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Gromov-Wasserstein Distances between Gaussian Distributions

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Abstract

The Gromov-Wasserstein distances were proposed a few years ago to compare distributions which do not lie in the same space. In particular, they offer an interesting alternative to the Wasserstein distances for comparing probability measures living on Euclidean spaces of different dimensions. In this paper, we focus on the Gromov-Wasserstein distance with a ground cost defined as the squared Euclidean distance and we study the form of the optimal plan between Gaussian distributions. We show that when the optimal plan is restricted to Gaussian distributions, the problem has a very simple linear solution, which is also solution of the linear Gromov-Monge problem. We also study the problem without restriction on the optimal plan, and provide lower and upper bounds for the value of the Gromov-Wasserstein distance between Gaussian distributions.

Keywords — optimal transport, Wasserstein distance, Gromov-Wasserstein distance, Gaussian distributions


1 Introduction

Optimal transport (OT) theory has become nowadays a major tool to compare probability distributions. It has been increasingly used over the last past years in various applied fields such as economy [11], image processing [20, 21], machine learning [4, 5] or more generally data science [18], with applications to domain adaptation [9] or generative models [3, 12], to name just a few.

Given two probability distributions \(\mu\) and \(\nu\) on two Polish spaces \((\mathcal{X}, d_\mathcal{X})\) and \((\mathcal{Y}, d_\mathcal{Y})\) and a positive lower semi-continuous cost function \(c : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+\), optimal transport focuses on solving the following optimization problem

\[
\inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y), \tag{1.1}
\]

where \(\Pi(\mu, \nu)\) is the set of measures on \(\mathcal{X} \times \mathcal{Y}\) with marginals \(\mu\) and \(\nu\). When \(\mathcal{X}\) and \(\mathcal{Y}\) are equal and Euclidean, typically \(\mathbb{R}^d\), and \(c(x, y) = \|x - y\|^p\) with \(p \geq 1\), Equation \(1.1\) induces a distance over the set of measures with finite moment of order \(p\), known as the \(p\)-Wasserstein distance \(W_p\):

\[
W_p(\mu, \nu) = \left( \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^p d\pi(x, y) \right)^{1/p}, \tag{1.2}
\]

or equivalently

\[
W_p(\mu, \nu) = \inf_{X \sim \mu, Y \sim \nu} \mathbb{E}[\|X - Y\|^p], \tag{1.3}
\]

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where the notation $X \sim \mu$ means that $X$ is a random variable with probability distribution $\mu$. It is known that Equation (1.1) always admits a solution $\pi$ \footnote{We say that $(\mathcal{X}, d_X, \mu)$ is strongly isomorphic to $(\mathcal{Y}, d_Y, \nu)$ if it exists a bijection $\phi : \mathcal{X} \to \mathcal{Y}$ such that $\phi$ is an isometry $(\phi^{-1}(\phi(y)), \phi(y')) = d_X(x, x')$, and $\phi \# \mu = \nu$.}, i.e. the infimum is always reached. Moreover, in the case of $W_2$, it is known \footnote{2-Wasserstein distance $W_2$ admits a closed-form expression \cite{10, 12, 17} when $\mu = N(m_0, \Sigma_0)$ and $\nu = N(m_1, \Sigma_1)$ are two Gaussian measures with means $m_0 \in \mathbb{R}^d$, $m_1 \in \mathbb{R}^d$ and covariance matrices $\Sigma_0 \in \mathbb{R}^{d \times d}$ and $\Sigma_1 \in \mathbb{R}^{d \times d}$, that is given by $W_2^2(\mu, \nu) = ||m_1 - m_0||^2 + \text{tr} \left( \Sigma_0 + \Sigma_1 - 2 \left( \Sigma_0^{1/2} \Sigma_1^{1/2} \right)^2 \right),$ (1.4) for any symmetric semi-definite positive $M$, $M^{1/2}$ is the unique symmetric semi-definite positive squared root of $M$. Moreover, if $\Sigma$ is non-singular, then the optimal transport map $T$ is affine and is given by $\forall x \in \mathbb{R}^d, \ T(x) = m_1 + \Sigma_0^{-1/2} \left( \Sigma_0^{1/2} \Sigma_1^{1/2} \right)^{-1} \Sigma_0^{-1/2} (x - m_0), \quad (1.5)$ and the corresponding optimal transport plan $\pi^*$ is a degenerate Gaussian measure.}

the fundamental metric properties of $G$ is not invariant to rotations and translations and more generally to isometries. Thus, when for instance $\mu$ is a measure on $\mathbb{R}^2$ and $\nu$ a measure on $\mathbb{R}^3$, it is not straightforward to design a cost function $c : \mathbb{R}^2 \times \mathbb{R}^3 \to \mathbb{R}$ and so one cannot define easily an OT distance to compare $\mu$ with $\nu$. To overcome these limitations, several extensions of OT have been proposed \cite{1, 7, 17}. Among them, the most famous one is probably the Gromov-Wasserstein (GW) problem \cite{16}: given two Polish spaces $(\mathcal{X}, d_X)$ and $(\mathcal{Y}, d_Y)$, each endowed respectively with probability measures $\mu$ and $\nu$, and given two measurable functions $c_X : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and $c_Y : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$, it aims at finding $GW_p(c_X, c_Y, \mu, \nu) = \left( \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{Y}} |c_X(x, x') - c_Y(y, y')|^p d\pi(x, y)d\pi(x', y') \right)^{1/p}, \quad (1.6)$

with $p \geq 1$. As for classic OT, it can be shown that Equation (1.6) always admits a solution (see \cite{25}). The GW problem can be seen as a quadratic optimization problem in $\pi$, as opposed to OT, which is a linear optimization problem in $\pi$. When $c_X = d_X^p$ and $c_Y = d_Y^q$, with $q \geq 1$, then $GW_p$ induces a distance over the space of metric measure spaces (i.e. the triplets $(\mathcal{X}, d_X, \mu)$) quotiented by the strong isomorphisms \cite{13, 23, 24}. The fundamental metric properties of $GW_p$ have been studied in depth in \cite{24, 16, 8}. In the Euclidean setting, when $\mathcal{X} = \mathbb{R}^m$, $\mathcal{Y} = \mathbb{R}^n$, with $m$ not necessarily being equal to $n$, and for the natural choice of costs $c_X = ||x||_{\mathbb{R}^m}$ and $c_Y = ||y||_{\mathbb{R}^n}$, where $||.||_{\mathbb{R}^m}$ means the Euclidean norm on $\mathbb{R}^m$, it can be easily shown that $GW_2(c_X, c_Y, \mu, \nu)$ is invariant to isometries. With a slight abuse of notations, we will note in the following $GW_2(\mu, \nu)$ instead of $GW_2(||.||_{\mathbb{R}^m}, ||.||_{\mathbb{R}^n}, \mu, \nu)$.

In this work, we focus on the problem of Gromov-Wasserstein between Gaussian measures. Given $\mu = N(m_0, \Sigma_0)$, $m_0 \in \mathbb{R}^m$ and with covariance matrix $\Sigma_0 \in \mathbb{R}^{m \times m}$, and $\nu = N(m_1, \Sigma_1)$, with $m_1 \in \mathbb{R}^n$ and with covariance matrix $\Sigma_1 \in \mathbb{R}^{n \times n}$, we aim to solve $GW_2^2(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int \left( ||x - x'||_{\mathbb{R}^m}^2 - ||y - y'||_{\mathbb{R}^n}^2 \right)^2 d\pi(x, y)d\pi(x', y'), \quad (GW)$

or equivalently $GW_2^2(\mu, \nu) = \inf_{X, Y, X', Y' \sim \pi \otimes \pi} \mathbb{E} \left[ \left( ||X - X'||_{\mathbb{R}^m}^2 - ||Y - Y'||_{\mathbb{R}^n}^2 \right)^2 \right], \quad (1.7)$
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where for \( x, x' \in \mathbb{R}^m \) and \( y, y' \in \mathbb{R}^n \), \((\pi \otimes \pi)(x, y, x', y') = \pi(x, y)\pi(x', y')\). In particular, can we find equivalent formulas to (1.4) and (1.5) in the case of Gromov-Wasserstein? In Section 2, we derive an equivalent formulation of the Gromov-Wasserstein problem. This formulation is not specific to Gaussian measures but to all measures with finite order 4 moment. It takes the form of a sum of two terms depending respectively on co-moments of order 2 and 4 of \( \pi \). Then in Section 3, we derive a lower bound by simply optimizing both terms separately. In Section 4, we show that the problem restricted to Gaussian optimal plans admits an explicit solution and this solution is closely related to Principal Components Analysis. This yields an upper bound to the general problem. In Section 5, we study the tightness of the bounds found in the previous sections and we exhibit a particular case where these upper and lower bounds coincide, which provides an exact computation of \( GW^2_2(\mu, \nu) \) and the optimal plan \( \pi^* \) which achieves it. Finally, Section 6 discusses the form of the solution in the general case, and the possibility that the optimal plan between two Gaussian distributions is always Gaussian.

Notations

We define in the following some of the notations that will be used in the paper.

- The notation \( Y \sim \mu \) means that \( Y \) is a random variable with probability distribution \( \mu \).
- If \( \mu \) is a positive measure on \( \mathcal{X} \) and \( T : \mathcal{X} \to \mathcal{Y} \) is an application, \( T \# \mu \) stands for the push-forward measure of \( \mu \) by \( T \), i.e. the measure on \( \mathcal{Y} \) such that \( \forall A \in \mathcal{Y}, (T \# \mu)(A) = \mu(T^{-1}(A)) \).
- If \( X \) and \( Y \) are random vectors on \( \mathbb{R}^m \) and \( \mathbb{R}^n \), we denote \( \text{Cov}(X, Y) \) the matrix of size \( m \times n \) of the form \( E[(X - E[X])(Y - E[Y])^T] \).
- the notation \( \text{tr}(M) \) denotes the trace of a matrix \( M \).
- \( \|M\|_F \) stands for the Frobenius norm of a matrix \( M \), i.e. \( \|M\|_F = \sqrt{\text{tr}(M^T M)} \).
- \( \text{rk}(M) \) stands for the rank of a matrix \( M \).
- \( I_n \) is the identity matrix of size \( n \).
- \( \tilde{I}_n \) stands for any matrix of size \( n \) of the form \( \text{diag}((\pm 1)_{i \leq n}) \).
- Suppose \( n \leq m \). For \( A \in \mathbb{R}^{m \times m} \), we denote \( A^{(n)} \in \mathbb{R}^{n \times n} \) the submatrix containing the \( n \) first rows and the \( n \) first columns of \( A \).
- Suppose \( n \leq m \). For \( A \in \mathbb{R}^{n \times n} \), we denote \( A^{[m]} \in \mathbb{R}^{m \times m} \) the matrix of the form \( \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix} \).
- We denote \( S_n(\mathbb{R}) \) the set of symmetric matrices of size \( n \), \( S_n^+(\mathbb{R}) \) the set of semi-definite positive matrices, and \( S_n^{++}(\mathbb{R}) \) the set of definite positive matrices.
- \( 1_{n,m} = (1)_{i \leq n, j \leq m} \) denotes the matrix of ones with \( n \) rows and \( m \) columns.
- \( \|x\|_{\mathbb{R}^n} \) stands for the Euclidean norm of \( x \in \mathbb{R}^n \). We will denote \( \|x\| \) when there is no ambiguity about the dimension.
- \( \langle x, x' \rangle_n \) stands for the Euclidean inner product in \( \mathbb{R}^n \) between \( x \) and \( x' \).
2 Derivation of the general problem

In this section, we derive an equivalent formulation of problem \( GW \) which takes the form of a functional of co-moments of order 2 and 4 of \( \pi \). This formulation is not specific to Gaussian measures but to all measures with finite 4th order moment.

