Covariance matrix estimation under data–based loss

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Outline

Introduction

Model

Let consider the multivariate linear regression model

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

where

- Y is an observed $n \times p$ matrix, X is an $n \times q$ matrix of known constants such that

$$\mathrm{rank}(X) = q \leq n. \tag{1.2}$$

- β is a $q \times p$ matrix of unknown parameters.
- $\mathcal{E}$ is an $n \times p$ elliptically symmetric noise.

We assume that $\mathcal{E}$ has a density, w.r.t the Lebesgue measure in $\mathbb{R}^{pn}$, of the form

$$\varepsilon \mapsto |\Sigma|^{-n/2} f\big(\mathrm{tr}(\varepsilon\,\Sigma^{-1}\varepsilon^{\top})\big)\,, \tag{1.3}$$

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

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

The canonical form

Although the matrix of regression coefficients β is also unknown, we are interested in estimating the invertible scale matrix Σ.

We address this problem under a decision–theoretic framework through a canonical form of the model (1.1).

The canonical form

Thanks to (1.2), the QR decomposition of X is of the form

$$X = Q_1 T^\top ,$$

where

- Q_1 is a $n \times q$ semi-orthogonal matrix.
- T a $q \times q$ lower triangular matrix with positive diagonal elements.

There exists an $n \times (n - q)$ semi-orthogonal matrix Q_2 such that

$$Q_2^\top X \beta = Q_2^\top Q_1 T^\top \beta = 0 .$$

Completes Q_1 with Q_2 such that $Q = (Q_1 Q_2)$ is an $n \times n$ orthogonal matrix. Then, we have

$$\begin{pmatrix} Q_1^\top \\ Q_2^\top \end{pmatrix} Y = \begin{pmatrix} Z \\ U \end{pmatrix} = \begin{pmatrix} Q_1^\top \\ Q_2^\top \end{pmatrix} X \beta + Q^\top \mathcal{E} = \begin{pmatrix} \theta \\ 0 \end{pmatrix} + Q^\top \mathcal{E} , \qquad (1.4)$$

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Recall that

$$\begin{pmatrix} Q_1^\top \\ Q_2^\top \end{pmatrix} Y = \begin{pmatrix} Z \\ U \end{pmatrix} = \begin{pmatrix} \theta \\ 0 \end{pmatrix} + Q^\top \mathcal{E}\,.$$

Inference on the $p \times p$ scale matrix Σ relies on the $(n-q) \times p$ matrix U which is of low dimension than the $n \times p$ observed matrix Y.

Note that

$$S = U^\top U$$

is a sufficient statistic for Σ and may serve as an estimate of Σ.

Note also that S is invertible when $p \leq n-q$ and is non-invertible when $p > n-q$.

In the following we set $m = n - q$

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Recall that

$$\varepsilon \mapsto |\Sigma|^{-n/2} f\big(\mathrm{tr}(\,\varepsilon\,\Sigma^{-1}\varepsilon^{\top})\big)\,.$$

The density of $Q^{\top}\mathcal{E}$ is the same as that of $\mathcal{E}$. It follows that the density of $(Z^{\top}\,U^{\top})^{\top} = Q^{\top}Y$ is

$$(z,u) \mapsto |\Sigma|^{-n/2} f\big(\,\mathrm{tr}\,(z-\theta)\,\Sigma^{-1}\,(z-\theta)^{\top} + \mathrm{tr}\,u\,\Sigma^{-1}\,u^{\top}\,\big). \tag{1.5}$$

Bellow $E_{\theta,\Sigma}$ will be the expectation w.r.t (1.5) and $E^{*}_{\theta,\Sigma}$ the expectation w.r.t

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

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What is wrong with the usual estimators ?

The usual estimators are of the form

$$\hat{\Sigma}_a = a\,S, \quad \text{where} \quad a > 0.$$

In the Gaussian case $\hat{\Sigma}_{1/m}$ correspond respectively to the unbiased estimator.

In the standard asymptotic setting, when p is fixed and $m \to \infty$ the unbiased estimator $\hat{\Sigma}_{1/m}$ is a *good* estimator ; in particular, it is a *consistent* and invertible estimator.

