 4.2. Let

$$f(t) \propto \frac{\exp(-\beta t - \gamma)}{(1+\exp(-\beta\, t - \gamma))^2}$$

where $\beta > 0$ and $\gamma > 0$. For that function we have

$$c = \frac{1}{2\beta} \quad \text{and} \quad b = \frac{1+e^{-\gamma}}{2\beta}.$$

Example 4.3. Let

$$f(t) \propto \frac{1}{\cosh(\beta\, t + \gamma)}$$

where $\beta > 0$ and $\gamma > 0$. For that function we have

$$c = \frac{1}{2\beta} \quad \text{and} \quad b = \frac{1}{\beta} \arctan(e^{-\gamma}) \cosh(\gamma).$$

Example 4.4. Let

$$f(t) \propto (t+A) \exp\left(-\frac{t}{2}\right)$$

with $A > 2$. For that function we have

$$c = 1 \quad \text{and} \quad b = 1 + \frac{2}{A}.$$

Now we provide here a last example (which is not in Fourdrinier, Mezoued and Strawderman [17]) for which the ratio $F(t)/f(t)$ is not monotone.

Example 4.5. Let

$$f(t) \propto \frac{1}{t^2 - 2\,t + 2} \exp\left(-\frac{1}{2}\arctan(t-1)\right) \mathbb{1}_{[0,A]}$$

with $A > 1$. It can be checked that

$$\frac{F(t)}{f(t)} = t^2 - 2\,t + 2$$

which is nonincreasing on the interval $[0, 1]$ and nondecreasing on $[1, A]$. Then it can be seen that $c \le F(t)/f(t) \le b$ with $c = F(1)/f(1) = 1$ and $b = \max\big(2, F(A)/f(A)\big)$.

5. Concluding remarks

In this paper, we have considered estimation of the inverse scatter matrix under quadratic loss and have derived risk expressions under a wide class of elliptically symmetric distribution. We proposed a unified approach that can deal with both singular and nonsingular S. As a by product of our derivations, we developed a new and more general Stein–Haff identity for the high-dimensional elliptically symmetric distribution setting.

Kubokawa and Inoue [25] consider general types of ridge estimators of the precision matrix and derive asymptotic expansions of their risk functions. They also suggest ridge function examples so that the second order terms of risks are smaller than those of standard estimators. Unfortunately, the type of ridge estimators they examined do not fall into our class of estimators, namely, estimators of the forms $a\,S^+ + S\,G(X,S)$ or $H_1\,\Psi(L)\,H_1^\top$. This seems to be the reason that Kubokawa and Inoue need to use asymptotic arguments rather than the exact forms as developed here. We plan to examine the numerical performance of our proposed estimators, for various elliptically symmetric distributions, with other precision matrix estimators. A comparison with ridge-type estimators would be particularly informative. As pointed out in Section 4, in order to develop these comparisons some further numerical work is needed to select optimal value of the multiplicative constant a, for a particular elliptically symmetric distribution.

Our new proof techniques and Stein–Haff identity for the singular elliptically contoured distributions in (1.1) can be applied to a number of setting. First, the results of Konno [23] for estimating large covariance matrices of multivariate normal distributions when the dimension of the variables is larger than the number of samples can be extended to the case of elliptically symmetric distribution. Next the analysis of the high dimensional James–Stein estimator in Chételat and Wells [8] can also be adapted to elliptically contoured distributions. The key technical tool in both of these extensions will be an application of Lemma 2.1.

Another direction would be to consider the problem of the estimation of discriminant coefficients, which arises in linear discriminant analysis when Fisher's linear discriminant function is viewed as the posterior log-odds under the assumption that two classes differ in mean but have a common scatter matrix. The improved inverse scatter matrix estimates developed in this article will likely give rise to improved discriminant coefficients under the quadratic loss function for the elliptically symmetric distributions in the case where the number of the variables is larger than the number of samples. Results on the improved discriminant coefficient estimation are given in Tsukuma and Konno [42] for the normal distribution when the number of the variables is smaller than the number of samples.

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Appendix

A.1. Differential expressions I

Let U and T be $p \times p$ matrices, the elements of which being functions of $S = (S_{ij})$ and let $\tilde{\mathcal{D}}_S$ be a $p \times p$ matrix, the elements of which being linear combinations of $\partial/\partial S_{ij}$. Tsukuma and Konno [42] recall the following result from Haff:

$$\tilde{\mathcal{D}}_S \, U \, T = \{\tilde{\mathcal{D}}_S \, U\} \, T + \left(U^\top \, \tilde{\mathcal{D}}_S^\top\right)^\top T. \tag{A.1}$$

In the particular case where $\tilde{\mathcal{D}}_S = \mathcal{D}_S$ with $(\mathcal{D}_S)_{ij} = 1/2\,(1+\delta_{ij})\,\partial/\partial S_{ij}$, we have $\mathcal{D}_S^\top = \mathcal{D}_S$ so that, if U is symmetric,

$$\mathcal{D}_S \, U \, T = \{\mathcal{D}_S \, U\} \, T + \left(U \, \mathcal{D}_S\right)^\top T. \tag{A.2}$$

Note that

$$\mathcal{D}_S \, S = \frac{p+1}{2} \, I_p \tag{A.3}$$

since

$$\begin{aligned}
\left(\mathcal{D}_S \, S\right)_{ik} &= \sum_{j=1}^{p} \frac{1}{2} \, (1+\delta_{ij}) \, \frac{\partial S_{jk}}{\partial S_{ij}} \\
&= \frac{\partial S_{ik}}{\partial S_{ii}} + \frac{1}{2} \sum_{j \neq i}^{p} \frac{\partial S_{jk}}{\partial S_{ij}} \\
&= \delta_{ki} + \frac{1}{2} \sum_{j \neq i}^{p} \delta_{ki} \\
&= \delta_{ki} + \frac{p-1}{2} \, \delta_{ki} \\
&= \frac{p+1}{2} \, \delta_{ki}.
\end{aligned}$$

Hence, as S is symmetric, applying (A.2) with $U = S$ and $T = S^+$ gives

$$\mathcal{D}_S \, S \, S^+ = \left\{\mathcal{D}_S \, S\right\} S^+ + \left(S \, \mathcal{D}_S\right)^\top S^+ = \frac{p+1}{2} \, S^+ + \left(S \, \mathcal{D}_S\right)^\top S^+, \tag{A.4}$$

thanks to (A.3).

A.2. Stein–Haff lemma type and differential operators

We give a concise proof of Lemma 2.1 in this subappendix. Note that a similar lemma has been provided in the elliptical case by Fourdrinier, Strawderman and Wells [18] through the Haff operator. However two features are different: they only considered the case where the matrix S is invertible and presented a lengthy proof. Nevertheless, we follow their lines being able to considerably shorten their proof. Also note that the invertibility of S does not play any role in the proof below.

