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Maximum likelihood covariance matrix estimation from two possibly mismatched data sets

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A B S T R A C T

We consider estimating the covariance matrix from two data sets, one whose covariance matrix \( R_1 \) is the sought one and another set of samples whose covariance matrix \( R_2 \) slightly differs from the sought one, due e.g. to different measurement configurations. We assume however that the two matrices are rather close, which we formulate by assuming that \( R_1^{1/2} R_2^{1/2} R_1^{1/2} \) follows a Wishart distribution around the identity matrix. It turns out that this assumption results in two data sets with different marginal distributions, hence the problem becomes that of covariance matrix estimation from two data sets which are distribution-mismatched. The maximum likelihood estimator (MLE) is derived and is shown to depend on the values of the number of samples in each set. We show that it involves whitening of one data set by the other one, shrinkage of eigenvalues and colorization, at least when one data set contains more samples than the size \( p \) of the observation space. When both data sets have less than \( p \) samples but the total number is larger than \( p \), the MLE again entails eigenvalues shrinkage but this time after a projection operation. Simulation results compare the new estimator to state of the art techniques.

1. Problem statement

Analysis or processing of multichannel data most often relies on the covariance matrix, which is a fundamental tool e.g., for principal component analysis, spectral analysis, adaptive filtering, detection, direction of arrival estimation among others [1–3]. In practical applications, the \( p \times p \) covariance matrix \( R \) needs to be estimated from a finite number \( n \) of samples. When the latter are independent and Gaussian distributed, the maximum likelihood estimator of \( R \) is \( n^{-1}S \) where \( X \) is the \( p \times n \) data matrix and \( S = XX^T \) is the sample covariance matrix (SCM) [1]. However, in low sample support or when deviation from the Gaussian assumption is at hand, the SCM tends to behave poorly. In particular it was observed that the sample covariance matrix is usually less well-conditioned than the true covariance matrix, and therefore considerable effort has been dedicated to regularizing it with a view to improve its performance.

One of the most important approach in this respect is due to Stein [4–6] who, instead of maximizing the likelihood function, advocated to minimize a meaningful loss function within a given class of estimators. Stein hence introduced the concept of admissible estimation and minimax estimators under the so-called Stein’s loss. He showed that the SCM-based estimator is not minimax and derived minimax estimators in two important classes, namely estimators of the form \( \hat{R} = GDG^T \) where \( D \) is a diagonal matrix and \( G \) is the Cholesky factor of \( S \), or of the form \( \hat{R} = U \text{diag}(\varphi(\lambda)) U^T \) where \( U \text{diag}(\lambda) U^T \) is the eigenvalue decomposition of \( S \) and \( \varphi(\lambda) \) is a non-linear function of \( \lambda \). This seminal work of Stein gave rise to a great number of studies, see for instance [7–13] and references therein. A second class of robust estimates is based on linear shrinkage of the SCM to a target matrix (an approach which can be interpreted as an empirical Bayes technique), i.e., estimates of the form \( \hat{R} = \alpha R_1 + \beta S \) where \( R_1 = I \) is the most widely spread choice, see e.g., [14–20]. Note that these techniques applied with \( R_1 = I \) achieve an affine transformation of the eigenvalues of \( S \), while retaining the eigenvectors, and therefore bear resemblance with Stein’s method, although the selection of \( \alpha, \beta \) may not be driven by the same principle. Robustness to a possibly non-Gaussian distribution has also been a topic of considerable interest and many papers have focused on robust estimation for elliptically distributed data, see e.g., [21–30] and references therein.

Most of the above cited works deal with estimation of a covariance matrix from a single data set. In this paper, we consider a situation where two data sets \( X_1 \) and \( X_2 \) are available, with respective covariance matrices \( R_1 \) and \( R_2 \). This situation typically arises in radar applications when one wishes to detect a target buried in clutter with unknown statistics [31,32]. In order to infer the latter, training samples are generally used, which hopefully share the

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same statistics as the clutter in the cell under test (CUT). However, it has been evidenced that clutter is most often heterogeneous \[31\], with a discrepancy compared to the CUT that may grow with the distance to the CUT \[33\]. Therefore, one is led to use some clustering that separates training samples, either based on their proximity to the CUT or by means of some statistical criterion, such as the power selected training \[34\]. The samples so selected are deemed to be representative of the clutter in the CUT while others are less reliable, which corresponds to the situation considered herein. A second example is in the field of synthetic aperture radar in the case where a scene is imaged on two consecutive days, with possible changes in between \[35\]. Finally, in hyperspectral imagery, the problem of target or anomaly detection leads to a very similar framework. Indeed, the background in a pixel under test has to be estimated from the local pixels around and pixels located further apart \[36\]. In the present paper, we assume that R2 is close to R1, the covariance matrix we wish to estimate. Since R2 differs from but is close to R1, we investigate using both X1 and X2 to estimate R1. The reason for using also X2 is that despite its covariance matrix is not R1, it is close to. Additionally, one might face situations where the number of samples in X1 is very small. This paper constitutes a first approach to this specific problem and we focus herein on the most natural approach, namely maximum likelihood estimation. The objective is to figure out the pros and cons of the latter and the conditions under which it is an accurate estimator. The paper is organized as follows. In section 2 we formulate the statistical assumptions: more precisely, we assume that R1 \(\sim R_1 \sim W(1)^2\) is a random matrix with a Wishart distribution around the identity matrix, and we derive the joint distribution of (X1, X2). Section 3 is devoted to the derivation of the maximum likelihood estimator of R1 from (X1, X2), taking into account the possible configurations regarding the number of samples in each data set. Numerical simulations illustrate the performance of the MLE and compare it with existing alternatives in section 4. Conclusions and possible extensions of the present work are drawn in section 5.

