Covariance matrix estimation under data-based loss

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ABSTRACT

In this paper, we consider the problem of estimating the $p \times p$ scale matrix Σ of a multivariate linear regression model $Y = X \beta + \mathcal{E}$ when the distribution of the observed matrix Y belongs to a large class of elliptically symmetric distributions. After deriving the canonical form $(Z^{\top}U^{\top})^{\top}$ of this model, any estimator $\hat{\Sigma}$ of Σ is assessed through the data-based loss tr $(S^{+}\Sigma(\Sigma^{-1}\hat{\Sigma} - I_p)^2)$ where $S = U^{\top}U$ is the sample covariance matrix and S^+ is its Moore-Penrose inverse. We provide alternative estimators to the usual estimators a S, where a is a positive constant, which present smaller associated risk. Compared to the usual quadratic loss tr $(\Sigma^{-1}\hat{\Sigma} - I_p)^2$, we obtain a larger class of estimators and a wider class of elliptical distributions for which such an improvement occurs. A numerical study illustrates the theory.

1. Introduction

Let consider the multivariate linear regression model, with p responses and n observations,

$$Y = X \beta + \mathcal{E}, \tag{1.1}$$

where Y is an $n \times p$ matrix, X is an $n \times q$ matrix of known constants of rank $q \le n$ and β is a $q \times p$ matrix of unknown parameters. We assume that the $n \times p$ noise matrix \mathcal{E} has an elliptically symmetric distribution with density, with respect to the Lebesgue measure in \mathbb{R}^{pn} , of the form

$$\varepsilon \mapsto |\Sigma|^{-n/2} f\left(\operatorname{tr}(\varepsilon \,\Sigma^{-1} \varepsilon^{\mathsf{T}})\right),\tag{1.2}$$

where Σ is a $p \times p$ unknown positive definite matrix and $f(\cdot)$ is a non–negative unknown function.

The model (1.1) has been considered by various authors such as Kubokawa and Srivastava (1999, 2001), who estimated Σ and β respectively in the context (1.2), and Tsukuma and Kubokawa (2016) who estimated Σ in the Gaussian setting. A common alternative representation of this model is $Y = M + \mathcal{E}$, where \mathcal{E} is as above and M is in the column space of X, has been also considered in the literature. See for instance Canu and Fourdrinier (2017) and Candès, Sing-Long and Trzasko (2013).

Although the matrix of regression coefficients β is also unknown, we are interested in estimating the scale matrix Σ . We address this problem under a decision-theoretic framework through a canonical form of the model (1.1), which allows to use a sufficient statistic $S = U^{\top}U$ for Σ , where U is an $(n - q) \times p$ matrix (see Section 2 for more details). In this context, the natural estimators of Σ are of the form

$$\hat{\Sigma}_a = a S \,, \tag{1.3}$$

for some positive constants *a*.

As pointed out by James and Stein (1961), the estimators of the form (1.3) perform poorly in the Gaussian setting. In fact, larger (smaller) eigenvalues of Σ are overestimated (underestimated) by those estimators. Thus we may expect to improve these estimators by shrinking the eigenvalues of S, which gives rise to the class of orthogonaly invariant

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estimators (see Takemura (1984)). Since the seminal work of James and Stein (1961), this problem has been largely considered in the Gaussian setting. See, for instance, Tsukuma and Kubokawa (2016), Tsukuma (2016) and Chételat and Wells (2016). However, the elliptical setting has been considered by a few authors such as Kubokawa and Srivastava (1999), Haddouche, Fourdrinier and Mezoued (2021).

In this paper, the performance of any estimator $\hat{\Sigma}$ of Σ is assessed through the data-based loss

$$L_{S}(\hat{\Sigma}, \Sigma) = \operatorname{tr}\left(S^{+}\Sigma\left(\Sigma^{-1}\hat{\Sigma} - I_{p}\right)^{2}\right)$$
(1.4)

and its associated risk

$$R(\hat{\Sigma}, \Sigma) = E_{\theta, \Sigma} \left[\operatorname{tr} \left(S^+ \Sigma \left(\Sigma^{-1} \hat{\Sigma} - I_p \right)^2 \right) \right], \tag{1.5}$$

where $E_{\theta,\Sigma}$ denotes the expectation with respect to the density specified below in (2.3) and where S^+ is the Moore– Penrose inverse of S. Note that, when p > n - q, S is non–invertible and, when $p \le n - q$, S is invertible so that S^+ coincides with the regular inverse S^{-1} . This type of loss is called data–based loss in so far as it contains a part of the observation U through $S = U^{\top}U$. The notion of data–based loss was introduced by Efron and Morris (1976) when estimating a location parameter. Likewise, Fourdrinier and Strawderman (2015) showed the interest of considering such a data–based loss with respect to the usual quadratic losses. Also, the data–based loss (1.4) was considered, in a Gaussian setting, by Tsukuma and Kubokawa (2015) who were motivated by the difficulty to handle with the standard quadratic loss

$$L(\hat{\Sigma}, \Sigma) = \operatorname{tr}\left(\Sigma^{-1}\hat{\Sigma} - I_p\right)^2.$$
(1.6)

See Haff (1980) and Tsukuma (2016) for more details. Thus the loss in (1.4) is a data-based variant of the (1.6), through which we aim to improve on the estimators $\hat{\Sigma}_a$ in (1.3) by alternative estimators, focusing on improved orthogonally invariant estimators. Note that most improvement results in the Gaussian case were derived thanks to Stein–Haff types identities. Here, we specifically use the Stein–Haff type identity given by Haddouche et al. (2021), in the elliptical case, to establish our dominance result, which is well adapted to our unified approach of the cases *S* invertible and *S* non–invertible.

The rest of this paper is structured as follows. In Section 2, we give improvement conditions of the proposed estimators over the usual estimators. In Section 3, we assess the quality of the proposed estimators through a simulation study in the context of the t–distribution. We also compare numerically our results with those of Konno (2009) in the Gaussian setting. Finally, we give in an Appendix all the proofs of our findings.