In the general asymptotic setting, when $m, p \to \infty$ with $p/m \to c > 0$, $\hat{\Sigma}_{1/m}$ perform poorly and is non-invertible for $c > 1$.

[5] O. Ledoit and M. Wolf, *A well-conditioned estimator for large-dimensional covariance matrices, 2004.*

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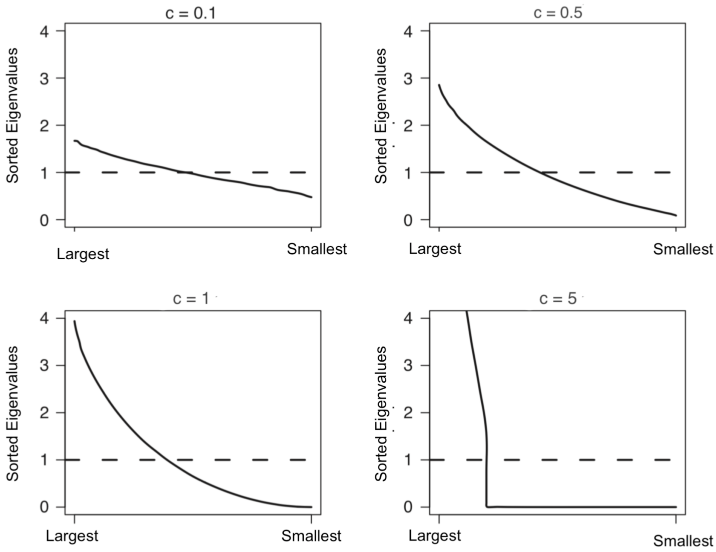

In the Gaussian setting, James and Stein

[3] W. James and C. Stein, Estimation with Quadratic Loss. Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, 1961.

show that the usual estimators of the form

$$\hat{\Sigma}_a = a\,S\,, \qquad \text{where} \qquad a > 0,$$

are inadmissible in the general asymptotic setting, when $m, p \to \infty$ with $p/m \to c > 0$.

This phenomenon extends to the elliptical case.

In the following we set $r = \min(m, p)$.

Our objective

Based on the eigenvalue decomposition of $S = H L H^\top$, where

- H is a $p \times r$ semi–orthogonal matrix of eigenvectors.
- $L = \mathrm{diag}(l_1, \ldots, l_r)$, with $l_1 >, \ldots, > l_r$, is the diagonal matrix of the r positive corresponding eigenvalues of S.

We aim to *improve*

$$\hat{\Sigma}_a = a\,S\,, \qquad \text{where} \qquad a > 0,$$

by alternative estimators of the form

$$\hat{\Sigma}_\Psi = a\left(S + H\,L\,\Psi(L)\,H^\top\right) = a\,H\,L\left(I_r + \Psi(L)\right)H^\top\,,$$

with $\Psi(L) = \mathrm{diag}(\psi_1(L), \ldots, \psi_r(L))$, where $\psi_i = \psi_i(L)$ $(i = 1, \ldots, r)$ is a differentiable function of L, which are usually called orthogonally invariant estimators.

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The performance of any estimators $\hat{\Sigma}$ is assessed through the data–based loss

$$L_S(\hat{\Sigma}, \Sigma) = \mathrm{tr}\left(S^+ \Sigma \left(\Sigma^{-1}\hat{\Sigma} - I_p\right)^2\right) \tag{1.6}$$

and its associated risk

$$R(\hat{\Sigma}, \Sigma) = E_{\theta,\Sigma}\left[L_S(\hat{\Sigma}, \Sigma)\right],$$

where

- $E_{\theta,\Sigma}$ denotes the expectation w.r.t. the density specified below in (1.5).
- S^+ is the Moore–Penrose inverse of S. Note that, when $c > 1$, S is non–invertible and, when $c < 1$, S is invertible so that S^+ coincides with the regular inverse S^{-1}.

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- S^{+} is the Moore–Penrose inverse of S. Note that, when $c > 1$, S is non–invertible and, when $c < 1$, S is invertible so that S^{+} coincides with the regular inverse S^{-1}.