**Theorem 2.1.** Let \( \mu \) be a probability measure on \( \mathbb{R}^m \) with mean vector \( m_0 \in \mathbb{R}^m \) and covariance matrix \( \Sigma_0 \in \mathbb{R}^{m \times m} \) such that \( \int \|x\|^4 d\mu < +\infty \) and \( \nu \) a probability measure on \( \mathbb{R}^n \) with mean vector \( m_1 \) and covariance matrix \( \Sigma_1 \in \mathbb{R}^{n \times n} \) such that \( \int \|y\|^4 d\nu < +\infty \). Let \( P_0, D_0 \) and \( P_1, D_1 \) be respective diagonalizations of \( \Sigma_0(= P_0 D_0 P_0^T) \) and \( \Sigma_1(= P_1 D_1 P_1^T) \). Let us define \( T_0 : x \in \mathbb{R}^m \mapsto P_0^T (x - m_0) \) and \( T_1 : y \in \mathbb{R}^n \mapsto P_1^T (y - m_1) \). Then problem \( GW \) is equivalent to problem

\[
\sup_{X \sim T_0 \# \mu, Y \sim T_1 \# \nu} \sum_{i,j} \text{Cov}(X_i^2, Y_j^2) + 2 \| \text{Cov}(X, Y) \|_F^2,
\]

where \( X = (X_1, X_2, \ldots, X_m)^T \), \( Y = (Y_1, Y_2, \ldots, Y_n)^T \), and \( \| \cdot \|_F \) is the Frobenius norm. More precisely, \( (X, Y) \) is optimal for \( \text{supCOV} \) if and only if the law of \( (T_0^{-1}(X), T_1^{-1}(Y)) \) is optimal for \( GW \).

This theorem is a direct consequence of the two following intermediary results.

**Lemma 2.1.** We denote \( O_m = \{ O \in \mathbb{R}^{m \times m} \mid O^T O = I_m \} \) the set of orthogonal matrices of size \( m \). Let \( \mu \) and \( \nu \) be two probability measures on \( \mathbb{R}^m \) and \( \mathbb{R}^n \). Let \( T_m : x \mapsto O_m x + x_m \) and \( T_n : y \mapsto O_n y + y_n \) be two affine applications with \( x_m \in \mathbb{R}^m \), \( O_m \in O_m \), \( y_n \in \mathbb{R}^n \), and \( O_n \in O_n \). Then \( GW_2(T_m \# \mu, T_n \# \nu) = GW_2(\mu, \nu) \).

**Lemma 2.2 (Vayer, 2020, [25]).** Suppose there exist some scalars \( a, b, c \) such that \( cX(x, x') = a\|x\|_R^2 + b\|x'\|_R^2 + c(x, x')_m \), where \( (\cdot, \cdot)_m \) denotes the inner product on \( \mathbb{R}^m \), and \( cY(y, y') = a\|y\|_R^2 + b\|y'\|_R^2 + c(y, y')_n \). Let \( \mu \) and \( \nu \) be two probability measures respectively on \( \mathbb{R}^m \) and \( \mathbb{R}^n \). Then

\[
GW_2(cX, cY, \mu, \nu) = C_{\mu, \nu} - 2 \sup_{\pi \in \Pi(\mu, \nu)} Z(\pi),
\]

where \( C_{\mu, \nu} = \int c_X^2 d\mu d\mu + \int c_Y^2 d\nu d\nu - 4ab \int \|x\|_R^2 \|y\|_R^2 d\pi(x, y) + c^2 \left( \int xy^T d\pi(x, y) \right)^2
\]

\[
+ (a + b)c \int \left( \int \|x\|_R^2 \langle \mathbb{E}_{X \sim \mu}[Y], y \rangle_n + \int \|y\|_R^2 \langle \mathbb{E}_{Y \sim \nu}[X], x \rangle_m \right) d\pi(x, y).
\]

**Proof of Theorem 2.1.** Using Lemma 2.1, we can focus without any loss of generality on centered Gaussian measures with diagonal covariance matrices. Thus, defining \( T_0 : x \in \mathbb{R}^m \mapsto P_0^T (x - m_0) \) and \( T_1 : y \in \mathbb{R}^n \mapsto P_1^T (y - m_1) \) and then applying Lemma 2.2 on \( GW_2(T_0 \# \mu, T_1 \# \nu) \) with \( a = 1, b = 1, \) and \( c = -2 \) while remarking that the last term in Equation (2.2) is null because \( \mathbb{E}_{X \sim T_0 \# \mu}[X] = 0 \) and \( \mathbb{E}_{Y \sim T_1 \# \nu}[Y] = 0 \), it follows that problem \( GW \) is equivalent to

\[
\sup_{\pi \in \Pi(T_0 \# \mu, T_1 \# \nu)} \left\| \int \|x\|_R^2 \|y\|_R^2 d\pi(x, y) + 2 \left\| \int xy^T d\pi(x, y) \right\|_F^2 \right. \].
\]

Since \( T_0 \# \mu \) and \( T_1 \# \nu \) are centered, we have that \( \int xy^T d\pi(x, y) = \text{Cov}(X, Y) \) where \( X \sim T_0 \# \mu \) and \( Y \sim T_1 \# \nu \). Furthermore, it can be easily computed that

\[
\int \|x\|_R^2 \|y\|_R^2 d\pi(x, y) = \sum_{i,j} \text{Cov}(X_i^2, Y_j^2) + \sum_{i,j} \mathbb{E}[X_i^2]\mathbb{E}[Y_j^2].
\]

Since the second term doesn’t depend on \( \pi \), we get that problem \( GW \) is equivalent to problem \( \text{supCOV} \).
3 Study of the general problem

Since problem $\text{supCOV}$ is hard to solve because of its dependence on co-moments of order 2 and 4 of $\pi$, one can optimize both terms separately in order to find a lower bound of $GW_2(\mu, \nu)$. In the rest of the paper we suppose for convenience and without any loss of generality that $n \leq m$.

**Theorem 3.1.** Suppose without any loss of generality that $n \leq m$. Let $\mu = \mathcal{N}(m_0, \Sigma_0)$ and $\nu = \mathcal{N}(m_1, \Sigma_1)$ be two Gaussian measures on $\mathbb{R}^m$ and $\mathbb{R}^n$. Let $P_0, D_0$ and $P_1, D_1$ be the respective diagonalizations of $\Sigma_0 (= P_0 D_0 P_0^T)$ and $\Sigma_1 (= P_1 D_1 P_1^T)$ which sort eigenvalues in decreasing order. We suppose that $\Sigma_0$ is non-singular. A lower bound for $GW_2(\mu, \nu)$ is then

$$GW_2^2(\mu, \nu) \geq LGW_2^2(\mu, \nu), \quad (3.1)$$

where

$$LGW_2^2(\mu, \nu) = 4 (\text{tr}(D_0) - \text{tr}(D_1))^2 + 4 (\|D_0\|_F - \|D_1\|_F)^2 + 4 \|D_0^{(n)} - D_1\|_F^2 + 4 \left(\|D_0\|_F^2 - \|D_0^{(n)}\|_F^2\right). \quad (LGW)$$

The proof of this theorem is divided in smaller intermediary results. First we recall the Isserlis lemma (see [14]), which allows to derive the co-moments of order 4 of a Gaussian distribution as a function of its co-moments of order 2.

**Lemma 3.1 (Isserlis, 1918, [14]).** Let $X$ be a zero-mean Gaussian vector of size $n$. Then

$$\forall i, j, k, l \leq n, \ E[X_i X_j X_k X_l] = E[X_i X_j] E[X_k X_l] + E[X_i X_k] E[X_j X_l] + E[X_i X_l] E[X_j X_k]. \quad (3.2)$$

Then we derive the following general optimization lemmas. The proofs of these two lemmas are postponed to the Appendix (Section 5).

**Lemma 3.2.** Suppose that $n \leq m$. Let $\Sigma$ be a semi-definite positive matrix of size $m + n$ of the form

$$\Sigma = \begin{pmatrix} \Sigma_0 & K \\ K^T & \Sigma_1 \end{pmatrix},$$

with $\Sigma_0 \in S_m^+(\mathbb{R}), \Sigma_1 \in S_n^+(\mathbb{R})$ and $K \in \mathbb{R}^{m \times n}$. Let $P_0, D_0$ and $P_1, D_1$ be the respective diagonalisations of $\Sigma_0 (= P_0^T D_0 P_0)$ and $\Sigma_1 (= P_1^T D_1 P_1)$ which sort the eigenvalues in decreasing order. Then

$$\max_{\Sigma_1 - K^T \Sigma_0^{-1} K \in S_n^+(\mathbb{R})} \|K\|_F^2 = \text{tr}(D_0^{(n)} D_1), \quad (3.3)$$

and is achieved at any

$$K^* = P_0^T \left( \hat{I}_n (D_0^{(n)})^{\frac{1}{2}} D_1^{\frac{1}{2}} \right) P_1, \quad (\text{opK1})$$

where $\hat{I}_n$ is of the form $\text{diag}(\pm 1)_{i \leq n}$.
Lemma 3.3. Suppose that \( n \leq m \). Let \( \Sigma \) be a semi-definite positive matrix of size \( m+n \) of the form:

\[
\Sigma = \begin{pmatrix} \Sigma_0 & K \\ K^T & \Sigma_1 \end{pmatrix},
\]

where \( \Sigma_0 \in S^{++}_m(\mathbb{R}) \), \( \Sigma_1 \in S^+_n(\mathbb{R}) \), and \( K \in \mathbb{R}^{m \times n} \). Let \( A \in \mathbb{R}^{n \times m} \) be a matrix with rank 1. Then

\[
\max_{\Sigma_1 - K^T \Sigma_0^{-1} K \in S^+_n(\mathbb{R})} \text{tr}(KA) = \sqrt{\text{tr}(A \Sigma_0 A^T \Sigma_1)}.
\] (3.4)