2. Main results

Although we are interested in estimating the scale matrix Σ , recall that β is a $q \times p$ matrix of unknown parameters. Note that, since X has full column rank, the least square estimator of β is $\hat{\beta} = (X^{\top}X)^{-1} X^{\top}Y$; this is the maximum likelihood estimator in the Gaussian setting. Natural estimators of the scale matrix Σ are based on the residual sum of squares given by

$$S = Y^{+} (I_n - P_X) Y, (2.1)$$

where $P_X = X (X^{\top}X)^{-1} X^{\top}$ is the orthogonal projector onto the subspace spanned by the columns of X.

Following the lines of Kubokawa and Srivastava (1999) and Tsukuma and Kubokawa (2020b), we derive the canonical form of the model (1.1) which allows a suitable treatment of the estimation of Σ . Let $X = Q_1 T^{\mathsf{T}}$ be the QRdecomposition of X where Q_1 is a $n \times q$ semi-orthogonal matrix and T a $q \times q$ lower triangular matrix with positive diagonal elements. Setting m = n - q, there exists a $n \times m$ semi-orthogonal matrix Q_2 which completes Q_1 such that $Q = (Q_1 Q_2)$ is an $n \times n$ orthogonal matrix. Then, since

$$Q_2^{\mathsf{T}} X \beta = Q_2^{\mathsf{T}} Q_1 T^{\mathsf{T}} \beta = 0$$

we have

$$Q^{\mathsf{T}}Y = \begin{pmatrix} Z \\ U \end{pmatrix} = \begin{pmatrix} Q_1^{\mathsf{T}} \\ Q_2^{\mathsf{T}} \end{pmatrix} X \beta + Q^{\mathsf{T}}\mathcal{E} = \begin{pmatrix} \theta \\ 0 \end{pmatrix} + Q^{\mathsf{T}}\mathcal{E}, \qquad (2.2)$$

where $Q_1^{\top} X \beta = \theta$ and where Z and U are, respectively, $q \times p$ and $m \times p$ matrices. As $X = Q_1 L^{\top}$, the projection matrix P_X satisfies $P_X = Q_1 L^{\top} (L^{\top} L)^{-1} L Q_1^{\top} = Q_1 Q_1^{\top}$ so that $I_n - P_X = Q_2 Q_2^{\top}$. It follows that (2.1) becomes

$$S = Y^{\mathsf{T}} Q_2 Q_2^{\mathsf{T}} Y = U^{\mathsf{T}} U,$$

according to (2.2), which is a sufficient statistic for Σ .

The orthogonal matrix Q provides a linear reduction from n to q observations within each of the p responses. In addition, according to (1.2), the density of $Q^{\mathsf{T}}\mathcal{E}$ is the same as that of \mathcal{E} , and hence, $(Z^{\mathsf{T}}U^{\mathsf{T}})^{\mathsf{T}}$ has an elliptically symmetric distribution about the matrix $(\theta^{\mathsf{T}}0^{\mathsf{T}})^{\mathsf{T}}$ with density

$$(z,u) \mapsto |\Sigma|^{-n/2} f\left(\operatorname{tr} (z-\theta) \Sigma^{-1} (z-\theta)^{\mathsf{T}} + \operatorname{tr} u \Sigma^{-1} u^{\mathsf{T}}\right),$$

$$(2.3)$$

where θ and Σ are unknown. In this sense, the model (2.2) is the canonical form of the multivariate linear regression model (1.1). Note that the marginal distribution of $U = Q_2^{\top} Y$ is elliptically symmetric about 0 with covariance matrix proportional to $I_m \otimes \Sigma$ (see Fang and Zhang (1990)). This implies that $S = U^{\top} U$ have a generalized Wishart distribution (see Díaz-Gacía and Gutiérrez-Jámez (2011)), which coincides with the standard (singular or non-singular) Wishart distribution in the Gaussian setting (see Srivastava (2003)).

As mentioned in Section 1, the usual estimators of $\hat{\Sigma}_a$ in (1.3) perform poorly. We propose alternative estimators of the form

$$\hat{\Sigma}_J = a\left(S+J\right),\tag{2.4}$$

where J = J(Z, S) is a correction matrix. The improvement over the class of estimators $\hat{\Sigma}_a$ can be done by improving the best estimator $\hat{\Sigma}_{a_o} = a_o S$ within this class, namely, the estimator which minimizes the risk (1.5). It is proved in the Appendix that

$$\hat{\Sigma}_{a_o} = a_o S$$
, with $a_o = \frac{1}{K^* v}$ and $v = \max\{p, m\}$, (2.5)

where K^* is the normalizing constant (assumed to be finite) of the density defined by

$$(z,u) \mapsto \frac{1}{K^*} |\Sigma|^{-n/2} F^* \left(\operatorname{tr} \left(z - \theta \right) \Sigma^{-1} \left(z - \theta \right)^\top + \operatorname{tr} u \Sigma^{-1} u^\top \right),$$
(2.6)

where, for any $t \ge 0$,

$$F^*(t) = \frac{1}{2} \int_t^\infty f(v) \, dv \, .$$

Note that under de quadratic loss function (1.6) the optimal constant is $1/K^*(p+m+1)$. Of course, this risk optimality has sense only if the risk of $\hat{\Sigma}_{a_o}$ is finite. As shown in Haddouche (2019), this is the case as soon as $E_{\theta,\Sigma}[\operatorname{tr}(\Sigma^{-1}S)] < \infty$ and $E_{\theta,\Sigma}[\operatorname{tr}(\Sigma S^+)] < \infty$.