Why this data–based loss ?

As shown by various authors such as Haddouche et al. (2021, [1]), Konno (2009, [4]) and (1980, Haff [2]), it is difficult to handle on the usual quadratic loss

two Σ^{-1}

$$L(\Sigma, \hat{\Sigma}) = \mathrm{tr}\left((\Sigma^{-1}\hat{\Sigma} - I_p)^2 \right) = \mathrm{tr}(\Sigma^{-1}\hat{\Sigma}\,\Sigma^{-1}\hat{\Sigma}) - 2\,\mathrm{tr}(\Sigma^{-1}\hat{\Sigma}) + p \,. \qquad (1.7)$$

We introduce the data, which give rise to the data–based loss

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Improved estimators

Our approach

Consider the data–based risk function

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

When $\hat{\Sigma} = \hat{\Sigma}_a = a\,S$, the best constant a is given by

$$a_o = \frac{1}{v\,K^*}, \qquad \text{where} \qquad v = \max(p, m). \tag{2.1}$$

Consider alternative estimators of the form

$$\hat{\Sigma}_\Psi = a_o\,H\,L\,(I_r + \Psi(L))\,H^\top. \tag{2.2}$$

The estimators $\hat{\Sigma}_\Psi$ improves over $\hat{\Sigma}_{a_o}$ as soon as

$$\Delta(G) = R(\hat{\Sigma}_\Psi, \Sigma) - R(\hat{\Sigma}_{a_o}, \Sigma) \leq 0$$

for all Σ, with strict inequality for some Σ.

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Our approach

The risk difference between $\hat{\Sigma}_\Psi$ and $\hat{\Sigma}_{a_o}$ is given by

$$\Delta(\Psi) = a_o^2 \, E_{\theta,\Sigma} \left[\mathrm{tr} \left(\Sigma^{-1} H L (2\,\Psi + \Psi^2) H^\top \right) \right] - 2\, a_o \, E_{\theta,\Sigma} \left[\mathrm{tr} \, (\Psi) \right] . \tag{2.3}$$

Replacing the integrand term of $\Delta(\Psi)$ by a random matrix $\delta(\Psi)$, which does not depends on Σ^{-1} such that

$$\Delta(\Psi) \leq E^*_{\theta,\Sigma}[\delta(\Psi)] .$$

A sufficient condition for $\Delta(\Psi)$ to be non–positive is that $\delta(\Psi)$ is non–positive.

To this end, we rely on the following Stein–Haff type identity.

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A Stein–Haff type identity

Lemma 1

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

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

Dominance results

Theorem 1

Assume that $E_{\theta,\Sigma}\left[\mathrm{tr}(S)\right],\ E_{\theta,\Sigma}\left[\mathrm{tr}(S^{+})\right],\ E_{\theta,\Sigma}\left[\|HL\Psi(L)\,H^{\top}\|_F^2\right]$ *and* $E_{\theta,\Sigma}\left[\|H\Psi(L)H^{\top}\|_F^2\right]$ *are finite. Let* $\Psi(L) = \mathrm{diag}(\psi_1, \ldots, \psi_r)$ *with* $\mathrm{tr}\big(\Psi(L)\big) \geq \lambda$, *for a fixed positive constant* λ. *Then an upper bound of the risk difference in* (2.3) *is given by*

$$\Delta(\Psi(L)) \leq a_o^2\, K^{*}\, E^{*}_{\theta,\Sigma}\left[g(\Psi)\right],$$

where

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Dominance results

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Assume that $E_{\theta,\Sigma}\left[\operatorname{tr}(S)\right]$, $E_{\theta,\Sigma}\left[\operatorname{tr}(S^{+})\right]$, $E_{\theta,\Sigma}\left[\|HL\Psi(L)\,H^{\top}\|_F^2\right]$ *and* $E_{\theta,\Sigma}\left[\|H\Psi(L)H^{\top}\|_F^2\right]$ *are finite. Let* $\Psi(L)=\operatorname{diag}(\psi_1,\ldots,\psi_r)$ *with* $\operatorname{tr}\big(\Psi(L)\big)\geq\lambda$, *for a fixed positive constant* λ. *Then an upper bound of the risk difference in* (2.3) *is given by*