2. Data model

Let us assume that we have two sets of measurements X1(p \(\times n_1\)) and X2(p \(\times n_2\)) which are distributed according to \(X_1 \sim \mathcal{N}(R_1, I)\) and \(X_2 \sim \mathcal{N}(0, R_2, I)\) where \(X(\mathcal{N}, \Sigma, \Omega)\) denotes the matrix-variate normal distribution whose density is

\[
(2\pi)^{-p(n_1+n_2)/2} |\Omega|^{-p/2} \exp\left(-\frac{1}{2} X' \Sigma^{-1} X \right)
\]

where \(|\Sigma|\) is the determinant andetr(\(\cdot\)) is the exponential of the trace of a matrix. Note that we consider real-valued data here whereas in radar applications it is customary to consider complex-valued signals. In Appendix A we show how the results below can be readily extended to the complex case. Our goal in this paper is to estimate R1, using both X1 and X2 even if R1 \(\neq R_2\). However, we assume that the two matrices are close to each other. In order to define a model that can reflect the proximity between R1 and R2, we note that the natural distance between them is given by \(d^2(R_1, R_2) = \sum_{k,l} \log^2 \lambda_k(G_k R_k G_k' + G_k' R_k G_k)
\[37,38\]
where \(G_k\) is a square-root of \(\Sigma\), i.e., \(G_k G_k' = \Sigma\), and \(\lambda_k(G_k R_k G_k' + G_k' R_k G_k)\) stands for the kth eigenvalue of \(G_k R_k G_k' + G_k' R_k G_k\). This matrix is pivotal in adaptive detection problems also. More precisely, in the case of a covariance mismatch between the training samples and the data under test, it is shown in \[39\] that the performance of the well-known adaptive matched filter depends essentially on this matrix. Therefore, it becomes natural to encapsulate the difference between R1 and R2 through the matrix \(W = G_k R_k G_k' + G_k' R_k G_k\) and its proximity to the identity matrix. There are of course different ways to translate this constraint in the model. For instance a frequentist approach may be advocated where the joint probability density function of (X1, X2) would be maximized under the constraint that the distance between W and I is smaller than some value. Alternatively, and this is what we elect here, one can resort to an empirical Bayes approach where the random matrix W follows some prior distribution rather concentrated around I. For mathematical tractability, we choose a conjugate prior for W and we assume that W follows a Wishart distribution with v degrees of freedom and parameter matrix \(\mu^{-1} I\), i.e., \(W \sim \mathcal{W}_p(v, \mu^{-1} I)\). Of course, this is a rather strong assumption whose validity would be difficult to check, e.g., on real data. However, it is in accordance with the mere knowledge we have about the relation between R1 and R2, and it allows for tractable derivations.

Using the fact that X1|R1 and X2|R2 are independent and Gaussian distributed with respective covariance matrices R1 and R2, and since R2 = G1W−1G1', we thus assume the following stochastic model:

\[
p(X_1, X_2| R_1, W) = (2\pi)^{-p(n_1+n_2)/2} |R_1|^{-n_1/2} |W^{-1} R_1|^{-n_2/2} \times \text{etr}\left(-\frac{1}{2} X_1' R_1^{-1} X_1 - \frac{1}{2} X_2' G_1^{-1} W G_1' X_2\right)
\]

(1a)

\[
p(W) = \frac{\mu^{v/2}}{2^{v/2} \Gamma_p(v/2)} |W|^{(v-1)/2} \text{etr}\left(-\frac{1}{2} \mu W\right)
\]

(1b)

Note that \(E(W^{-1}) = (v - p - 1)\mu I\) so that \(E(R_2) = E[G_1 W^{-1} G_1'] = (v - p - 1)\mu R_1\); therefore, for \(E(R_2)\) to be equal to \(R_1\), one must select \(\mu = v - p - 1\). Observe also that W comes closer to I as \(v\) grows large. Indeed, \(E(W) = \mu (v - p - 1)^{-1} I\) which goes to zero as \(v \rightarrow \infty\) \[40\].

The marginal distribution of (X1, X2) is obtained by integrating (1) with respect to W, which results in

\[
p(X_1, X_2) = \int_{W=0} \int_{W} p(X_1, X_2| R_1, W) p(W) dW
\]

\[
= \frac{(2\pi)^{-p(n_1+n_2)/2} \mu^{v/2}}{2^{v/2} \Gamma_p(v/2)} |R_1|^{-n_1/2} \text{etr}\left(-\frac{1}{2} X_1' R_1^{-1} X_1\right) \times \int_{W=0} |W|^{(v+n_2-1)/2} \text{etr}\left(-\frac{1}{2} \mu W\right) dW
\]

\[
= \frac{(2\pi)^{-p(n_1+n_2)/2} \mu^{v/2}}{2^{v/2} \Gamma_p(v/2)} \times \int_{R_1} |R_1|^{-n_1/2} \text{etr}\left(-\frac{1}{2} X_1' R_1^{-1} X_1\right) \times \int_{W=0} |W|^{(v+n_2-1)/2} \text{etr}\left(-\frac{1}{2} \mu W\right) dW
\]

\[
= (2\pi)^{-p(n_1+n_2)/2} |R_1|^{-n_1/2} \text{etr}\left(-\frac{1}{2} X_1' R_1^{-1} X_1\right) \times \frac{(2\pi)^{-p(n_1+n_2)/2} \mu^{v/2}}{2^{v/2} \Gamma_p(v/2)} \times \frac{\mu (v+n_2)^{v-n_2/2}}{\Gamma_p(v/2)}
\]

(2)

In order to obtain the third equality, we made use of the fact that, if S \(\sim \mathcal{W}_p(v, \Sigma)\),

\[
\int_{S=0} p(S) dS = 1 \Rightarrow \int_{S=0} |S|^{(v-1)/2} \text{etr}\left(-\frac{1}{2} \Sigma S^{-1}\right) dS = 2^{v/2} \Gamma_p(v/2) |\Sigma|^{v/2}
\]

(3)