In order to give a unified dominance result of $\hat{\Sigma}_J$ over $\hat{\Sigma}_{a_o}$ for the two cases where S is non-invertible and where S is invertible, we consider, as a correction matrix in (2.4), the projection of a matrix function G(Z, S) = G on the subspace spanned by the columns of SS^+ , namely,

$$J = SS^+G. ag{2.7}$$

In addition to the risk finiteness conditions of $\hat{\Sigma}_{a_o}$, it can be shown that the risk of $\hat{\Sigma}_J$ is finite as soon as the expectations $E_{\theta,\Sigma}[\|\Sigma^{-1}SS^+G\|_F^2]$ and $E_{\theta,\Sigma}[\|S^+G\|_F^2]$ are finite, where $\|\cdot\|_F$ denotes the Frobenius norm. Under these conditions, the risk difference between $\hat{\Sigma}_J$ and $\hat{\Sigma}_{a_o}$ is

$$\Delta(G) = a_o^2 E_{\theta,\Sigma} \left[\operatorname{tr} \left(\Sigma^{-1} S S^+ G \{ I_p + S^+ G + S S^+ \} \right) \right] - 2 a_o E_{\theta,\Sigma} \left[\operatorname{tr} \left(S^+ G \right) \right].$$
(2.8)

Noticing that the first integrand term in (2.8) depends on the unknown parameter Σ^{-1} , our approach consists in replacing this integrand term by a random matrix $\delta(G)$, which does not depend on Σ^{-1} , such that $\Delta(G) \leq E^*_{\theta, \Sigma}[\delta(G)]$ where $E^*_{\theta, \Sigma}$ denotes the expectation with respect to the density (2.6). Clearly, a sufficient condition for $\Delta(G)$ to be non–positive (and hence, for $\hat{\Sigma}_J$ to improve over $\hat{\Sigma}_{a_o}$) is that $\delta(G)$ is non–positive. To this end, we rely on the following Stein–Haff type identity.

Lemma 2.1 (Haddouche et al. (2021)). Let G(z, s) be a $p \times p$ matrix function such that, for any fixed z, G(z, s) is weakly differentiable with respect to s. Assume that $E_{\theta, \Sigma}[|\operatorname{tr}(\Sigma^{-1}S S^+ G)|] < \infty$. Then we have

$$E_{\theta,\Sigma} \left[\operatorname{tr} \left(\Sigma^{-1} S S^{+} G \right) \right] = K^{*} E_{\theta,\Sigma}^{*} \left[\operatorname{tr} \left(2 S S^{+} \mathcal{D}_{s} \{ S S^{+} G \}^{\top} + (m - r - 1) S^{+} G \right) \right],$$
(2.9)

where $r = \min\{p, m\}$ and $\mathcal{D}_{s}\{\cdot\}$ is the Haff operator whose generic element is $\frac{1}{2}(1 + \delta_{ij})\frac{\partial}{\partial S_{ij}}$, with $\delta_{ij} = 1$ if i = j and $\delta_{ij} = 0$ if $i \neq j$.

Note that the existence of the expectations in (2.9) is implied by the above risk finiteness conditions. An original Stein–Haff identity was derived independently by Stein (1986) and Haff (1979) in the Gaussian setting where S is invertible. This identity was extended to the class of elliptically symmetric distributions in (2.3) Kubokawa and Srivastava (1999) and also by Bodnar and Gupta (2009). Here, we use the new Stein–Haff type identity recently derived by Haddouche et al. (2021) in the elliptical framework (2.3) dealing with both cases S non–invertible and S invertible.

Applying Lemma 2.1 to the term depending on Σ^{-1} in the right-hand side of (2.8) gives

$$\Delta(G) = a_o^2 K^* E_{\theta,\Sigma}^* \Big[(m - r - 1) \operatorname{tr} \left(S^+ G + (S^+ G)^2 + S^+ G S S^+ \right) \\ + 2 \operatorname{tr} \left(S S^+ D_s \{ S S^+ G + S S^+ G S^+ G + S S^+ G S S^+ \}^\top \right) \Big] - 2 a_o E_{\theta,\Sigma} \Big[\operatorname{tr} \left(S^+ G \right) \Big].$$
(2.10)

It is worth noticing that the risk difference in (2.10) depends on the $E_{\theta,\Sigma}$ and $E_{\theta,\Sigma}^*$ expectations (which coincide in the Gaussian setting since $F^* = f$). Thus, in order to derive a dominance result, we need to compare these two expectations. A possible approach consists to restrict us to the subclass of densities verifying $c \leq F^*(t)/f(t) \leq b$, for some positive constants c and b (see Berger (1975) for the class where $c \leq F^*(t)/f(t)$). Due to the complexity of the use of the quadratic loss in (1.6) (which necessitates a twice application of the Stein–Haff type identity (2.9)), this subclass was considered by Haddouche et al. (2021). Here, thanks to the data–based loss (1.4), we are able to avoid such a restriction, and hence, to deal with a larger class of elliptically symmetric distributions in (2.3) (subject to the moment conditions induced by the above finiteness conditions).

Following the suggestion to shrink the eigenvalues of S mentioned in Section 1, we consider as a correction matrix a matrix SS^+G with G orthogonally invariant in the following sense. Let $S = H L H^{\top}$ the eigenvalue decomposition of S where H is a $p \times r$ semi-orthogonal matrix of eigenvectors and $L = \text{diag}(l_1, \ldots, l_r)$, with $l_1 > \ldots > l_r$, is the diagonal matrix of the r positive corresponding eigenvalues of S (see Kubokawa and Srivastava (2008) for more details). Then set $G = H L \Psi(L) H^{\top}$, with $\Psi(L) = \text{diag}(\psi_1(L), \ldots, \psi_r(L))$ where $\psi_i = \psi_i(L)$ ($i = 1, \ldots, r$) is a differentiable function of L. Consequently, by semi-orthogonality of H, we have $SS^+H = H H^{\top}H = H$, so that the correction matrix in (2.7) is

$$J = SS^+G = G = H L\Psi(L) H^\top.$$

Thus the alternative estimators that we consider are of the form

$$\hat{\Sigma}_{\Psi} = a_o \left(S + H L \Psi(L) H^{\mathsf{T}} \right) = a_o H L \left(I_r + \Psi(L) \right) H^{\mathsf{T}}, \qquad (2.11)$$

which are usually called orthogonally invariant estimators (i.e. equivariant under orthogonal transformations). See for instance Takemura (1984).

