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Luigi Malagò
Montrucchio
Giovanni Pistone

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Wasserstein Riemannian Geometry of Positive-definite Matrices*

Luigi Malagò[†], Luigi Montrucchio[‡], and Giovanni Pistone[§]

Abstract. The Wasserstein distance on multivariate non-degenerate Gaussian densities is a Riemannian distance. After reviewing the properties of the distance and the metric geodesic, we derive an explicit form of the Riemannian metrics on positive-definite matrices and compute its tensor form with respect to the trace scalar product. The tensor is a matrix, which is the solution of a Lyapunov equation. We compute explicit form for the Riemannian exponential, the normal coordinates charts, the Riemannian gradient, and discuss the gradient flow of the entropy. Finally, the Levi-Civita covariant derivative is computed in matrix form together with the differential equation for the parallel transport. While all computations are given in matrix form, nonetheless we discuss the use of a special moving frame. Applications are briefly discussed.

Key words. Gaussian distribution, Wasserstein distance, Riemannian metrics, Natural gradient, Riemannian Exponential, Normal coordinates, Levi-Civita covariant derivative, Optimization on positive-definite symmetric matrices, Information Geometry.

AMS subject classifications. 15B48, 53C23, 53C25, 60D05

1. Introduction and overview. Given two Gaussian distributions $N_n(\mu_i, \Sigma_i)$, $i = 1, 2$, consider the Gaussian vector (X_1, X_2) where each block has an assigned distribution. The use of the number

$$(1) \quad G^2 = \inf \mathbb{E} \left(\|X_1 - X_2\|^2 \right)$$

as an index of dissimilarity between distributions has been considered by many classical authors, C. Gini (1914), P. Levy, and M. R. Fréchet. There is a considerable contemporary literature on this problem, where the index is called L^2 -Wasserstein distance and it is discussed in general, outside our special case of Gaussian distributions. Among the literature most relevant for the approach used in this paper we mention Y. Brenier [9], R. J. McCann [22], F. Otto [24]. The explicit computation of the value of W^2 is known, together with an explicit formula for the metric geodesic.

The value of the index of Eq. (1) as a function of means and dispersion matrices has been computed by some authors, in particular I. Olkin and F. Pukelsheim [23], D. C. Dowson and B. V. Landau [12], C. R. Givens and R. M. Shortt [15], M. Gelbrich [14], R. Bhatia et al. [8].

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[†]Romanian Institute of Science and Technology (malago@rist.ro).

[‡]Collegio Carlo Alberto, Piazza Vincenzo Arbarello 8, 10122 Torino, Italy (luigi.montrucchio@unito.it).

[§]de Castro Statistics, Collegio Carlo Alberto, Piazza Vincenzo Arbarello 8, 10122 Torino, Italy (giovanni.pistone@carloalberto.org).

They found

$$(2) \quad G^2 = \|\mu_1 - \mu_2\|^2 + \text{Tr} \left(\Sigma_1 + \Sigma_2 - 2 \left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \right)$$

$$(3) \quad = \|\mu_1 - \mu_2\|^2 + \text{Tr} \left(\Sigma_1 + \Sigma_2 - 2 (\Sigma_1 \Sigma_2)^{1/2} \right) .$$

The W^2 index is actually the square of a distance, hence a measure of divergence between distribution. We can mimic the argument of a famous paper by Amari [3], which derives the notion of both Fisher metric and natural gradient from the second-order approximation of the Kullback-Leibler divergence. In fact, we show that for small H such that the divergence of $\Sigma + H$ and Σ is constant it holds

$$(4) \quad \text{Tr} \left(\Sigma + (\Sigma + H) - 2 \left(\Sigma^{1/2} (\Sigma + H) \Sigma^{1/2} \right)^{1/2} \right) \simeq \frac{1}{2} \text{Tr} (\mathcal{L}_\Sigma [H] H) ,$$

where $\mathcal{L}_\Sigma [H] \Sigma + \Sigma \mathcal{L}_\Sigma [H] = H$. According to a standard argument, for any smooth function f , as $H \rightarrow 0$, the increment $f(\Sigma + H) - f(\Sigma)$ is maximized in the direction

$$(5) \quad \text{grad } f(\Sigma) = \nabla f(\Sigma) \Sigma + \Sigma \nabla f(\Sigma) .$$

The quadratic form in Eq. (4) is the natural candidate for the Riemannian metric associated to the given distance and the gradient in Eq. (5) is the natural gradient.

The fact that the distance L^2 -Wasserstein geometry is actually Riemannian on a suitable subset of distribution has been stated in general in [24, §4] and has been developed in the Gaussian case by A. Takatsu [27]. In the present paper, we proceed along these lines by deriving explicit forms of the Riemannian metrics, the Riemannian exponential, and the Levi-Civita (covariant) derivative, Riemannian parallel transport, and the Riemannian Hessian. The perspective is dictated by the authors' interests in Machine Learning, Manifold Optimization, and Information Geometry. Further relevant, more technical, references are cited in the text when needed.

1.1. Overview. In Sec. 2 we review the properties of the space of symmetric matrices we are going to use in particular, the trace norm, Riccati equation, Lyapunov equation, and the calculus of the mapping $\sigma: A \mapsto AA^*$, where A is a non-singular square matrix.

The set of positive-definite matrices is seen as an elementary manifold, as it is an open set of an Euclidean space. In this context, the mapping σ is a submersion and we compute horizontal vectors at each point. The manifold we deal with is finite dimensional. However, all operations of interest being matrix operations, there is no need of choosing a basis, so we use the language of non-parametric differential geometry of W. Klingenberg [17] and S. Lang [18]. A short review of the matrix algebra we need is given in Sec. 2

In Sec. 3 we review for reference purposes well-known results about the metric geometry induced by the dissimilarity index. We re-state the result as Prop. 3.2 and, for sake of completeness, we provide in Appendix a further proof inspired by [12]. The index itself turns out to be a distance. Its value is attained on a joint degenerate distribution, and, it is possible to write down an explicit metric geodesic, if the distributions at end-points are not both

singular. This has been done by R. J. McCann [22, Example 1.7] and it is restated as Prop. 3.4.