Note that \(p(X_1, X_2| R_1)\) in (2) can be factored as \(p(X_1, X_2| R_1) = f_1(X_1| R_1) \times f_2(X_2| R_1)\) which shows that X1 and X2 are marginally independent and that \(p(X_1, X_2| R_1) = p(X_1| R_1) p(X_2| R_1)\) with \(p(X_1| R_1) \propto \text{etr}\left(-\frac{1}{2} X_1' R_1^{-1} X_1\right)\) and \(p(X_2| R_1) \propto |1 + (X_1' R_1^{-1} X_1)^{-1/2}|^{-(v+n_2)/2}\). Due to the model adopted for the random matrix \(W = G_1 R_1 G_1'\), X2 follows a matrix variate Student distribution \[41\]. Therefore, the fact that \(R_2 \neq R_1\) results here in two data sets with different distributions: one set
\(X_1\) is Gaussian distributed with covariance matrix \(R_1\) while the uncertainty in \(R_3\) leads to a Student distribution for \(X_0\). This is a rather original situation where one has to carry covariance matrix estimation from two data sets which are mismatched in their distributions. This peculiarity will result in new schemes compared to the conventional case of a single set with given distribution, as detailed now.

### 3. Maximum likelihood estimation

In this section we address estimation of \(R_1\) from \((X_1, X_2)\) and we focus on the most natural estimator, i.e., the maximum likelihood estimator. From (2), the log-likelihood function is, up to an additive and constant term

\[
\ell(R_1) = -\frac{n_1 + n_2}{2} \log |R_1| - \frac{v + n_2}{2} \log |I + \mu^{-1}S_1| - \frac{1}{2} \text{Tr}[R_1^{-1}S_1]
\]

where \(S_1 = X_1X_1^\top\) and \(S_2 = X_2X_2^\top\). Differentiating the previous equation and using the fact that \(d|R| = |R| \text{det} dR\) and \(dR^{-1} = -R^{-1}(dR)R^{-1}\), we obtain the following equation that the ML solution satisfies

\[
(v - n_1)R_1^{-1} - (v + n_2)(I + \mu^{-1}S_1)^{-1} + R_1^{-1}S_1R_1^{-1} = 0
\]

In order to solve (5), we must investigate various configurations for \((n_1, n_2)\) as the solution will depend on them. Before going to the technical details of each case, we give an overview of the results obtained.

#### 3.1. Summary of results

As is illustrated below, the expression of the maximum likelihood estimator depends on the respective values of \(n_1\) and \(n_2\). In the sequel three cases will be distinguished: a first situation where \(n_1 < p\) and \(n_2 \geq p\), a second one which is the mirror situation, namely \(n_1 \geq p\) and \(n_2 < p\), and finally a third more challenging case where \(n_1 < p\), \(n_2 < p\) and \(n_1 + n_2 \geq p\).

In the first (respectively second) case, the ML solution is given by (11) [resp. (21)]: it will be shown that the estimation process entails whitening of \(X_1\) [resp. \(X_2\)] by the inverse of the square-root of the sample covariance matrix of \(X_2\) [resp. \(X_1\)], followed by shrinkage of eigenvalues and finally colorization by the square-root of the sample covariance matrix of \(X_2\) [resp. \(X_1\)]. The technique of eigenvalue shrinkage is rather well known but usually applied to the SCM of a single set: herein, due to the presence of two data sets, this technique is applied to one data set after it has been whitened by the second one. Interestingly enough, the ML solution can also be written as (14) [resp. (22)], that is as a weighted sum of the SCM of each data set, where the whitening matrix is diagonal for one set of samples, and non diagonal for the other set.

Finally, when \(n_2 < p\), \(p < n_1\) and \(n_1 + n_2 \geq p\), the procedure includes a partitioning between the subspace spanned by the columns of \(X_2\) and its orthogonal complement. In the former, shrinkage of eigenvalues is used while, in the latter, projection of the SCM of \(X_1\) is retained.

#### 3.2. Case \(n_1 < p\) and \(n_2 \geq p\)

We consider first the case where \(n_1 < p\) and \(n_2 \geq p\), i.e., \(n_1\) is not large enough for \(S_1\) to be positive definite and one needs to use \(X_2\) in order to estimate \(R_1\), even though \(R_2 \neq R_1\). Eq. (5) can be rewritten as

\[
(v - n_1)R_1^{-1}(R_1 + \mu^{-1}S_1) - (v + n_2)I + R_1^{-1}S_1R_1^{-1} - (R_1 + \mu^{-1}S_1) = 0
\]

\Rightarrow -(n_1 + n_2)I + (v - n_1)\mu^{-1}S_2 + R_1^{-1}S_1 + \mu^{-1}S_1R_1^{-1} - S_2 = 0

\Rightarrow R_1R_2 - \left[\frac{v - n_1}{\mu(n_1 + n_2)}I + \frac{1}{n_1 + n_2}S_2R_2^{-1}\right]R_1

- \frac{1}{\mu(n_1 + n_2)}S_1 = 0

\]
A comment is also in order regarding the behavior of the MLE when $\nu$ grows large, i.e., when $W$ comes closer to $I$. Indeed, with $\mu = \nu - p - 1$, one has

$$\lim_{n \to \infty} \frac{\xi_k}{n_1 + n_2} \Rightarrow \lim R_{12} = \frac{1}{n_1 + n_2} \left[ S_1 + I \right]$$

$$\lim_{n \to \infty} R_1 = \frac{1}{n_1 + n_2} L_2^{-1} S_2 L_2^{-T} + I \left[ \frac{1}{n_1 + n_2} \right]$$

$$= \frac{1}{n_1 + n_2} \left[ S_1 + S_2 \right]$$

(13)

which shows that, as $W$ comes closer to $I$, i.e., as $R_2$ comes closer to $R_1$, the MLE is simply the sample covariance matrix of the whole data, as may be expected.