In particular, if \( \Sigma_0 = \text{diag}(\alpha) \) and \( \Sigma_1 = \text{diag}(\beta) \) with \( \alpha \in \mathbb{R}^m \) and \( \beta \in \mathbb{R}^n \), then

\[
\max_{\Sigma_1 - K^T \Sigma_0^{-1} K \in S^+_n(\mathbb{R})} \text{tr}(K \mathbb{1}_{n,m}) = \sqrt{\text{tr}((\Sigma_0)\text{tr}(\Sigma_1))},
\] (3.5)

with \( \mathbb{1}_{n,m} = (1)_{i \leq n, j \leq m} \), and is achieved at

\[
K^* = \frac{\alpha \beta^T}{\text{tr}(\Sigma_0)\text{tr}(\Sigma_1)}.
\] (opK2)

Proof of theorem 3.1. For \( \mu = \mathcal{N}(m_0, \Sigma_0) \) and \( \nu = \mathcal{N}(m_1, \Sigma_1) \), we note \( P_0, D_0 \) and \( P_1, D_1 \) the respective diagonalizations of \( \Sigma_0 \) and \( \Sigma_1 \) which sort the eigenvalues in decreasing order. Let \( T_0 : x \in \mathbb{R}^m \mapsto P_0^T (x - m_0) \) and \( T_1 : y \in \mathbb{R}^n \mapsto P_1^T (y - m_1) \). For \( \pi \in \Pi(T_0 \# \mu, T_1 \# \nu) \) and \( (X,Y) \sim \pi \), we denote \( \Sigma \) the covariance matrix of \( \pi \) and \( \Sigma \) the covariance matrix of \( (X^2, Y^2) \) with \( X^2 := ([XX^T]_{i,i})_{i \leq m} \) and \( Y^2 := ([YY^T]_{j,j})_{j \leq n} \). Using Isserlis lemma to compute \( \text{Cov}(X^2, X^2) \) and \( \text{Cov}(Y^2, Y^2) \), it follows that \( \Sigma \) and \( \Sigma \) are of the form:

\[
\Sigma = \begin{pmatrix} D_0 & K \\ K^T & D_1 \end{pmatrix} \quad \text{and} \quad \Sigma = \begin{pmatrix} 2D_0^2 & \tilde{K} \\ \tilde{K}^T & 2D_1^2 \end{pmatrix},
\] (3.6)

In order to find a supremum for each term of \( \text{(supCov)} \), we use a necessary condition for \( \pi \) to be in \( \Pi(T_0 \# \mu, T_1 \# \nu) \) which is that \( \Sigma \) and \( \Sigma \) must be semi-definite positive. To do so, we can use the equivalent condition that the Schur complements of \( \Sigma \) and \( \Sigma \), namely \( D_1 - K^T D_0^{-1} K \) and \( 2D_0^2 + \frac{1}{2} K^T D_0^{-2} K \), must also be semi-definite positive. Remarking that the left-hand term in \( \text{(supCov)} \) can be rewritten \( \text{tr}(K \mathbb{1}_{n,m}) \), we have the two following inequalities

\[
\sup_{X \sim T_0 \# \mu, Y \sim T_1 \# \nu} \sum_{i,j} \text{Cov}(X^2_i, Y^2_j) \leq \max_{\tilde{K} \in S^+_n(\mathbb{R})} \text{tr}(\tilde{K} \mathbb{1}_{n,m}),
\] (3.7)

and

\[
\sup_{X \sim T_0 \# \mu, Y \sim T_1 \# \nu} ||\text{Cov}(X,Y)||_F^2 \leq \max_{\tilde{K} \in S^+_n(\mathbb{R})} ||\tilde{K}||_F^2.
\] (3.8)

Applying Lemmas 3.2 and 3.3 on both right-hand terms, we get on one hand:

\[
\sup_{X \sim T_0 \# \mu, Y \sim T_1 \# \nu} \text{Cov}(X,Y) \leq (D_0^{(n)} D_1),
\] (3.9)

and on the other hand:

\[
\sum_{i,j} \text{Cov}(X^2_i, Y^2_j) \leq 2 \sqrt{\text{tr}(D_0^2)\text{tr}(D_1^2)}
\] (3.10)

\[
= 2\|D_0\|_F\|D_1\|_F.
\]
Furthermore, using Lemma 2.2 it follows that
\[
GW_2^2(\mu, \nu) = C_{\mu, \nu}
\]
\[
-4 \sup_{X \sim T_0 \# \mu, Y \sim T_1 \# \nu} \left( \sum_{i,j} \text{Cov}(X_i^2, Y_j^2) + \sum_{i,j} \mathbb{E}[X_i^2] \mathbb{E}[X_j^2] + 2 \|\text{Cov}(X, Y)\|^2_F \right)
\]
\[
\geq C_{\mu, \nu} - 8 \sqrt{\text{tr}(D_0^2)\text{tr}(D_1^2)} - 4\text{tr}(D_0)\text{tr}(D_1) - 8\text{tr}(D_0^{(n)}D_1),
\]
where
\[
C_{\mu, \nu} = \mathbb{E}_{U \sim \mathcal{N}(0,2D_0)}[\|U\|^4_F] + \mathbb{E}_{V \sim \mathcal{N}(0,2D_1)}[\|V\|^4_F] - 4\mathbb{E}_{X \sim \mu}[\|X\|^2_F] \mathbb{E}_{Y \sim \nu}[\|Y\|^2_F]
\]
\[
= 8\text{tr}(D_0^2) + 4(\text{tr}(D_0))^2 + 8\text{tr}(D_0^2) + 4(\text{tr}(D_1))^2 - 4\text{tr}(D_0)\text{tr}(D_1).
\]
Finally
\[
GW_2^2(\mu, \nu) \geq 4(\text{tr}(D_0))^2 + 4(\text{tr}(D_1))^2 - 8\text{tr}(D_0)\text{tr}(D_1) + 8\text{tr}(D_0^2) + 8\text{tr}(D_1^2)
\]
\[
-8 \sqrt{\text{tr}(D_0^2)\text{tr}(D_1^2)} - 8\text{tr}(D_0^{(n)}D_1)
\]
\[
= L GW_2^2(\mu, \nu).
\]

Inequality (3.7) becomes an equality if there exists a plan \( \pi \in \Pi(T_0 \# \mu, T_1 \# \nu) \) such that for \((X, Y) \sim \pi, \sum \text{Cov}(X_i^2, Y_j^2) = 2\|D_0\|_F D_1\|D_0\|_F\) \thanks{3.3}. Thanks to lemma \(3.3\) we know that \(\text{tr}(K^*_{\#n,m}) = 2\|D_0\|_F\|D_1\|_F\) for
\[
K^* = \frac{2\alpha^2(\beta^2)^T}{\|D_0\|_F\|D_1\|_F},
\]
where \(\alpha^2 = (\alpha_1^2, \alpha_2^2, \ldots, \alpha_m^2)\) and \(\beta^2 = (\beta_1^2, \beta_2^2, \ldots, \beta_n^2)\) are the diagonal vectors of \(D_0^2\) and \(D_1^2\). However, it seems not straightforward to exhibit a plan \( \pi \in \Pi(T_0 \# \mu, T_1 \# \nu) \) such that for \((X, Y) \sim \pi, \text{Cov}(X^2, Y^2) = K^*\). An important point to mention is that it can be shown, thanks to Isserlis Lemma, that does not exist a Gaussian plan in \(\Pi(T_0 \# \mu, T_1 \# \nu)\) with such symmetric co-moments of order 4.

On the other hand, it can be easily seen that inequality (3.8) is in fact an equality since the maximal value of \(\|\text{Cov}(X, Y)\|_F^2\) is reached when the law of \((X, Y)\) is Gaussian and \(\text{Cov}(X, Y)\) is of the form \(\text{opK}^1\). Moreover, the following lemma shows that if \(\text{Cov}(X, Y)\) is of the form \(\text{opK}^1\), then the law of \((X, Y)\) is necessarily Gaussian and \((X, Y)\) is in general sub-optimal for the left-hand term in \(\text{supCOV}\) \thanks{3.4}. The proof is postponed to the Appendix (Section 8).

\begin{lemma} Suppose that \(n \leq m\). Let \(X \sim \mathcal{N}(0, D_0)\) and \(Y \sim \mathcal{N}(0, D_1)\) be two Gaussian vectors of respective size \(m\) and \(n\) with diagonal covariance matrices. If \(\text{Cov}(X, Y)\) is of the form
\[
\text{Cov}(X, Y) = \begin{pmatrix} \tilde{I}_n(D_0^{(n)})^{\frac{1}{2}} D_1^{\frac{1}{2}} \\ 0_{m-n, n} \end{pmatrix},
\]
\end{lemma}
then
\[
Y = \begin{pmatrix} \tilde{I}_n D_1^{\frac{1}{2}} (D_0^{(n)})^{-\frac{1}{2}} \\ 0_{n, m-n} \end{pmatrix} X,
\]
and so \((X, Y)\) is a Gaussian vector and
\[
\sum_{i,j} \text{Cov}(X_i^2, Y_j^2) = 2\text{tr}(D_0^{(n)}D_1),
\]
where \(X = (X_1, X_2, \ldots, X_m)^T\) and \(Y = (Y_1, Y_2, \ldots, Y_n)^T\).
Thus, there doesn’t exist a plan $\pi \in \Pi(T_0 \# \mu, T_1 \# \mu_1)$ with co-moments of order 2 of the form $\text{opK1}$ and with symmetric co-moments of order 4 of the form $\text{opK2}$, since the former requires $\pi$ to be Gaussian and the latter requires $\pi$ not to be Gaussian. However, the solutions exhibited in Lemmas 3.2 and 3.3 are not unique so it may exist a plan $\pi$ which is optimal for both terms of $\text{supCOV}$ but with co-moments of order 2 of a different form than $\text{opK1}$ or with symmetric co-moments of order 4 of a different form than $\text{opK2}$. Thus, we cannot conclude whether $GW_2(\mu, \nu) = LGW_2(\mu, \nu)$ or $GW_2(\mu, \nu) > LGW_2(\mu, \nu)$.

4 Problem restricted to Gaussian transport plans

In this section, we study the following problem, where we constrain the optimal transport plan to be Gaussian.

$$GGW_2^2(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu) \cap \mathcal{N}_{m+n}} \int \int (\|x - x'\|_F^2 - \|y - y'\|_F^2) d\pi(x,y)d\pi(x',y'), \quad (\text{GaussGW})$$

where $\mathcal{N}_{m+n}$ is the set of Gaussian measures on $\mathbb{R}^{m+n}$.

Since $GGW_2$ is the Gromov-Wasserstein problem restricted to Gaussian transport plans, it is clear that $\text{supCOV}$ is an upper bound of $\text{GW}$. Combining this result with Theorem 3.1, we get the following simple but important proposition.

**Proposition 4.1.** If $\mu = \mathcal{N}(m_0, \Sigma_0)$ and $\nu = \mathcal{N}(m_1, \Sigma_1)$, with $\Sigma_0$ non-singular, then

$$LGW_2^2(\mu, \nu) \leq GW_2^2(\mu, \nu) \leq GGW_2^2(\mu, \nu). \quad (4.1)$$

We exhibit in the following a solution of $\text{GaussGW}$, which yields an explicit form for the upper bound $GGW_2^2(\mu, \nu)$.