Proof of Lemma 2.1. As $U = (U_1, \dots, U_n)$ and $S = UU^\top$, we have

$$\begin{aligned}\operatorname{tr}\left(\Sigma^{-1} S\, G(X,S)\right) &= \operatorname{tr}\left(G(X,S)\,\Sigma^{-1} S\right)\\ &= \operatorname{tr}\left(G(X,S)\,\Sigma^{-1}\sum_{i=1}^{n} U_i\, U_i^\top\right)\\ &= \sum_{i=1}^{n}\operatorname{tr}\left(U_i^\top\, G(X,S)\,\Sigma^{-1}\, U_i\right)\\ &= \sum_{i=1}^{n} U_i^\top\, G(X,S)\,\Sigma^{-1}\, U_i. \end{aligned}\tag{A.5}$$

Now, using the argument in Lemma 1(i) of Fourdrinier, Strawderman and Wells [18], it follows from (A.5) that

$$\begin{aligned}E_{\theta,\Sigma}\left[\operatorname{tr}\left(\Sigma^{-1} S\, G(X,S)\right)\right] &= k\sum_{i=1}^{n} E^*_{\theta,\Sigma}\left[\operatorname{div}_{U_i}(G^\top(X,S)\,U_i)\right]\\ &= k\,E^*_{\theta,\Sigma}\left[A_1 + A_2\right],\end{aligned}\tag{A.6}$$

where

$$\begin{aligned}A_1 &= \sum_{i=1}^{n}\sum_{j=1}^{p}\sum_{m=1}^{p}\frac{\partial U_{mi}}{\partial U_{ji}}\, G^\top_{jm}\\ &= \sum_{i=1}^{n}\sum_{j=1}^{p}\sum_{m=1}^{p}\delta_{jm}\, G^\top_{jm}(X,S)\\ &= n\sum_{j=1}^{p} G^\top_{jj}(X,S)\\ &= n\operatorname{tr}(G(X,S))\end{aligned}\tag{A.7}$$

and

$$\begin{aligned}A_2 &= \sum_{i=1}^{n}\sum_{j=1}^{p}\sum_{m=1}^{p} U_{mi}\,\frac{\partial G^\top_{jm}(X,S)}{\partial U_{ji}}\\ &= \sum_{i=1}^{n}\sum_{m=1}^{p} U_{mi}\sum_{j=1}^{p}\frac{\partial G^\top_{jm}(X,S)}{\partial U_{ji}}\\ &= \sum_{i=1}^{n}\sum_{m=1}^{p} U_{mi}(\nabla_{U^\top} G^\top(X,S))_{im}\\ &= \sum_{m=1}^{p}(U\nabla_{U^\top} G^\top(X,S))_{mm}\\ &= \operatorname{tr}(U\,\nabla_{U^\top}\, G^\top(X,S)).\end{aligned}\tag{A.8}$$

Finally, combining (A.6)–(A.8), we obtain the desired result. □

To deal with the term $\operatorname{tr}(U\,\nabla_{U^\top}\, G^\top(X,S))$ it may be convenient to use the Haff operator and the following lemma, where we give a link between the differential expressions $D^*_{1/2} S\, G(X,S)$ and $\operatorname{tr}\left(U\,\nabla_{U^\top}\, G^\top(X,S)\right)$.

Lemma A.1. *For any $p \times p$ matrix function $G(x,s)$ differentiable with respect to s for any x,*

$$2\,D^*_{1/2}\left(S\, G(X,S)\right) = (p+1)\operatorname{tr}\left(G(X,S)\right) + \operatorname{tr}\left(U\,\nabla_{U^\top}\, G^\top(X,S)\right).\tag{A.9}$$

Proof. Firstly, we express $\operatorname{tr}\left(U\,\nabla_{U^\top}\, G^\top(X,S)\right)$ in terms of S, we have

$$\begin{aligned}(U\,\nabla_{U^\top}\, G^\top(X,S))_{ii} &= \sum_{j=1}^{n}\sum_{k=1}^{p} U_{ij}\,(\nabla_{U^\top})_{jk}\,(G^\top(X,S))_{ki}\\ &= \sum_{j=1}^{n}\sum_{k=1}^{p} U_{ij}\,\frac{\partial (G^\top(X,S))_{ki}}{\partial U_{kj}}\end{aligned}$$

$$= \sum_{j=1}^{n} \sum_{k=1}^{p} U_{ij} \sum_{r \le l}^{p} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{rl}} \frac{\partial S_{rl}}{\partial U_{kj}}$$

$$= \sum_{j=1}^{n} \sum_{k=1}^{p} U_{ij} \sum_{r \le l}^{p} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{rl}} (\delta_{rk} U_{lj} + \delta_{lk} U_{rj}), \tag{A.10}$$

since $S = U\,U^\top$. From (A.10) we can write

$$(U\,\nabla_{U^\top}\,G^\top(X,S))_{ii} = A + B + C \tag{A.11}$$

where

$$\begin{aligned} A &= \sum_{j=1}^{n} \sum_{k=1}^{p} U_{ij} \sum_{r=l}^{p} 2\,\delta_{rk} U_{rj} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{rr}} \\ &= 2 \sum_{j=1}^{n} \sum_{k=1}^{p} U_{ij}\,U_{kj} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{kk}} \\ &= 2 \sum_{k=1}^{p} S_{ik} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{kk}}, \end{aligned} \tag{A.12}$$

$$B = \sum_{j=1}^{n} U_{ij} \sum_{k<l}^{p} U_{lj} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{kl}},$$

and

$$C = \sum_{j=1}^{n} U_{ij} \sum_{k>r}^{p} U_{rj} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{rk}}.$$

Now it is clear that

$$\begin{aligned} B + C &= \sum_{j=1}^{n} U_{ij} \sum_{k \ne l}^{p} U_{lj} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{kl}} \\ &= \sum_{k \ne l}^{p} S_{lj} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{kl}}. \end{aligned} \tag{A.13}$$

Then, substituting (A.12) and (A.13) in (A.11), it follows that

$$\operatorname{tr}\left(U\,\nabla_{U^\top}\,G^\top(X,S)\right) = 2 \sum_{i=1}^{p} \left\{ \sum_{k=1}^{p} S_{ik} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{kk}} + \frac{1}{2} \sum_{k \ne l}^{p} S_{lj} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{kl}} \right\}. \tag{A.14}$$

Secondly, we have

$$\begin{aligned} 2\,D^*_{1/2}\big(S\,G(X,S)\big) &= 2 \sum_{i=1}^{p} \frac{\partial (S\,G(X,S))_{ii}}{\partial S_{ii}} + \sum_{i \ne j} \frac{\partial (S\,G(X,S))_{ij}}{\partial S_{ij}} \\ &= 2 \sum_{i=1}^{p} \left(G_{ii}(X,S) + \sum_{k=1}^{p} S_{ik} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{ii}} \right) + \sum_{i \ne j}^{p} \left(G_{jj}(X,S) + \sum_{k=l}^{p} S_{ik} \frac{\partial (G^\top(X,S))_{kj}}{\partial S_{ij}} \right) \\ &= (p+1)\operatorname{tr}(G(X,S)) + 2 \sum_{k=1}^{p} \left\{ \sum_{i=1}^{p} S_{ik} \frac{\partial (G^\top(X,S))_{ki}}{\partial S_{ii}} + \frac{1}{2} \sum_{i \ne j}^{p} S_{ik} \frac{\partial (G^\top(X,S))_{kj}}{\partial S_{ij}} \right\} \\ &= (p+1)\operatorname{tr}\big(G(X,S)\big) + \operatorname{tr}\left(U\,\nabla_{U^\top}\,G^\top(X,S)\right), \end{aligned} \tag{A.15}$$

according to (A.14) for the last equality in (A.15). $\square$

We now deal with the term $\operatorname{tr}\left(Q_0\, \mathcal{D}_S\, S\, S^+\right)$ considered in Section 3. As partial derivatives with respect to the S_{ij} are involved, recall (see, for instance, Chételat and Wells [8]) that

$$\frac{\partial S^+}{\partial S_{ij}} = -S^+\, \frac{\partial S}{\partial S_{ij}}\, S^+ + (I_p - S\, S^+)\, \frac{\partial S}{\partial S_{ij}}\, S^+\, S^+ + S^+\, S^+\, \frac{\partial S}{\partial S_{ij}}\, (I_p - S\, S^+). \tag{A.16}$$

