# Random Matrix-Improved Estimation of the Wasserstein Distance between two Centered Gaussian Distributions 

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#### Abstract

This article proposes a method to consistently estimate functionals $\frac{1}{p} \sum_{i=1}^{p} f\left(\lambda_{i}\left(C_{1} C_{2}\right)\right)$ of the eigenvalues of the product of two covariance matrices $C_{1}, C_{2} \in \mathbb{R}^{p \times p}$ based on the empirical estimates $\lambda_{i}\left(\hat{C}_{1} \hat{C}_{2}\right)\left(\hat{C}_{a}=\frac{1}{n_{a}} \sum_{i=1}^{n_{a}} x_{i}^{(a)} x_{i}^{(a) \mathrm{T}}\right)$, when the size $p$ and number $n_{a}$ of the (zero mean) samples $x_{i}^{(a)}$ are similar. As a corollary, a consistent estimate of the Wasserstein distance (related to the case $f(t)=\sqrt{t}$ ) between centered Gaussian distributions is derived.

The new estimate is shown to largely outperform the classical sample covariance-based "plug-in" estimator. Based on this finding, a practical application to covariance estimation is then devised which demonstrates potentially significant performance gains with respect to state-of-the-art alternatives.


## I. Introduction

Many machine learning and signal processing applications require an adequate framework to compare statistical objects, starting with probability distributions. The Wasserstein distance, initially inspired by Monge [1] and later by Kantorovich [2] in a transport theory analogy, provides a natural notion of dissimilarity for probability measures and finds a wide spectrum of applications in image analysis [3], shape matching [4], computer vision [5], etc.

However, computing the Wasserstein distance is expensive as it requires to minimize a cost function taking the form of an integral over the space of probability measures. Despite recent advances [6], where regularized approximations that reduce this numerical cost are proposed, the latter is still involved in general. Special cases exist for which the Wasserstein distance assumes a closed form, particularly when the underlying distributions are zero-mean Gaussian with covariance matrices $C_{1}$ and $C_{2}$. The closed-form formula however involves the eigenvalues of $C_{1} C_{2}$ and thus depends on the unknown population covariance matrices $C_{1}$ and $C_{2}$. Assuming the observation of $n_{1}, n_{2} \gg p$ samples with covariances $C_{1}, C_{2}$, respectively, $C_{1} C_{2}$ is conventionally approximated by its empirical version $\hat{C}_{1} \hat{C}_{2}$. As we will show, this induces a dramatic estimation bias in practical applications where $p$ is rather large or, equivalently, $n_{1}, n_{2}$ rather small, a standard assumption in big data applications.

Based on recent advances in random matrix theory, this article proposes a new consistent estimate for the Wasserstein distance between two centered Gaussian distributions when the dimension $p$ of the samples is of the same order of magnitude as their numbers $n_{1}, n_{2}$. This work enters the scope of Mestre's seminal ideas [7] on the estimation of
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functionals $\frac{1}{p} \sum_{i=1}^{p} f\left(\lambda_{i}(C)\right)$ of the eigenvalue distribution of population covariance matrices $C$, which can be related to the (limiting) eigenvalue distribution of the sample estimates $\hat{C}$ via a complex integration trick. We recently extended this work to the estimation of functionals of the eigenvalue distribution of F -matrices in [8], i.e., matrices of the form $C_{1}^{-1} C_{2}$, and applied to the estimation of the natural geodesic Fisher distance, Battacharrya distance, and Rényi/KullbachLeibler divergences between Gaussian distributions.

Our main contribution is the extension of [7], [8] to functionals $f$ of the eigenvalues of products $C_{1} C_{2}$ of population covariance matrices. The Wasserstein distance falls within this scope for $f(t)=\sqrt{t}$. Unlike [8], where the functionals of interest $\left(f(t)=t, \log (t), \log ^{2}(t)\right)$ are amenable to explicit evaluations of the complex integrals, the present $f(t)=\sqrt{t}$ scenario is more technically involved and gives rise to real non-explicit, yet numerically computable, integrals.

In the remainder of the article, Section $\Pi$ introduces the main model and assumptions, Section III provides our key technical result and its corollary to the Wasserstein distance estimation, and a practical application to covariance matrix estimation is finally proposed in Section IV.
Reproducibility. Matlab codes for the various estimators introduced and studied in this article are available at https://github.com/maliktiomoko/RMTWasserstein

## II. Model and Main Objective

For $a \in\{1,2\}$, let $X_{a}=\left[x_{1}^{(a)}, \ldots, x_{n_{a}}^{(a)}\right]$ be $n_{a}$ independent and identically distributed random vectors with $x_{i}^{(a)}=C_{a}^{\frac{1}{2}} \tilde{x}_{i}^{(a)}$, where $\tilde{x}_{i}^{(a)} \in \mathbb{R}^{p}$ has zero mean, unit variance and finite fourth order moment entries. This holds in particular for $x_{i}^{(a)} \sim \mathcal{N}\left(0, C_{a}\right)$. In order to control the growth rates of $n_{1}, n_{2}, p$, we make the following assumption:

Assumption 1 (Growth Rates). As $n_{a} \rightarrow \infty, p / n_{a} \rightarrow c_{a} \in$ $(0,1)$ and $\lim \sup _{p} \max \left\{\left\|C_{a}^{-1}\right\|,\left\|C_{a}\right\|\right\}<\infty$ for $\|\cdot\|$ the operator norm.