**Theorem 4.1.** Suppose without any loss of generality that $n \leq m$. Let $\mu = \mathcal{N}(m_0, \Sigma_0)$ and $\nu = \mathcal{N}(m_1, \Sigma_1)$ be two Gaussian measures on $\mathbb{R}^m$ and $\mathbb{R}^n$. Let $P_0, D_0$ and $P_1, D_1$ be the respective diagonalizations of $\Sigma_0 (= P_0 D_0 P_0^T)$ and $\Sigma_1 (= P_1 D_1 P_1^T)$ which sort eigenvalues in decreasing order. We suppose that $\Sigma_0$ is non-singular ($\mu$ is not degenerate). Then problem $\text{GaussGW}$ admits a solution of the form $\pi^* = (I_m, T) \# \mu$ with $T$ affine of the form

$$\forall x \in \mathbb{R}^m, \quad T(x) = m_1 + P_1 A P_0^T (x - m_0). \quad (4.2)$$

where $A \in \mathbb{R}^{n \times m}$ is written

$$A = \left( \tilde{I}_n D_1^\frac{1}{2} (D_0^{(n)})^{-\frac{1}{2}} \ 0_{n,m-n} \right), \quad (4.3)$$

where $\tilde{I}_n$ is of the form $\text{diag}((\pm 1)_{i \leq n})$. Moreover

$$GGW_2^2(\mu, \nu) = 4(\text{tr}(D_0) - \text{tr}(D_1))^2 + 8\|D_0^{(n)} - D_1\|_2^2 + 8 \left( \|D_0\|_2^2 - \|D_0^{(n)}\|_2^2 \right). \quad (\text{GGW})$$

**Proof.** Since the problem is restricted to Gaussian plans, the left-hand term in equation $\text{supCOV}$ can be rewritten $2\|\text{Cov}(X, Y)\|_2^2$ thanks to Lemma 3.1 (Isserlis) and so problem $\text{supCOV}$ becomes in that case

$$\sup_{X \sim T_0 \# \mu, \ Y \sim T_1 \# \nu} 4\|\text{Cov}(X, Y)\|_2^2. \quad (4.4)$$

Applying Lemma 3.2, we can exhibit a Gaussian optimal plan $\tilde{\pi}^* \in \Pi(T_0 \# \mu, T_1 \# \nu)$ with covariance matrix $\Sigma$ of the form:

$$\Sigma = \left( \begin{array}{cc} D_0 & K^* \\ K^* & D_1 \end{array} \right), \quad (4.5)$$
with
\[ K^* = \left( I_n(D_0(n))^{-1/2}D_1^{-1/2} \right)_{m-n,n} \] (4.6)

Thus, applying Lemma 3.4, it follows directly that \( \tilde{\pi}^* \) is of the form \( (I_m, \tilde{T})\#T_0\#\mu \), with \( \tilde{T} \) linear of the form
\[ \forall x \in \mathbb{R}^m, \quad \tilde{T}(x) = Ax, \] (4.7)
with \( A \) of the form
\[ A = \left( I_nD_1^{1/2}(D_0(n))^{-1/2} 0_{n,m-n} \right). \] (4.8)

Then, we can deduce the form of the optimal Gaussian plan \( \pi^* \in \Pi(\mu, \nu) \):
\[ \pi^* = (T_0^{-1}, T_1^{-1})\#\tilde{\pi}^* \]
\[ = (T_0^{-1}, T_1^{-1})\#(I_m, \tilde{T})\#T_0\#\mu \]
\[ = (I_m, T_1^{-1}\#\tilde{T}\#T_0)\#\mu \]
\[ = (I_m, T)\#\mu \] (4.9)

where \( T \) is affine of the form
\[ \forall x \in \mathbb{R}^m, \quad T(x) = T_1^{-1} \circ \tilde{T} \circ T_0(x) = m_1 + P_1AP_0^T(x - m_0). \] (4.10)

Moreover, using Lemmas 2.2 and 3.2, it follows that
\[ GGW_2^2(\mu, \nu) = C_{\mu, \nu} - 16 \sup_{X \sim T_0\#\mu, Y \sim T_1\#\nu} \|\text{Cov}(X, Y)\|_F^2 \]
\[ = 8\text{tr}(D_0^2) + 4(\text{tr}(D_0))^2 + 8\text{tr}(D_1^2) + 4(\text{tr}(D_1))^2 - 4\text{tr}(D_0)\text{tr}(D_1) - 16\text{tr}(D_0(n)D_1) \]
\[ = 4(\text{tr}(D_0) - \text{tr}(D_1))^2 + 8\left((D_0(n) - D_1)^2\right) + 8\left(\text{tr}(D_0^2) - \text{tr}(D_0(n)^2)\right). \] (4.11)

**Link with Gromov-Monge** The previous result generalizes Theorem 4.2.6 in [25], which studies the solutions of the linear Gromov-Monge problem between Gaussian distributions
\[ \inf_{T\#\mu = x, T \text{ linear}} \int \int \left( \|x - x'\|_{\mathbb{R}^m}^2 + \|T(x) - T(x')\|_{\mathbb{R}^n}^2 \right) d\mu(x)d\mu(x'). \] (4.12)

Indeed, solutions of \([4.12]\) necessarily provide linear transport plans \( \pi = (I_m, T)\#\mu \) if \( T \) is linear. Conversely, Theorem 4.1 shows that restricting the optimal plan to be Gaussian in Gromov-Wasserstein between two Gaussian distributions yields an optimal plan of the form \( \pi = (I_m, T)\#\mu \) with a linear \( T \), whatever the dimensions \( m \) and \( n \) of the two Euclidean spaces.

**Link with Principal Component Analysis** We can easily draw connections between \( GGW_2^2 \) and PCA. Indeed, we can remark that the optimal plan can be derived by performing PCA on both distributions \( \mu \) and \( \nu \) in order to obtain distributions \( \tilde{\mu} \) and \( \tilde{\nu} \) with zero mean vectors and diagonal covariance matrices with eigenvalues in decreasing order (\( \tilde{\mu} = T_0\#\mu \) and \( \tilde{\nu} = T_1\#\nu \)), then by keeping only the \( n \) first components in \( \tilde{\mu} \) and finally by deriving the optimal transport plan which achieves \( W_2^2 \) between the obtained truncated distribution and \( \tilde{\nu} \). In other terms, noting \( P_n : \mathbb{R}^m \to \mathbb{R}^n \) the linear mapping which, for \( x \in \mathbb{R}^m \) keeps only its \( n \) first components (\( n \)-frame), \( T_{W_2} \) the optimal transport map such that \( \pi_{W_2} = (I_n, T_{W_2})\#P_n\#\tilde{\mu} \) achieves \( W_2(P_n\#\tilde{\mu}, \tilde{\nu}) \), it follows that the optimal plan \( \pi_{GGW_2} \) which achieves \( GGW_2(\tilde{\mu}, \tilde{\nu}) \) can be written
\[ \pi_{GGW_2} = (I_m, \tilde{I_n}\#T_{W_2}\#P_n)\#\tilde{\mu}, \] (4.13)
Gromov-Wasserstein Distance between Gaussian Distributions

where, with an abuse of notation, we write $I_m$ (resp. $\tilde{I}_n$) the map on $\mathbb{R}^m$ (resp. $\mathbb{R}^n$) represented by the similarly denoted matrix.

An example of $\pi_{GGW_2}$ can be found in Figure 1 when $m = 2$ and $n = 1$.

![Figure 1: transport plan $\pi_{GGW_2}$ solution of problem (GaussGW) with $m = 2$ and $n = 1$. In that case, $\pi_{GGW_2}$ is the degenerate Gaussian distribution supported by the affine plane of equation $y = T_{W_2}(x)$, where $T_{W_2}$ is the classic $W_2$ optimal transport map when the distributions are rotated and centered first.](image)

**Case of equal dimensions** When $m = n$, the optimal plan $\pi_{GGW_2}$ which achieves $GGW_2(\mu, \nu)$ is closely related to the optimal transport plan $\pi_{W_2} = (I_m, T_{W_2})\#T_0\#\mu$. Indeed, $\pi_{GGW_2}$ can be simply derived by applying the transformations $T_0$ and $T_1$ to respectively $\mu$ and $\nu$, then by computing $\pi_{W_2}$ between $T_0\#\mu$ and $T_1\#\nu$, and finally by applying the inverse transformations $T_0^{-1}$ and $T_1^{-1}$. In other terms, $\pi_{GGW_2}$ can be written

$$\pi_{GGW_2} = (I_m, T_1^{-1}\#\tilde{I}_n\#T_{W_2}\#T_0)\#\mu.$$  

(4.14)

An example of transport between two Gaussians measures in dimension 2 in Figure 2.

As illustrated in Figure 3, the $GGW_2$ optimal transport map $T_{GGW_2}$ defined in Equation (4.2) is not equivalent to the $W_2$ optimal transport map $T_{W_2}$ defined in (1.5) even when the dimensions $m$ and $n$ are equal. More precisely, if $\Sigma_0$ and $\Sigma_1$ can be diagonalized in the same orthonormal basis with eigenvalues in the same order (decreasing or increasing), then $T_{W_2}$ and $T_{GGW_2}$ are equivalent (top of Figure 3). On the other hand, if $\Sigma_0$ and $\Sigma_1$ can be diagonalized in the same orthonormal basis but with eigenvalues not in the same order, $T_{W_2}$ and $T_{GGW_2}$ will have very different behaviors (bottom of Figure 3). Between those two extreme cases, we can say that the closer the columns of $P_0$ will be collinear to the columns of $P_1$ (with the eigenvalues in decreasing order), the more $T_{W_2}$ and $T_{GGW_2}$ will tend to have similar behaviors (middle of Figure 3).

**Link with Gromov-Wasserstein with inner product as cost function** If $\mu$ and $\nu$ are centered Gaussian measures, let us consider the following problem

$$GW_2^2(\langle.,.\rangle_m, \langle.,.\rangle_n, \mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int \int (\langle x, x' \rangle_n - \langle y, y' \rangle_n)^2 d\pi(x, y) d\pi(x', y').$$  

(innerGW)

Notice that the above problem is not restricted to Gaussian plans, but the following proposition shows that in fact its solution is Gaussian.

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Figure 2: Solution of (GaussGW) between two Gaussians measures in dimension 2. First the distributions are centered and rotated. Then a classic $W_2$ transport is applied between the two aligned distributions.