As a preliminary result note that for any $p \times p$ matrices A, B and C, we have

$$\sum_{l=1}^{p} \sum_{i=1}^{p} C_{li} \sum_{j=1}^{p} \frac{1}{2}\, (1+\delta_{ij}) \left(A\, \frac{\partial S}{\partial S_{ij}}\, B\right)_{jl} = \frac{1}{2}\operatorname{tr}\big(\operatorname{diag}(A)\, \operatorname{diag}(B\,C)\big) + \frac{1}{2}\operatorname{tr}(A)\operatorname{tr}(B\,C), \tag{A.17}$$

where, for any $p \times p$ matrix M, $\operatorname{diag}(M)$ is the diagonal matrix formed with the diagonal elements of M. Indeed, denoting by τ the left hand-side of (A.17), this term can be expanded as

$$\begin{aligned} \tau &= \sum_{l=1}^{p} \sum_{i=1}^{p} C_{li} \sum_{j=1}^{p} \frac{1}{2}\, (1+\delta_{ij}) \sum_{q=1}^{p} A_{jq} \sum_{k=1}^{p} \frac{\partial S_{qk}}{\partial S_{ij}}\, B_{kl} \\ &= \sum_{l=1}^{p} \sum_{i=1}^{p} C_{li} \left(\sum_{j=1}^{p} \frac{1}{2}\, (1+\delta_{ij})\, A_{jj} \right) B_{il}, \end{aligned}$$

since

$$\frac{\partial S_{qk}}{\partial S_{ij}} = \delta_{qj}\, \delta_{ki}.$$

Then, expressing the sum with respect to j, gives

$$\begin{aligned} \tau &= \sum_{l=1}^{p} \sum_{i=1}^{p} C_{li}\, \frac{1}{2} \big(A_{ii} + \operatorname{tr}(A)\big)\, B_{il} \\ &= \frac{1}{2} \sum_{i=1}^{p} A_{ii} \sum_{l=1}^{p} C_{li}\, B_{il} + \frac{1}{2}\operatorname{tr}(A) \sum_{i=1}^{p} \sum_{l=1}^{p} C_{li}\, B_{il} \\ &= \frac{1}{2} \sum_{i=1}^{p} A_{ii}\, (B\,C)_{ii} + \frac{1}{2}\operatorname{tr}(A) \sum_{i=1}^{p} (B\,C)_{ii}, \end{aligned}$$

which is (A.17).

From the above, the following lemma can be derived.

Lemma A.2. *For Q_0 as in the first paragraph of Section 3, we have*

$$\begin{aligned} \operatorname{tr}\left(Q_0\, \mathcal{D}_S\, S\, S^+\right) = {} & \frac{p+1-(n \wedge p)}{2} \operatorname{tr}\left(Q_0\, S^+\right) + \frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S^+)\, \operatorname{diag}(Q_0)\right) + \frac{q}{2}\operatorname{tr}\left(S^+\right) \\ & - \frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S^+)\, \operatorname{diag}(Q_0\, S\, S^+)\right) - \frac{1}{2}\operatorname{tr}\left(S^+\right)\, \operatorname{tr}\left(Q_0\, S\, S^+\right) \\ & - \frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S\, S^+)\, \operatorname{diag}(Q_0\, S^+)\right). \end{aligned} \tag{A.18}$$

Furthermore, if S is noninvertible, we have

$$\operatorname{tr}\left(Q_0\, \mathcal{D}_S\, S\, S^+\right) \geq 0 \tag{A.19}$$

as soon as

$$p \geq q \geq 2\, n. \tag{A.20}$$

Proof. First note that when S is invertible the left hand-side of (A.18) equals 0, this agrees with the fact that the right hand-side of (A.18) does not depend on S.

According to (A.4), we have

$$\operatorname{tr}\left(Q_0\, \mathcal{D}_S\, S\, S^+\right) = \frac{p+1}{2}\operatorname{tr}\left(Q_0\, S^+\right) + \operatorname{tr}\left(Q_0\, \{S\, \mathcal{D}\}^{\top}\, S^+\right), \tag{A.21}$$

the second term of (A.21) being expressed as

$$\begin{aligned}\operatorname{tr}\left(Q_0\,\{S\,\mathcal{D}\}^\top S^+\right) &= \sum_{l=1}^{p}\sum_{i=1}^{p}(Q_0)_{li}(\{S\,\mathcal{D}\}^\top S^+)_{il}\\ &= \sum_{l=1}^{p}\sum_{i=1}^{p}(Q_0)_{li}\sum_{j=1}^{p}\frac{1}{2}\,(1+\delta_{ij})\left(S\,\frac{\partial S^+}{\partial S_{ij}}\right)_{jl}. \end{aligned} \tag{A.22}$$

Applying (A.16) it follows that

$$\begin{aligned} S\,\frac{\partial S^+}{\partial S_{ij}} &= -S\,S^+\,\frac{\partial S}{\partial S_{ij}}\,S^+ + (S - S\,S\,S^+)\,\frac{\partial S}{\partial S_{ij}}\,S^+\,S^+ + S\,S^+\,S^+\,\frac{\partial S}{\partial S_{ij}}\,(I_p - S\,S^+)\\ &= -S\,S^+\,\frac{\partial S}{\partial S_{ij}}\,S^+ + S^+\,\frac{\partial S}{\partial S_{ij}} - S^+\,\frac{\partial S}{\partial S_{ij}}\,S\,S^+, \end{aligned} \tag{A.23}$$

since $S\,S\,S^+ = S\,S^+\,S = S$ and $S\,S^+\,S^+ = S^+\,S\,S^+ = S^+$. Hence, from (A.21) and (A.23),

$$\begin{aligned}\operatorname{tr}\left(Q_0\,\{S\,\mathcal{D}\}^\top S^+\right) &= \sum_{l=1}^{p}\sum_{i=1}^{p}(Q_0)_{li}\sum_{j=1}^{p}\frac{1}{2}\,(1+\delta_{ij})\left(-S\,S^+\,\frac{\partial S}{\partial S_{ij}}\,S^+ + S^+\,\frac{\partial S}{\partial S_{ij}} - S^+\,\frac{\partial S}{\partial S_{ij}}\,S\,S^+\right)_{jl}\\ &= -\frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S\,S^+)\operatorname{diag}(Q_0\,S^+)\right) - \frac{1}{2}\operatorname{tr}\left(S\,S^+\right)\operatorname{tr}\left(Q_0\,S^+\right)\\ &\quad+\frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S^+)\operatorname{diag}(Q_0)\right) + \frac{1}{2}\operatorname{tr}\left(S^+\right)\operatorname{tr}(Q_0)\\ &\quad-\frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S\,S^+)\operatorname{diag}(Q_0\,S^+)\right) - \frac{1}{2}\operatorname{tr}\left(S\,S^+\right)\operatorname{tr}\left(Q_0\,S^+\right) \end{aligned} \tag{A.24}$$

by applying (A.17) with $C = Q_0$ and, successively, $A = -S\,S^+$, $A = S^+$, $A = -S^+$, and $B = S^+$, $B = I_p$, $B = S\,S^+$. Recalling that $\operatorname{tr}(Q_0) = q$ and $\operatorname{tr}\left(S\,S^+\right) = n \wedge p$ and gathering (A.21) and (A.24) give (A.18).

As for Inequality (A.19), note that

$$\operatorname{tr}(\operatorname{diag}(A)\operatorname{diag}(B)) \le \operatorname{tr}(A)\operatorname{tr}(B), \tag{A.25}$$

for any positive semidefinite matrices A and B. As S is noninvertible, (A.18) becomes

$$\begin{aligned}\operatorname{tr}\left(Q_0\,\mathcal{D}_S\,S\,S^+\right) &= \frac{p+1-n}{2}\operatorname{tr}\left(Q_0\,S^+\right) + \frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S^+)\operatorname{diag}(Q_0)\right) + \frac{q}{2}\operatorname{tr}\left(S^+\right)\\ &\quad-\frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S^+)\operatorname{diag}(Q_0\,S\,S^+)\right) - \frac{1}{2}\operatorname{tr}\left(S^+\right)\operatorname{tr}\left(Q_0\,S\,S^+\right)\\ &\quad-\frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S\,S^+)\operatorname{diag}(Q_0\,S^+)\right) \end{aligned} \tag{A.26}$$

and applying (A.25) in (A.26) successively with $A = S^+$, $B = Q_0\,S\,S^+$ and $A = S\,S^+$, $B = Q_0\,S^+$ gives

$$\begin{aligned}\operatorname{tr}\left(Q_0\,\mathcal{D}_S\,S\,S^+\right) &\ge \frac{p+1-n}{2}\operatorname{tr}\left(Q_0\,S^+\right) + \frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S^+)\operatorname{diag}(Q_0)\right) + \frac{q}{2}\operatorname{tr}\left(S^+\right)\\ &\quad-\operatorname{tr}\left(S^+\right)\operatorname{tr}\left(Q_0\,S\,S^+\right) - \frac{1}{2}\operatorname{tr}\left(S\,S^+\right)\operatorname{tr}\left(Q_0\,S^+\right)\\ &\ge \left(\frac{p+1}{2} - n\right)\operatorname{tr}\left(Q_0\,S^+\right) + \frac{1}{2}\operatorname{tr}\left(\operatorname{diag}(S^+)\operatorname{diag}(Q_0)\right) + \left(\frac{q}{2} - n\right)\operatorname{tr}\left(S^+\right), \end{aligned} \tag{A.27}$$

gathering the common terms and using the fact that

$$\operatorname{tr}\left(Q_0\,S\,S^+\right) = \operatorname{rk}\left(Q_0\,S\,S^+\right) \le \min(q, n) \le n.$$