We define the sample covariance estimate $\hat{C}_{a}$ of $C_{a}$ as

$$
\hat{C}_{a} \equiv \frac{1}{n_{a}} X_{a} X_{a}^{\top}=\frac{1}{n_{a}} \sum_{i=1}^{n_{a}} x_{i}^{(a)} x_{i}^{(a) \top}
$$

The Wasserstein distance $D_{W}\left(C_{1}, C_{2}\right)$ between two zeromean Gaussian distributions with covariances $C_{1}$ and $C_{2}$, respectively, assumes the form [9, Remark 2.31]:

$$
\begin{equation*}
D_{W}\left(C_{1}, C_{2}\right)=\operatorname{tr}\left(C_{1}\right)+\operatorname{tr}\left(C_{2}\right)-2 \operatorname{tr}\left[\left(C_{1}^{\frac{1}{2}} C_{2} C_{1}^{\frac{1}{2}}\right)^{\frac{1}{2}}\right] \tag{1}
\end{equation*}
$$

It is easily shown that, under Assumption 1 ,

$$
\frac{1}{p} \operatorname{tr} \hat{C}_{a}-\frac{1}{p} \operatorname{tr} C_{a} \rightarrow 0
$$

almost surely. But estimating $\operatorname{tr}\left(C_{1}^{\frac{1}{2}} C_{2} C_{1}^{\frac{1}{2}}\right)^{\frac{1}{2}}$ is more involved: this is the focus of the article. Up to a normalization by $p$, this term can be written under the functional form:

$$
\begin{equation*}
\frac{1}{p} \operatorname{tr}\left(C_{1}^{\frac{1}{2}} C_{2} C_{1}^{\frac{1}{2}}\right)^{\frac{1}{2}}=\frac{1}{p} \sum_{i=1}^{n} \sqrt{\lambda_{i}\left(C_{1} C_{2}\right)} \equiv D\left(C_{1}, C_{2} ; \sqrt{\cdot}\right) \tag{2}
\end{equation*}
$$

with $\lambda_{i}(X)$ the $i$-th smallest eigenvalue of $X$.
Our objective is to estimate the more generic form

$$
\begin{equation*}
D\left(C_{1}, C_{2} ; f\right) \equiv \frac{1}{p} \sum_{i=1}^{n} f\left(\lambda_{i}\left(C_{1} C_{2}\right)\right) \tag{3}
\end{equation*}
$$

for $f: \mathbb{R} \rightarrow \mathbb{R}$ a real function admitting a complexanalytic extension. To this end, we shall relate the eigenvalues $\lambda_{i}\left(C_{1} C_{2}\right)$ to $\lambda_{i}\left(\hat{C}_{1} \hat{C}_{2}\right)$ through the Stieltjes transform $\left(m_{\theta}(z) \equiv \int \frac{d \theta(\lambda)}{\lambda-z}\right.$ for measure $\theta$ and $z \in \mathbb{C}$ ) of their associated normalized counting measures

$$
\mu_{p}=\frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_{i}\left(\hat{C}_{1} \hat{C}_{2}\right)}, \quad \nu_{p}=\frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_{i}\left(C_{1} C_{2}\right)}
$$

In particular, $m_{\mu_{p}}(z)=\frac{1}{p} \sum_{i=1}^{p} \frac{1}{\lambda_{i}-z}$ for $\lambda_{i}=\lambda_{i}\left(\hat{C}_{1} \hat{C}_{2}\right)$.
With these notations, we are in position to introduce our main results.

## III. Main Results

The following theorem provides a consistent estimate for the metric $D\left(C_{1}, C_{2} ; f\right)$ defined in (3).
Theorem 1. Let $\Gamma \subset\{z \in \mathbb{C}$, $\operatorname{real}[z]>0\}$ be a contour surrounding $\cup_{p=1}^{\infty} \operatorname{supp}\left(\mu_{p}\right)$. Then, under Assumption 1

$$
D\left(C_{1}, C_{2} ; f\right)-\hat{D}\left(X_{1}, X_{2} ; f\right) \xrightarrow{\text { a.s. }} 0
$$

where
$\hat{D}\left(X_{1}, X_{2} ; f\right)=\frac{n_{2}}{2 \pi i p} \oint_{\Gamma} f\left(\frac{\varphi_{p}(z)}{\psi_{p}(z)}\right)\left[\frac{\varphi_{p}^{\prime}(z)}{\varphi_{p}(z)}-\frac{\psi_{p}^{\prime}(z)}{\psi_{p}(z)}\right] \psi_{p}(z) d z$ and, recalling $m_{\mu_{p}}(z)=\frac{1}{p} \sum_{i=1}^{p} \frac{1}{\lambda_{i}-z}$ for $\lambda_{i}=\lambda_{i}\left(\hat{C}_{1} \hat{C}_{2}\right)$, $\varphi_{p}(z)=\frac{z}{1-\frac{p}{n_{1}}-\frac{p}{n_{1}} z m_{\mu_{p}}(z)}, \psi_{p}(z) \stackrel{1}{=}-\frac{p}{n_{2}}-\frac{p}{n_{2}} z m_{\mu_{p}}(z)$.