The space of nondegenerate Gaussian measures (or, equivalently, the space of positive definite matrices) can be endowed with a Riemann structure that induces the L^2 -Wasserstein distance. This is discussed in Sec. 4. We use the presentation given by in [27], cf. also [8], which in turn adapts to the Gaussian case the original work [24, §4]. We add a detailed explanation of the “coordinate system” associated with the Riemannian geometry. We show that the Wasserstein Riemannian metrics is given at each dispersion matrix Σ by

$$(6) \quad W_{\Sigma}(U, V) = \text{Tr}(\mathcal{L}_{\Sigma}[U] \Sigma \mathcal{L}_{\Sigma}[V]) = \frac{1}{2} \text{Tr}(\mathcal{L}_{\Sigma}[U] V) ,$$

where U, V are symmetric matrices and $\mathcal{L}_{\Sigma}[U]$ is the solution X of the matrix equation $X\Sigma + \Sigma X = U$.

The form of the Riemannian exponential is derived in Sec. 5. The natural gradient and some applications to optimization and the example of the gradient flow of the entropy are discussed in Sec. 6.

The analysis of the second-order geometry is treated in Sec. 7, where we compute the Levi-Civita covariant derivative, the Riemannian Hessian, and other related topics.

2. Symmetric matrices. Given a mean vector $\mu \in \mathbb{R}^n$ and a symmetric $n \times n$ non-negative definite dispersion matrix $\Sigma \in \text{Sym}^+(n)$, there exists a unique Gaussian distribution on \mathbb{R}^n , denoted $N_n(\mu, \Sigma)$, with the given parameters, and conversely. The set \mathcal{G}^n of Gaussian distributions on \mathbb{R}^n is in 1-to-1 correspondence with the space of its parameters,

$$(7) \quad \mathcal{G}^n \ni N_n(\mu, \Sigma) \leftrightarrow (\mu, \Sigma) \in \mathbb{R}^n \times \text{Sym}^+(n) .$$

Moreover, \mathcal{G}^n is closed for weak convergence and the identification is continuous in both directions. A reference for Gaussian distributions is T. W. Anderson [5].

For ease of later reference, we review below a few results on spaces of matrices. General references are the monographs by P. R. Halmos [16], J. R. Magnus and H. Neudecker [19], and R. Bhatia [7].

The vector space of $n \times m$ real matrices is denoted by $M(n \times m)$, while square matrices are denoted $M(n) = M(n \times n)$. It is an Euclidean space of dimension nm and the vectorization mapping $M(n \times m) \ni A \mapsto \text{vec}(A) \in \mathbb{R}^{nm}$ is an isometry, $\langle A, B \rangle = (\text{vec}(A))^*(\text{vec}(B)) = \text{Tr}(AB^*)$. The norm is denoted by $\|A\| = \sqrt{\text{Tr}(AA^*)}$.

Symmetric matrices $\text{Sym}(n)$ form a vector subspace of $M(n)$ whose orthogonal complement is the vector space of anti-symmetric matrices $\text{Sym}^{\perp}(n)$. We will find it convenient to use, with reference to symmetric matrices, the equivalent scalar product $\langle A, B \rangle_2 = \frac{1}{2} \text{Tr}(AB^*)$ e.g., see Eq. (6).

The closed pointed cone of non-negative-definite symmetric matrices is $\text{Sym}^+(n)$ and its interior, the open cone of the positive-definite symmetric matrices, is $\text{Sym}^{++}(n)$.

Given $A, B \in \text{Sym}(n)$, the equation $TAT = B$ is called *Riccati equation*. If $A \in \text{Sym}^{++}(n)$ and $B \in \text{Sym}^+(n)$, then the equation $TAT = B$ has unique solution $T \in \text{Sym}^+(n)$. In fact, from $TAT = B$ it follows $A^{1/2}TA^{1/2}A^{1/2}TA^{1/2} = A^{1/2}BA^{1/2}$ and, in turn, $A^{1/2}TA^{1/2} =$

$(A^{1/2}BA^{1/2})^{1/2}$ because $T \in \text{Sym}^+(n)$ hence, the solution is

$$(8) \quad T = A^{-1/2} \left(A^{1/2}BA^{1/2} \right)^{1/2} A^{-1/2} .$$

Notice that $\det(T) = \det(A)^{-1/2} \det(B)^{1/2}$, hence $\det(T) > 0$ if $\det(B) > 0$. In terms of random variables, if $X \in \text{N}_n(0, A)$ and $Y = \text{N}_n(0, B)$, then T is the unique matrix in $\text{Sym}^+(n)$ such that $Y \sim TX$.

More compact closed-form solutions of the Riccati equation are available. Given $A \in \text{Sym}^{++}(n)$ and $B \in \text{Sym}^+(n)$, observe that $AB = A^{1/2}(A^{1/2}BA^{1/2})A^{-1/2}$. By similarity, we see that the eigenvalues of AB are non-negative, hence the square root

$$(9) \quad (AB)^{1/2} = A^{1/2}(A^{1/2}BA^{1/2})^{1/2}A^{-1/2}$$

is well defined, see [7, Ex. 4.5.2]. Now we can re-write Eq. (8) as

$$(10) \quad T = A^{-1}A^{1/2} \left(A^{1/2}BA^{1/2} \right)^{1/2} A^{-1/2} = A^{-1}(AB)^{1/2} .$$

As $AB = A(BA)A^{-1}$, the eigenvalues of AB and BA are the same, so that the same argument used before shows that

$$(11) \quad T = (BA)^{1/2}A^{-1} .$$

The square-of-the-matrix mapping $\sigma: A \mapsto A^2$ is an injection of $\text{Sym}^{++}(n)$ onto itself. The derivative is $d_X\sigma(A) = XA + AX$ and the derivative operator $d\sigma(A)$ is invertible. Alternative notation for the derivative we would occasionally find convenient to use are $d_X\sigma(A) = d\sigma(A)[X]$.