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Recall that

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

In order to the rid of Σ^{-1} in the integrand term, we apply the Stein–Haff type identity in Lemma 1. Then we have

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Examples

Note that Theorem 1 is well adapted to deal with:

- The James Stein (1961, [3]) estimator where

$$\psi_i(L) = \frac{1}{(v + r - 2i + 1)},$$

for $i = 1, \ldots, r$, since

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- The Efron-Morris-Dey estimator, considered by Tsukuma and Kubokawa (2020, [6]), where

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Haff estimators : the Gaussian case

When $c \leq 1$, Haff (1980, [2]) considered an empirical Bayes estimation of Σ.

Let a prior of Σ^{-1} be

$$\Sigma^{-1} \sim \mathcal{W}_p(p+1, \gamma^{-1} I_p),$$

where γ is an unknown hyperparameter.

The resulting posterior distribution of Σ^{-1} given S is

$$\Sigma^{-1} | S \sim \mathcal{W}_p(m+p+1, (S+\gamma I_p)^{-1}).$$

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The hyperparameter γ is estimated from the marginal density of S proportional to

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The resulting maximum likelihood estimator is

$$\hat{\gamma} = \frac{p(p+1)}{m+p+1}\frac{1}{\mathrm{tr}(S^{-1})} .$$

Thus we obtain an empirical Bayes estimator of the form

$$\hat{\Sigma}^{EB} = \frac{1}{m}(S+\hat{\gamma}\, I_p) = \frac{1}{m} H\, L\left(I_p + \frac{p(p+1)}{m+p+1}\frac{L^{-1}}{\mathrm{tr}(L^{-1})}\right) H^{\top}$$

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Taking into account both cases where $c \leq 1$ and $c > 1$, we define a Haff type estimators as

$$\hat{\Sigma}_{\alpha,b} = a_o \, H \left(I_r + b \frac{L^{-\alpha}}{\mathrm{tr}(L^{-\alpha})} \right) H^\top \,, \quad \text{where} \quad \alpha \geq 1 \text{ and } b > 0 \,. \qquad (2.4)$$

For $\alpha = 1$, this is the estimator considered by Konno (2009, [4]), who deals with the Gaussian case and the quadratic loss

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Proposition 1

Assume that the expectations $E_{\theta,\Sigma}\left[\mathrm{tr}(S^+)\right]$ and $E_{\theta,\Sigma}\left[\mathrm{tr}^2(S)\right]$ are finite. Then the Haff type estimators $\hat{\Sigma}_{\alpha,b}$ in (2.4) *improves on the usual estimator $\hat{\Sigma}_{a_o}$ in* (2.1) *under the data–based loss* (1.6) *as soon as*

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Sketch of Proof 1/3

Applying Theorem 1, an upper bound of the risk difference is given by

$$\Delta(\Psi) \leq a_o^2 \, K^* \, E^*_{\theta,\Sigma}\big(g(\Psi)\big)\,, \tag{2.5}$$

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

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

and

$$g_2(\Psi) = 4 l_i b \left(1 + b \frac{l_i^{-\alpha}}{\mathrm{tr}(L^{-\alpha})}\right) \frac{\partial}{\partial l_i} \left(\frac{l_i^{-\alpha}}{\mathrm{tr}(L^{-\alpha})}\right) + \frac{2b}{\mathrm{tr}(L^{-\alpha})} \sum_{i=1}^{r} \sum_{j \neq i}^{r} \frac{l_i^{1-\alpha} - l_j^{1-\alpha}}{l_i - l_j}$$
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$$\Delta(\Psi) \leq a_o^2\,b\,K^*\,E^*_{\theta,\Sigma}\big[-2\,(r-1) \;+ (v-r+1)\,b\big]\,.$$

Therefore, $\hat{\Sigma}_{\alpha,b}$ improves over $\hat{\Sigma}_{a_o}$ under the data-based loss (1.6) as soon as $0 < b \leq b_0 = 2\,(r-1)/(v-r+1)$.