Finally, another interpretation of the MLE can be obtained by rewriting the MLE in another form. Noting that the range space of $L_1^{-1} X_1$ coincides with the range space of $u_1, \ldots, u_{n_1}$, it follows that $u_k = L_2^{-1} X_1 \eta_k$ for some vector $\eta_k$. Therefore, (11) can be rewritten as

$$R_1 = X_1 \left[ \sum_{k=1}^{n_1} \left( \xi_k - \frac{\nu - n_1}{\mu(1 + n_2)} \right) \eta_k \eta_k^T \right] X_1^T + \frac{\nu - n_1}{\mu(1 + n_2)} S_2$$

$$= X_1 \Gamma_1 X_1^T + \frac{\nu - n_1}{\mu(1 + n_2)} X_1 X_2^T$$

(14)

Consequently, the MLE is a weighted version of the sample covariance matrices of each data set. In fact, it can be shown (we omit the details) that if a solution to (5) is sought which is of the form (14), then $\Gamma_1$ is solution to the equation

$$\begin{align*}
\Gamma_1^2 + &\left[ \frac{\nu - n_1}{\mu(1 + n_2)} \right] (X_1 S_2^T X_1)^{-1} - \frac{1}{n_1 + n_2} \right] \Gamma_1 \\
&\frac{\nu + n_2}{\mu(1 + n_2)} (X_1 S_2^T X_1)^{-1} = 0
\end{align*}$$

(15)

It ensues that $\Gamma_1$ and $X_1^T S_1^T X_1$ share the same eigenvalues, which are indeed the right singular vectors $v_k$ of $L_2^{-1} X_1$. Moreover, the eigenvalues $\gamma_k^2$ of $\Gamma_1$ satisfy

$$\gamma_k^2 + \frac{\nu - n_1}{\mu(1 + n_2)} \sigma_k^{-2} - \frac{1}{n_1 + n_2} \right] \gamma_k^2 - \frac{(\nu + n_2)}{(\mu(1 + n_2))^2} = 0$$

(16)

To summarize, the MLE of $R_1$, can either be written as in (11) where the eigenvalues $\xi_k$ are related to the eigenvalues $\lambda_k$ of $L_2^{-1} S_1 L_2^{-T}$ by (9), or as in (14) where $\Gamma_1$ is given by (15).

3.3 Case $n_2 < p$ and $n_1 \geq p$

We now consider a situation where $n_2 < p$ and $n_1 \geq p$ under which one has a sufficient number of “good” samples $X_1$ for $S_1$ to be full-rank. Yet, it might be of interest to use $X_2$ even though its covariance matrix $R_2 \neq R_1$. The derivation of the MLE follows along the same lines as in the previous case, except that now $S_2$ is rank-deficient and $S_1$ is full-rank. Starting from the ML Eq. (5), on can write

$$(\nu - n_1) R_1^{-1} (R_1 + \mu^{-1} S_2) - (\nu + n_2) I + R_1^{-1} S_1 R_1^{-1} (R_1 + \mu^{-1} S_2) = 0$$

$$\Rightarrow - (n_1 + n_2) I + (\nu - n_1) \mu^{-1} R_1^{-1} S_1 R_1^{-1} S_1 + \mu^{-1} R_1^{-1} S_1 R_1^{-1} S_1 = 0$$

$$\Rightarrow - (n_1 + n_2) R_2 S_1 R_2^{-1} S_1 R_2^{-1} + (\nu - n_1) \mu^{-1} R_1^{-1} S_1 R_1^{-1} S_1 = 0$$

$$\Rightarrow R_2 S_1^{-1} R_2^{-1} - \frac{1}{(\mu (n_1 + n_2))} S_1 = 0$$

(17)

Let $S_1 = L_1 L_1^{-T}$ and let us define $R_{11} = L_1^{-1} R_1 L_1^{-T}$ and $S_2 = L_1^{-1} L_2^{-1}$. Then, taking the transpose of the previous equation, post-multiplying by $L_1^{-1}$ and post-multiplying by $L_1^{-1}$, we obtain

$$R_{11}^{-1} - \frac{1}{(\mu (n_1 + n_2))} S_2 = 0$$

(18)

As before, it can be seen that $R_{11}$ and $S_2$ share the same eigenvalues. The $p - n_2$ eigenvectors of $S_2$ associated with zero eigenvalue will correspond to a constant eigenvalue for $R_{11}$ equal to $1$. A strictly positive eigenvalue $\zeta$ of $R_{11}$ is related to its counterpart $\lambda$ of $S_2$ by

$$\zeta^2 - \zeta \left[ \frac{\lambda (\nu - n_1)}{\mu(1 + n_2)} + \frac{1}{n_1 + n_2} \right] - \frac{\lambda}{\mu (n_1 + n_2)} = 0$$

(19)

Now, if we let $L_1^{-1} X_2 = Y \Theta Z^T = \sum_{k=1}^{n_2} \theta_k y_k z_k^T$ be the singular value decomposition of $L_1^{-1} X_2$, we have

$$\begin{align*}
R_{11} &= \sum_{k=1}^{n_2} \zeta_k y_k y_k^T + \frac{1}{n_1 + n_2} \sum_{k=1}^{p} y_k y_k^T \\
&= \sum_{k=1}^{n_2} \left( \zeta_k - \frac{1}{n_1 + n_2} \right) y_k y_k^T + \frac{1}{n_1 + n_2} I
\end{align*}$$

(20)

where $\zeta_k$ is the positive root of (19) with $\lambda$ substituted for $\theta_k^2$. The MLE of $R_1$ becomes

$$R_1 = \sum_{k=1}^{n_2} \left( \zeta_k - \frac{1}{n_1 + n_2} \right) L_1 y_k y_k^T L_1^{-1} + \frac{1}{n_1 + n_2} S_1$$

(21)

Again, since the range space of $L_1^{-1} X_2$ is spanned by $y_1, \ldots, y_{n_2}$, one has $y_k = L_1^{-1} X_2 \hat{X}_k$ and hence

$$R_1 = X_1 \left[ \sum_{k=1}^{n_2} \left( \zeta_k - \frac{1}{n_1 + n_2} \right) X_1 \right] X_1^T + \frac{1}{n_1 + n_2} X_1 X_1^T$$

(22)