Now, adapting the risk finiteness conditions mentioned above, we are in a position to give our dominance result of the alternative estimators in (2.11) over the optimal estimator in (2.5), under the data–based loss (1.4).

Theorem 2.1. Assume that the following expectations $E_{\theta,\Sigma}[\operatorname{tr}(\Sigma^{-1}S)]$, $E_{\theta,\Sigma}[\operatorname{tr}(\Sigma S^+)]$, $E_{\theta,\Sigma}[\|\Sigma^{-1}HL\Psi(L)H^{\top}\|_F^2]$ and $E_{\theta,\Sigma}[\|H\Psi(L)H^{\top}\|_F^2]$ are finite. Let $\Psi(L) = \operatorname{diag}(\psi_1, \dots, \psi_r)$ where $\psi_i = \psi_i(L)$ $(i = 1, \dots, r)$ is differentiable function of L with $\operatorname{tr}(\Psi(L)) \geq \lambda$, for a fixed positive constant λ .

Then an upper bound of the risk difference between $\hat{\Sigma}_{\Psi}$ and $\hat{\Sigma}_{a_{\alpha}}$ under the loss function (1.4) is given by

$$\Delta(\Psi(L)) \le a_o^2 K^* E_{\theta, \Sigma}^* [g(\Psi)],$$

where

$$g(\Psi) = \sum_{i=1}^{r} \left\{ 2(v-r+1)\psi_i + (v-r+1)\psi_i^2 + 4l_i(1+\psi_i)\frac{\partial\psi_i}{\partial l_i} + \sum_{j\neq i}^{r} \frac{l_i(2\psi_i + \psi_i^2) - l_j(2\psi_j + \psi_i^2)}{l_i - l_j} - 2v\lambda \right\}.$$
(2.12)

Also $\hat{\Sigma}_{\Psi}$ in (2.11) improves over $\hat{\Sigma}_{a_0}$ in (2.5) as soon as $g(\Psi) \leq 0$.

The proof of Theorem 2.1 is given in the Appendix. Note that, although the expectation $E_{\theta,\Sigma}^*$ is associated to the generating function $f(\cdot)$ in (1.2), the function $g(\Psi)$ does not depend on $f(\cdot)$, and hence, the improvement result in Theorem 2.1 is robust in that sense. Note also that Theorem 2.1 is well adapted to deal with the James and Stein (1961) estimator where $\psi_i(L) = 1/(v + r - 2i + 1)$, for i = 1, ..., r, since $tr(\Psi(L)) > \lambda = 1/(v + r - 1)$ and the Efron-Morris-Dey estimator, considered by Tsukuma and Kubokawa (2020a), where $\psi_i(L) = 1/(1 + b l_i^{\alpha}/tr(L^{\alpha}))v$, for i = 1, ..., r and for positive constants b and α , since $tr(\Psi(L)) > \lambda = r/(b + 1)v$.

In the following, we consider a new class of estimators which is an extension of the Haff (1980) class, that is, estimators of the form

$$\hat{\Sigma}_{\alpha,b} = a_o \left(S + H L \Psi(L) H^{\top} \right) \text{ with, for } \alpha \ge 1 \text{ and } b > 0, \ \Psi(L) = b \frac{L^{-\alpha}}{\operatorname{tr}(L^{-\alpha})},$$
(2.13)

where a_o is given in (2.5). For $\alpha = 1$, this is the estimator considered by Konno (2009), who deals with the Gaussian case and the quadratic loss (1.6), while Tsukuma and Kubokawa (2020a) used an extended Stein loss. An elliptical setting was also considered by Haddouche et al. (2021) under the quadratic loss (1.6).

It is proved in the Appendix that, for the entire class of elliptically symmetric distributions in (2.3), any estimator $\hat{\Sigma}_{a,b}$ in (2.13) improves on the optimal estimator $\hat{\Sigma}_{a,c}$ in (2.5), under the data-based loss (1.4), as soon as

$$0 < b \le \frac{2(r-1)}{v-r+1}.$$
(2.14)

It worth noting that Tsukuma and Kubokawa (2020a) gave Condition (2.14) as an improvement condition although their loss was different.

3. Numerical study

Let the elliptical density in (1.2) be a variance mixture of normal distributions where the mixing variable, with density *h*, has the inverse–gamma distribution $\mathcal{IG}(k/2, k/2)$ with shape and scale parameters both equal to k/2 for k > 2. Thus, for any $t \ge 0$, the generating function *f* in (1.2) has the form

$$f(t) = \int_0^\infty \frac{1}{(2\nu\pi)^{np/2}} \exp\left(\frac{-t}{2\nu}\right) h(\nu) \, d\nu,$$

which corresponds to the *t*-distribution with *k* degrees of freedom. Then the primitive F^* of *f* in (2.6) is, for any $t \ge 0$,

$$F^*(t) = \frac{1}{2} \int_t^\infty \int_0^\infty \frac{1}{(2\nu\pi)^{np/2}} \exp\left(\frac{-w}{2\nu}\right) h(\nu) \, d\nu \, dw = \int_0^\infty \frac{\nu}{(2\nu\pi)^{np/2}} \exp\left(\frac{-t}{2\nu}\right) h(\nu) \, d\nu \, d\nu.$$

by Fubini's theorem. Therefore the normalizing constant K^* in (2.6) is

$$K^* = \int_{\mathbb{R}^{pn}} \int_0^\infty \frac{|\Sigma|^{-n/2}}{(2 \mathrm{v} \pi)^{np/2}} \mathrm{v} \exp\left(\frac{-1}{2\mathrm{v}} \left(\mathrm{tr} \left(z-\theta\right) \Sigma^{-1} \left(z-\theta\right)^\top + \mathrm{tr} \Sigma^{-1} u^\top u\right) \right) h(\mathrm{v}) \, d\mathrm{v} \, dz \, du \,,$$