Figure 3: Comparison between $W_2$ and $GGW_2$ mappings between empirical distributions. Left: 2D source distribution (colored) and target distribution (transparent). Middle: resulting mapping of Wasserstein $T_{W_2}$. Right: resulting mapping of Gaussian Gromov-Wasserstein $T_{GGW_2}$. The colors are added in order to visualize where each sample has been sent.
Proposition 4.2. Suppose \( m \leq n \). Let \( \mu = \mathcal{N}(0, \Sigma_0) \) and \( \nu = \mathcal{N}(0, \Sigma_1) \) be two centered Gaussian measures respectively on \( \mathbb{R}^m \) and \( \mathbb{R}^n \). Then the solution of problem \((\text{GaussGW})\) exhibited in Theorem 4.1 is also solution of problem \((\text{innerGW})\).

Proof. The proof of this proposition is a direct consequence of lemma 2.2: indeed, applying it with \( a = 0, b = 0, \) and \( c = 1 \), it follows that problem \((\text{innerGW})\) is equivalent to

\[
\sup_{\pi \in \Pi(\mu, \nu)} \left\| \int xy^T d\pi(x, y) \right\|_F^2.
\]

(4.15)

Since \( \mu \) and \( \nu \) are centered, it follows that problem \((\text{innerGW})\) is equivalent to

\[
\sup_{X \sim \mu, Y \sim \nu} \|\text{Cov}(X, Y)\|_F^2.
\]

(4.16)

Applying Lemma 3.2, it follows that the solution exhibited in Theorem 4.1 is also solution of problem \((\text{innerGW})\).

\[\blacksquare\]

5 Tightness of the bounds and particular cases

5.1 Bound on the difference

Proposition 5.1. Suppose without loss of generality that \( n \leq m \), if \( \mu = \mathcal{N}(m_0, \Sigma_0) \) and \( \nu = \mathcal{N}(m_1, \Sigma_1) \), then

\[
\text{GGW}_2^2(\mu, \nu) - \text{LGW}_2^2(\mu, \nu) \leq 8\|\Sigma_0\|_F\|\Sigma_1\|_F \left(1 - \frac{1}{\sqrt{m}}\right).
\]

(5.1)

To prove this proposition, we will use the following technical result (the proof is postponed to the Appendix (Section 8)):

Lemma 5.1. Let \( u \in \mathbb{R}^m \) and \( v \in \mathbb{R}^m \) be two unit vectors with non-negative coordinates ordered in decreasing order. Then

\[
u^T u \geq \frac{1}{\sqrt{m}},
\]

(5.2)

with equality if \( u = \left(\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}, \ldots\right)^T \) and \( v = (1, 0, \ldots)^T \).

Proof of Proposition 5.1. By subtracting \((\text{LGW})\) from \((\text{GGW})\), it follows that

\[
\text{GGW}_2^2(\mu, \nu) - \text{LGW}_2^2(\mu, \nu) = 8 \left\|D_0\|_F\|D_1\|_F - \text{tr}(D_0^{(m)} D_1)\right\|
\]

(5.3)

where \( D_1^{[m]} = \begin{pmatrix} D_1 & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{R}^{m \times m} \). Noting \( \alpha \in \mathbb{R}^m \) and \( \beta \in \mathbb{R}^m \) the vectors of eigenvalues of \( D_0 \) and \( D_1^{[m]} \), it follows that

\[
\text{GGW}_2^2(\mu, \nu) - \text{LGW}_2^2(\mu, \nu) = 8\|\alpha\|\|\beta\| - \alpha^T \beta) = 8\|\alpha\|\|\beta\|(1 - u^T v),
\]

(5.4)

where \( u = \frac{\alpha}{\|\alpha\|} \) and \( v = \frac{\beta}{\|\beta\|} \). Applying lemma 5.1, we get directly that

\[
\text{GGW}_2^2(\mu, \nu) - \text{LGW}_2^2(\mu, \nu) \leq 8\|D_0\|_F\|D_1^{[m]}\|_F \left(1 - \frac{1}{\sqrt{m}}\right),
\]

(5.5)

\[\blacksquare\]
The difference between $GGW^2_2(\mu, \nu)$ and $LGW^2_2(\mu, \nu)$ can be seen as the difference between the right and left terms of the Cauchy-Schwarz inequality applied to the two vectors of eigenvalues $\alpha \in \mathbb{R}^m$ and $\beta \in \mathbb{R}^m$. The difference is maximized when the vectors $\alpha$ and $\beta$ are the least collinear possible. This happens when the eigenvalues of $D_0$ are all equal and $n = 1$ or $\nu$ is degenerate of true dimension 1. On the other hand, this difference is null when $\alpha$ and $\beta$ are collinear. Between those two extremal cases, we can say that the difference between $GGW^2_2(\mu, \nu)$ and $LGW^2_2(\mu, \nu)$ will be relatively small if the last $m - n$ eigenvalues of $D_0$ are small compared to the $n$ first eigenvalues and if the $n$ first eigenvalues are close to be proportional to the eigenvalues of $D_1$. An example in the case where $m = 2$ and $n = 1$ can be found in Figure 4.

![Figure 4](image-url)  

“Figure 4: plot of $GGW^2_2(\mu, \nu)$ and $LGW^2_2(\mu, \nu)$ in function of $\alpha_2$ for $\mu = \mathcal{N}(0, \text{diag}(\alpha))$, $\nu = \mathcal{N}(0, \beta_1)$, $\alpha = (\alpha_1, \alpha_2)^T$, for $(\alpha_1, \beta_1) = (1, 1)$ (left), $(\alpha_1, \beta_1) = (1, 2)$ (middle), $(\alpha_1, \beta_1) = (1, 10)$ (right). One can easily compute using (GGW) and (LGW) that $GGW^2_2(\mu, \nu) = 12\alpha_2^2 + 8\alpha_2(\alpha_1 - \beta_1) + 12(\alpha_1 - \beta_1)^2$ and $LGW^2_2(\mu, \nu) = 12\alpha_2^2 + 8\alpha_2(\alpha_1 - \beta_1) - 4\sqrt{\alpha_2^2 + \alpha_1^2\beta_1} + 12(\alpha_1 - \beta_1)^2 + 8\alpha_1\beta_1$.”

### 5.2 Explicit case

As seen before, the difference between $GGW^2_2(\mu, \nu)$ and $LGW^2_2(\mu, \nu)$, with $\mu = \mathcal{N}(m_0, \Sigma_0)$ and $\nu = \mathcal{N}(m_1, \Sigma_1)$, is null when the two vectors of eigenvalues of $\Sigma_0$ and $\Sigma_1$ (sorted in decreasing order) are collinear. When we suppose $\Sigma_0$ non-singular, it implies that $m = n$ and that the eigenvalues of $\Sigma_1$ are proportional to the eigenvalues of $\Sigma_0$ (rescaling). This case includes the more particular case where $m = n = 1$. In that case $\mu = \mathcal{N}(m_0, \sigma_0^2)$ and $\nu = \mathcal{N}(m_1, \sigma_1^2)$, because $\sigma_1$ is always proportional to $\sigma_0$.

**Proposition 5.2.** Suppose $m = n$. Let $\mu = \mathcal{N}(m_0, \Sigma_0)$ and $\nu = \mathcal{N}(m_1, \Sigma_1)$ two Gaussian measures on $\mathbb{R}^m = \mathbb{R}^n$. Let $P_0$, $D_0$ and $P_1$, $D_1$ be the respective diagonalizations of $\Sigma_0(= P_0D_0P_0^T)$ and $\Sigma_1(= P_1D_1P_1^T)$ which sort eigenvalues in non-increasing order. Suppose $\Sigma_0$ is non-singular and that it exists a scalar $\lambda \geq 0$ such that $D_1 = \lambda D_0$. In that case, $GW^2_2(\mu, \nu) = GW^2_2(\mu, \nu) = LGW^2_2(\mu, \nu)$ and the problem admits a solution of the form $(I_m, T) \# \mu$ with $T$ affine of the form:

$$
\forall x \in \mathbb{R}^m, \quad T(x) = m_1 + \sqrt{\lambda}P_1\tilde{I}_mP_0^T(x - m_0),
$$

where $\tilde{I}_m$ of the form $\text{diag}((\pm 1)_{i \leq m})$. Moreover

$$
GW^2_2(\mu, \nu) = (\lambda - 1)^2 (4(\text{tr}(\Sigma_0))^2 + 8\|\Sigma_0\|_F^2).
$$

**Proof.** From [5.3], we have

$$
GGW^2_2(\mu, \nu) - LGW^2_2(\mu, \nu) = 8(\|D_0\|_F\|D_1\|_F - \text{tr}(D_0D_1)).
$$

Noting $\alpha \in \mathbb{R}^m$ and $\beta \in \mathbb{R}^m$ the eigenvalues vectors of $D_0$ and $D_1$, it follows that

$$
GGW^2_2(\mu, \nu) - LGW^2_2(\mu, \nu) = 8(\|\alpha\|\|\beta\| - \alpha^T\beta).
$$

Since it exists $\lambda \geq 0$ such that $D_1 = \lambda D_0$, we have $\beta = \lambda \alpha$, and so $\alpha^T\beta = \|\alpha\|\|\beta\|$. Thus $GGW^2_2(\mu, \nu) - LGW^2_2(\mu, \nu) = 0$ and using Proposition 4.1, we get that $GW^2_2(\mu, \nu) = GW^2_2(\mu, \nu) = LGW^2_2(\mu, \nu)$. We get (5.6) and (5.7) by simply reinserting in (4.2) and (GGW). 

\[\square\]
Corollary 5.1. Let $\mu = \mathcal{N}(m_0, \sigma_0^2)$ and $\nu = \mathcal{N}(m_1, \sigma_1^2)$ be two Gaussian measures on $\mathbb{R}$. Then
\[
GW^2_2(\mu, \nu) = 12(\sigma_0^2 - \sigma_1^2)^2,
\]
and the optimal transport plan $\pi^*$ has the form $(I_1, T)\#\mu$ with $T$ affine of the form:
\[
\forall x \in \mathbb{R}, \ T(x) = m_1 \pm \frac{\sigma_1}{\sigma_0}(x - m_0).
\]
Thus, the solution of $W^2_2(\mu, \nu)$ is also solution of $GW^2_2(\mu, \nu)$.

5.3 Case of degenerate measures
In all the results exposed above, we have supposed $\Sigma_0$ non-singular, which means that $\mu$ is not degenerate. Yet, if $\Sigma_0$ is not full rank, one can easily extend the previous results thanks to the following proposition.