Finally, it is clear from Condition (A.20) that the first term and the third term of the right hand-side of (A.27) are nonnegative. As the second term is nonnegative as well, we obtain Inequality (A.19). □

A.3. Differential expressions II

In this subappendix, we present a unified approach to calculus on eigenstructure for singular and nonsingular sample scatter matrices necessary to develop Stein–Haff identities for the elliptically symmetric distributions. Results similar to these are given in Konno [23]. We treat both the singular and nonsingular cases in a unified manner as well as fill-in many of the analytic details of the delicate proofs.

Recall, from (2.14) in Section 2, that the sample covariance matrix S has the eigenvalue decomposition $S = H_1 L H_1^\top$ where H_1 is a matrix such that $H_1^\top H_1 = I_{n\wedge p}$. When $p \leq n$, H_1 is a $p\times p$ matrix in $\mathcal{O}_p(\mathbb{R})$ (i.e. $H_1^\top H_1 = I_p$) while, when $p > n$, H_1 is a $p \times n$ semi-orthogonal matrix (i.e. $H_1^\top H_1 = I_n$). In the case where $p > n$, we complete the semi-orthogonal matrix H_1 by a $p \times (p-n)$ matrix H_2 such that $H = (H_1\ H_2)$ is a $p\times p$ matrix in $\mathcal{O}_p(\mathbb{R})$ (see Srivastava [39]). Then, setting

$$\tilde{L} = \begin{pmatrix} L & 0_{n\times(p-n)} \\ 0_{(p-n)\times n} & 0_{(p-n)\times(p-n)} \end{pmatrix},$$

we have

$$H\tilde{L}H^\top = H_1 L H_1^\top = S. \tag{A.28}$$

Note that, by orthogonality of H, it follows that

$$I_p = HH^\top = (H_1\, H_2)\begin{pmatrix} H_1^\top \\ H_2^\top \end{pmatrix} = H_1H_1^\top + H_2H_2^\top$$

which implies

$$H_2H_2^\top = I_p - H_1H_1^\top. \tag{A.29}$$

In the case where $p \leq n$, there is no matrix H_2 to consider so that we set $H = H_1$ and we have $\tilde{L} = L$.

Note also that, expressing the (i, j) term of the matrices, for any $p\times p$ matrix A, we have

$$(A\tilde{L})_{ij} = \begin{cases} A_{ij}\, l_j & \text{if } j = 1,\dots,n\wedge p \\ 0 & \text{if } p > n \text{ and } j = n+1,\dots,p \\ 0 & \text{if } i,j = 1,\dots,p \text{ and } i \neq j. \end{cases} \tag{A.30}$$

and

$$(\tilde{L}A)_{ij} = \begin{cases} l_i\, A_{ij} & \text{if } i = 1,\dots,n\wedge p \\ 0 & \text{if } p > n \text{ and } i = n+1,\dots,p \\ 0 & \text{if } i,j = 1,\dots,p \text{ and } i \neq j. \end{cases} \tag{A.31}$$

Furthermore,

$$(H^\top AH)_{ij} = \begin{cases} (H_1^\top AH_1)_{ij} & \text{if } i,j = 1,\dots,n\wedge p \\ (H_2^\top AH_1)_{ij} & \text{if } p > n,\ i = n+1,\dots,p \text{ and } j = 1,\dots,n \\ (H_1^\top AH_2)_{ij} & \text{if } p > n,\ j = n+1,\dots,p \text{ and } i = 1,\dots,n. \end{cases} \tag{A.32}$$

Finally upon differentiating and by orthogonality of H, we have

$$0 = d(I_p) = d(H^\top H) = d(H^\top)H + H^\top d(H) = 0$$

so that

$$d(H^\top)H = -H^\top d(H). \tag{A.33}$$

Recall that, for two $p\times n$ matrices A and B such that B is a differentiable function of A, $d(B)$ is the exterior product of the elements of B so that, dA_{ij} being the dual basis of $\partial/\partial A_{ij}$, we have

$$d(B)_{kl} = \sum_{i=1}^{p}\sum_{j=1}^{n} \frac{\partial B_{kl}}{\partial A_{ij}}\, dA_{ij}, \tag{A.34}$$

for $1 \leq k \leq p$ and $1 \leq l \leq n$ (see Muirhead [35, Chapter 2]).

In the following lemma, we give expressions of the generic elements of the matrix $H^\top d(H)$ in (A.33).

Lemma A.3. *Let $i, j = 1,\dots,p$. For $i = j$, we have*

$$(H^\top d(H))_{ii} = 0. \tag{A.35}$$

For $i \neq j$, we have that $(H^\top d(H))_{ij}$ equals

$$\begin{cases} \dfrac{1}{l_j - l_i}\left[H_1^\top \{d(U)\,U^\top + U\,d(U^\top)\}\,H_1\right]_{ij} & \text{if } i,j = 1,\dots,n\wedge p \\ \dfrac{1}{l_j}\left[H_2^\top \{d(U)\,U^\top + U\,d(U^\top)\}\,H_1\right]_{ij} & \text{if } p > n, i = n+1,\dots,p \text{ and } j = 1,\dots,n \\ \dfrac{1}{l_i}\left[H_1^\top \{d(U)\,U^\top + U\,d(U^\top)\}\,H_2\right]_{ij} & \text{if } p > n, j = n+1,\dots,p \text{ and } i = 1,\dots,n. \end{cases} \tag{A.36}$$

Proof. First, as the diagonal elements of a matrix are those of its transpose, for any $i = 1, \ldots, p$, we have

$$\big(H^\top d(H)\big)_{ii} = \big(\{H^\top d(H)\}^\top\big)_{ii} = \big(d(H^\top)H\big)_{ii} = -\big(H^\top d(H)\big)_{ii},$$

according to (A.33). Hence (A.35) holds, which is the first result of Lemma A.3.

Now, thanks to (A.28), we have

$$d(S) = d(H)\,\tilde{L}\,H^\top + Hd(\tilde{L})H^\top + H\,\tilde{L}\,d(H^\top). \tag{A.37}$$

Then, multiplying respectively by $H^\top$ and by H the left hand-side and the right hand-side of (A.37), we obtain

$$\begin{aligned} H^\top d(S)\,H &= H^\top d(H)\,\tilde{L} + d(\tilde{L}) + \tilde{L}\,d(H^\top)\,H \\ &= H^\top d(H)\,\tilde{L} + d(\tilde{L}) - \tilde{L}\,H^\top d(H), \end{aligned} \tag{A.38}$$

according to (A.33). To express the (i, j) term of the matrices in (A.38), use (A.30) and (A.31) with $A = H^\top d(H)$ and the fact that

$$d\tilde{L}_{ij} = \begin{cases} dl_i & \text{if } i = j \text{ and } i = 1, \ldots, n \wedge p \\ 0 & \text{if } i \neq j \text{ or, when } p > n,\ i = n+1, \ldots, p \text{ or } j = n+1, \ldots, p. \end{cases}$$