The result of Theorem 1 is very similar to [8, Theorem 1] established for functionals of the eigenvalues of $C_{1}^{-1} C_{2}$. The main difference lies in the expression of the function $\varphi_{p}(z)$.

Proof. The proof of Theorem 1 is based on the same approach as for [10, Theorem 1]. One first creates a link between the Stieltjes transform $m_{\nu_{p}}$ and $D\left(C_{1}, C_{2} ; f\right)$ using Cauchy's integral formula:

$$
\begin{align*}
\frac{1}{p} \sum_{i=1}^{p} f\left(\lambda_{i}\left(C_{1} C_{2}\right)\right) & =\int f(t) d \nu_{p}(t) \\
& =\frac{1}{2 \pi i} \int\left[\oint_{\Gamma_{\nu}} \frac{f(z)}{z-t} d z\right] d \nu_{p}(t) \\
& =\frac{-1}{2 \pi i} \oint_{\Gamma_{\nu}} f(z) m_{\nu_{p}}(z) d z \tag{4}
\end{align*}
$$

with $\Gamma_{\nu}$ a contour surrounding the support $\operatorname{supp}\left(\nu_{p}\right)$ of $\nu_{p}$. To relate the unknown $m_{\nu_{p}}$ to the observable $m_{\mu_{p}}$, we proceed as follows. By first conditioning on $\hat{C}_{1}, \hat{C}_{1}^{\frac{1}{2}} \hat{C}_{2} \hat{C}_{1}^{\frac{1}{2}}$ is seen as a sample covariance matrix for the samples $\hat{C}_{1}^{\frac{1}{2}} C_{2}^{\frac{1}{2}} \tilde{x}_{i}^{(2)}$, for which [11] allows one to relate $m_{\mu_{p}}$ to the Stieltjes transform of the eigenvalue distribution $\zeta_{p}$ of $C_{2}^{\frac{1}{2}} \hat{C}_{1} C_{2}^{\frac{1}{2}}$. The latter is yet another sample covariance matrix for the samples $C_{2}^{\frac{1}{2}} C_{1}^{\frac{1}{2}} \tilde{x}_{i}^{(1)}$; exploiting [11] again creates the connection from $m_{\zeta_{p}}$ to $m_{\nu_{p}}$. This entails the two equations:

$$
\begin{align*}
m_{\mu_{p}}(z) & =\varphi_{p}(z) m_{\zeta_{p}}\left(\varphi_{p}(z)\right)+o_{p}(1)  \tag{5}\\
m_{\nu_{p}}\left(\frac{z}{\Psi_{p}(z)}\right) & =m_{\zeta_{p}}(z) \Psi_{p}(z)+o_{p}(1) \tag{6}
\end{align*}
$$

where $\Psi_{p}(z) \equiv 1-\frac{p}{n_{2}}-\frac{p}{n_{2}} z m_{\zeta_{p}}(z)$. Successively plugging (5)-(6) into (4) by means of two successive appropriate changes of variables, we obtain Theorem 1 .

Theorem 1 takes the form of a complex integral which, for generic choices of $f$, needs be numerically evaluated. In the specific case of present interest where $f(z)=\sqrt{z}$, this complex integral can be evaluated as follows.
Theorem 2. Let $\lambda_{1} \leq \ldots \leq \lambda_{p}$, with $\lambda_{i} \equiv \lambda_{i}\left(\hat{C}_{1} \hat{C}_{2}\right)$, and define $\left\{\xi_{i}\right\}_{i=1}^{p}$ and $\left\{\eta_{i}\right\}_{i=1}^{p}$ the (increasing) eigenvalues of $\Lambda-\frac{1}{n_{1}} \sqrt{\lambda} \sqrt{\lambda}^{\top}$ and $\Lambda-\frac{1}{n_{2}} \sqrt{\lambda} \sqrt{\lambda}^{\top}$, respectively, where $\lambda=\left(\lambda_{1}, \ldots, \lambda_{p}\right)^{\top}, \Lambda=\operatorname{diag}(\lambda)$ and $\sqrt{ }$. is understood entry wise. Then, under Assumption 1,

$$
D\left(C_{1}, C_{2} ; \sqrt{\cdot}\right)-\hat{D}\left(X_{1}, X_{2} ; \sqrt{\cdot}\right) \xrightarrow{\text { a.s. }} 0
$$