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$$= \int_0^\infty \mathbf{v} \int_{\mathbb{R}^{pn}} \frac{|\Sigma|^{-n/2}}{(2\,\mathbf{v}\pi)^{np/2}} \exp\left(\frac{-1}{2\mathbf{v}} \left(\operatorname{tr}\left(z-\theta\right)\Sigma^{-1}\left(z-\theta\right)^\top + \operatorname{tr}\Sigma^{-1}u^\top u\right)\right) dz \, du \, h(\mathbf{v}) \, d\mathbf{v}$$
(3.1)

by Fubini's theorem. Clearly the most inner integral in (3.1) equals 1 so that

$$K^* = \int_0^\infty v h(v) \, dv = \frac{k}{k-2},$$

by propriety of $\mathcal{IG}(k/2, k/2)$. Note that, when k goes to ∞ , $\mathcal{IG}(k/2, k/2)$ goes to the multivariate Gaussian distribution (for which $K^* = 1$ since $f = F^*$) with covariance matrix $I_n \otimes \Sigma$.

In the following, we study numerically the performance of the alternative estimators in (2.13) expressed as

$$\hat{\Sigma}_{\alpha,b} = a_o \left(S + \frac{b}{\operatorname{tr}(L^{-\alpha})} H L^{1-\alpha} H^{\top} \right) \quad \text{where} \quad 0 \le b \le b_0 = \frac{2(r-1)}{v-r+1} \quad \text{and} \quad \alpha \ge 1.$$
(3.2)

As mentioned above, Konno (2009) consider the case $\alpha = 1$, in the Gaussian setting and under the quadratic loss (1.6), for which its improvement condition is

$$0 \le b \le b_1 = \frac{2(r-1)(v+r+1)}{(v-r+1)(v-r+3)}$$

Note that, although $b_0 < b_1$, the improvement condition in (3.2) is valid fo any $\alpha \ge 1$ and all the class of elliptically symmetric distributions (2.3). However it was shown numerically by Haddouche et al. (2021) that b_1 is optimal in the Gaussian context.

We consider the following structures of Σ : (i) the identity matrix I_p and (ii) an autoregressive structure with coefficient 0.9 (i.e. a $p \times p$ matrix where the (i, j)th element is $0.9^{|i-j|}$). To assess how an alternative estimator $\hat{\Sigma}_{\alpha,b}$ improves over $\hat{\Sigma}_{\alpha,c}$, we compute the Percentage Reduction In Average Loss (PRIAL) defined as

$$PRIAL(\hat{\Sigma}_{\alpha,b}) = \frac{\text{average loss of } \hat{\Sigma}_{a_o} - \text{average loss of } \hat{\Sigma}_{\alpha,b}}{\text{average loss of } \hat{\Sigma}_{a_o}}$$

and based on 1000 independent Monte–Carlo replications for some couples (p, m).

In Figure 1, we study the effect of the constant *b* in (3.2) on the prial's in the non–invertible ((p, m) = (25, 10)) and the invertible ((p, m) = (10, 25)) cases. The Gaussian setting is investigated for the structure (i) of Σ . Note that, when $0 \le b \le b_0$, the best prial (around 7% in both invertible and non–invertible cases) is reported for $b = b_0 = 1.125$ (for (v, r) = (25, 20)). For this reason, in the following, we consider the estimators $\hat{\Sigma}_{a,b_0}$ with

$$b_0 = \frac{2(r-1)}{v-r+1} \,.$$

Note also that, for $b > b_0$, the estimators $\hat{\Sigma}_{\alpha,b}$ still improve over Σ_{a_o} and that the maximum value of the prial is around 50%. This shows that there exists a larger range of values of *b* than the one our theory provides for which $\hat{\Sigma}_{\alpha,b}$ improves over $\hat{\Sigma}_{a_o}$.

In Figure 2, we study the effect of α on the prial's of the estimator $\hat{\Sigma}_{\alpha,b_0}$ over $\hat{\Sigma}_{a_o} = S/v$ when the sampling distribution is Gaussian ($K^* = 1$ in (2.5)), and over $\hat{\Sigma}_{a_o} = S(k-2)/vk$ when it is the *t*-distribution ($K^* = (k-2)/k$ in (2.5)) with *k* degrees of freedom. For the structure (i) of Σ , note that, for $\alpha \ge 6$, the prial's stabilize at 12.5%, in the Gaussian case, and at 8.5%, in the Student case. Similarly, the prial's are better in the Gaussian setting for the structure (i) and may be negative for the structure (ii).

In Figure 3, under the Gaussian assumption, we provide the prial's of $\hat{\Sigma}_{\alpha,b_0}$ with respect to $\hat{\Sigma}_{a_o} = S/v$ under the data-based loss (1.4) and the prial's of $\hat{\Sigma}_{\alpha,b_1}$ with respect to $\hat{\Sigma}_{a_o} = S/(v+r+1)$ under the quadratic loss (1.6). For the two structures (i) and (ii) of Σ , the prial's are better under the data-based loss. For the structure (i) with $\alpha = 1$ (which coincide with the Konno's estimator), we observe a prial equal to 1.73% which is similar to that of Konno (2009). Note that, under the data-based loss the prial is much better since it equals 13.42%. We observe similar behaviors for the structure (i) than for the structure (i), but with lower prial's.

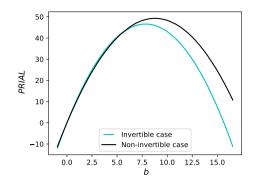


Fig. 1: Effect of *b* on the PRIAL of $\hat{\Sigma}_{\alpha,b}$, with $\alpha = 1$, under data-based loss in the Gaussian setting. The structure (i) of Σ is considered for the invertible case with (p, m) = (10, 25) and the non-invertible case with (p, m) = (25, 10).