Note that (22) differs from (14) in that the weighting matrix applied between $X_1$ and $X_2$ is now diagonal while that applied between $X_2$ and $X_1$ is no longer diagonal. Furthermore, if one looks for a solution of the form (22), then $\Gamma_2$ is the solution to

$$\begin{align*}
\Gamma_2^2 &+ \left[ \frac{\nu - n_1}{\mu(1 + n_2)} \right] (X_2 S_1^{-1} X_2)^{-1} - \frac{1}{n_1 + n_2} \right] \Gamma_2 \\
&\frac{\nu + n_2}{\mu(1 + n_2)} (X_2 S_1^{-1} X_2)^{-1} = 0
\end{align*}$$

(23)

$\Gamma_2$ and $X_2 S_1^{-1} X_2$ share the same eigenvectors (actually $z_k$) and the eigenvalue $\gamma_k^2$ of $\Gamma_2$ is obtained as the positive solution to

$$\gamma_k^2 + \frac{\nu - n_1}{\mu(1 + n_2)} \sigma_k^{-2} - \frac{1}{n_1 + n_2} \right] \gamma_k^2 - \frac{(\nu + n_2)}{(\mu(1 + n_2))^2} = 0$$

(24)

Remark 1. When $n_1 \geq p$ and $n_2 \geq p$, the previous techniques can still be used, with slight variations. In this case, $S_1$ and $S_2$ are now full-rank, and therefore the MLE of $R_1$ is given by (11) but with the first sum extended to $p$ eigenvectors ($S_1$ has now $p$ non-zero eigenvalues), and the second term vanishes. The ML solution is also given by (21) with the first term extended to $p$ eigenvectors and the second term vanishing.

3.4 Case $n_2 < p$, $n_2 < p$ and $n_1 + n_2 \geq p$

We now consider the more challenging case where neither of the two data sets contains enough samples for their respective sample covariance matrices to be full-rank, and thus it becomes mandatory to combine both sets. This situation is a bit trickier and requires some carefulness. Going back to (5), the MLE of $R_1$ should satisfy

$$\begin{align*}
(n - n_1) R_1^{-1} - (n + n_2) (R_1 + \mu^{-1} S_2)^{-1} + R_1^{-1} S_1 R_1^{-1} &= 0 \\
\Rightarrow (n - n_1) R_1^{-1} + R_1^{-1} S_1 R_1^{-1}
\end{align*}$$
\[-(v + n_2) \left[ R_1^{-1} - \mu^{-1} R_1^{-1} X_2 (I + \mu^{-1} X_1^T R_1^{-1} X_2)^{-1} X_1^T R_1^{-1} \right] = 0 \]
\[\Rightarrow (n_1 + n_2) R_1 = (v + n_2) \mu^{-1} X_2 (I + \mu^{-1} X_1^T R_1^{-1} X_2)^{-1} X_1^T + X_1 \]
(25)

Before pursuing, it is worthy looking at the previous equation to get some insight. We observe that the projection of $R_1$ onto the subspace orthogonal to $X_2$ will be equal to the projection of $S_1$ on this same subspace. This suggests to use a decomposition that splits data in $R(X_2)$ and its orthogonal complement. To do so, let us consider the SVD of $X_2$ as $X_2 = C D \tilde{E} F = [C \quad D \quad \tilde{E}]$, where $C$ is a $(p \times p)$ matrix, $D$ is a $(p \times n_2)$ matrix and $\tilde{E}$ is the $n_2 \times n_2$ diagonal matrix of singular values. Let us also operate a change of coordinates and define
\[\Sigma = C^T R_1 C = \begin{bmatrix} C^T R_1 & C^T D \tilde{E} & 0 \\ C^T D & C^T D \tilde{E} & 0 \\ 0 & 0 & \Sigma_{bb} \end{bmatrix} = \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ab} & \Sigma_{bb} \end{bmatrix} \]
(26)

With these definitions, it is straightforward to show that $X_2^T R_1^{-1} X_2 = \bar{E} \Sigma_{aa} \bar{E}^T$ where $\Sigma_{aa} = \Sigma_{aa} - \Sigma_{ab} \Sigma_{bb}^{-1} \Sigma_{ba}$ and thus
\[X_2^T (I + \mu^{-1} X_1^T R_1^{-1} X_2)^{-1} X_1^T = C^T D \bar{E} \Sigma_{aa} \bar{E}^T \]
\[-D \Sigma_{bb}^{-1} \]
\[= C^T D \bar{E} \Sigma_{aa} \bar{E}^T \]
(27)

Therefore, pre-multiplying (25) by $C^T$ and post-multiplying it by $C$, we obtain
\[(n_1 + n_2) \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ab} & \Sigma_{bb} \end{bmatrix} \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ab} & \Sigma_{bb} \end{bmatrix} = (v + n_2) \mu^{-1} \begin{bmatrix} D \Sigma_{bb}^{-1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} D \Sigma_{bb}^{-1} & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} C^T S_1 C_a & C^T S_1 C_b \\ C^T S_1 C_a & C^T S_1 C_b \end{bmatrix} \]
(28)

which immediately implies that
\[(n_1 + n_2) \Sigma_{aa} = C^T S_1 C_a \]
\[(n_1 + n_2) \Sigma_{ab} = C^T S_1 C_b \]
(29)

This corroborates the comments we made after Eq. (25) since one has
\[(n_1 + n_2) C_b \Sigma_{ab} C_b^T = (n_1 + n_2) C_a C_b^T / C_a C_b^T = \lambda \]
\[= C_a C_b^T \]
(30)