Proposition 5.3. Let $\mu = \mathcal{N}(0, D_0)$ and $\nu = \mathcal{N}(0, D_1)$ be two centered Gaussian measures on $\mathbb{R}^n$ and $\mathbb{R}^n$ with diagonal covariance matrices $D_0$ and $D_1$ with eigenvalues in decreasing order. We denote $r = rk(D_0)$ the rank of $D_0$ and we suppose that $r < m$. Let us define $P_r = (I_r \quad 0_{r,m-r}) \in \mathbb{R}^{n \times m}$. Then
\[
GW^2_2(\mu, \nu) = GW^2_2(P_r \# \mu, \nu),
\]
Proof. For $r < m$, we denote $\Gamma_r(\mathbb{R}^m)$ the set of vectors $x = (x_1, \ldots, x_m)^T$ of $\mathbb{R}^m$ such that $x_{r+1} = \cdots = x_m = 0$. For $\pi \in \Pi(\mu, \nu)$, one can remark that for any borel set $A \subset \mathbb{R}^m \setminus \Gamma_r(\mathbb{R}^m)$, and any borel set $B \subset \mathbb{R}^n$, we have $\pi(A, B) = 0$ and so
\[
GW^2_2(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^m \times \mathbb{R}^n} \left(\|x - x'\|_{\mathbb{R}^m}^2 + \|y - y'\|_{\mathbb{R}^n}^2 \right) d\pi(x, y) dx dy
\]
\[
= \inf_{\pi \in \Pi(\mu, \nu)} \int_{\Gamma_r(\mathbb{R}^m) \times \mathbb{R}^n} \left(\|x - x'\|_{\mathbb{R}^m}^2 + \|y - y'\|_{\mathbb{R}^n}^2 \right) d\pi(x, y) dx dy
\]
\[
= \inf_{\pi \in \Pi(\mu, \nu)} \int_{\Gamma_r(\mathbb{R}^m) \times \mathbb{R}^n} P_r(x - x') \|\|y - y'\|_{\mathbb{R}^n}^2 \right) d\pi(x, y) dx dy
\]
Now, observe that for $\pi \in \Pi(\mu, \nu)$, $(P_r, I_n)\#\pi \in \Pi(P_r \# \mu, \nu)$. It follows that
\[
GW^2_2(\mu, \nu) \leq \inf_{\pi \in \Pi(P_r \# \mu, \nu)} \int_{\mathbb{R}^r \times \mathbb{R}^n} \left(\|x - x'\|_{\mathbb{R}^r}^2 + \|y - y'\|_{\mathbb{R}^n}^2 \right) d\pi(x, y) dx dy
\]
\[
= GW^2_2(P_r \# \mu, \nu).
\]
Conversely, since $\mu$ has no mass outside of $\Gamma_r(\mathbb{R}^m)$, $P_r^T P_r \# P_r \# \mu = \mu$, which implies that for $\pi \in \Pi(P_r \# \mu, \nu)$, $(P_r^T, I_n)\#\pi \in \Pi(\mu, \nu)$. It follows that
\[
GW^2_2(P_r \# \mu, \nu) = \inf_{\pi \in \Pi(P_r \# \mu, \nu)} \int_{\mathbb{R}^r \times \mathbb{R}^n} \left(\|x - x'\|_{\mathbb{R}^r}^2 + \|y - y'\|_{\mathbb{R}^n}^2 \right) d\pi(x, y) dx dy
\]
\[
= \inf_{\pi \in \Pi(P_r \# \mu, \nu)} \int_{\mathbb{R}^r \times \mathbb{R}^n} \left(\|P_r^T(x - x')\|_{\mathbb{R}^r}^2 + \|y - y'\|_{\mathbb{R}^n}^2 \right) d\pi(x, y) dx dy
\]
\[
\leq \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^r \times \mathbb{R}^n} \left(\|x - x'\|_{\mathbb{R}^r}^2 + \|y - y'\|_{\mathbb{R}^n}^2 \right) d\pi(x, y) dx dy
\]
\[
\leq GW^2_2(\mu, \nu).
\]
The exact same reasoning can be made in the case of $GGW_2$. Morover, it can be easily seen when looking at $[\text{LGW}]$ that $LGW^2_2(\mu, \nu) = LGW^2_2(P_r \# \mu, \nu)$. \qed
Thus, when $\Sigma_0$ is not full rank, one can apply Proposition 5.3 and consider directly the Gromov-Wasserstein distance between the projected (non-degenerate) measure $P_\tau\#\mu$ on $\mathbb{R}^r$ and $\nu$ and so Proposition 4.1 still holds when $\mu$ is degenerate.

In the case of $GGW_2$, an explicit optimal transport plan can still be exhibited. In the following, we denote $r_0$ and $r_1$ the ranks of $\Sigma_0$ and $\Sigma_1$, and we suppose without loss of generality that $r_0 \geq r_1$, but this time not necessarily that $m \geq n$. If $\mu = \mathcal{N}(m_0, \Sigma_0)$ and $\nu = \mathcal{N}(m_1, \Sigma_1)$ are two Gaussian measures on $\mathbb{R}^m$ and $\mathbb{R}^n$, and $(P_0, D_0)$ and $(P_1, D_1)$ are the respective diagonalizations of $\Sigma_0(= P_0D_0P_0^T)$ and $\Sigma_1(= P_1D_1P_1^T)$ which sort the eigenvalues in decreasing order, an optimal transport plan which achieves $GGW_2(\mu, \nu)$ is of the form $\pi^* = (I_m, T)\#\mu$ with

$$\forall x \in \mathbb{R}^m, \quad T(x) = m_1 + P_1AP_1^T(x - m_0), \quad (5.15)$$

where $A \in \mathbb{R}^{n \times m}$ is of the form

$$A = \begin{pmatrix} I_{r_1}&(D_1^{(r_1)})^\frac{1}{2}(D_0^{(r_1)})^{-\frac{1}{2}}&0_{n-r_1,m-r_1} \\ 0_{n-r_1,r_1}&0_{n-r_1,m-r_1} & \end{pmatrix},$$

where $I_{r_1}$ is any matrix of the form $\text{diag}((\pm 1)_{i \leq r_1})$.

### 6 Behavior of the empirical solution

In this section, we perform a simple experiment to illustrate the behavior of the solution of the Gromov Wasserstein problem. In this experiment, we draw independently $k$ samples $(X_j)_{j \leq k}$ and $(Y_i)_{i \leq k}$ from respectively $\mu = \mathcal{N}(0, \text{diag}(\alpha))$ and $\nu = \mathcal{N}(0, \text{diag}(\beta))$ with $\alpha \in \mathbb{R}^m$ and $\beta \in \mathbb{R}^n$. Then we compute the Gromov-Wasserstein distance between the two histograms $X$ and $Y$ with the algorithm proposed in [19] using the Python Optimal Transport library. In Figure 5, we plot the first coordinates of the samples $Y_i$ in function of the first coordinate of the samples $X_j$ they have been assigned to by the algorithm (blue dots). We draw also the line of equation $y = \pm \sqrt{3}x$ to compare with the theoretical solution of the Gaussian restricted problem (orange line) for $k = 2000$, $\alpha = (1,0,1)^T$ and $\beta = 2$ (top left), $k = 2000$, $\alpha = (1,0.1)^T$ and $\beta = (2,0.3)^T$ (top right), $k = 2000$, $\alpha = (1,0.1,0.01)^T$ and $\beta = 2$ (middle right), $k = 7000$, $\alpha = (1,0.3)$ and $\beta = 2$ (bottom right). Observe that the empirical solution seems to be behaving exactly in the same way as the theoretical solution exhibited in Theorem 4.1 as soon as $\alpha$ and $\beta$ are close to be collinear. However, when $\alpha$ and $\beta$ are further away from collinearity, determining the behavior of the empirical solution becomes more complex. Solving Gromov-Wasserstein numerically, even approximately, is a particularly hard task, therefore we cannot conclude if the empirical solution does not behave in the same way as the theoretical solution exhibited in theorem 4.1 or if the algorithm has not converged in these more complex cases. This second assumption seems to be more likely because it seems that increasing the number of points $k$ reduces the gap between the blue dots and the orange line. Thus, we conjecture that the optimal plan which achieves $GGW_2(\mu, \nu)$ is also solution of the non-restricted problem $GW_2(\mu, \nu)$ and that $GW_2(\mu, \nu) = GGW_2(\mu, \nu)$.

### 7 Conclusion

In this paper, we have exhibited lower and upper bounds for the Gromov-Wasserstein distance (with a squared ground distance) between Gaussian measures living on different Euclidean spaces. We have also studied the tightness of the provided bounds, both theoretically and numerically. The upper bound is obtained through the study of the problem with the additional restriction that the optimal plan itself is Gaussian. We have shown that this particular case has a very simple closed-form solution,

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<sup>3</sup>The library is accessible here: https://pythonot.github.io/index.html
Gromov-Wasserstein Distance between Gaussian Distributions

Figure 5: plot of the first coordinate of samples $Y_i$ in function of the the first coordinate of their assigned samples $X_j$ (blue dots) and line of equation $y = \pm \sqrt{\beta} x$ (orange line) for $k = 2000$, $\alpha = (1, 0.1)^T$ and $\beta = 2$ (top left), $k = 2000$, $\alpha = (1, 0.1)^T$ and $\beta = (2, 0.3)^T$ (top right), $k = 2000$, $\alpha = (1, 0.1, 0.01)^T$ and $\beta = 2$ (middle left), $k = 7000$, $\alpha = (1, 0.3)$ and $\beta = 2$ (middle right), $k = 7000$, $\alpha = (1, 0.1)^T$, and $\beta = (2, 1)^T$ (bottom left), and $k = 7000$ and $\alpha = (1, 0.3, 0.1)$ and $\beta = 2$ (bottom right).

which can be described as first performing PCA on both distributions and then deriving the optimal linear plan between these aligned distributions. We conjecture that the linear solution exhibited when adding this restriction might also be the solution of the unconstrained problem.
8 Appendix: proof of the lemmas

8.1 Proof of Lemma 3.2

Proof. The proof is inspired from the proof of Equation (1.4) provided in [13]. We want to maximize \( \text{tr}(K^T K) \) with the constraint that \( \Sigma \) is semi-definite positive. Let \( S = \Sigma_1 - K^T \Sigma_0^{-1} K \) (Schur complement). Problem (3.3) can be written in the following way

\[
\min_{S \in S_n^+(\mathbb{R})} -\text{tr}(K^T K). \tag{8.1}
\]

For a given \( S \), the set of feasible \( K \) is the set of \( K \) such that \( K^T \Sigma_0^{-1} K = \Sigma_1 - S \). Since \( \Sigma_0 \in S_m^+(\mathbb{R}) \), \( K^T \Sigma_0^{-1} K \in S_n^+(\mathbb{R}) \) and so \( \Sigma_1 - S \in S_n^+(\mathbb{R}) \). We note \( r \) the rank of \( K^T \Sigma_0^{-1} K \). One can observe that

\[
r \leq n \leq m,
\]

where the left-hand side inequality follows from the fact that \( \text{rk}(AB) \leq \min\{\text{rk}(A), \text{rk}(B)\} \). Then, \( \Sigma_1 - S \) can be diagonalized

\[
\Sigma_1 - S = K^T \Sigma_0^{-1} K = U \Lambda^2 U^T = U_r \Lambda_r^2 U_r^T, \tag{8.2}
\]

with \( \Lambda^2 = \text{diag}(\lambda_1^2, \ldots, \lambda_r^2, 0, \ldots, 0) \), \( \Lambda_r^2 = \text{diag}(\lambda_1^2, \lambda_2^2) \), and \( U_r \in \mathcal{V}_r(\mathbb{R}^n) := \{ M \in \mathbb{R}^{n \times r} | M^T M = I_r \} \) (Stiefel Manifold [15]) such that \( U = \begin{pmatrix} U_r & U_{n-r} \end{pmatrix} \). From (8.2), we can deduce that

\[
(\Sigma_0^{-\frac{1}{2}} K U_r \Lambda_r^{-1})^T \Sigma_0^{-\frac{1}{2}} K U_r \Lambda_r^{-1} = I_r. \tag{8.3}
\]