For $i \neq j$, we have

$$(H^\top d(S)\,H)_{ij} = \begin{cases} (H^\top d(H))_{ij}\,(l_j - l_i) & \text{if } i, j = 1, \ldots, n \wedge p \\ (H^\top d(H))_{ij}\,l_j & \text{if } p > n,\ j = n+1, \ldots, p \text{ and } i = 1, \ldots, n \\ (H^\top d(H))_{ij}\,l_i & \text{if } p > n,\ i = n+1, \ldots, p \text{ and } j = 1, \ldots, n \\ 0 & \text{if } p > n,\ i, j = n+1, \ldots, p, \end{cases}$$

so that it follows that

$$(H^\top d(H))_{ij} = \begin{cases} \dfrac{1}{l_j - l_i}(H_1^\top d(S)\,H_1)_{ij} & \text{if } i, j = 1, \ldots, n \wedge p \\ \dfrac{1}{l_j}(H_2^\top d(S)\,H_1)_{ij} & \text{if } p > n,\ i = n+1, \ldots, p \text{ and } j = 1, \ldots, n \\ \dfrac{1}{l_i}(H_1^\top d(S)\,H_2)_{ij} & \text{if } p > n,\ j = n+1, \ldots, p \text{ and } i = 1, \ldots, n. \end{cases} \tag{A.39}$$

As $S = U\,U^\top$, replacing $d(S)$ by $d(U)\,U^\top + U\,d(U^\top)$ in (A.39), gives (A.36). □

Lemma A.3 is applied to obtain the partial derivatives of the diagonal elements of L and of the elements of H with respect to the generic elements of U.

Lemma A.4. *For $1 \le m \le n \wedge p$, $1 \le j \le n$ and $1 \le i \le p$, we have*

$$\frac{\partial l_m}{\partial U_{ij}} = 2\sum_{k=1}^{p}(H_1)_{im}U_{kj}(H_1)_{km}. \tag{A.40}$$

Also, for $1 \le c, a, k \le p$ and $1 \le l \le n$, we have

$$\frac{\partial H_{ak}}{\partial U_{cl}} = \begin{cases} A + B & \text{if } p > n \\ A & \text{if } p \le n \end{cases} \tag{A.41}$$

where

$$A = \sum_{i \neq k}^{n \wedge p}\sum_{m=1}^{p}\frac{H_{ai}\,[H_{ci}\,H_{mk} + H_{ck}\,H_{mi}]\,U_{ml}}{l_k - l_i} \tag{A.42}$$

and

$$B = \sum_{i=n+1}^{p}\sum_{m=1}^{p}\frac{H_{ai}\,[H_{ci}\,H_{mk} + H_{ck}\,H_{mi}]\,U_{ml}}{l_k}. \tag{A.43}$$

Proof. Let $1 \le m \le n \wedge p$. Using (A.28) and $d(S) = d(U)\,U^\top + U\,d(U^\top)$ we have

$$\begin{aligned}
dL_{mm} &= (H_1^\top\, d(S)\, H_1)_{mm} \\
&= (H_1^\top\, [d(U)\, U^\top + U\, d(U^\top)]\, H_1)_{mm} \\
&= (H_1^\top\, d(U)\, U^\top\, H_1)_{mm} + (\{H_1^\top\, U\, d(U^\top)\, H_1\}^\top)_{mm} \\
&= 2\,(H_1^\top\, d(U)\, U^\top\, H_1)_{mm} \\
&= 2 \sum_{i=1}^{p} \sum_{j=1}^{n} \sum_{k=1}^{p} (H_1^\top)_{mi}\, (dU)_{ij}\, (U^\top)_{jk}\, (H_1)_{km} \\
&= 2 \sum_{i=1}^{p} \sum_{j=1}^{n} \sum_{k=1}^{p} (H_1)_{im}\, U_{kj}\, (H_1)_{km}\, dU_{ij} \\
&= \sum_{i=1}^{p} \sum_{j=1}^{n} \left\{ 2 \sum_{k=1}^{p} (H_1)_{im}\, U_{kj}\, (H_1)_{km} \right\} dU_{ij}.
\end{aligned}$$

As, for $1 \le m \le n \wedge p$, we have $L_{mm} = l_m$, Equality (A.40) follows, for any $1 \le j \le n$ and any $1 \le i \le p$, according to (A.34).

Now, since $HH^\top = I_p$, we can write

$$dH_{ak} = (HH^\top d(H))_{ak} = \sum_{i=1}^{p} H_{ai}(H^\top d(H))_{ik}, \tag{A.44}$$

which can be expressed, in the case where $p > n$, as

$$dH_{ak} = \sum_{i=1}^{n} H_{ai}(H^\top d(H))_{ik} + \sum_{i=n+1}^{p} H_{ai}(H^\top d(H))_{ik}. \tag{A.45}$$

In this last case, applying (A.35) and (A.36) in Lemma A.3, we have

$$dH_{ak} = A + B \tag{A.46}$$

where

$$A = \sum_{i \neq k}^{n} H_{ai} \left\{ \frac{1}{l_k - l_i} \left[(H^\top d(U) U^\top H)_{ik} + (H^\top\, U\, d(U^\top)\, H)_{ik} \right] \right\} \tag{A.47}$$

and

$$B = \sum_{i=n+1}^{p} H_{ai} \left\{ \frac{1}{l_k} \left[(H^\top d(U) U^\top H)_{ik} + (H^\top\, U\, d(U^\top)\, H)_{ik} \right] \right\}. \tag{A.48}$$

Now, expanding (A.47) gives

$$\begin{aligned}
A &= \sum_{i \neq k}^{n} H_{ai} \left\{ \frac{1}{l_k - l_i} \sum_{c=1}^{p} \sum_{l=1}^{n} \sum_{m=1}^{p} [H_{ci}\, dU_{cl}\, U_{ml}\, H_{mk} + H_{ck}\, dU_{cl}\, U_{ml}\, H_{mi}] \right\} \\
&= \sum_{c=1}^{p} \sum_{l=1}^{n} \left\{ \sum_{i \neq k}^{n} \sum_{m=1}^{p} \frac{1}{l_k - l_i}\, H_{ai}\, [H_{ci} H_{mk} + H_{ck}\, H_{mi}]\, U_{ml} \right\} dU_{cl}
\end{aligned} \tag{A.49}$$

while (A.48) equals

$$B = \sum_{c=1}^{p} \sum_{l=1}^{n} \left\{ \sum_{i=n+1}^{p} \sum_{m=1}^{p} \frac{1}{l_k}\, H_{ai}\, [H_{ci}\, H_{mk} + H_{ck}\, H_{mi}]\, U_{ml} \right\} dU_{cl}. \tag{A.50}$$

Finally, by combining (A.49) and (A.50), we obtain that dH_{ak} equals

$$\sum_{c=1}^{p} \sum_{l=1}^{n} \left\{ \sum_{\substack{i=1 \\ i \neq k}}^{n} \sum_{m=1}^{p} \frac{H_{ai}[H_{ci} H_{mk} + H_{ck} H_{mi}] U_{ml}}{l_k - l_i} + \sum_{i=n+1}^{p} \sum_{m=1}^{p} \frac{H_{ai}[H_{ci} H_{mk} + H_{ck} H_{mi}] U_{ml}}{l_k} \right\} dU_{cl}$$

which is (A.41) in the case where $p > n$, according to (A.34).

The result for the case $p \le n$ is easily deduced by following the same steps and using (A.44) instead of (A.45) for the differential operator dH_{ak}. $\square$

An application of Lemma A.4 to the critical term $(U\nabla_{U^\top})^\top H_1\,\varphi(L)\,H_1^\top$ gives the following result.