For each assigned matrix $V \in \text{Sym}(n)$, the matrix $X = (d\sigma(A))^{-1}V$ is the unique solution X in the space $\text{Sym}(n)$ to the *Lyapunov equation*

$$(12) \quad V = XA + AX .$$

We will write $X = \mathcal{L}_A[V]$. In the paper, we are going to use the obvious equations

$$(13) \quad V = \mathcal{L}_A[V]A + A\mathcal{L}_A[V] ,$$

$$(14) \quad X = \mathcal{L}_A[XA + AX] .$$

The Lyapunov operator itself can be seen as a derivative. In fact, the inverse of the mapping σ is $\sigma^{-1}: \Sigma \rightarrow \Sigma^{1/2}$. By the derivative-of-the-inverse rule

$$(15) \quad d_V\sigma^{-1}(\Sigma) = (d\sigma(\sigma^{-1}(\Sigma)))^{-1}[V] = \mathcal{L}_A[V] , \quad \Sigma^{1/2} = A .$$

If Σ is the dispersion of a non-singular Gaussian distribution, then $C = \Sigma^{-1} \in \text{Sym}^{++}(n)$ is the concentration matrix and represents an alternative and useful parameterization. From the Lyapunov equation $V = X\Sigma + \Sigma X$ we obtain $\Sigma^{-1}V\Sigma^{-1} = \Sigma^{-1}X + X\Sigma^{-1}$, hence

$$(16) \quad \mathcal{L}_\Sigma[V] = \mathcal{L}_{\Sigma^{-1}}[\Sigma^{-1}V\Sigma^{-1}] \quad \text{and} \quad \mathcal{L}_{\Sigma^{-1}}[U] = \mathcal{L}_\Sigma[\Sigma U \Sigma] .$$

In a similar way, we obtain another useful equation,

$$(17) \quad \mathcal{L}_\Sigma [V] = \Sigma^{-1/2} \mathcal{L}_\Sigma \left[\Sigma^{-1/2} V \Sigma^{-1/2} \right] \Sigma^{-1/2} .$$

There is a relation between the Lyapunov equation and the trace. From $X\Sigma + \Sigma X = V$, we get $\Sigma^{-1}X\Sigma + X = \Sigma^{-1}V$, then

$$(18) \quad \text{Tr} (\mathcal{L}_\Sigma [V]) = \frac{1}{2} \text{Tr} (\Sigma^{-1}V) .$$

We will need later the derivative of $A \mapsto \mathcal{L}_A [V]$ for a fixed V . We compute it by differentiating in the direction U , with respect A , the identity (13). We have

$$(19) \quad 0 = d_U \mathcal{L}_A [V] A + \mathcal{L}_A [V] U + U \mathcal{L}_A [V] + A d_U \mathcal{L}_A [V] .$$

Hence $d_U \mathcal{L}_A [V]$ is the solution to the Lyapunov equation

$$(20) \quad d_U \mathcal{L}_A [V] A + A d_U \mathcal{L}_A [V] = -(\mathcal{L}_A [V] U + U \mathcal{L}_A [V]) ,$$

so that

$$(21) \quad d_U \mathcal{L}_A [V] = -\mathcal{L}_A [\mathcal{L}_A [V] U + U \mathcal{L}_A [V]] .$$

We shall need also the second derivative of the function $\sigma^{-1}: \Sigma \mapsto \Sigma^{1/2}$. From Eq. (15) we have $d\sigma^{-1}(\Sigma)[V] = \mathcal{L}_{\Sigma^{1/2}} [V]$, then, from

$$(22) \quad d^2\sigma^{-1}(\Sigma)[U, V] = \mathcal{L}_{\Sigma^{1/2}} [\mathcal{L}_{\Sigma^{1/2}} [V] U + U \mathcal{L}_{\Sigma^{1/2}} [V]] .$$

Lyapunov equation is of crucial importance for us, as the linear operator \mathcal{L}_A enters in the expression of the Riemannian metric of interest with respect to the standard scalar product, see Eq. (6). In fact, the numerical implementation of the scalar product $W_\Sigma(U, V)$ requires the computation of the matrix $\mathcal{L}_\Sigma [U]$.

There are many ways to write down the closed-form solution to Eq. (12). The integral form solution is

$$(23) \quad \mathcal{L}_A [V] = \int_0^\infty dt e^{-tA} V e^{-tA} .$$

The vectorized form of the Lyapunov equation (12) is

$$(24) \quad \text{vec} (V) = (A \otimes I + I \otimes A) \text{vec} (X) ,$$

and so

$$(25) \quad \mathcal{L}_A [V] = \text{bind} \left((A \otimes I + I \otimes A)^{-1} \text{vec} (V) \right) .$$

A solution based on the spectral decomposition $A = O\Lambda O^*$, $\Lambda = \text{diag} (\lambda_j : j = 1, \dots, n)$ and $O^*O = I$, is computed using Hadamard's matrix product $[a_{ij}] \circ [b_{ij}] = [a_{ij}b_{ij}]$ as

$$(26) \quad O^* X O = \left[\frac{1}{\lambda_i + \lambda_j} \right]_{i,j=1}^d \circ (O^* V O) .$$

This closed form solutions are discussed in [7]. Efficient numerical solutions are not based on the closed forms above, but rely on specialized numerical algorithms as discussed by E. L. Wachspres [28] and by V. Simoncini [26].