where, if $n_{1} \neq n_{2}$,

$$
\begin{aligned}
\hat{D}\left(X_{1}, X_{2} ; \sqrt{\cdot}\right) & =2 \sqrt{n_{1} n_{2}} \frac{1}{p} \sum_{j=1}^{p} \sqrt{\lambda_{j}} \\
& +\frac{2 n_{2}}{\pi p} \sum_{j=1}^{p} \int_{\xi_{j}}^{\eta_{j}} \sqrt{-\frac{\varphi_{p}(x)}{\psi_{p}(x)}} \psi_{p}^{\prime}(x) d x
\end{aligned}
$$

with $\varphi_{p}, \psi_{p}$ defined in Theorem 11 and, if $n_{1}=n_{2}$,

$$
\hat{D}\left(X_{1}, X_{2} ; \sqrt{\cdot}\right)=\frac{2 n_{1}}{p} \sum_{j=1}^{p}\left(\sqrt{\lambda_{j}}-\sqrt{\xi_{j}}\right)
$$

While still assuming an integral form (when $n_{1} \neq n_{2}$ ), this formulation no longer requires the arbitrary choice of a contour $\Gamma$ and significantly reduces the computational time to estimate $D\left(C_{1}, C_{2}, \sqrt{ } \cdot\right)$. For $n_{1}=n_{2}$, a case of utmost practical interest, the expression is completely explicit and computationally only requires to evaluate the eigenvalues $\xi_{j}$ of $\Lambda-\frac{1}{n_{1}} \sqrt{\lambda} \sqrt{\lambda}^{\top}$. The latter being a (negative definite) rank1 perturbation of $\Lambda$, by Weyl's interlacing lemma [12], the $\xi_{j}$ 's are interlaced with the $\lambda_{j}$ 's as

$$
\xi_{1} \leq \lambda_{1} \leq \xi_{2} \leq \ldots \leq \xi_{p} \leq \lambda_{p}
$$

As the $\lambda_{j}$ 's are of order $O(1)$ with respect to $p, \mid \lambda_{j}-$ $\xi_{j}\left|\leq\left|\lambda_{j}-\lambda_{j-1}\right|=O\left(p^{-1}\right)\right.$, therefore explaining why the expression of $\hat{D}\left(X_{1}, X_{2} ; \sqrt{ }\right)$ is of order $O(1)$.


Fig. 1. Deformation of the initial contour $\Gamma$ (in black) into the new contour $\tilde{\Gamma}$ (in blue). The branch cuts are represented in green (i.e., real $z$ 's for which the argument of $\varphi(z) \psi(z)$ is negative).

Proof. The $\xi_{i}$ and $\eta_{i}$, as defined in the theorem statement, are the respective zeros of the rational functions $1-\frac{p}{n_{1}}-$ $\frac{p}{n_{1}} z m_{\tilde{\mu}_{p}}(z)$ and $1-\frac{p}{n_{2}}-\frac{p}{n_{2}} z m_{\tilde{\mu}_{p}}(z)$ (see [10, Appendix B]). Thus, $\varphi_{p}$ and $\psi_{p}$ can be expressed under the rational form:

$$
\varphi_{p}(z)=z \frac{\prod_{i=1}^{p} z-\lambda_{i}}{\prod_{i=1}^{p} z-\eta_{i}}, \quad \psi_{p}(z)=\frac{\prod_{i=1}^{p} z-\xi_{i}}{\prod_{i=1}^{p} z-\lambda_{i}}
$$

Evaluating the estimate from Theorem 1 for $f(z)=\sqrt{z}$ then requires to evaluate a complex integral involving rational functions and square roots of rational functions. Since the complex square root is multivalued, a careful control of "branch-cuts" is required. To perform this calculus, we deform the integration contour $\Gamma$ of Theorem 1 into $\tilde{\Gamma}$ as per Figure 1. In the case $n_{1} \neq n_{2}$, the closed null-integral contour $\tilde{\Gamma}$ (blue in Figure 1) is the sum of the sought-for integral over $\Gamma$ and of four extra components:

1) Integrals over $\epsilon$-radius circles around $\xi_{i}$ : those are null in the limit $\epsilon \rightarrow 0$, as confirmed by a change of variable $z=\xi_{i}+\epsilon e^{\imath \theta}$ which allows one to bound the integrand;
2) Integrals over the real axis (in the $\epsilon \rightarrow 0$ limit):