It now remains to find $\Sigma_{ab}$ or equivalently $\Sigma_{aa,b}$. Towards this end, note that
\[(n_1 + n_2) \Sigma_{ab} = (n_1 + n_2) \begin{bmatrix} \Sigma_{aa} + \Sigma_{ab} \Sigma_{bb}^{-1} \Sigma_{ab} + C_a C_b \end{bmatrix} \]
\[= (n_1 + n_2) \Sigma_{ab} + (C_a C_b (C_a C_b)^{-1} (C_a C_b)^{-1}) \]
\[(n_1 + n_2) \Sigma_{ab} \]
(32)

which leads to
\[(n_1 + n_2) \Sigma_{ab} = (v + n_2) \mu^{-1} \begin{bmatrix} D \Sigma_{bb}^{-1} & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} C^T S_1 C_b \end{bmatrix} \]
(33)

For the sake of notational convenience, let us denote $F = [C^T S_1 C_b]$. Post-multiplying the previous equation by $\begin{bmatrix} D \Sigma_{bb}^{-1} & 0 \end{bmatrix}$ results in
\[(n_1 + n_2) \Sigma_{aa,b} \Sigma_{ab} = (v + n_2) \mu^{-1} \begin{bmatrix} F D \Sigma_{bb}^{-1} F^T & \mu^{-1} F \Sigma_{bb}^{-1} F^T \end{bmatrix} + \begin{bmatrix} C^T S_1 C_b \end{bmatrix} \]
(34)

where $\Sigma_{aa,b} = D \Sigma_{bb}^{-1} D \Sigma_{bb}^{-1}$ and $F = D \Sigma_{bb}^{-1} F$. Similarly to what was done before, $\Sigma_{aa,b}$ and $F$ share the same eigenvectors. When the eigenvalue $\lambda$ of $F$ is zero (there are actually $p - n_1$ of them [45]) the corresponding eigenvalue $\phi$ of $\Sigma_{aa,b}$ is $\frac{\phi}{\lambda}$. For each of the $r = n_1 + n_2 - p$ non-zero $\lambda$, the corresponding $\phi$ is the unique positive root of
\[\phi^2 \left[ 1 - \frac{\phi}{\lambda} + \frac{\mu}{\mu(n_1 + n_2)} \right] = 0 \]
(35)

Therefore, if $\hat{u}_k$ are the eigenvectors of $\hat{F}$, $\hat{\Sigma}_{aa,b}$ is given by
\[\Sigma_{aa,b} = \sum_{k=1}^{r} \phi_k \hat{u}_k \hat{u}_k^T + \frac{v - n_1}{\mu(n_1 + n_2)} \sum_{k=r+1}^{p} \hat{u}_k \hat{u}_k^T \]
(36)

Once $\Sigma_{aa,b}$ is computed, $\Sigma_{aa,b} = D \Sigma_{aa,b} D$ and $\Sigma_{bb}$ can be obtained from (32). Finally, the MLE of $R_1$ is given by $\Sigma_{aa,b} C^T$.

We now present an alternative way to compute the solution. From (25), it appears that $R_1$ can be written as $R_1 = X_1 X_2 X_1 X_2 X_1 X_2$, where $X_2 = (v + n_2) \mu^{-1} (I + \mu^{-1} X_2 R_1^{-1} X_2)$. Let $X = [X_1 X_2]$ and let $X^T = QR$ be the QR decomposition of $X^T$ with $Q$ a $(n_1 + n_2) \times p$ semi-unitary matrix, i.e., $Q^T Q = I_p$. Let us partition $Q$ as $Q = \begin{bmatrix} Q_a & Q_b \end{bmatrix}$ so that $X_2 = Q_a R$ and $X_2 = Q_b R$. Then, one has
\[(n_1 + n_2) R_1 = X_1 X_2 X_1 X_2 X_1 X_2 = Q_a [Q_a Q_b + Q^T a] \]
and therefore
\[(n_1 + n_2)^{-1} X_1 X_2 X_1 X_2 X_1 X_2 = Q_a [Q_a Q_b + Q^T a]^{-1} Q_a^T \]
\[= Q_a [I + Q_b] (Q_b - I) [Q_b - I]^{-1} Q_a^T \]
\[= Q_a Q_a^T - Q_a [I + Q_b] (Q_b - I) [I + Q_b]^{-1} Q_a^T \]
\[= \left[ Q_a Q_a^T \right]^{-1} - \left[ I + Q_a Q_a^T \right]^{-1} \]
(37)

Consequently, if we define $B_2 = \begin{bmatrix} Q_a Q_b \end{bmatrix}$, we have
\[\Gamma_2^{-1} = (v + n_2)^{-1} [I + \mu^{-1} X_2 R_1^{-1} X_2] \]
\[= (v + n_2)^{-1} \mu I + (v + n_2)^{-1} X_2 R_1^{-1} X_2 \]
\[= (v + n_2)^{-1} \mu I + (v + n_2)^{-1} (n_1 + n_2) (G_2 + B_2)^{-1} \]
(38)

Pre-multiplying the previous equation by $(\Gamma_2 + B_2)$ and post-multiplying by $\Gamma_2$, we obtain the following second-order polynomial equation:
\[\Gamma_2 + [B_2 - \frac{v - n_1}{\mu} I] \Gamma_2 - \frac{v + n_2}{\mu} B_2 = 0 \]
(39)

It follows that $\Gamma_2$ and $B_2$ share the same eigenvectors. If $\lambda$ is a non-zero eigenvalue of $B_2$, then $\Gamma_2$ is the unique positive root of the following polynomial equation:
\[\lambda^2 - \frac{v - n_1}{\mu} \lambda - \frac{v + n_2}{\mu} = 0 \]
(40)
Fig. 1. Average distance between $\hat{R}_1$ and $R_1$ in case 1.

(a) $n_1 + n_2 = p$

(b) $n_1 + n_2 = 3p/2$

(c) $n_1 + n_2 = 2p$

Fig. 2. Average distance between $\hat{R}_1$ and $R_1$ in case 2.