We study now the square-of-a-matrix operation when acting on general invertible matrices. We show in the next proposition that this operation is a *submersion*. We recall the definition, see [11, Ch. 8, Ex. 8–10] or [18, §II.2]. Let \mathcal{O} be an open set of the Hilbert space H , and $f: \mathcal{O} \rightarrow \mathcal{N}$ a smooth surjection from the Hilbert space H onto a manifold \mathcal{N} , i.e., assume that for each $A \in \mathcal{O}$ the derivative at A , $df(A): H \rightarrow T_{f(A)}\mathcal{N}$ is surjective. In such a case, for each $C \in \mathcal{N}$, the fiber $f^{-1}(C)$ is a sub-manifold. Given a point $A \in f^{-1}(C)$, a vector $U \in H$ is called *vertical* if it is tangent to the manifold $f^{-1}(C)$. Each such a tangent vector U is the velocity at $t = 0$ of some smooth curve $t \mapsto \gamma(t)$ with $\gamma(0) = A$ and $\dot{\gamma}(0) = U$. Precisely, from $f(\gamma(t)) = C$ for all t we derive the characterization of vertical vectors. We have $df(A)[\dot{\gamma}(0)] = 0$ i.e., the tangent space at A is $T_A f^{-1}(f(A)) = \text{Ker}(df(A))$. The orthogonal space to the tangent space $T_A f^{-1}(f(A))$ is called the space of *horizontal* vectors at A ,

$$(27) \quad \mathcal{H}_A = \text{Ker}(df(A))^\perp = \text{Im}(df(A)^*) .$$

Let us apply the general theory to our case of interest. We denote by $\text{GL}(n) \subset \text{M}(n)$ the open set of invertible matrices; $\text{O}(n)$ is the subgroup of $\text{GL}(n)$ of orthogonal matrices; $\text{Sym}^\perp(n)$ is the subspace of $\text{M}(n)$ of anti-symmetric matrices; and $\text{Sym}^*(n) = \text{Sym}(n) \cap \text{GL}(n)$. We are going to show that the mapping

$$(28) \quad \sigma: \text{GL}(n) \ni A \mapsto AA^* \in \text{Sym}^{++}(n)$$

is indeed a submersion. The fiber $\sigma^{-1}(C) = \{A \in \text{GL}(n) \mid AA^* = C\}$ is characterized as follows. From $AA^* = C = C^{1/2}C^{1/2}$, we get

$$(29) \quad C^{-1/2}AA^*C^{-1/2} = I ,$$

hence there exists an orthogonal matrix $R = A^*C^{-1/2} \in \text{O}(n)$ such that $A = C^{1/2}R^*$. Conversely, $AA^* = C$ if $A = C^{1/2}R^*$.

Proposition 2.1. 1) For each given $A \in \text{GL}(n)$ we have the orthogonal splitting

$$(30) \quad \text{M}(n) = \text{Sym}(n) A \oplus \text{Sym}^\perp(n) (A^*)^{-1} .$$

2) The mapping

$$(31) \quad \sigma: \text{GL}(n) \ni A \mapsto AA^* \in \text{Sym}^{++}(n)$$

is a submersion with fibers

$$(32) \quad \sigma^{-1}(C) = \left\{ C^{1/2}R \mid R \in \text{O}(n) \right\}$$

and its differential at A is $d_X\sigma(A) = XA^* + AX^*$. The kernel of the differential is

$$(33) \quad \text{Ker}(d\sigma(A)) = \text{Sym}^\perp(n) (A^*)^{-1}$$

and its orthogonal complement, $\mathcal{H}_A = \text{Ker}(d\sigma(A))^\perp$, is

$$(34) \quad \mathcal{H}_A = \text{Sym}(n) A .$$

3) The orthogonal projection of $X \in \text{M}(n)$ onto \mathcal{H}_A is $\mathcal{L}_{AA^*}[XA^* + AX^*]$.

Proof. 1) Assume $\langle B, CA \rangle = 0$, for all $C \in \text{Sym}(n)$ that is, $CA \in \text{Sym}^+(A)$. Then $\text{Tr}(BA^*C) = 0$, so that $BA^* \in \text{Sym}^\perp(n)$ that is, $B \in \text{Sym}^\perp(n)(A^*)^{-1}$.

2) Consider the matrix A as a point in the fiber manifold $\sigma^{-1}(AA^*)$. The derivative of σ at A , $X \mapsto d_X\sigma(A) = XA^* + AX^*$, is surjective, because for each $W \in \text{Sym}(n)$ we have $d\sigma(A) \left[\frac{1}{2}W(A^*)^{-1} \right] = W$, hence σ is a surjection and the fiber $\sigma^{-1}(AA^*)$ is a sub-manifold of $\text{GL}(n)$. Let us compute the splitting of $M(n)$ into the kernel of $d\sigma(A)$ and its orthogonal, $M(n) = \text{Ker}(d\sigma(A)) \oplus \mathcal{H}_A$. As the vector space tangent to $\sigma^{-1}(AA^*)$ at A is the kernel of the derivative at A :

$$\begin{aligned} \text{Ker}(d\sigma(A)) &= \{X \in M(n) \mid XA^* + AX^* = 0\} \\ &= \{X \in M(n) \mid (AX^*)^* = -AX^*\}. \end{aligned}$$

Hence, $X \in \text{Ker}(d\sigma(A)) \iff AX^* \in \text{Sym}^\perp(n)$. Namely, $\text{Ker}(d\sigma(A)) = \text{Sym}^\perp(n)(A^*)^{-1}$. But we have just proved that this implies $\mathcal{H}_A = \text{Sym}(n)A$.