Sketch of Proof 3/3

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

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

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

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Numerical study

Case of a t-distribution

Let the elliptical density in (1.3) be a variance mixture of normal distributions where the mixing variable, with density h, has the inverse–gamma distribution $\mathcal{IG}(k/2, k/2)$

Thus, for any $t \geq 0$, the generating function f in (1.3) has the form

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

which corresponds to the t–distribution with k degrees of freedom.

Then the primitive F^* of f in is, for any $t \geq 0$,

$$F^*(t) = \int_0^\infty \frac{\mathrm{v}}{(2\mathrm{v}\pi)^{np/2}} \exp\left(\frac{-t}{2\mathrm{v}}\right) h(\mathrm{v})\, d\mathrm{v}\,.$$

The normalizing constant K^* is given by

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Improved estimators

We study numerically the performance of

$$\hat{\Sigma}_{\alpha,b} = a_o\, H \left(I_r + b \frac{L^{-\alpha}}{\operatorname{tr}(L^{-\alpha})} \right) H^\top \,, \tag{3.1}$$

where

$$0 \leq b \leq b_0 = \frac{2\,(r-1)}{v-r+1} \quad \text{and} \quad \alpha \geq 1.$$

Konno (2009, [4]) consider the case $\alpha = 1$, in the Gaussian setting and under the usual quadratic loss, for which its improvement condition is $0 \leq b \leq b_1 = 2\,(r-1)\,(v+r+1)/(v-r+1)\,(v-r+3)$. Although $b_0 < b_1$, the improvement condition in (3.1) is valid for any $\alpha \geq 1$ and all the class of elliptically symmetric distributions.

It was shown numerically by Haddouche et al. (2021, [1]) that b_1 is optimal in the Gaussian context.

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The considered structures of Σ

We consider the following structures of Σ :

- (i) the identity matrix I_p
- (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 $\hat{\Sigma}_{a_o}$, we compute the Percentage Relative Improvement in Average Loss (PRIAL) defined as

$$PRIAL(\hat{\Sigma}_{\alpha,b}) = \frac{R(\hat{\Sigma}_{a_o},\Sigma) - R(\hat{\Sigma}_{\alpha,b},\Sigma)}{R(\hat{\Sigma}_{a_o},\Sigma)} \times 100$$

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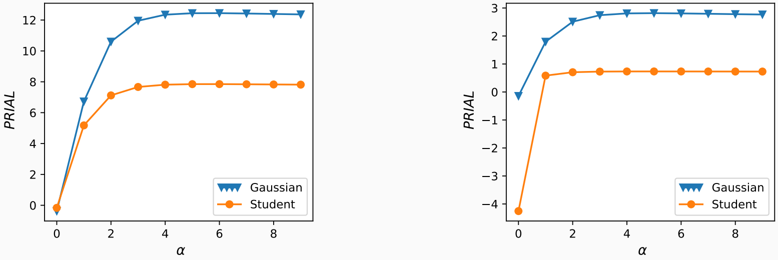
Effect of α

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,
- $\hat{\Sigma}_{a_o} = S(k-2)/vk$ when it is the t–distribution (K^* in (2.1) equals $(k-2)/k$).

We consider the non–invertible case where $p/m = c > 1$, with $(p, m) = (50, 20)$, for the structures (i) and (ii) of Σ for the t–distribution, with $k = 5$, and the Gaussian distribution

The data–based loss



(i) (ii)

Fig. 2 – PRIAL's of $\hat{\Sigma}_{\alpha, b_0}$ in (3.1) under the data–based loss (1.6).

- For the structure (i) of Σ, note that, for $\alpha \geq 6$, 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 (ii)
- When α is close to zero, the prial's are small for the structure (i) and may be negative for the structure (ii).