$$
\begin{aligned}
& A_{2}=\frac{n_{2}}{\pi p} \sum_{j=1}^{p} \int_{\xi_{j}+\epsilon}^{\eta_{j}-\epsilon} \sqrt{-\left(\varphi_{p} \psi_{p}\right)(x)}\left[2 \frac{\psi_{p}^{\prime}(z)}{\psi_{p}(z)}\right. \\
& \left.-\left(\frac{\varphi_{p}^{\prime}(z)}{\varphi_{p}(z)}+\frac{\psi_{p}^{\prime}(z)}{\psi_{p}(z)}\right)\right] d x \\
& =\frac{2 n_{2}}{\pi p} \sum_{j=1}^{p} \int_{\xi_{j}}^{\eta_{j}} \sqrt{-\varphi_{p} \psi_{p}(x)}\left[\frac{\psi_{p}^{\prime}(z)}{\psi_{p}(z)}\right] d x \\
& -\frac{n_{2}}{\pi p} \sum_{j=1}^{p} \int_{\xi_{j}+\epsilon}^{\eta_{j}-\epsilon} \frac{\sqrt{-\varphi_{p} \psi_{p}(x)}}{\varphi_{p} \psi_{p}(x)}\left[\frac{d}{d x}\left(\varphi_{p}(x) \psi_{p}(x)\right)\right] d x \\
& =\frac{2 n_{2}}{\pi p} \sum_{j=1}^{p} \int_{\xi_{j}}^{\eta_{j}} \sqrt{-\frac{\varphi_{p}(x)}{\psi_{p}(x)} \psi_{p}^{\prime}(x) d x} \\
& -2 \frac{n_{2}}{\pi p} \sum_{j=1}^{p} \frac{1}{\sqrt{\epsilon \frac{d}{d x}\left(\frac{1}{\left(\varphi_{p} \psi_{p}(x)\right)}\right)\left(\eta_{j}\right)}}+o(\epsilon)
\end{aligned}
$$

3) Integrals over the $\epsilon$-radius circles around $\eta_{j}$, with $\epsilon \rightarrow 0$

$$
A_{3}=2 \frac{n_{2}}{\pi p} \sum_{j=1}^{p} \frac{1}{\sqrt{\epsilon \frac{d}{d x}\left(\frac{1}{\left(\varphi_{p} \psi_{p}(x)\right)}\right)\left(\eta_{j}\right)}}+o(\epsilon)
$$

which thus compensates the last ( $\epsilon$-diverging) term in $A_{2}$. 4) Residues in the $\lambda_{j}$ poles

$$
A_{4}=2 \frac{n_{2}}{p} \lim _{z \rightarrow \lambda_{j}} \sum_{j=1}^{p} \sqrt{\left(\varphi_{p} \psi_{p}\right)(z)}=2 \frac{n_{2}}{p} \sqrt{\frac{n_{1}}{n_{2}}} \sum_{j=1}^{p} \sqrt{\lambda_{j}}
$$

Putting these terms together entails the result of the theorem for the case where $n_{1} \neq n_{2}$. For $n_{1}=n_{2}$, it suffices to take the limit of the expression as $\xi_{j} \rightarrow \eta_{j}$. This yields:

$$
\begin{aligned}
\hat{D}\left(X_{1}, X_{2} ; \sqrt{\cdot}\right) & =\frac{2 n_{1}}{p} \sum_{j=1}^{p} \sqrt{\lambda_{j}} \\
& +\frac{2 n_{1}}{p} \sum_{j=1}^{p} \frac{1}{\pi} \lim _{t \rightarrow \xi_{j}} \int_{\xi_{j}}^{t} \sqrt{-\frac{\varphi_{p}(x)}{\psi_{p}(x)}} \psi_{p}^{\prime}(x) d x \\
& =\frac{2 n_{1}}{p} \sum_{j=1}^{p} \sqrt{\lambda_{j}} \\
& -\frac{2 n_{1}}{p} \sum_{j=1}^{p} \frac{1}{2 \pi \imath} \lim _{\epsilon \rightarrow 0} \oint_{\Gamma_{\xi_{j}}^{\epsilon}} \sqrt{-\varphi_{p} \psi_{p}(x)} \frac{\psi_{p}^{\prime}(x)}{\psi_{p}(x)} d x
\end{aligned}
$$

where $\Gamma_{\xi_{j}}^{\epsilon}$ is an $\epsilon$-radius circular contour around $\xi_{j}$. The second equality is obtained by deforming the real integral in the complex plane (see [13] for complex analysis details). The result unfolds by letting $z=\xi_{i}+\epsilon e^{2 \theta}$.

Consequently, we obtain the following $n, p$-consistent estimate for the Wasserstein distance $D_{W}\left(C_{1}, C_{2}\right)$ of (1).
Corollary 1 (Consistent Estimate of $D_{W}\left(C_{1}, C_{2}\right)$ ). Under Assumption 1 ,
$\frac{1}{p} D_{W}\left(C_{1}, C_{2}\right)-\left[\frac{1}{p} \operatorname{tr}\left(\hat{C}_{1}+\hat{C}_{2}\right)-2 \hat{D}\left(X_{1}, X_{2} ; \sqrt{ } \cdot\right)\right] \xrightarrow{\text { a.s. }} 0$
for $\hat{D}\left(X_{1}, X_{2} ; \sqrt{\cdot}\right)$ given by Theorem 2 .
Remark 1 (Estimation of $\left\|C_{1}-C_{2}\right\|_{F}^{2}$ ). The Frobenius distance between two covariance matrices also falls under the scope of the present article for the function $f(z)=z$. Indeed,
$D_{F}\left(C_{1}, C_{2}\right)=\left\|C_{1}-C_{2}\right\|_{F}^{2}=\operatorname{tr}\left(C_{1}^{2}+C_{2}^{2}\right)-2 \operatorname{tr}\left(C_{1} C_{2}\right)$.
Then under Assumption 1 and along with the fact that $\frac{1}{p} \operatorname{tr} C_{1}^{2}$ can be estimated consistently from $\frac{1}{p} \operatorname{tr} \hat{C}_{1}^{2}-\frac{1}{n_{1} p}\left(\operatorname{tr} \hat{C}_{1}\right)^{2}$,