Lemma A.5. *For any diagonal matrix $\varphi(L) = \mathrm{diag}(\varphi_1(L), \ldots, \varphi_{n\wedge p}(L))$ and for $1 \le i,j \le p$, the generic term $B_{ij} = \left\{U\,\nabla_{U^\top}\,H_1\,\varphi(L)\,H_1^\top\right\}_{ij}$ of the matrix $U\,\nabla_{U^\top}\,H_1\,\varphi(L)\,H_1^\top$ equals*

$$\begin{cases} \displaystyle\sum_{q=1}^{n} H_{iq}H_{jq}\left\{2l_q\frac{\partial\varphi_q(L)}{\partial l_q} + \sum_{b\neq q}^{n}\frac{l_b\varphi_q(L) - l_b\varphi_b(L)}{l_q - l_b}\right\} + \sum_{b=n+1}^{p} H_{ib}H_{jb}\sum_{q=1}^{n}\varphi_q(L) & \text{if } p > n \\ \displaystyle\sum_{q=1}^{p} H_{iq}H_{jq}\left\{2l_q\frac{\partial\varphi_q(L)}{\partial l_q} + \sum_{b\neq q}^{p}\frac{l_b\varphi_q(L) - l_b\varphi_b(L)}{l_q - l_b}\right\} & \text{if } p \le n. \end{cases}$$

Proof. First, we deal with the case $p > n$. For $1 \le i,j \le p$, we have

$$\left\{(U\nabla_{U^\top})^\top H_1\varphi H_1^\top\right\}_{ij} = \sum_{k=1}^{p}(U\nabla_{U^\top})_{ki}(H_1\varphi H_1^\top)_{kj} = S_1 + S_2 + S_3,$$

where

$$S_1 = \sum_{k=1}^{p}\sum_{l,q=1}^{n} U_{kl}\,(H_1)_{kq}\,\frac{\partial\varphi_q(L)}{\partial U_{il}}\,(H_1)_{jq} \tag{A.51}$$

$$S_2 = \sum_{k=1}^{p}\sum_{l,q=1}^{n} U_{kl}\,\frac{\partial(H_1)_{kq}}{\partial U_{il}}\,\varphi_q(L)\,(H_1)_{jq}, \tag{A.52}$$

and

$$S_3 = \sum_{k=1}^{p}\sum_{l,q=1}^{n} U_{kl}\,(H_1)_{kq}\,\varphi_q(L)\,\frac{\partial(H_1)_{jq}}{\partial U_{il}}. \tag{A.53}$$

To expand the S_i's terms, we use the decomposition $L = H^\top S\,H$ and the fact that

$$L_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ l_i & \text{if } i = j \\ 0 & \text{if } i \ge n+1. \end{cases} \tag{A.54}$$

First, as for (A.51), we have

$$S_1 = \sum_{k=1}^{p}\sum_{l,q=1}^{n} U_{kl}(H_1)_{kq}\sum_{m=1}^{n}\frac{\partial\varphi_q(L)}{\partial l_m}\frac{\partial l_m}{\partial U_{il}}(H_1)_{jq},$$

so that, using (A.40) in Lemma A.4, we can write

$$\begin{aligned} S_1 &= \sum_{k=1}^{p}\sum_{l,q,m=1}^{n} U_{kl}(H_1)_{kq}\frac{\partial\varphi_q(L)}{\partial l_m}2\sum_{q_3=1}^{p}(H_1)_{im}U_{q_3 l}(H_1)_{q_3 m}(H_1)_{jq} \\ &= 2\sum_{k,q_3=1}^{p}\sum_{q,m=1}^{n}(H_1)_{kq}S_{kq_3}(H_1)_{im}(H_1)_{jq}\frac{\partial\varphi_q(L)}{\partial l_m} \\ &= 2\sum_{q,m=1}^{n} L_{qm}\,(H_1)_{im}\,(H_1)_{jq}\,\frac{\partial\varphi_q(L)}{\partial l_m} \\ &= 2\sum_{m=1}^{n} l_m\,\frac{\partial\,\varphi_m(L)}{\partial l_m}(H_1)_{im}\,(H_1)_{jm} \end{aligned} \tag{A.55}$$

since $S = UU^\top$ and thanks to (A.54).

As for S_2 in (A.52), applying (A.41) in Lemma A.4, we have

$$
\begin{aligned}
S_2 &= \sum_{k=1}^{p}\sum_{l,q=1}^{n} U_{kl}\,(H_1)_{jq}\,\varphi_q(L)\left\{\sum_{q_1\neq q}^{n}\sum_{q_2=1}^{p}\frac{[H_{kq_1}H_{iq_1}H_{q_2q}+H_{kq_1}H_{iq}H_{q_2q_1}]U_{q_2l}}{l_q-l_{q_1}}\right.\\
&\quad\left.+\sum_{q_1=n+1}^{p}\sum_{q_2=1}^{p}\frac{[H_{kq_1}H_{iq_1}H_{q_2q}+H_{kq_1}H_{iq}H_{q_2q_1}]U_{q_2l}}{l_q}\right\}\\
&= \sum_{k=1}^{p}\sum_{q=1}^{n}(H_1)_{jq}S_{kq_2}\varphi_q(L)\left\{\sum_{q_1\neq q}^{n}\sum_{q_2=1}^{p}\frac{[H_{kq_1}H_{iq_1}H_{q_2q}+H_{kq_1}H_{iq}H_{q_2q_1}]}{l_q-l_{q_1}}\right.\\
&\quad\left.+\sum_{q_1=n+1}^{p}\sum_{q_2=1}^{p}\frac{[H_{kq_1}H_{iq_1}H_{q_2q}+H_{kq_1}H_{iq}H_{q_2q_1}]}{l_q}\right\}\\
&= \sum_{k=1}^{p}\sum_{q=1}^{n}\left\{\sum_{q_1\neq q}^{n}\sum_{q_2=1}^{p}\frac{\varphi_q(L)}{l_q-l_{q_1}}[H_{jq}S_{kq_2}H_{kq_1}H_{iq_1}H_{q_2q}+H_{jq}S_{kq_2}H_{kq_1}H_{iq}H_{q_2q_1}]\right.\\
&\quad\left.+\sum_{q_1=n+1}^{p}\sum_{q_2=1}^{p}\frac{\varphi_q(L)}{l_q}[H_{jq}S_{kq_2}H_{kq_1}H_{iq_1}H_{q_2q}+H_{jq}S_{kq_2}H_{kq_1}H_{iq}H_{q_2q_1}]\right\}\\
&= \sum_{q=1}^{n}\sum_{q_1\neq q}^{n}\frac{\varphi_q(L)}{l_q-l_{q_1}}[L_{q_1q}H_{jq}H_{iq_1}+L_{q_1q_1}H_{jq}H_{iq}]\\
&\quad+\sum_{q=1}^{n}\sum_{q_1=n+1}^{p}\frac{\varphi_q(L)}{l_q}[L_{q_1q}H_{jq}H_{iq_1}+l_{q_1}H_{jq}H_{iq}].
\end{aligned}
$$

Then, using (A.54), we can see that S_2 reduces to

$$
S_2=\sum_{q=1}^{n}\sum_{q_1\neq q}^{n}\frac{H_{jq}H_{iq}l_{q_1}\varphi_q(L)}{l_q-l_{q_1}}=\sum_{q=1}^{n}\sum_{q_1\neq q}^{n}H_{iq_1}H_{iq_1}\frac{l_q\varphi_{q_1}(L)}{l_{q_1}-l_q}. \tag{A.56}
$$