3) Consider the decomposition of X into the horizontal and the vertical part, $X = CA + D(A^*)^{-1}$ with $C \in \text{Sym}(n)$ and $D \in \text{Sym}^\perp(n)$. By transposition, we get $X^* = A^*C - A^{-1}D$. From the previous two equations, we obtain the two equations $XA^* = C(AA^*) + D$ and $AX^* = (AA^*)C - D$. The sum of the two previous equations is $XA^* + AX^* = C(AA^*) + (AA^*)C$, which is a Lyapunov equation. \blacksquare

3. Wasserstein distance. The aim of this section is to present the derivation of the Wasserstein distance in the Gaussian case and equation for the metric geodesic.

3.1. Block-Gaussian. Let us consider the case where the dispersion matrix $\Sigma \in \text{Sym}^+(2n)$ is partitioned into $n \times n$ blocks, we consider random variables X and Y such that

$$(35) \quad \begin{bmatrix} X \\ Y \end{bmatrix} \sim N_{2n}(\mu, \Sigma), \quad \Sigma = \begin{bmatrix} \Sigma_1 & K \\ K^* & \Sigma_2 \end{bmatrix},$$

so that $K_{ij} = \text{Cov}(X_i, Y_j)$ if $i = 1, \dots, n$ and $j = (n+1), \dots, 2n$. It follows that $K_{ij}^2 \leq (\Sigma_1)_{ii}(\Sigma_2)_{jj}$, which in turn imply the bounds

$$(36) \quad \|K\|_2^2 \leq \text{Tr}(\Sigma_1) \text{Tr}(\Sigma_2) \quad \text{and} \quad \sup_{ij} |K_{ij}| \leq \frac{1}{2}(\text{Tr}(\Sigma_1) + \text{Tr}(\Sigma_2)).$$

Assigned the mean vectors $\mu_1, \mu_2 \in \mathbb{R}^2$ and dispersion matrices $\Sigma_1, \Sigma_2 \in \text{Sym}^+(n)$, we define the set of jointly Gaussian distributions with given marginals to be

$$(37) \quad \mathcal{G}((\mu_1, \Sigma_1), (\mu_2, \Sigma_2)) = \left\{ N_{2n} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_1 & K \\ K^* & \Sigma_2 \end{bmatrix} \right) \right\},$$

and the *Gini dissimilarity index* to be

$$(38) \quad G^2((\mu_1, \Sigma_1), (\mu_2, \Sigma_2)) = \inf \left\{ \mathbb{E} \left[\|X - Y\|^2 \right] \mid \begin{bmatrix} X \\ Y \end{bmatrix} \sim \gamma, \quad \gamma \in \mathcal{G}((\mu_1, \Sigma_1), (\mu_2, \Sigma_2)) \right\} = \|\mu_1 - \mu_2\|^2 + \text{Tr}(\Sigma_1) + \text{Tr}(\Sigma_2) - 2 \sup_K \left\{ \text{Tr}(K) \mid \begin{bmatrix} \Sigma_1 & K \\ K^* & \Sigma_2 \end{bmatrix} \in \text{Sym}^+(2n) \right\}$$

Actually, because of the bound in Eq. (36), the set $\mathcal{G}((\mu_1, \Sigma_1), (\mu_2, \Sigma_2))$ is compact and the inf is attained.

It is easy to verify that the relation

$$(39) \quad G((\mu_1, \Sigma_1), (\mu_2, \Sigma_2)) = \sqrt{\min \left\{ \mathbb{E} \left[\|X - Y\|^2 \mid \begin{bmatrix} X \\ Y \end{bmatrix} \sim \gamma, \gamma \in \mathcal{G}((\mu_1, \Sigma_1), (\mu_2, \Sigma_2)) \right] \right\}}$$

defines a distance on $\mathcal{G}_n \simeq \mathbb{R}^n \times \text{Sym}^+(n)$.

Actually, the symmetry of G is clear as well as the triangle inequality is easily obtained by considering Gaussian distributions on $\mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n$ with given marginals. To conclude, assume that the min is reached at some $\bar{\gamma}$. Then

$$(40) \quad 0 = G((\mu_1, \Sigma_1), (\mu_2, \Sigma_2)) = \mathbb{E}_{\bar{\gamma}} \left[|X - Y|^2 \right] \Leftrightarrow \mu_1 = \mu_2 \quad \text{and} \quad \Sigma_1 = \Sigma_2 .$$

A further observation is that distance G is homogeneous i.e.,

$$(41) \quad G((\lambda\mu_1, \lambda^2\Sigma_1), (\lambda\mu_2, \lambda^2\Sigma_2)) = \lambda G((\mu_1, \Sigma_1), (\mu_2, \Sigma_2)), \quad \lambda \geq 0 .$$

3.2. Computing the quadratic dissimilarity index. Now we proceed to determine the Gini index for multivariate Gaussian distributions. We will present a proof as given by Dowson and Landau [12] but with some corrections.

Given $\Sigma_1, \Sigma_2 \in \text{Sym}^+(n)$, each admissible K 's in (38) belong to a compact set of $M(n)$ because of the bound (36), so the maximum of the function $2 \text{Tr}(K)$ is reached. So we are led to study:

$$(42) \quad \begin{cases} \alpha(\Sigma_1, \Sigma_2) = \max_{K \in M(n)} 2 \text{Tr}(K) \\ \text{subject to} \\ \Sigma = \begin{bmatrix} \Sigma_1 & K \\ K^* & \Sigma_2 \end{bmatrix} \in \text{Sym}^+(2n) \end{cases}$$

Similarly, the value of the min problem will be denoted by $\beta(\Sigma_1, \Sigma_2)$.

Next result provides a solution to problem (42).