$$
\begin{aligned}
\frac{1}{p} D_{F}\left(C_{1}, C_{2}\right)- & {\left[\frac{1}{p} \operatorname{tr}\left(\hat{C}_{1}^{2}+\hat{C}_{2}^{2}\right)-\frac{p}{n_{1}}\left(\frac{1}{p} \operatorname{tr} \hat{C}_{1}\right)^{2}\right.} \\
& \left.-\frac{p}{n_{2}}\left(\frac{1}{p} \operatorname{tr} \hat{C}_{2}\right)^{2}-2 \hat{D}\left(X_{1}, X_{2} ; \cdot\right)\right] \xrightarrow{\text { a.s. }} 0 .
\end{aligned}
$$

In this case, $\hat{D}\left(X_{1}, X_{2} ; \cdot\right)$ assumes the simple expression

$$
\hat{D}\left(X_{1}, X_{2} ; \cdot\right)=\frac{1}{p} \sum_{j=1}^{p} \lambda_{j}=\frac{1}{p} \operatorname{tr} \hat{C}_{1} \hat{C}_{2}
$$

which follows from $\frac{1}{p} \operatorname{tr} \hat{C}_{1} \hat{C}_{2}-\frac{1}{p} \operatorname{tr} C_{1} C_{2} \xrightarrow{\text { a.s. }} 0$ (by elementary probability arguments) or equivalently from a residue calculus based on Theorem 1 for $f(z)=z$.

## IV. Simulations and Applications

In this section, we first corroborate our theoretical findings by comparing the classical plug-in estimator to our proposed estimator on synthetic Gaussian data. We then provide an application of our results to improved covariance matrix estimation based on few samples.

## A. Confirmation of our results on synthetic data

We here compare the classical plug-in estimate of the Wasserstein distance (that is (1) with $C_{a}$ replaced by $\hat{C}_{a}, a=$ 1,2 ) with our proposed estimate in Corollary 1 Table $\square$ lists the results obtained for Toeplitz matrices $C_{1}, C_{2}$ estimated based on various values of $p, n_{1}, n_{2}$. While our proposed estimator is designed under a large $p, n_{1}, n_{2}$ assumption (as per Assumption 11), it achieves competitive performances even for small values of $p$, corroborating here our findings in [8] for other classes of covariance matrix distances.

| $p$ | $D_{\mathrm{W}}\left(C_{1}, C_{2}\right)$ | Classical | Proposed |
| ---: | ---: | ---: | ---: |
| 2 | 0.0110 | 0.0127 | 0.0120 |
| 4 | 0.0175 | 0.0198 | 0.0183 |
| 8 | 0.0208 | 0.0232 | 0.0206 |
| 16 | 0.0225 | 0.0280 | 0.0227 |
| 32 | 0.0233 | 0.0339 | 0.0234 |
| 64 | 0.0237 | $\mathbf{0 . 0 4 5 1}$ | 0.0240 |
| 128 | 0.0239 | $\underline{\underline{\mathbf{0 . 0 6 6 7}}}$ | 0.0244 |
| 256 | 0.0240 | $\underline{\underline{\mathbf{0 . 1 0 9 2}}}$ | 0.0244 |
| 512 | 0.0241 | $\underline{\underline{\mathbf{0 . 1 9 5 3}}}$ | 0.0245 |

$($ error $<5 \%)($ error $>\mathbf{5 0 \%}) \underline{(\text { error }>\mathbf{1 0 0 \%})} \underline{\underline{(\text { error }>\mathbf{3 0 0 \%})}}$
TABLE I
Estimators of the Wasserstein distance between $C_{1}$ and $C_{2}$ WITH $\left[C_{1}\right]_{i j}=.2^{|i-j|},\left[C_{2}\right]_{i j}=.4^{|i-j|}, x_{i}^{(a)} \sim \mathcal{N}\left(0, C_{a}\right) ; n_{1}=1024$ AND $n_{2}=2048$ FOR DIFFERENT $p$. AVERAGED OVER 100 TRIALS.

## B. Application to covariance matrix estimation

As a concrete application, Theorem 1 may be used to improve the actual estimation of covariance matrices under a small number $n \sim p$ of sample data, as similarly performed in [14] for other covariance matrix distances.

The idea is as follows: we first particularize Theorem 1 and Theorem 2 to the case where one of the covariance matrices, say $C_{1}$, is known by taking $c_{1}=0$ (i.e., $n_{1} \rightarrow \infty$ for all fixed $p)$. This gives access to estimates for $D_{W}\left(M, C_{2} ; \sqrt{ } \cdot\right)$ for all deterministic positive definite matrix $M$. We then minimize this estimated distance over $M$ in order to estimate $C_{2}$ by means of a gradient descent approach.