(a) $n_1 + n_2 = p$

(b) $n_1 + n_2 = 3p/2$

(c) $n_1 + n_2 = 2p$
If $\lambda = 0$ then $\gamma = (v - n_2)\mu^{-1}$. Finally, the solution $\Gamma_2$ is given by

$$
\Gamma_2 = \sum_{k=1}^{r} \gamma_k b_k b_k^T + \frac{v - n_1}{\mu} \sum_{k=r+1}^{n_2} \gamma_k b_k b_k^T
$$

$$
= \sum_{k=1}^{r} \left[ \gamma_k - \frac{v - n_1}{\mu} \right] b_k b_k^T + \frac{v - n_1}{\mu} I
$$

where $b_k$ are the eigenvectors of $B_2$. Note that

$$
B_2 b = \lambda b \Rightarrow (Q_2 Q_2^T)^{-1} b - b = \lambda b
$$

$$
= (Q_2 Q_2^T)^{-1} b = (1 + \lambda) b
$$

and hence $b$ is an eigenvector of $Q_2 Q_2^T$ associated with eigenvalue $(1 + \lambda)^{-1}$, or equivalently a right singular vector of $Q_2$. Observe also that, since $X_2 = Q_2 R$ and $XX^T = R^T Q_2^T Q_2 R$, one has

$Q_2 Q_2^T = X_2^T R^{-1} X_2 = X_2^T (R^T R)^{-1} X_2$

$= X_2^T (XX^T)^{-1} X_2 = X_2^T (X_1 X_1^T + X_2 X_2^T)^{-1} X_2$

Hence, if we let $S = X_1 X_1^T + X_2 X_2^T = LL^T$, then $Q_2^T$ and $L^{-1} X_2$ share the same right singular vectors.

### 4. Numerical simulations

In this section, we evaluate numerically the performance of the MLE presented above through Monte-Carlo simulations. We consider a scenario where the size of the observation space is $p = 128$. Three cases will be considered for the covariance matrix $R_1$, which correspond to different kind of processes. In the first case the $(k, \ell)$ element is $R_1(k, \ell) = P_{\rho}^{|k-\ell|} + \delta(k, \ell)$ with $\rho = 0.7$. The second case assumes that $R_2(k, \ell) = P e^{-0.5(2\pi \sigma_f |k-\ell|)^2} + \delta(k, \ell)$ with $\sigma_f = 0.02$. In the third case, $R_3(k, \ell) = r_{AR}(|k - \ell|) + \delta(k, \ell)$ where $r_{AR}(|k - \ell|)$ corresponds to the correlation of an autoregressive process whose poles are located at $0.95 e^{\pm i2\pi0.05}$, $0.9 e^{\pm i2\pi0.15}$, $0.9 e^{\pm i2\pi0.18}$. Finally $P = 100$ and $r_{AR}(0) = 100$. The corresponding processes are rather lowpass in case 1 and 2, while case 3 concerns processes with sharp peaks in their spectrum. In each simulation $X_1$ is generated from a Gaussian distribution with covariance matrix $R_1$. Then $W$ is generated from a Wishart distribution with $v = p + 2$ degrees of freedom and parameter matrix $(v - p - 1)^{-1} I$ and $R_2$ is computed as $R_2 = G_0 W^{-1} G_0^T$. Then $X_2$ is generated from a Gaussian distribution with covariance matrix $R_2$.

The MLE is compared with four competitors. The first is the sample covariance matrix based on all samples, i.e., $(n_1 + n_2)^{-1} S$ where $S = X_1 X_1^T + X_2 X_2^T$. The second is of the form $G_{SCM} D_{SCM}^T$, where $G_{SCM}$ is the Cholesky factor of $S$, and $D$ is a diagonal matrix which is chosen to minimize Stein’s loss and is given by $D_{SCM} = 1/(n_1 + n_2 + p - 2k + 1)$. The third is of the same form but is meant at minimizing the natural distance between $R_1$ and its estimate: as shown in [13], it amounts to choosing $D_{SCM} = \exp \left\{ -E \left[ \log \gamma_{n_1 + n_2 + 1}^2 \right] \right\}$. Finally, we consider the class of orthogonally invariant estimators of the form $U_{SCM} \text{diag}(\varphi(\lambda)) U_{SCM}^T$ where $S = U_{SCM} \text{diag}(\lambda) U_{SCM}^T$ is the eigenvalue decomposition of $S$ and $\varphi(\lambda) = \left[ \varphi_1(\lambda), \ldots, \varphi_p(\lambda) \right]$. Stein showed that the choice $\varphi_k = \lambda_k/n_1 + n_2 + p - 1 + 2\lambda_k \sum_{j \neq k} (\lambda_k - \lambda_j)^{-1}$ is the best with respect to Stein’s loss. However this choice has two drawbacks: it can result in some $\varphi_k < 0$ and it does not preserve the order of the eigenvalues $\lambda_k$, which is a problem [41]. In order to overcome these problems, Stein proposed an isotonizing scheme that guarantees $\varphi_k > 0$ and preserves order, see [46] for details of this scheme. We consider this improved estimator as the fourth alternative. The figure of merit for all estimators will be the natural
distance between the true and the estimated covariance matrices $d^2(\hat{R}_1, \hat{R}_2) = \sum_{k=1}^{p} \log^2 \hat{\lambda}_k(R^{-1}_1 R^{-1}_2)$.

The simulation results are shown in Figs. 1-4 where we consider different values for the total number of samples $n = n_1 + n_2$, namely $n = p$, $n = 3p/2$ and $n = 2p$. The main conclusions regarding these simulations are the following:

- the MLE is shown to outperform its competitors when $n_1$ is small and $n$ is large enough, typically it has the best performance for $n = 3p/2$ and $n = 2p$. One can observe that the improvement achieved by the MLE is more important when $n = 2p$ and $n_1$ is small, i.e., when one has few samples drawn from $R_1$ and a large majority of samples drawn from $R_2$.
- in contrast, when $n = p$ the other methods can perform better than the MLE, especially when $n_1$ is above a threshold, i.e., when the number of “good” samples is large enough.
- among the Stein-like methods, that based on eigenvalue decomposition (with isotonizing) is the best, but the method based on Cholesky factorization and minimization of the geodesic distance comes very close.