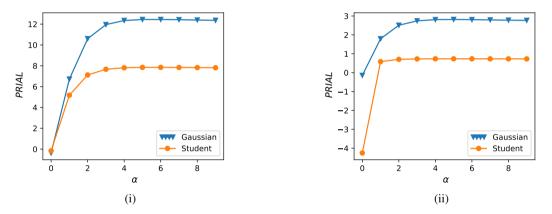


Fig. 2: PRIAL's of $\hat{\Sigma}_{\alpha,b_0}$ under the data-based loss. The non-invertible case is considered, with (p,m) = (50, 20), for the structures (i) and (ii) of Σ for the t-distribution, with k = 5 degrees of freedom, and the Gaussian distribution.

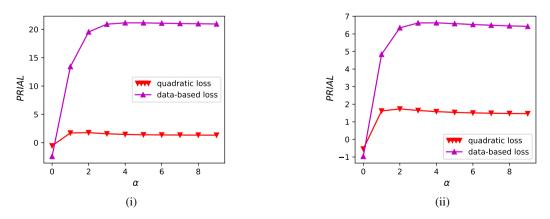


Fig. 3: PRIAL's of $\hat{\Sigma}_{a,b_0}$ under data-based loss and PRIAL's of $\hat{\Sigma}_{a,b_1}$ under quadratic loss. The non-invertible case is considered, with (p,m) = (20, 10), for the structures (i) and (ii) of Σ under the Gaussian distribution.

4. Conclusion and perspective

For a wide class of elliptically symmetric distributions, we provide a large class of estimators of the scale matrix Σ of the elliptical multivariate linear model (1.1) which improve over the usual estimators *a S*. We highlight that the use of the data-based loss (1.4) is more attractive than the use of the classical quadratic loss (1.6). Indeed, (1.4) brings more improved estimators and their improvement is valid within a larger class of distributions. This means that (1.4) is more discriminant than (1.6) to exhibit improved estimators.

While in (2.10) the risk difference between $\hat{\Sigma}_J = a_o(S + J)$ with $J = SS^+G(Z, S)$ and $\hat{\Sigma}_{a_o} = a_o S$, the dominance result in Theorem 2.1 is given for a correction matrix $G(Z, S) = HL\Psi(L)H^{\top}$ which depends only on S. Recently, Tsukuma (2016) consider, in the Gaussian case, alternative estimators where G(Z, S) depends on S and on the information contained in the sample mean Z. This class of estimators merits future investigations in an elliptical setting.

5. Appendix

We give in the following corollary an adaptation of Lemma (2.9) to an orthogonally invariant matrix function *G*, that is, of the form $G = H L \Phi(L) H^{\top}$ where $\Phi(L) = \text{diag}(\phi_1, \dots, \phi_r)$ with $\phi_i = \phi_i(L)$ $(i = 1, \dots, r)$ is differentiable function of *L*

Corollary 5.1. Let $\Phi(L) = \operatorname{diag}(\phi_1, \dots, \phi_r)$ where $\phi_i = \phi_i(L)$ $(i = 1, \dots, r)$ is differentiable function of L. Assume that $E_{\theta \Sigma} \left[|\operatorname{tr}(\Sigma^{-1}H L \Phi(L) H^{\mathsf{T}})| \right] < \infty$. Then we have

$$E_{\theta,\Sigma}\left[\operatorname{tr}(\Sigma^{-1} H L \Phi(L) H^{\top})\right] = K^* E_{\theta,\Sigma}^* \left[\sum_{i=1}^r \left((v-r+1) \phi_i + 2l_i \frac{\partial \phi_i}{\partial l_i} + \sum_{j\neq i}^r \frac{l_i \phi_i - l_j \phi_j}{l_i - l_j} \right)\right].$$

Proof. Let $G = H L \Phi(L) H^{\top}$, $S^+ = H L^{-1} H^{\top}$ and $SS^+ = H H^{\top}$. Then,

$$SS^+G = H H^\top H L \Phi(L) H^\top = H L \Phi(L) H^\top = G,$$

since H is semi–orthogonal. Assuming that $E_{\theta \Sigma} \left[|\operatorname{tr}(\Sigma^{-1} H L \Phi(L) H^{\mathsf{T}})| \right] < \infty$, we have from Lemma 2.1

$$E_{\theta,\Sigma}\left[\operatorname{tr}\left(\Sigma^{-1} H L \Phi(L) H^{\top}\right)\right] = K^* E_{\theta,\Sigma}^* \left[2 \operatorname{tr}\left(H H^{\top} \mathcal{D}_s\{H L \Phi(L) H^{\top}\}\right) + (m - r - 1) \operatorname{tr}\left(H \Phi(L) H^{\top}\right)\right].$$
(5.1)

Firstly, using Lemma A.4.2 in Haddouche et al. (2021), we have

$$\mathcal{D}_{s}\left\{H L \Phi(L) H^{\mathsf{T}}\right\} = H \Phi^{(1)}(L) H^{\mathsf{T}} + \frac{1}{2} \operatorname{tr}\left(\Phi(L)\right) \left(I_{p} - H H^{\mathsf{T}}\right),$$
(5.2)

where $\Phi^{(1)}(L) = \text{diag}(\phi_1^{(1)}, ..., \phi_r^{(1)})$, with

$$\phi_i^{(1)} = \frac{1}{2}(p - r + 2)\phi_i + l_i \frac{\partial\phi_i}{\partial l_i} + \frac{1}{2}\sum_{j \neq i}^r \frac{l_i \phi_i - l_j \phi_j}{l_i - l_j}.$$
(5.3)

for i = 1 ... r.