For $C_{1}$ known, we redefine $\mu_{p}=\frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_{i}\left(C_{1} \hat{C}_{2}\right)}$ and obtain, as a corollary of Theorem 1 .
Theorem 3. Let $\Gamma \subset\{z \in \mathbb{C}, \operatorname{real}[z]>0\}$ a contour surrounding $\cup_{p=1}^{\infty} \operatorname{supp}\left(\mu_{p}\right)$. Then,

$$
D\left(C_{1}, C_{2} ; f\right)-\frac{1}{2 \pi i c_{2}} \oint_{\Gamma} F\left(-m_{\tilde{\mu}_{p}}(z)\right) d z \xrightarrow{\text { a.s. }} 0
$$

with $m_{\tilde{\mu}_{p}}(z)=\frac{p}{n_{2}} m_{\mu_{p}}(z)+\frac{p-n_{2}}{n_{2} z}$ and $F^{\prime}(z)=f\left(\frac{1}{z}\right)$.

Proof. For $C_{1}$ known $\left(c_{1} \rightarrow 0\right), \varphi_{p}(z)=z$, and the estimator of Theorem 1 yields:
$\hat{D}\left(X_{1}, X_{2} ; f\right)=\frac{1}{2 \pi i} \oint_{\Gamma} f\left(\frac{z}{\psi_{p}(z)}\right)\left[\frac{\psi_{p}^{\prime}(z)}{\psi_{p}(z)}-\frac{1}{z}\right] \frac{\psi_{p}(z) d z}{c_{2}}$.
Using the relation $m_{\tilde{\mu}_{p}}(z)=-\frac{\psi_{p}(z)}{z}$, we then get

$$
\hat{D}\left(X_{1}, X_{2} ; f\right)=-\frac{1}{2 \pi i c_{2}} \oint_{\Gamma} f\left(-\frac{1}{m_{\tilde{\mu}_{p}}(z)}\right) m_{\tilde{\mu}_{p}}^{\prime}(z) z d z
$$

and the result is immediate after an integration by parts.

For $f(z)=\sqrt{z}$, one has $F(z)=2 \sqrt{z}$ and we obtain, with a similar proof as for Theorem 2,

$$
\begin{aligned}
& D\left(C_{1}, C_{2} ; \sqrt{\cdot}\right)-\hat{D}\left(C_{1}, X_{2} ; \sqrt{\cdot}\right) \xrightarrow{\text { a.s. }} 0 \\
& \hat{D}\left(C_{1}, X_{2} ; \sqrt{\cdot}\right)=\frac{2}{\pi c_{2}} \sum_{j=1}^{p} \int_{\xi_{j}}^{\lambda_{j}} \sqrt{m_{\tilde{\mu}_{p}(x)}} d x .
\end{aligned}
$$

Our objective is now to exploit the fact that

$$
\begin{equation*}
C_{2}=\operatorname{argmin}_{M \succ 0} D_{W}\left(M, C_{2}\right) \tag{8}
\end{equation*}
$$

where the minimization is over the open cone of positive definite matrices. Using the approximation $D\left(M, C_{2} ; \sqrt{\cdot}\right) \simeq$ $\hat{D}\left(M, X_{2} ; \sqrt{ } \cdot\right)$, we are then tempted to minimize $\frac{1}{p} \operatorname{tr}(M+$ $\left.\hat{C}_{2}\right)-2 \hat{D}\left(M, X_{2} ; \sqrt{\cdot}\right)$ in place of $D_{W}\left(M, C_{2}\right)$. The former quantity however has a non zero probability to be negative, and we thus instead propose to estimate $C_{2}$ as:

$$
\begin{aligned}
\check{C}_{2} & =\operatorname{argmin}_{M} h(M) \\
h(M) & =\left[\frac{1}{p} \operatorname{tr}\left(M+\hat{C}_{2}\right)-2 \hat{D}\left(M, X_{2} ; \sqrt{\cdot}\right)\right]^{2} .
\end{aligned}
$$

To compute the gradient $\nabla h(M)$ of $h$ at position $M$, one needs to evaluate the differential $\mathrm{D} h(M)[\xi]$, at $M$ and in the direction $\xi$, in the Riemmanian manifold of $p \times p$ symmetric positive definite matrices (see [15], [14] to further technical details). We then use the relation $\mathrm{D} h(M)[\xi]=$ $\langle\nabla h(M), \xi\rangle_{M}$ where $\langle\cdot, \cdot\rangle$. is the Riemmanian metric defined as $\langle\eta, \xi\rangle_{M}=\operatorname{tr}\left(M^{-1} \eta M^{-1} \xi\right)$. We obtain the relation