In a final simulation, we evaluate the influence of $\nu$: recall that, as $\nu$ increases, $W$ is closer to $I$ and thus $R_2$ is closer to $R_1$, which means that $X_2$ should be nearly as informative as $X_1$. In Fig. 4 we display the average distance as a function of $\nu$ in case 1 with $n_1 + n_2 = 2p$. It is observed that, as $\nu$ increases, the performance of all estimators improve. The proposed MLE is no longer the most accurate above a threshold, where it is dominated by the Stein’s estimator based on the eigenvalues of the whole sample covariance matrix. However, the proposed MLE still performs better than all other estimators.

### 5. Conclusions

In this paper, we considered the problem of estimating a covariance matrix $R_1$ from two data sets, one set $X_1$ whose covariance matrix is actually $R_1$, and another set $X_2$ whose covariance matrix $R_2$ is different but close to $R_1$. Since the distance between $R_1$ and $R_2$ depends on the eigenvalues of $W = G_1^{-1}R_1^{-1}G_1$, we embedded the latter in a statistical model and assumed that it followed a Wishart distribution around the identity matrix. We showed that the problem is that of estimating $R_1$ from two data sets with different distributions. The maximum likelihood estimator was derived and its expression was shown to depend on the number of samples in $X_1$ and $X_2$. The MLE was shown to perform quite well, as compared to state of the art algorithms, at least when the number of samples in $X_1$ is small and the total number of samples $n$ is large enough. However, as in a classical framework with a single data set, there is room from improvement of the MLE, especially in low sample support. Therefore, future work should be devoted to improving the MLE in this situation. For instance, one could study how the MLE could be regularized or could investigate whether a Stein-like approach is possible for this two data sets framework. Alternatively, a frequentist approach where joint estimation of $R_1$ and $W$ is performed under some constraints constitutes a worthy path of investigation.

### Declaration of Competing Interest

None.

### Appendix A. Extension to complex-valued data

In this appendix, we briefly show that the derivations concerning the maximum likelihood estimator can be extended in a straightforward manner to the complex case. Let us assume here that $X_1|R_1 \sim \mathcal{CN}(0, R_1, I)$ and $X_2|R_2 \sim \mathcal{CN}(0, R_2, I)$ are complex-valued data and distributed according to a circularly symmetric complex-valued matrix-variate normal distribution. Let $R_1 = G_1^{-1}H_1$—where $H_1$ stands for the Hermitian transpose— and $R_2 = G_2^{-1}H_2$, where $W \sim \mathcal{CN}_{p}(\nu, \mu^{-1}I)$ follows a complex Wishart distribution. The statistical (complex-valued) model is thus

$$p(X_1, X_2|R_1, W) = \pi^{-(n_1+n_2)}|R_1|^{-n_1}|W^{-1}R_1|^{-n_2} \times \text{etr}
\left[-X_1^H R_1^{-1} X_1 - X_2^H G_1^{-1}H_1^{-1} X_2 \right]$$ (A.1a)

$$p(W) = \frac{\mu^{|p|}}{\Gamma_p(v)} |W|^{-p} \text{etr}(-\mu W)$$ (A.1b)

Note that, in the complex case, $\mathbb{E}[W^{-1}] = (\nu - p - 1)\mu I$ [40] so that $\mathbb{E}[R_1] = \mathbb{E}[G_1 W^{-1} G_1^H] = (\nu - p - 1)\mu R_1$. Therefore, for $\mathbb{E}[R_2]$ to be equal to $R_1$, one must have $\mu = \nu - p - 1$ in the real case.

The marginal distribution of $(X_1, X_2)$ is now

$$p(X_1, X_2|R_1) = \int_{W>0} p(X_1, X_2|R_1, W) p(W)dW$$

$$= \pi^{-(n_1+n_2)}\frac{\mu^{|p|}}{\Gamma_p(v)} |R_1|^{-n_1-n_2} \text{etr}
\left[-X_1^H R_1^{-1} X_1 \right] \times \int_{W>0} |W|^{v+n_2} \text{etr}
\left[-W[\mu I + G_1^{-1}X_1X_1^H G_1^{-1}H_1^{-1}] \right]dW$$

$$= \pi^{-(n_1+n_2)}\frac{\mu^{|p|}}{\Gamma_p(v)} |R_1|^{-n_1-n_2} \times \text{etr}
\left[-X_1^H R_1^{-1} X_1 \right] |\mu I + G_1^{-1}X_1X_1^H G_1^{-1}H_1^{-1}|^{-(n_1+n_2)}$$

$$= \pi^{-(n_1+n_2)}\frac{\mu^{|p|}}{\Gamma_p(v)} |R_1|^{-n_1-n_2} \times \text{etr}
\left[-X_1^H R_1^{-1} X_1 \right] |\mu I + G_1^{-1}X_1X_1^H G_1^{-1}H_1^{-1} + \mu R_1^{-1} X_1|^{-(n_1+n_2)}$$ (A.2)

and we recover the fact that $X_1|R_1$ is Gaussian distributed and that $X_2|R_2$ is Student distributed. From (A.2), the log-likelihood function is, up to an additive and constant term

$$f(R_1) = -(n_1+n_2) \log |R_1| - (\nu + n_2) \log |\mu I + R_1^{-1}S_2| - \text{Tr}[R_1^{-1}S_1]$$

$$= (\nu - n_1) \log |R_1| - (\nu + n_2) \log |R_1 + \mu^{-1}S_2| - \text{Tr}[R_1^{-1}S_1]$$ (A.3)
where $S_1 = X_1X_1^H$ and $S_2 = X_2X_2^H$. Differentiating the previous equation, it follows that the maximum likelihood estimator of $R_1$ should satisfy

$$(v - n_1)R_1^{-1} - (v + n_2)(R_1 + \mu^{-1}S_2)^{-1} + R_1^{-1}S_1R_1^{-1} = 0$$

(A.4)

which is exactly (5), the equation in the real case. From there, all previous derivations follow simply by replacing the transpose by the Hermitian transpose.

References