wher

Secondly, using the fact that $H^{\top}H = I_r$, we have from (5.2)

$$H H^{\mathsf{T}} \mathcal{D}_{s} \left\{ H L \Phi(L) H^{\mathsf{T}} \right\} = H \Phi^{(1)}(L) H^{\mathsf{T}} .$$

$$(5.4)$$

Then, putting (5.4) in (5.1), we obtain

$$E_{\theta,\Sigma}\left[\operatorname{tr}\left(\Sigma^{-1} H L \Phi(L) H^{\top}\right)\right] = K^* E_{\theta,\Sigma}^*\left[2\operatorname{tr}\left(\Phi^{(1)}(L)\right) + (m-r-1)\operatorname{tr}\left(\Phi(L)\right)\right].$$

Finally, using (5.3), we have

$$E_{\theta,\Sigma} \left[\operatorname{tr} \left(\Sigma^{-1} H L \Phi(L) H^{\mathsf{T}} \right) \right] = K^* E_{\theta,\Sigma}^* \left[\sum_{i=1}^r \left((p+m-2r+1) \phi_i + 2 l_i \frac{\partial \phi_i}{\partial l_i} + \sum_{j \neq i}^r \frac{l_i \phi_i - l_j \phi_j}{l_i - l_j} \right) \right],$$

e $(p+m-2r+1) = (v-r)$.

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The optimal constat a_o in (2.5). Let $\hat{\Sigma}_a = aS$ where a > 0. Assume that the expectations $E_{\theta,\Sigma}[\operatorname{tr}(\Sigma^{-1}S)]$ and $E_{\theta,\Sigma}[\operatorname{tr}(\Sigma S^+)]$ are finite. Then, the risk of $\hat{\Sigma}_{a_o}$ relating to the data-based loss (1.4) is given by

$$R(\hat{\Sigma}_{a}, \Sigma) = E_{\theta, \Sigma} \left[\operatorname{tr} \left(S^{+} \Sigma \left(\Sigma^{-1} \hat{\Sigma}_{a} - I_{p} \right)^{2} \right) \right] = a^{2} E_{\theta, \Sigma} \left[\operatorname{tr} \left(\Sigma^{-1} S S^{+} S \right) \right] - 2 a E_{\theta, \Sigma} \left[\operatorname{tr} \left(S S^{+} \right) \right] + E_{\theta, \Sigma} \left[\operatorname{tr} \left(S^{+} \Sigma \right) \right].$$
(5.5)

Applying the Stein-Haff type identity in Corollary (5.1), with $\Psi(L) = I_r$, to the first term in the right-hand side of (5.5), we obtain

$$E_{\theta,\Sigma} \left[\operatorname{tr} \left(\Sigma^{-1} S S^{+} S \right) \right] = E_{\theta,\Sigma} \left[\operatorname{tr} \left(\Sigma^{-1} H L H^{\top} \right) \right] = K^{*} E_{\theta,\Sigma}^{*} \left[\sum_{i=1}^{r} \left((v - r + 1) + \sum_{j \neq i}^{r} \frac{l_{i} - l_{j}}{l_{i} - l_{j}} \right) \right]$$

= $K^{*} \left[r(v - r + 1) + r(r - 1) \right] = K^{*} r v.$ (5.6)

Now, using the fact that $tr(S^+ S) = tr(H H^{\top}) = r$ and thanks to (5.6), we have

$$R(\hat{\Sigma}_a, \Sigma) = a^2 K^* r v - 2 a r + E_{\theta, \Sigma} [\operatorname{tr} (S^+ \Sigma)].$$

Therefore, choosing $a = 1/K^* v$ is optimal under the risk (1.5).

Proof of Theorem 2.1. Let $\hat{\Sigma}_{\Psi} = a_o \left(S + H L \Psi(L) H^{\mathsf{T}} \right)$ where $\Psi(L) = \operatorname{diag}(\psi_1, \dots, \psi_r)$ such that $\psi_i = \psi_i(L)$ $(i = 1, \dots, r)$ is differentiable function of L and $\operatorname{tr}(\Psi(L)) \geq \lambda > 0$. Hence, using the fact that $H^{\mathsf{T}}H = I_r$, the involving terms in the risk difference (2.8) becomes

$$J = SS^+G = G = HL\Psi(L)H^\top$$
 and $S^+G = H\Psi(L)H^\top$.

Then, the risk difference between $\hat{\Sigma}_{\Psi}$ and $\hat{\Sigma}_{a_{\alpha}}$ is given by

$$\Delta(\Psi) = a_o^2 E_{\theta,\Sigma} \left[\operatorname{tr} \left(\Sigma^{-1} H L \left(2\Psi + \Psi^2 \right) H^{\mathsf{T}} \right) \right] - 2 a_o E_{\theta,\Sigma} \left[\operatorname{tr} \left(\Psi \right) \right].$$
(5.7)

Now, applying the Stein-Haff type identity in Corollary (5.1) to the first term in the right hand side of (5.7), for $\Phi = 2\Psi + \Psi^2$, we have

$$\Delta(\Psi) = a_o^2 K^* E_{\theta,\Sigma}^* \left[\sum_{i=1}^r \left\{ (v - r + 1) \left(2\psi_i + \psi_i^2 \right) + 2l_i \frac{\partial(2\psi_i + \psi_i^2)}{\partial l_i} + \sum_{j \neq i}^r \frac{l_i \left(2\psi_i + \psi_i^2 \right) - l_j \left(2\psi_j + \psi_i^2 \right)}{l_i - l_j} \right\} \right] - 2a_0 E_{\theta,\Sigma} \left[\operatorname{tr} \left(\Psi \right) \right].$$

Therefore, using the fact that $tr(\Psi) \ge \lambda > 0$, an upper bound of the risk difference $\Delta(\Psi)$ is given by

$$\begin{split} \Delta(\Psi) &\leq a_o^2 \, K^* \, E_{\theta, \Sigma}^* \left[\sum_{i=1}^r \left\{ 2 \, (v-r+1) \, \psi_i + (v-r+1) \, \psi_i^2 + 4 \, l_i \, (1+\psi_i) \frac{\partial \psi_i}{\partial l_i} \right. \\ &+ \left. \sum_{j \neq i}^r \frac{l_i \, (2 \, \psi_i + \psi_i^2) - l_j \, (2 \, \psi_j + \psi_i^2)}{l_i - l_j} \right. - 2 (a_o \, K^*)^{-1} \lambda \Big\} \right] \,, \end{split}$$

where $(a_0 K^*)^{-1} = v$.