Proposition 3.1. 1) Let $\Sigma_1, \Sigma_2 \in \text{Sym}^+(n)$. Then

$$(43) \quad \alpha(\Sigma_1, \Sigma_2) = 2 \text{Tr} \left(\left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \right) \quad \text{and} \quad \beta(\Sigma_1, \Sigma_2) = -\alpha(\Sigma_1, \Sigma_2) .$$

2) If moreover $\det(\Sigma_1) > 0$, then

$$(44) \quad \alpha(\Sigma_1, \Sigma_2) = 2 \text{Tr} \left((\Sigma_1 \Sigma_2)^{1/2} \right) .$$

Proof. 1) The lengthy proof is gathered in a final App. 9.1.

2) From Eq. (9) we obtain

$$(45) \quad \text{Tr} \left(\left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \right) = \text{Tr} \left(\Sigma_1^{1/2} \left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \Sigma_1^{-1/2} \right) = \text{Tr} \left((\Sigma_1 \Sigma_2)^{1/2} \right) . \quad \blacksquare$$

The following result enables us to find easily the exact lower and upper bounds of $\mathbb{E} [\|X - Y\|^2]$.

Proposition 3.2. *Let X, Y be multivariate Gaussian random variables taking values in \mathbb{R}^n and having means μ_1 and μ_2 and dispersion matrices Σ_1 and Σ_2 respectively. Then*

$$\begin{aligned} \|\mu_1 - \mu_2\|^2 + \text{Tr} \left(\Sigma_1 + \Sigma_2 - 2 \left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \right) &\leq \mathbb{E} [\|X - Y\|^2] \leq \\ &\|\mu_1 - \mu_2\|^2 + \text{Tr} \left(\Sigma_1 + \Sigma_2 + 2 \left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \right). \end{aligned}$$

If $\det \Sigma_1 \neq 0$, then the extremal values are attained at the joint distribution of

$$(46) \quad \begin{bmatrix} X \\ \mu_2 \pm T(X - \mu_1) \end{bmatrix} \sim \text{N}_{2n} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_1 & \pm T \Sigma_1 \\ \pm \Sigma_1 T & \Sigma_2 \end{bmatrix} \right) = \text{N}_{2n} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_1 & \pm (\Sigma_2 \Sigma_1)^{1/2} \\ \pm (\Sigma_1 \Sigma_2)^{1/2} & \Sigma_2 \end{bmatrix} \right),$$

respectively, where $T \in \text{Sym}^+(n)$ is the solution to the Riccati equation $T \Sigma_1 T = \Sigma_2$.

Proof. From Proposition 3.1 and Eq. (38), it follows

$$\begin{aligned} \min [\|X - Y\|^2] &= \|\mu_1 - \mu_2\|^2 + \text{Tr}(\Sigma_1) + \text{Tr}(\Sigma_2) - 2 \text{Tr} \left(\left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \right), \\ \max [\|X - Y\|^2] &= \|\mu_1 - \mu_2\|^2 + \text{Tr}(\Sigma_1) + \text{Tr}(\Sigma_2) + 2 \text{Tr} \left(\left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \right). \end{aligned}$$

To check the extremal points it suffices to observe that, in view of relation (8):

$$(47) \quad \text{Tr}(T \Sigma_1) = \text{Tr} \left(\Sigma_1^{-1/2} \left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \Sigma_1^{1/2} \right) = \text{Tr} \left(\left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \right).$$

Hence it is verified that the extremal values are attained at $Y = \mu_2 \pm T(X - \mu_1)$. In the second form of the distribution we are using Eq. (10) and Eq. (11). \blacksquare

The fact that the Gini dissimilarity is a distance which makes $\mathbb{R}^n \times \text{Sym}^+(n)$ a metric space is formally claimed in the next Proposition.

Proposition 3.3. *The relation*

$$(48) \quad G((\mu_1, \Sigma_1), (\mu_2, \Sigma_2)) = \sqrt{\|\mu_1 - \mu_2\|^2 + \text{Tr} \left(\Sigma_1 + \Sigma_2 - 2 \left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \right)}$$

defines a distance on $\mathbb{R}^n \times \text{Sym}^+(n)$.

Let us now find the geodesic in the metric space $(\mathbb{R}^n \times \text{Sym}^{++}(n), G)$.

Proposition 3.4. *The geodesic from (μ_1, Σ_1) to (μ_2, Σ_2) , with $(\mu_1, \Sigma_1), (\mu_2, \Sigma_2) \in \mathbb{R}^n \times \text{Sym}^{++}(n)$, is the curve*

$$(49) \quad \Gamma: [0, 1] \ni t \mapsto (\mu(t), \Sigma(t)),$$

where $\mu(t) = (1-t)\mu_1 + t\mu_2$ and

$$(50) \quad \Sigma(t) = ((1-t)I + tT)\Sigma_1((1-t)I + tT) = \\ (1-t)^2\Sigma_1 + t^2\Sigma_2 + t(1-t) \left((\Sigma_1\Sigma_2)^{1/2} + (\Sigma_2\Sigma_1)^{1/2} \right),$$

where T is the (unique) non-negative definite solution to the Riccati equation $T\Sigma_1T = \Sigma_2$.