Similarly, S_3 in (A.53) can be expressed as

$$
\begin{aligned}
S_3 &= \sum_{k=1}^{p}\sum_{l,q=1}^{n} U_{kl}(H_1)_{kq}\varphi_q(L)\left\{\sum_{q_1\neq q}^{n}\sum_{q_2=1}^{p}\frac{[H_{jq_1}H_{iq_1}H_{q_2q}+H_{jq_1}H_{iq}H_{q_2q_1}]}{l_q-l_{q_1}}U_{q_2l}\right.\\
&\quad\left.+\sum_{q_1=n+1}^{p}\sum_{q_2=1}^{p}\frac{[H_{jq_1}H_{iq_1}H_{q_2q}+H_{jq_1}H_{iq}H_{q_2q_1}]}{l_q}U_{q_2l}\right\}\\
&= \sum_{k=1}^{p}\sum_{q=1}^{n}H_{kq}S_{kq_2}\varphi_q(L)\left\{\sum_{q_1\neq q}^{n}\sum_{q_2=1}^{p}\frac{[H_{jq_1}H_{iq_1}H_{q_2q}+H_{jq_1}H_{iq}H_{q_2q_1}]}{l_q-l_{q_1}}\right.\\
&\quad\left.+\sum_{q_1=n+1}^{p}\sum_{q_2=1}^{p}\frac{[H_{jq_1}H_{iq_1}H_{q_2q}+H_{jq_1}H_{iq}H_{q_2q_1}]}{l_q}\right\}\\
&= \sum_{k=1}^{p}\sum_{q=1}^{n}\sum_{q_1\neq q}^{n}\sum_{q_2=1}^{p}\frac{H_{kq}S_{kq_2}\varphi_q(L)H_{jq_1}H_{iq_1}H_{q_2q}}{l_q-l_{q_1}}\\
&\quad+\sum_{k=1}^{p}\sum_{q=1}^{n}\sum_{q_1\neq q}^{n}\sum_{q_2=1}^{p}\frac{H_{kq}S_{kq_2}\varphi_q(L)H_{jq_1}H_{iq}H_{q_2q_1}}{l_q-l_{q_1}}\\
&\quad+\sum_{k=1}^{p}\sum_{q=1}^{n}\sum_{q_1=n+1}^{p}\sum_{q_2=1}^{p}\frac{H_{kq}S_{kq_2}\varphi_q(L)H_{jq_1}H_{iq_1}H_{q_2q}}{l_q}\\
&\quad+\sum_{k=1}^{p}\sum_{q=1}^{n}\sum_{q_1=n+1}^{p}\sum_{q_2=1}^{p}\frac{H_{kq}S_{kq_2}\varphi_q(L)H_{jq_1}H_{iq}H_{q_2q_1}}{l_q}
\end{aligned}
$$

$$= \sum_{q=1}^{n} \sum_{q_1 \neq q}^{n} \frac{l_q H_{jq_1} H_{iq_1} \varphi_q(L)}{l_q - l_{q_1}} + \sum_{q=1}^{n} \sum_{q_1 \neq q}^{n} \frac{L_{qq_1} H_{jq_1} H_{iq} \varphi_q(L)}{l_q - l_{q_1}}$$
$$+ \sum_{q=1}^{n} \sum_{q_1=n+1}^{p} \frac{l_q H_{jq_1} H_{iq_1} \varphi_q(L)}{l_q} + \sum_{q=1}^{n} \sum_{q_1=n+1}^{p} L_{qq_1} \varphi_q(L) H_{jq_1} H_{iq}$$
$$= \sum_{q=1}^{n} \sum_{q_1 \neq q}^{n} H_{jq_1} H_{iq_1} \frac{l_q \varphi_q(L)}{l_q - l_{q_1}} + \sum_{q=1}^{n} \sum_{q_1=n+1}^{p} H_{jq_1} H_{iq_1} \varphi_q(L), \tag{A.57}$$

where the last equality is due to (A.54). Finally, gathering the above expressions of S_1, S_2 and S_3 in (A.55)–(A.57), we obtain the desired result when $p > n$. The case $p \leq n$ is easily deduced, following the same steps, by replacing "n" by "p" and by removing the sum $\sum_{q_1=n+1}^{p}$. $\square$

Thanks to Lemma A.5, the following proposition provides an expression for the quantity $\operatorname{tr}\big(n\, G(X,S) + U\, \nabla_{U^\top} G^\top(X,S)\big)$ in the case where $G(X,S) = H_1 L^{-1} \Psi(L) H_1^\top$.

Proposition A.1. *Let* $\Psi(L) = \operatorname{diag}(\psi_1(L), \ldots, \psi_{n\wedge p}(L))$ *and* $G(X,S) = H_1 L^{-1} \Psi(L) H_1^\top$. *We have*

$$\operatorname{tr}\big(n\, G(X,S) + U\, \nabla_{U^\top} G^\top(X,S)\big)$$
$$= \sum_{k=1}^{n\wedge p} \left\{ \big(|n-p| - 1\big) \frac{\psi_k(L)}{l_k} + 2 \frac{\partial \psi_k(L)}{\partial l_k} + \sum_{b\neq k}^{n\wedge p} \frac{\psi_k(L) - \psi_b(L)}{l_k - l_b} \right\}. \tag{A.58}$$

Proof. Note first that

$$\operatorname{tr}(G(X,S)) = \operatorname{tr}\big(L^{-1} \Psi(L)\big) = \sum_{k=1}^{n\wedge p} \frac{\psi_k(L)}{l_k}, \tag{A.59}$$

so that we will have to calculate

$$\operatorname{tr}\big(U\, \nabla_{U^\top} G^\top(X,S)\big) = \sum_{k=1}^{n\wedge p} B_{ii} \tag{A.60}$$

where, B_{ij} is defined in Lemma A.4 with $\varphi(L) = L^{-1} \Psi(L)$, that is, with $\varphi_k = \psi_k(L)/l_k$, for $1 \leq k \leq n \wedge p$. We have, according to Lemma A.4,

$$B_{ij} = \begin{cases} C_{ij} + D_{ij} & \text{if } p > n \\ C_{ij} & \text{if } p \leq n \end{cases} \tag{A.61}$$

where

$$C_{ij} = \sum_{k=1}^{n\wedge p} H_{ik} H_{jk} \left\{ 2 \left(\frac{\partial \psi_k(L)}{\partial l_k} - \frac{\psi_k(L)}{l_k} \right) + \sum_{b\neq k}^{n\wedge p} \frac{l_b\, \psi_k(L)\, l_k^{-1} - \psi_b(L)}{l_k - l_b} \right\} \tag{A.62}$$

and

$$D_{ij} = \sum_{b=n+1}^{p} H_{ib} H_{jb} \sum_{k=1}^{n} \psi_k(L)\, l_k^{-1}. \tag{A.63}$$

Note that, for $1 \leq k \leq n \wedge p$, the following bookkeeping identity holds

$$\sum_{b\neq k}^{n\wedge p} \frac{l_b\, \psi_k(L)\, l_k^{-1} - l_k\, \psi_b(L)\, l_k^{-1}}{l_k - l_b} = \sum_{b\neq k}^{n\wedge p} \frac{l_b\, \psi_k(L) - l_k\, \psi_b(L) + l_k\, \psi_k(L) - l_k\, \psi_k(L)}{l_k\,(l_k - l_b)}$$
$$= \sum_{b\neq k}^{n\wedge p} \frac{\psi_k(L) - \psi_b(L)}{l_k - l_b} - \sum_{b\neq k}^{n\wedge p} \frac{\psi_k(L)}{l_k}$$
$$= \sum_{b\neq k}^{n\wedge p} \frac{\psi_k(L) - \psi_b}{l_k - l_b} - [(n\wedge p) - 1]\, \frac{\psi_k(L)}{l_k}.$$

Therefore (A.62) equals

$$\begin{aligned} C_{ij} &= \sum_{k=1}^{n\wedge p} H_{ik}\, H_{jk} \left\{ 2\, \frac{\partial \psi_k(L)}{\partial l_k} - [(n\wedge p)+1]\, \frac{\psi_k(L)}{l_k} + \sum_{b\neq k}^{n\wedge p} \frac{\psi_k(L)-\psi_b(L)}{l_k-l_b} \right\} \\ &= \sum_{k=1}^{n\wedge p} H_{ik}\, \psi_k^*(L)\, H_{kj}^\top \\ &= (H_1\, \Psi^*(L)\, H_1^\top)_{ij}, \end{aligned} \tag{A.64}$$

where $\Psi^*(L) = \mathrm{diag}(\psi_1^*(L), \ldots, \psi_{n\wedge p}^*(L))$ with

$$\psi_k^*(L) = 2\, \frac{\partial \psi_k(L)}{\partial l_k} - [(n\wedge p)+1]\, \frac{\psi_k(L)}{l_k} + \sum_{b\neq k}^{n\wedge p} \frac{\psi_k(L)-\psi_b(L)}{l_k-l_b} \tag{A.65}$$

for $1 \le k \le n \wedge p$.