$$
\begin{aligned}
& \pi \imath p \frac{\nabla h(M)}{2 \sqrt{h(M)}}=\frac{1}{p} M^{2} \\
& +\sum_{j=1}^{p} \int_{\xi_{j}}^{\lambda_{j}} \sqrt{\frac{1}{m_{\tilde{\mu}_{p}}(x)}} \operatorname{sym}\left(M \hat{C}_{2}\left(M \hat{C}_{2}-x I_{p}\right)^{-2} M\right) d x
\end{aligned}
$$

where $\operatorname{sym}(A)=\frac{1}{2}\left(A+A^{\boldsymbol{\top}}\right)$ is the symmetric part of $A \in$ $\mathbb{R}^{p \times p}$. We can write the latter as:

$$
\nabla h(M)=2 \sqrt{h(M)}\left[\operatorname{sym}\left(V \Lambda_{\nabla} V^{-1}\right)+\frac{1}{p} M^{2}\right]
$$

where $V$ is the orthogonal matrix of the eigenvectors of $M \hat{C}_{2}$ and $\Lambda_{\nabla}$ is the diagonal matrix with

$$
\begin{aligned}
{\left[\Lambda_{\nabla}\right]_{k k} } & =\frac{1}{\pi p} \sum_{j \neq k} \int_{\xi_{j}}^{\lambda_{j}} \sqrt{\frac{1}{m_{\tilde{\mu}_{p}}(x)}} \frac{1}{\left(\lambda_{k}-x\right)^{2}} d x \\
& +\frac{1}{\pi p} \sum_{j \neq k} \int_{\xi_{k}}^{\lambda_{k}} \sqrt{\frac{1}{m_{\tilde{\mu}_{p}}(x)}} \frac{1}{\left(\lambda_{j}-x\right)^{2}} d x
\end{aligned}
$$

```
Algorithm 1 Proposed estimation algorithm.
Require Positive definite initialization \(M=M_{0}\).
```

Repeat $M \leftarrow M^{\frac{1}{2}} \exp \left(-t M^{-\frac{1}{2}} \nabla h(M) M^{-\frac{1}{2}}\right) M^{\frac{1}{2}}$ with $t$ either fixed or optimized by backtracking line search. Until Convergence.
Return $M$.

This finally entails the gradient descent Algorithm 1
Figure 2 depicts the results of the algorithm. There is displayed the Wasserstein distance $D_{W}(C, \cdot)$ between a matrix $C$ having four distinct eigenvalues of equal multiplicity (precisely, $\nu_{p}=\frac{1}{4}\left(\delta_{.1}+\delta_{3}+\delta_{4}+\delta_{5}\right)$ ) and various estimators of $C$ : the sample covariance matrix (SCM), the state-of-theart "non-linear shrinkage" estimators QuEST1 [16] (based on a Frobenius distance minimization) and QuEST2 [17] (based on a Stein loss minimization), and the result of the gradient descent approach proposed in this section. For fair comparison, the iterative QuEST1, QuEST2 and our proposed method are all initialized at $M_{0}$ the linear shrinkage estimator from [18]. Note that our proposed choice of $C$ is particularly suited to mimick an "optimal transport" problem of displacing the eigenvalues of $M_{0}$ to the discrete four positions of the eigenvalues of $C$.

In addition to the computational simplicity of our gradientdescent approach with respect to the QuEST estimators (see the numerical method details in [19]), the figure demonstrates significant gains brought by our proposed approach for large values of $p / n$, where the SCM particularly fails.

## V. Concluding Remarks

Interestingly, while the Fisher distance or Kullbach-Liebler divergence, which depend on logarithms of inverse of covariance matrices, are understandably difficult to estimate in the $n_{1}, n_{2}<p$ regime (see [10] for advanced discussions on this matter), the Wasserstein distance should not be confronted with this limitation. Yet, the invertibility of $C_{1}, C_{2}$ and the request for $c_{1}, c_{2} \in(0,1)$ (i.e., $\left.p<n_{1}, n_{2}\right)$ from Assumption 1 are fundamental to our proofs. Precisely, the variable changes exploited in the proof of Theorem 1 to reach a contour $\Gamma_{\nu}$ correctly surrounding $\operatorname{supp}\left(\nu_{p}\right)$ from a contour $\Gamma$ surrounding $\operatorname{supp}\left(\mu_{p}\right)$ are not satisfying if $c_{1}>1$ or $c_{2}>1$. These surprising difficulties need clarification.

Another point of interest lies in the comparative advantage of exploiting a particular covariance matrix distance in specific scenarios. For instance, it may seem that ill-conditioned matrices should be more tolerated by Wasserstein distance estimators than by Fisher distance estimators. Yet, this aspect is not obvious in our proofs and also deserves more insights.

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Fig. 2. Wasserstein distance $D_{W}(C, \cdot)$ between $C$ with $\nu_{p}=\frac{1}{4}\left(\delta_{.1}+\delta_{3}+\right.$ $\delta_{4}+\delta_{5}$ ) and (green) our proposed estimator, (blue) the sample covariance matrix, (red) and (light blue) the QuEST estimators proposed in [17], [16]; for $p=100$ and varying number of samples $n$ averaged over 10 realizations.
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