Proof. Clearly, $\Gamma(0) = (\mu_1, \Sigma_1)$ and $\Gamma(1) = (\mu_2, \Sigma_2)$. Let us compute the distance between $\Gamma(0)$ and the point

$$(51) \quad \Gamma(t) = (\mu(t), \Sigma(t)) = (\mu_1 + t(\mu_2 - \mu_1), ((1-t)I + tT)\Sigma_1((1-t)I + tT)).$$

We have

$$\begin{aligned} \Sigma_1^{1/2}\Sigma(t)\Sigma_1^{1/2} &= \Sigma_1^{1/2}((1-t)I + tT)\Sigma_1((1-t)I + tT)\Sigma_1^{1/2} \\ &= \left(\Sigma_1^{1/2}((1-t)I + tT)\Sigma_1^{1/2} \right) \left(\Sigma_1^{1/2}((1-t)I + tT)\Sigma_1^{1/2} \right), \end{aligned}$$

so that

$$(52) \quad \left(\Sigma_1^{1/2}\Sigma(t)\Sigma_1^{1/2} \right)^{1/2} = \Sigma_1^{1/2}((1-t)I + tT)\Sigma_1^{1/2},$$

and hence

$$(53) \quad \text{Tr} \left(\left(\Sigma_1^{1/2}\Sigma(t)\Sigma_1^{1/2} \right)^{1/2} \right) = \text{Tr} \left(\Sigma_1^{1/2}((1-t)I + tT)\Sigma_1^{1/2} \right) = (1-t) \text{Tr}(\Sigma_1) + t \text{Tr}(T\Sigma_1).$$

We have

$$\begin{aligned} \text{Tr}(\Sigma(t)) &= \text{Tr}(((1-t)I + tT)\Sigma_1((1-t)I + tT)) \\ &= (1-t)^2 \text{Tr}(\Sigma_1) + 2t(1-t) \text{Tr}(T\Sigma_1) + t^2 \text{Tr}(\Sigma_2) \end{aligned}$$

Collecting all the above results,

$$\begin{aligned} \text{Tr} \left(\Sigma_1 + \Sigma(t) - 2 \left(\Sigma_1^{1/2}\Sigma(t)\Sigma_1^{1/2} \right)^{1/2} \right) &= \text{Tr}(\Sigma_1) + \\ &= (1-t)^2 \text{Tr}(\Sigma_1) + 2t(1-t) \text{Tr}(T\Sigma_1) + t^2 \text{Tr}(\Sigma_2) - 2(1-t) \text{Tr}(\Sigma_1) - 2t \text{Tr}(T\Sigma_1) = \\ &= t^2 \text{Tr}(\Sigma_1) + t^2 \text{Tr}(\Sigma_2) - 2t^2 \text{Tr}(T\Sigma_1) = t^2 \text{Tr} \left(\Sigma_1 + \Sigma_2 - 2 \left(\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2} \right)^{1/2} \right). \end{aligned}$$

In conclusion,

$$G(\Gamma(0), \Gamma(t)) = \sqrt{\|\mu(0) - \mu(t)\|^2 + \text{Tr} \left(\Sigma(0) + \Sigma(t) - 2 \left(\Sigma(0)^{1/2}\Sigma(t)\Sigma(0)^{1/2} \right)^{1/2} \right)} = \\ tG(\Gamma(0), \Gamma(1)). \quad \blacksquare$$

A few remarks are of order.

1. Clearly Proposition 3.4 still holds under the only assumption that Σ_1 is not singular.
2. The definition of geodesic in metric spaces we use here is related to Merger convexity property, see [25, p. 78]. A stronger definition requires the proportionality of the distance between couple of points on the curve, i.e.,

$$(54) \quad G(\Gamma(s), \Gamma(t)) = |t - s| G(\Gamma(0), \Gamma(1)),$$

for $s, t \in [0, 1]$. It will be proved later that in fact our geodesic enjoy such a stronger property.

3.3. Degenerate distributions. A few results formulated in the previous section required the dispersion matrices to be nonsingular. It is interesting to analyze the opposite case in which both matrices Σ_1 and Σ_2 are singular.

The simplest case occurs when the two subspaces, $\text{Range } \Sigma_1$ and $\text{Range } \Sigma_2$, are orthogonal.

Under all joint distribution for the random vector (X, Y) , with marginals $X \sim N_2(0, \Sigma_1)$ and $Y \sim N_2(0, \Sigma_2)$, the values of X and Y will lie into orthogonal subspaces, so that $XY^* = 0$. Hence $\|X - Y\|^2 = \|X\|^2 + \|Y\|^2$, and

$$(55) \quad \mathbb{E} \|X - Y\|^2 = \mathbb{E} \|X\|^2 + \mathbb{E} \|Y\|^2 = \text{Tr}(\Sigma_1) + \text{Tr}(\Sigma_2).$$

So any joint distribution (X, Y) attains the optimal value $\sqrt{\text{Tr}(\Sigma_1) + \text{Tr}(\Sigma_2)}$.

If we now define $X(t) = (1 - t)X + tY$, then

$$(56) \quad \mathbb{E} [\|X - X(t)\|^2] = \mathbb{E} [t^2 \|X - Y\|^2] = t^2 [\text{Tr}(\Sigma_1) + \text{Tr}(\Sigma_2)],$$

and so we have the geodesic joining the two random vectors X and Y .

The previous example can be extended by taking two singular matrices

$$(57) \quad \Sigma_1 = \sigma_1^2 v v^* \text{ and } \Sigma_2 = \sigma_2^2 w w^*$$

where $v \neq w \in \mathbb{R}^n$ and $\|v\| = \|w\| = 1$. Clearly, $\text{Range } \Sigma_1 \cap \text{Range } \Sigma_2 = \{0\}$ and they are one-dimensional spaces spanned by vectors v and w , respectively (it is not restrictive to assume $v^*w \geq 0$, too). By (48), it follows that the distance between the two matrices is

$$(58) \quad G(\Sigma_1, \Sigma_2) = \sqrt{\sigma_1^2 + \sigma_2^2 - 2\sigma_1\sigma_2 v^*w}.$$