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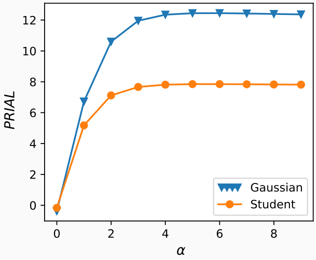

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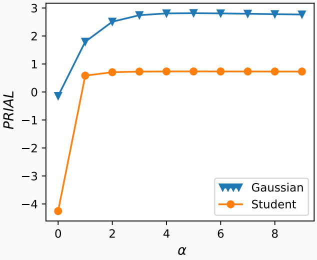

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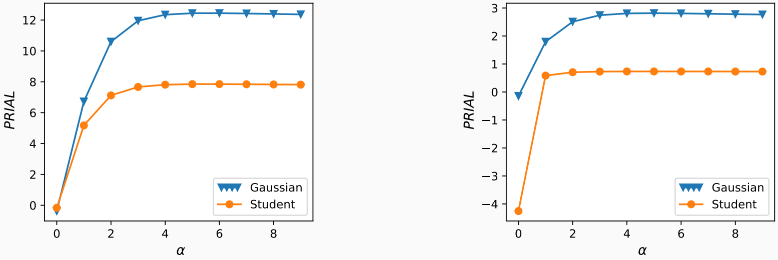

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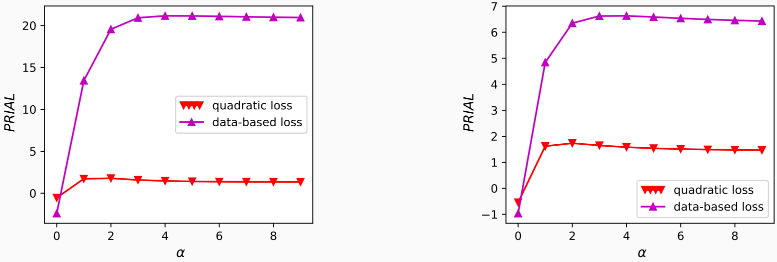
Loss functions comparison under the Gaussian assumption



(i) **(ii)**

Fig. 3 – PRIAL's of $\hat{\Sigma}_{\alpha,b_0}$ under data–based loss and PRIAL's of $\hat{\Sigma}_{\alpha,b_1}$ under quadratic loss.

- Prial's of $\hat{\Sigma}_{\alpha,b_0}$ w.r.t $\hat{\Sigma}_{a_o} = S/v$ under the data–based loss (1.6) and the prial's of $\hat{\Sigma}_{\alpha,b_1}$ w.r.t $\hat{\Sigma}_{a_o} = S/(v+r+1)$ under the quadratic loss (1.7).
- For (i) and (ii), the prial's are better under the data–based loss.
- For the structure (i) with $\alpha = 1$ (the Konno's estimator), we observe a prial equal to 1.73% which is similar to that of [4].

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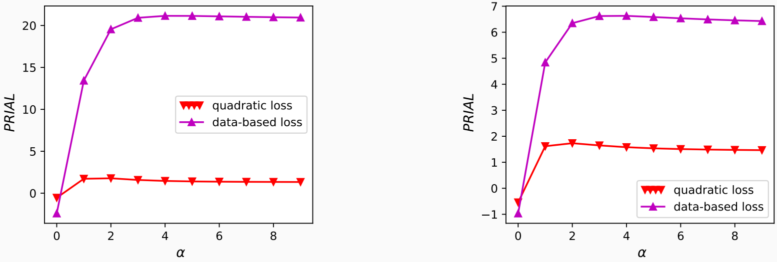

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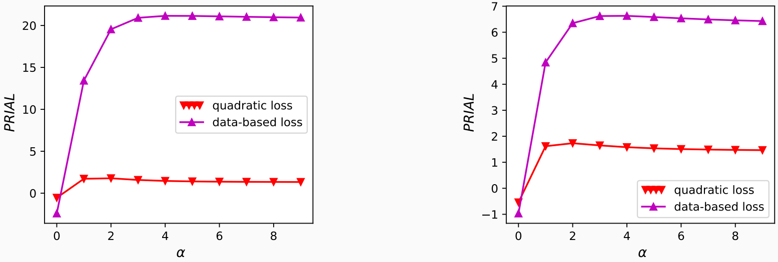

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Thank you for your attention !

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