We can set \( B_r = \Sigma_0^{-\frac{1}{2}} K U_r \Lambda_r^{-1} \) such that \( B_r \in \mathcal{V}_r(\mathbb{R}^m) \). One can deduce that

\[
K U_r = \Sigma_0^{\frac{1}{2}} B_r \Lambda_r.
\]

Moreover, since \( U_m^T K^T \Sigma_0^{-1} K U_m = 0 \) and \( \Sigma_0 \in S_m^+(\mathbb{R}) \), it follows that \( K U_{n-r} = 0 \) and so

\[
K = K U U^T = K U_r U_r^T = \Sigma_0^{\frac{1}{2}} B_r \Lambda_r U_r^T. \tag{8.4}
\]

We can write \( \text{tr}(K^T K) \) as a function of \( B_r \):

\[
\text{tr}(K^T K) = \text{tr}(U_r \Lambda_r B_r^T \Sigma_0 B_r \Lambda_r U_r^T) = \text{tr}(U_r U_r \Lambda_r B_r^T \Sigma_0 B_r \Lambda_r) = \text{tr}(\Lambda_r^2 B_r^T \Sigma_0 B_r), \tag{8.5}
\]

Thus, for a given \( S \), the set of \( K \) such that \( K^T \Sigma_0^{-1} K = \Sigma_1 - S \) is parametrized by the \( r \)-frame \( B_r \). We want to find \( B_r \) which maximizes \( \text{tr}(K^T K) \) for a given \( S \). This problem can be rewritten:

\[
\min_{B_r \in \mathcal{V}_r(\mathbb{R}^m)} -\text{tr}(\Lambda_r^2 B_r^T \Sigma_0 B_r). \tag{8.6}
\]

The following is a readaptation of the proof of the Proposition (3.1) in [2] when \( B_r \) is not a squared matrix. The Lagrangian of problem (8.6) can be written

\[
\mathcal{L}(B_r, C) = -\text{tr}(\Lambda_r^2 B_r^T \Sigma_0 B_r) + \text{tr}(C(B_r^T B_r - I_r)),
\]

where \( C \in S_r(\mathbb{R}) \) is the Lagrange multiplier associated to the constraint \( B_r^T B_r = I_r \) (\( C \) is symmetric because \( B_r^T B_r - I_r \) is symmetric). We can then derive the first-order condition

\[
-2\Sigma_0 B_r \Lambda_r^2 + 2 B_r C = 0,
\]
or equivalently
\[ \Sigma_0 B_r \Lambda_r^2 B_r^T = B_r C B_r^T. \] (8.7)

Since \( C \in S_r(\mathbb{R}) \), \( B_r C B_r^T \in S_m(\mathbb{R}) \) and \( \Sigma_0 B_r \Lambda_r^2 B_r^T \in S_m(\mathbb{R}) \). We can deduce that \( \Sigma_0 \) and \( B_r \Lambda_r B_r^T \) commute. Moreover, since \( \Sigma_0 \) and \( B_r \Lambda_r^2 B_r^T \) are both symmetric, they can be diagonalized in the same basis. Since \( B_r \in \mathcal{V}_r(\mathbb{R}^m) \), it can be seen as the \( r \) first vectors of an orthogonal basis of \( \mathbb{R}^m \). It means there exists a matrix \( B_{m-r} \) such that
\[ B_r \Lambda_r^2 B_r^T = B \Lambda_m B^T, \]
where \( \Lambda_m \in \mathbb{R}^{m \times m} = \text{diag}(\lambda_1^2, ..., \lambda_r^2, 0, ..., 0) \) and \( B = (B_r \ B_{m-r}) \). Thus the eigenvalues of \( B_r \Lambda_r^2 B_r^T \) are exactly the eigenvalues of \( \Lambda_m \). Since \( \Sigma_0 \) and \( B_r \Lambda_r^2 B_r^T \) can be diagonalized in the same basis, we get that \( \text{tr}(\Lambda_r^2 B_r^T \Sigma_0 B_r) = \text{tr}(\Sigma_0 B_r \Lambda_r^2 B_r^T) = \text{tr}(D_0 \tilde{\Lambda}_m) \) where \( \tilde{\Lambda}_m \) is a diagonal matrix with the same eigenvalues as \( \Lambda_m \), but in a different order. Now, it can be easily seen that the optimal value of (8.6) is reached when \( B_r \) is a permutation matrix which sorts the eigenvalues of \( \Lambda_m \) in decreasing order.

Thus, for a given \( S \), the maximum value of \( \text{tr}(K^T K) \) is \( \text{tr}(D_0 \tilde{\Lambda}_m(S)) \). We can now establish for which \( S \), \( \text{tr}(D_0 \tilde{\Lambda}_m(S)) \) is optimal. For a given \( S \), we denote \( \lambda_1, ..., \lambda_n \) the eigenvalues of \( \Sigma_1 - S \) and \( \beta_1, ..., \beta_n \) the eigenvalues of \( \Sigma_1 \) ordered in decreasing order. Since \( S \in S_n^+(\mathbb{R}) \), \( \forall x \in \mathbb{R}^n \), the following inequality holds:
\[ x^T (\Sigma_1 - S) x \leq x^T \Sigma_1 x. \] (8.8)

This inequality still holds when restricted to any subspace of \( \mathbb{R}^n \). Using the Courant-Fischer theorem, we can conclude that:
\[ \forall i \leq n, \quad \lambda_i \leq \beta_i. \] (8.9)

Thus, the optimal value of \( \text{tr}(D_0 \tilde{\Lambda}_m(S)) \) is reached when \( S = 0 \) and \( \tilde{\Lambda}_m(0) = \left( \begin{array}{cc} D_1 & 0 \\ 0 & 0 \end{array} \right) \) and so
\[ \text{tr}(D_0 \tilde{\Lambda}_m(0)) = \text{tr}(D_0(n) D_1). \]
Let \( A = \left( \begin{array}{c c c c} \mathcal{I}_n(D_0(n)) \mathcal{I}_n(D_0(n)) & \mathcal{I}_n(D_0(n)) \\ 0_{m-n,n} & 0 \end{array} \right) \) with \( \mathcal{I}_n \) of the form \( \text{diag}((\pm 1)_{i \leq n}) \). It can be easily verified that \( A^T D_0^{-1} A = D_1 \) and if \( K^* = P_0^T AP_1 \), \( K^* \Sigma_0^{-1} K^* = P_1^T A^T P_0 \Sigma_0^{-1} P_0^T A P_1 \). Dressing \( P^T A \) as \( \text{tr}(A^T A) = \text{tr}(D_0(n) D_1) \).

**8.2 Proof of Lemma 3.3**

In order to prove lemma 3.3 we will use the following lemma, demonstrated by Antreicher and Wolkowicz [2].

**Lemma 8.1.** (Antreicher and Wolkowicz, 1998, [2]) Let \( \Sigma_0 \) and \( \Sigma_1 \) be two symmetric matrices of size \( n \). We note \( \Sigma_0 = P_0 \Lambda_0 P_0^T \) and \( \Sigma_1 = P_1 \Lambda_1 P_1^T \) there respective diagonalization such that the eigenvalues of \( \Lambda_0 \) are sorted in non-increasing order and the eigenvalues of \( \Lambda_1 \) are sorted in increasing order. Then
\[ \min_{P P^T = I_n} \text{tr}(\Sigma_0 P \Sigma_1 P^T) = \text{tr}(\Lambda_0 \Lambda_1), \] (8.10)
and it is achieved for \( P^* = P_0 P_1^T \).

**Proof of Lemma 3.3** We proceed in the same way as before: first, we derive the expression of the optimal value for a given \( S = \Sigma_1 - K_T \Sigma_0^{-1} K \), then we determine for which \( S \) this expression is maximum. The start of the proof is exactly the same as the proof of [3.2] until formula [3.4]. We diagonalize \( \Sigma_1 - S = K_T \Sigma_0^{-1} K = U_r \Lambda_r U_r^T \) where \( r \) is the rank of \( K_T \Sigma_0^{-1} K \), then we set \( B_r = \Sigma_0^{-\frac{1}{2}} K U_r \Lambda_r^{-1} \) while observing that \( B_r \in \mathcal{V}_r(\mathbb{R}^m) \) and we deduce that \( K = \Sigma_0^{-\frac{1}{2}} B_r \Lambda_r U_r^T \). By reinjecting this expression, it follows that
\[ \text{tr}(KA) = \text{tr}(A^T K^T) = \text{tr}(A^T U_r \Lambda_r B_r^T \Sigma_0^{\frac{1}{2}}) = \text{tr}(\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r B_r^T). \] (8.11)
For a given $S$, the problem of finding the optimal value is parametrized by $B_r$ and is:

$$\min_{B_r \in \mathcal{V}_r(\mathbb{R}^m)} -\text{tr}(\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r B_r^T).$$  

(8.12)

The Lagrangian of this problem can be written:

$$\mathcal{L}(B_r, C) = -\text{tr}(\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r B_r^T) + \text{tr}(C(B_r^T B_r - I_r)),$$  

(8.13)

where $C \in S_r(\mathbb{R})$ is the Lagrangian multiplier associated to the constraint $B_r^T B_r = I_r$. We can then derive the first-order condition:

$$-\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r + 2B_r C = 0,$$

or equivalently:

$$\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r B_r^T = 2B_r C B_r^T.$$  

Since $C \in S_r(\mathbb{R})$, $2B_r C B_r^T \in S_m(\mathbb{R})$ and $\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r \in S_m(\mathbb{R})$, moreover, the rank of $\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r B_r^T$ is equal to 1 because $\text{rk}(A) = 1$ and $\text{rank}(\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r B_r^T) = 0$ would imply that $\text{tr}(KA) = 0$, which cannot be the maximum value of our problem. So there exists a vector $u_m \in \mathbb{R}^m$ such that:

$$\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r B_r^T = u_m u_m^T.$$  

(8.14)

Then we can reinject the value $B_r$ in the expression:

$$\Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r B_r^T = \Sigma_0^{\frac{1}{2}} A^T U_r \Lambda_r \Lambda_r^{-1} U_r^T K^T \Sigma_0^{-\frac{1}{2}}$$

$$= \Sigma_0^{\frac{1}{2}} A^T U_r U_r^T K^T \Sigma_0^{-\frac{1}{2}}$$

$$= \Sigma_0^{\frac{1}{2}} A^T K^T \Sigma_0^{-\frac{1}{2}},$$  

(8.15)

where we used the fact that $K = KUU^T = KU_r U_r^T$ because $KU_{n-r} = 0$. We have so on one hand:

$$\text{tr}(KA) = \text{tr}(\Sigma_0^{\frac{1}{2}} A^T K^T \Sigma_0^{-\frac{1}{2}}) = \text{tr}(u_m u_m^T) = u_m^T u_m,$$  