Now we deal with the quantity in (A.63) which involves $p > n$. Recalling the decomposition of H in (A.28), we have

$$D_{ij} = (H_2\, H_2^\top)_{ij}\, \mathrm{tr}(L^{-1}\, \psi(L)) = (I_p - H_1 H_1^\top)_{ij}\, \mathrm{tr}(L^{-1}\, \psi(L)), \tag{A.66}$$

according to (A.29).

Gathering (A.64) and (A.66) in (A.61) gives

$$B_{ij} = \begin{cases} (H_1\, \Psi^*(L)\, H_1^\top)_{ij} + (I_p - H_1 H_1^\top)_{ij}\, \mathrm{tr}(L^{-1}\, \Psi(L)) & \text{if } p > n \\ (H_1\, \Psi^*(L)\, H_1^\top)_{ij} & \text{if } p \le n \end{cases} \tag{A.67}$$

and hence (A.60) can be written as

$$\mathrm{tr}\left(U\, \nabla_{U^\top}\, G^\top(X,S)\right) = \begin{cases} \mathrm{tr}\left(\Psi^*(L)\right) + (p-n)\, \mathrm{tr}(L^{-1}\, \Psi(L)) & \text{if } p > n \\ \mathrm{tr}\left(\Psi^*(L)\right) & \text{if } p \le n, \end{cases}$$

which is equal, according to (A.65) and to (A.59), to

$$\begin{cases} \displaystyle\sum_{k=1}^{n} \left\{ 2\, \frac{\partial \psi_k(L)}{\partial l_k} + [-2\,n + p - 1]\, \frac{\psi_k(L)}{l_k} + \sum_{b\neq k}^{n} \frac{\psi_k(L)-\psi_b(L)}{l_k-l_b} \right\} & \text{if } p > n \\ \displaystyle\sum_{k=1}^{p} \left\{ 2\, \frac{\partial \psi_k(L)}{\partial l_k} - [p+1]\, \frac{\psi_k(L)}{l_k} + \sum_{b\neq k}^{p} \frac{\psi_k(L)-\psi_b(L)}{l_k-l_b} \right\} & \text{if } p \le n. \end{cases} \tag{A.68}$$

Finally, after simplifying, (A.59) and (A.68) yield (A.58), which is the desired result. □

Applying Proposition A.1 to $\Psi(L)$ in (2.20) gives rise to the following corollary.

Corollary A. *Let $\Psi(L)$ be as in (2.20). Then*

$$\begin{aligned} &[n - (|n-p| - 3)]\, \mathrm{tr}\,(G(X,S)) + \mathrm{tr}\left(U\, \nabla_{U^\top}\, G^\top(X,S)\right) \\ &= \sum_{k=1}^{n\wedge p} \left\{ \frac{2}{l_k}\, \frac{\partial \delta_k(L)}{\partial l_k} + \sum_{b\neq k}^{n\wedge p} \frac{\{\delta_k(L) - a\}/l_k - \{\delta_b(L) - a\}/l_b}{l_k - l_b} \right\}, \end{aligned} \tag{A.69}$$

which is nonnegative under Conditions (2.17), (2.18) and the second inequality in (2.22).

Proof. It follows from (A.58) and (A.59) that

$$\begin{aligned} &[n - (|n-p| - 3)]\, \mathrm{tr}\,(G(X,S)) + \mathrm{tr}\left(U\, \nabla_{U^\top}\, G^\top(X,S)\right) \\ &= \sum_{k=1}^{n\wedge p} \left\{ 2\, \frac{\psi_k(L)}{l_k} + 2\, \frac{\partial \psi_k(L)}{\partial l_k} + \sum_{b\neq k}^{n\wedge p} \frac{\psi_k(L)-\psi_b(L)}{l_k-l_b} \right\}. \end{aligned} \tag{A.70}$$

Now, by (2.20), for $k = 1, \ldots, n\wedge p$, $\psi_k(L) = (\delta_k(L) - a)/l_k$ so that

$$\frac{\partial \psi_k(L)}{\partial l_k} = \frac{1}{l_k}\, \frac{\partial \delta_k(L)}{\partial l_k} + \frac{a - \delta_k(L)}{l_k^2}$$

and the terms $\psi_k(L)/l_k$ cancel in (A.70), which gives (A.69).

As for the sign of (A.69), note first that, by Condition (2.18), the derivative terms on the right hand side of (A.69) are nonnegative. We will see that the other terms are nonnegative as well, so that the quantity in (A.69) is nonnegative. Indeed, for $k = 1, \ldots, p$ and for $b \neq k$, we have

$$\begin{aligned}
\frac{1}{l_k - l_b}\left[\frac{\delta_k(L) - a}{l_k} - \frac{\delta_b(L) - a}{l_b}\right] &= \frac{\delta_k(L)\, l_b - a\, l_b - \delta_b(L)\, l_k + a\, l_k}{l_k\, l_b\, (l_k - l_b)} \\
&= \frac{\delta_k(L)\, l_b - \delta_b(L)\, l_k}{l_k\, l_b\, (l_k - l_b)} + \frac{a}{l_k\, l_b} \\
&= \frac{l_b\, (\delta_k(L) - \delta_b(L)) - \delta_b(L)\, (l_k - l_b)}{l_k\, l_b\, (l_k - l_b)} + \frac{a}{l_k\, l_b} \\
&= \frac{\delta_k(L) - \delta_b(L)}{l_k\, (l_k - l_b)} + \frac{a - \delta_b(L)}{l_k\, l_b} \\
&\geq 0,
\end{aligned}$$

according to (2.15), (2.17) and the second inequality in (2.22). □

A.4. Matrix and trace inequalities

Through the singular value decomposition in (2.14), we have $S^+ = H_1\, L^{-1}\, H_1^\top$ and for any $p \times 1$ vector x it can be seen that

$$x^\top S^+ x = (H_1^\top x)^\top L^{-1}\, (H_1^\top x) = \sum_{i=1}^{p} \frac{1}{l_i}\, (H_1^\top x)_i^2 \geq \sum_{i=1}^{p} \frac{1}{\sum_{j=1}^{p} l_j}\, (H_1^\top x)_i^2 = x^\top \frac{H_1\, H_1^\top}{\mathrm{tr}(L)}\, x. \tag{A.71}$$

Therefore, it follows that

$$S^+ \geq \frac{H_1\, H_1^\top}{\mathrm{tr}(S)}, \tag{A.72}$$

and hence,

$$\mathrm{tr}(S^+) \geq \frac{\mathrm{tr}(H_1\, H_1^\top)}{\mathrm{tr}(S)} = \frac{n \wedge p}{\mathrm{tr}(S)}. \tag{A.73}$$

Similarly, we can show that

$$\mathrm{tr}(S^+\, Q_0) \geq \frac{\mathrm{tr}(H_1\, H_1^\top\, Q_0)}{\mathrm{tr}(S)} = \frac{\mathrm{tr}(S\, S^+\, Q_0)}{\mathrm{tr}(S)}. \tag{A.74}$$

Since $Q_0 = Q\, (Q^\top\, Q)^{-1}\, Q^\top$

$$\mathrm{tr}(S^+\, Q_0) = \mathrm{tr}([Q\, (Q^\top\, Q)^{-1/2}]^\top\, S^+\, [Q\, (Q^\top\, Q)^{-1/2}])$$

and since, setting $x = H_1^\top\, Q\, (Q^\top\, Q)^{-1/2}\, y$, for any $p \times 1$ vector y, it follows from (A.71) that

$$[Q\, (Q^\top\, Q)^{-1/2}]^\top\, S^+\, [Q\, (Q^\top\, Q)^{-1/2}] \geq \frac{[H_1^\top\, Q\, (Q^\top\, Q)^{-1/2}]^\top\, S^+\, [H_1^\top\, Q\, (Q^\top\, Q)^{-1/2}]}{\mathrm{tr}(S)}.$$

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