Improvement condition (2.14) of alternative estimators in (2.13). Let consider the class of alternative estimators $\hat{\Sigma}_{\alpha,b}$ in (2.13). Then, applying Theorem 2.1, an upper bound of the risk difference between $\hat{\Sigma}_{\alpha,b}$ and $\hat{\Sigma}_{a_{\alpha}}$ is given by

$$\Delta(\Psi) \le a_o^2 K^* E_{\theta, \Sigma}^* \left(g(\Psi) \right), \tag{5.8}$$

where the integrand term in (2.12) becomes

$$g(\Psi) = g_1(\Psi) + g_2(\Psi)$$

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 \square

with

$$g_1(\Psi) = -2(r-1)b \sum_{i=1}^r \frac{l_i^{-\alpha}}{\operatorname{tr}(L^{-\alpha})} + (v-r+1)b^2 \sum_{i=1}^r \frac{l_i^{-2\alpha}}{\operatorname{tr}^2(L^{-\alpha})},$$

since $\operatorname{tr}(\Psi(L)) = b$, and

$$g_{2}(\Psi) = 4l_{i}b\left(1 + b\frac{l_{i}^{-\alpha}}{\operatorname{tr}(L^{-\alpha})}\right)\frac{\partial}{\partial l_{i}}\left(\frac{l_{i}^{-\alpha}}{\operatorname{tr}(L^{-\alpha})}\right) + \frac{2b}{\operatorname{tr}(L^{-\alpha})}\sum_{i=1}^{r}\sum_{j\neq i}^{r}\frac{l_{i}^{1-\alpha} - l_{j}^{1-\alpha}}{l_{i} - l_{j}} + \frac{b^{2}}{\operatorname{tr}^{2}(L^{-\alpha})}\sum_{i=1}^{r}\sum_{j\neq i}^{r}\frac{l_{i}^{1-2\alpha} - l_{j}^{1-2\alpha}}{l_{i} - l_{j}}$$

The proof consist to prove that the integrand term $g_2(\Psi)$ is non-positive. To this end, it can be shown that, for $\alpha \ge 1$,

$$\sum_{i=1}^{r} \sum_{j \neq i}^{r} \frac{l_{i}^{1-\alpha} - l_{j}^{1-\alpha}}{l_{i} - l_{j}} = 2 \sum_{i}^{r} \sum_{j > i}^{r} \frac{l_{i}^{1-\alpha} - l_{j}^{1-\alpha}}{l_{i} - l_{j}} \le 0 \quad \text{and} \quad \sum_{i=1}^{r} \sum_{j \neq i}^{r} \frac{l_{i}^{1-2\alpha} - l_{j}^{1-2\alpha}}{l_{i} - l_{j}} = 2 \sum_{i=1}^{r} \sum_{j > i}^{r} \frac{l_{i}^{1-2\alpha} - l_{j}^{1-2\alpha}}{l_{i} - l_{j}} < 0.$$

since $L = \text{diag}(l_1 >, \dots, > l_r)$. Then

$$g_2(\Psi) \le 4 \, l_i \, b \, \left(1 + b \, \frac{l_i^{-\alpha}}{\operatorname{tr}(L^{-\alpha})}\right) \, \frac{\partial}{\partial l_i} \left(\frac{l_i^{-\alpha}}{\operatorname{tr}(L^{-\alpha})}\right) = 4 \, b \, \alpha \, \frac{l_i^{-\alpha}}{\operatorname{tr}(L^{-\alpha})} \left(1 + b \, \frac{l_i^{-\alpha}}{\operatorname{tr}(L^{-\alpha})}\right) \, \left(\frac{l_i^{-\alpha}}{\operatorname{tr}(L^{-\alpha})} - 1\right) \, ,$$

since

$$\frac{\partial}{\partial l_i} \left(\frac{l_i^{-\alpha}}{\operatorname{tr}(L^{-\alpha})} \right) = \alpha \frac{l_i^{-\alpha-1}}{\operatorname{tr}(L^{-\alpha})} \left(\frac{l_i^{-\alpha}}{\operatorname{tr}(L^{-\alpha})} - 1 \right) \,.$$

Therefore, since $l_i^{-\alpha} \leq \operatorname{tr}(L^{-\alpha})$, the integrand term $g_2(\Psi) \leq 0$. Then

$$g(\Psi) \le g_1(\Psi) = -2(r-1)b + (v-r+1)b^2 \frac{\operatorname{tr}(L^{-2\alpha})}{\operatorname{tr}^2(L^{-\alpha})}.$$

Now, using the fact that $tr(L^{-2\alpha}) \leq tr^2(L^{-\alpha})$, we have

$$g(\Psi) \leq -2(r-1)b + (v-r+1)b^2$$
.

since b > 0. Hence, an upper bound for the risk difference in (5.8) is given by

$$\Delta(\Psi) \le a_o^2 b K^* E_{\theta, \Sigma}^* \left[-2(r-1) + (v-r+1) b \right].$$

Therefore, $\hat{\Sigma}_{a,b}$ improves over $\hat{\Sigma}_{a_0}$ under the data-based loss (1.4) as soon as $0 < b \le b_0 = 2(r-1)/(v-r+1)$. \Box

CRediT authorship contribution statement

Dominique Fourdrinier: Conceptualization, Methodology, Supervision, Validation, Writing - review & editing, Writing - original draft, Software. **Anis M. Haddouche:** Conceptualization, Methodology, Supervision, Validation, Writing - review & editing, Writing - original draft, Software. **Fatiha Mezoued:** Conceptualization, Methodology, Supervision, Validation, Writing - review & editing, Writing - original draft, Software.

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