(8.16)

and on the other hand:

$$\Sigma_0^{\frac{1}{2}} A^T K^T \Sigma_0^{-\frac{1}{2}} (\Sigma_0^{\frac{1}{2}} A^T K^T \Sigma_0^{-\frac{1}{2}})^T = \Sigma_0^{\frac{1}{2}} A^T K^T \Sigma_0^{-1} KA \Sigma_0^{\frac{1}{2}}$$

$$= \Sigma_0^{\frac{1}{2}} A^T (\Sigma_1 - S) A \Sigma_0^{\frac{1}{2}}$$

$$= u_m^T u_m u_m^T u_m$$

$$= u_m^T u_m,$$  

(8.17)

and thus

$$\text{tr}(\Sigma_0^{\frac{1}{2}} A^T (\Sigma_1 - S) A \Sigma_0^{\frac{1}{2}}) = u_m^T u_m \text{tr}(u_m u_m^T) = (u_m^T u_m)^2 = (\text{tr}(KA))^2.$$  

(8.18)

Then we will determine for which $S$, $\text{tr}(\Sigma_0^{\frac{1}{2}} A^T (\Sigma_1 - S) A \Sigma_0^{\frac{1}{2}})$ is maximum:

$$\text{tr}(\Sigma_0^{\frac{1}{2}} A^T (\Sigma_1 - S) A \Sigma_0^{\frac{1}{2}}) = \text{tr}(A \Sigma_0 A^T (\Sigma_1 - S))$$

$$= \text{tr}(A \Sigma_0 A^T \Sigma_1) - \text{tr}(A \Sigma_0 A^T S).$$  

(8.19)

Let $B = A \Sigma_0 A^T$. We can observe that $B \in S_n^+(\mathbb{R})$ with rank 1. Moreover, since $S \in S_n^+(\mathbb{R})$, it can be diagonalized, and we denote $S = PDP^T$. As before, we will first determine the value of $\text{tr}(BS)$ for a given $D$, then we will determine which $D$ minimizes $\text{tr}(BS)$. For a given $D$, we want the optimal value of

$$\min_{P^T P = I_n} \text{tr}(BPDP^T).$$  

(8.20)
Since $B$ is symmetric with rank 1, it has only one non null eigenvalue which is equal to its trace. Using Lemma 8.1, we can deduce that

$$\min_{PP^T=I_n} \text{tr}(BPDP^T) = \text{tr}(B) \lambda_n,$$

(8.21)

where $\lambda_n$ is the smallest eigenvalue of $D$. Since $S \in S^+_n(\mathbb{R})$, the smallest possible value for $\lambda_n$ is 0.

If $\Sigma_0 = \text{diag}(\alpha)$, $\Sigma_1 = \text{diag}(\beta)$, it can be easily seen that $\text{tr}(I_{n,m}I_{n,m}^T\Sigma_1) = \text{tr}(\Sigma_0)\text{tr}(\Sigma_1)$. Thus, if $K = \frac{\alpha \beta^T}{\text{tr}(\Sigma_0)\text{tr}(\Sigma_1)} = \frac{\Sigma_0\Sigma_1}{\text{tr}(\Sigma_0)\text{tr}(\Sigma_1)}$, we can observe that

$$\text{tr}(K_{n,m}) = \text{tr}(I_{n,m}K) = \frac{\text{tr}(I_{n,m}\Sigma_0\Sigma_1)}{\text{tr}(\Sigma_0)\text{tr}(\Sigma_1)} = \frac{\text{tr}(\Sigma_0)\text{tr}(\Sigma_1)}{\text{tr}(\Sigma_0)\text{tr}(\Sigma_1)},$$

(8.22)

Now we must show that $S = \Sigma_1 - K^T\Sigma_0^{-1}K \in S^+_n(\mathbb{R})$. To do so, we will show that $\forall i \leq n$, the determinant of the principal minor $S^{(i)}$ is positive. We can derive that

$$S = \Sigma_1 - \frac{\beta}{\text{tr}(\Sigma_0)\text{tr}(\Sigma_1)}\Sigma_0^{-1}\alpha \beta^T = \Sigma_1 - \frac{\beta}{\text{tr}(\Sigma_0)\text{tr}(\Sigma_1)}\Sigma_0\Sigma_1 = \Sigma_1 - \frac{\beta}{\text{tr}(\Sigma_1)}\Sigma_1.$$

(8.23)

Using the matrix determinant lemma, it follows that

$$\forall i \leq n, \ \det(S^{(i)}) = \prod_k \beta_k \left(1 - \frac{\text{tr}(\Sigma_1^{(i)})}{\text{tr}(\Sigma_1)}\right).$$

(8.24)

Thus, $\forall i < n$, $\det(S^{(i)}) > 0$, and $\det(S) = 0$. We conclude that $S \in S^+_n(\mathbb{R})$ and the smallest eigenvalue of $S$ is 0. \hfill \Box

8.3 Proof of Lemma 3.4

Proof. for any $i \leq m$ and any $j \leq n$, the Cauchy-Schwarz inequality tells us that

$$|\text{Cov}(X_i, Y_j)| \leq \sqrt{\mathbb{E}[X_i^2]\mathbb{E}[Y_j^2]},$$

(8.25)

with equality if and only if $Y_j = \lambda X_i$ with $\lambda \in \mathbb{R}$. If $\text{Cov}(X, Y)$ is of the form $(\hat{I}_nD_0^{(n)}D_1^T)$, then

$$\forall i \leq n, \ |\text{Cov}(X_i, Y_i)| = \sqrt{\alpha_i\beta_i},$$

(8.26)

where $\alpha_i = \mathbb{E}[X_i^2]$ and $\beta_i = \mathbb{E}[Y_i^2]$. Thus, for all $i \leq n$, $Y_i = \lambda_i X_i$ with $\lambda_i \in \mathbb{R}$. Since $X_i \sim \mathcal{N}(0, \alpha_i)$ and $Y_i \sim \mathcal{N}(0, \beta_i)$, it follows that $\lambda_i = \pm \sqrt{\frac{\beta_i}{\alpha_i}}$ and that

$$Y = \left(\hat{I}_nD_1^T(D_0^{(n)})^{-\frac{1}{2}}0_{n,m-n}\right)X.$$

(8.27)

Since $Y$ depends linearly on $X$, it follows that $(X, Y)$ is a Gaussian vector. Thus, using Isserlis Lemma, we can compute that

$$\text{Cov}(X_i^2, Y_j) = \begin{cases} 2\alpha_i\beta_i & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

(8.28)

So that $\sum_{i,j} \text{Cov}(X_i^2, Y_j) = 2\text{tr}(D_0^{(n)}D_1)$. \hfill \Box
8.4 Proof of Lemma 5.1

**Proof.** For $m \geq 1$, let $\Gamma_{m}$ denote the set of vectors $v = (v_{1}, \ldots, v_{m})$ of $\mathbb{R}^{m}$ such that $v_{1} \geq v_{2} \geq \ldots \geq v_{m} \geq 0$ and $\sum_{i=1}^{m} v_{i}^{2} = 1$. We want to prove that

$$
\forall u, v \in \Gamma_{m}, \quad \sum_{i=1}^{m} u_{i}v_{i} \geq \frac{1}{\sqrt{m}}.
$$

We proceed by induction on $m$. For $m = 1$, it’s obviously true since $\Gamma_{1} = \{1\}$. Assume now $m > 1$, and the result true for $m - 1$. Let $u, v \in \Gamma_{m}$, then using the result for $(u_{2}, \ldots, u_{m})/(\sum_{i=2}^{m} u_{i}^{2})^{1/2}$ and $(v_{2}, \ldots, v_{m})/(\sum_{i=2}^{m} v_{i}^{2})^{1/2}$ that both belong to $\Gamma_{m-1}$, we have

$$
\sum_{i=1}^{m} u_{i}v_{i} = u_{1}v_{1} + \sum_{i=2}^{m} u_{i}v_{i} \geq u_{1}v_{1} + \frac{1}{\sqrt{m-1}} \left( \sum_{i=2}^{m} u_{i}^{2} \right)^{1/2} \left( \sum_{i=2}^{m} v_{i}^{2} \right)^{1/2}
$$

$$
= u_{1}v_{1} + \frac{1}{\sqrt{m-1}} \sqrt{1 - u_{1}^{2}} \sqrt{1 - v_{1}^{2}}.
$$

Now since $u, v \in \Gamma_{m}$, we have $u_{1}, v_{1} \in [\frac{1}{\sqrt{m}}, 1]$. Let us denote $F(u_{1}, v_{1}) = u_{1}v_{1} + \frac{1}{\sqrt{m-1}} \sqrt{1 - u_{1}^{2}} \sqrt{1 - v_{1}^{2}}$.

We have for all $v_{1} \in [\frac{1}{\sqrt{m}}, 1] :

$$
F(1, v_{1}) = v_{1} \geq \frac{1}{\sqrt{m}} \quad \text{and} \quad F\left(\frac{1}{\sqrt{m}}, v_{1}\right) = \frac{\sqrt{1 - v_{1}^{2}} + v_{1}}{\sqrt{m}} \geq \frac{1 - v_{1}^{2} + v_{1}}{\sqrt{m}} \geq \frac{1}{\sqrt{m}}.
$$

And computing the partial derivative of $F$ with respect to $u_{1}$, we get

$$
\frac{\partial F}{\partial u_{1}}(u_{1}, v_{1}) = v_{1} - \frac{u_{1} \sqrt{1 - v_{1}^{2}}}{\sqrt{m-1} \sqrt{1 - u_{1}^{2}}}.
$$

This is a decreasing function of $u_{1}$, with value $v_{1}$ at $u_{1} = 0$ and value that goes to $-\infty$ when $u_{1}$ goes to 1. Therefore the function $F(\cdot, v_{1})$ on $[0, 1]$ is first increasing and then decreasing, showing that

$$
\forall u_{1} \in [\frac{1}{\sqrt{m}}, 1], \quad F(u_{1}, v_{1}) \geq \min \left( F\left(\frac{1}{\sqrt{m}}, v_{1}\right), F(1, v_{1}) \right) \geq \frac{1}{\sqrt{m}}.
$$

Finally we thus have proved that

$$
\sum_{i=1}^{m} u_{i}v_{i} \geq \frac{1}{\sqrt{m}},
$$

and moreover the equality is achieved when the vectors $u$ and $v$ are the vectors $(1, 0, \ldots, 0)$ and $(\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}, \ldots, \frac{1}{\sqrt{m}})$.

\[\square\]

References