Despite singularity of these matrices, it can be directly found the point realizing the minimum in (38). It is given by the singular matrix in $\text{Sym}^+(2n)$:

$$(59) \quad \begin{bmatrix} \sigma_1^2 v v^* & \sigma_1 \sigma_2 v w^* \\ \sigma_1 \sigma_2 w v^* & \sigma_2^2 w w^* \end{bmatrix} = \begin{bmatrix} \sigma_1 v \\ \sigma_2 w \end{bmatrix} \begin{bmatrix} \sigma_1 v^* & \sigma_2 w^* \end{bmatrix}.$$

4. Wasserstein Riemannian geometry. We have seen how to compute the geodesic of the distance given by the Gini dissimilarity. As the component \mathbb{R}^n carries the standard Euclidean geometry, we focus on the geometry of the matrix part i.e., we shall restrict our analysis to 0-mean distributions $N_n(0, \Sigma)$. Moreover, we consider positive definite dispersion matrices. The purpose of this section is to endow the open set $\text{Sym}^{++}(n)$ with a structure of Riemannian manifold by deriving a metric whose distance is equal to the Wasserstein distance. The Riemannian metric is obtained by pushing forward the Euclidean geometry of square matrices to the space of dispersion matrices via the mapping $\sigma: A \mapsto AA^* = \Sigma$, cf. [27].

In view of Prop. 2.1, the mapping $\sigma: \text{GL}(n) \rightarrow \text{Sym}^{++}(n) \subset \text{M}(n)$, is a submersion, the space $\text{Sym}^\perp(n) (A^*)^{-1}$ is the space of the vertical vectors at A , and the space $\mathcal{H}_A = \text{Sym}(n) A$ is the set of horizontal vectors at A .

We recall that a submersion $f: \text{GL}(n) \rightarrow \text{Sym}^{++}(n)$ is called Riemannian if for all A the differential restricted to horizontal vectors $df(A): \mathcal{H}_A \rightarrow T_{f(A)} \text{Sym}^{++}(n)$ is an isometry i.e.,

$$(60) \quad U, V \in \mathcal{H}_A \Rightarrow \langle df(A)[U], df(A)[V] \rangle_{f(A)} = \langle U, V \rangle .$$

A linear isometry is always 1-to-1 and, if it is onto, we can write backward that

$$(61) \quad X, Y \in T_{f(A)} \text{Sym}^{++}(n) \Rightarrow \langle X, Y \rangle_{f(A)} = \left\langle \left(df(A)|_{\mathcal{H}_A} \right)^{-1} X, \left(df(A)|_{\mathcal{H}_A} \right)^{-1} Y \right\rangle .$$

A Riemannian submersion preserves the length of curves. Let $[0, 1] \ni t \mapsto \gamma(t)$ be a smooth curve in H and consider its image $[0, 1] \ni t \mapsto f(\gamma(t))$. The velocity of the image is $t \mapsto df(\gamma(t))[\dot{\gamma}(t)]$ and its length is

$$(62) \quad \int_0^1 dt \|df(\gamma(t))[\dot{\gamma}(t)]\|_{f(\gamma(t))} = \int_0^1 dt \|\dot{\gamma}(t)\|_H$$

Fix a matrix $A \in \text{GL}(n)$ such that $\sigma(A) = AA^* = \Sigma$, and consider the open convex cone

$$(63) \quad \mathcal{H}_A^{++} = \text{Sym}^{++}(n) A \subset \mathcal{H}_A .$$

We denote by σ_A the restriction to \mathcal{H}_A^{++} of σ .

Proposition 4.1. *The mapping*

$$(64) \quad \sigma_A: \mathcal{H}_A^{++} \ni B \mapsto BB^* = C \in \text{Sym}^{++}(n)$$

is globally invertible, the solution to $\sigma_A(B) = C$ being

$$(65) \quad B = C^{-1/2} (C^{1/2} \Sigma C^{1/2})^{1/2} C^{-1/2} A .$$

Proof. For each $C \in \text{Sym}^{++}(n)$, the equation

$$(66) \quad C = BB^* = (BA^{-1}A)(BA^{-1}A)^* = (BA^{-1})\Sigma(BA^{-1})^*$$

is a Riccati equation for BA^{-1} . As $B \in \text{Sym}^{++}(n) A$, we have $BA^{-1} \in \text{Sym}^{++}(n)$ and

$$(67) \quad BA^{-1} = C^{-1/2} (C^{1/2} \Sigma C^{1/2})^{1/2} C^{-1/2}$$

is the unique solution. ■

We come now to the point, i.e., the construction of a metric based on horizontal vectors at a point.

Proposition 4.2. *The scalar product*

$$(68) \quad \langle U, V \rangle_{\Sigma} \equiv W_{\Sigma}(U, V) = \text{Tr} [\mathcal{L}_{\Sigma}(U) \Sigma \mathcal{L}_{\Sigma}(V)], \quad U, V \in \text{Sym}(n),$$

is the isometric push-forward of the metric on $\text{Sym}^*(n)$ by the mapping $\sigma: A \mapsto AA^* = \Sigma$.

Proof. Let $X \in M(n)$ and consider the decomposition of $X = X_V + X_H$ with X_V vertical at A and X_H horizontal at A . Then $d\sigma(A)[X] = d\sigma(A)[X_H]$ and the restriction of the derivative $d\sigma(A)$ to the vector space \mathcal{H}_A of horizontal vectors at A is 1-to-1 onto the tangent space of $\text{Sym}^{++}(n)$ at AA^* , that is, $\text{Sym}(n)$. For such a restriction, we have, for each $H \in \mathcal{H}_A$,

$$\begin{aligned} U = d\sigma(A)[H] &= HA^* + AH^* = HA^{-1}AA^* + A(HA^{-1}A)^* \\ &= (HA^{-1})AA^* + AA^*(HA^{-1})^* = (HA^{-1})AA^* + AA^*(HA^{-1}), \end{aligned}$$

so that the inverse mapping of the restriction is given by

$$(69) \quad H = \left(d\sigma(A)|_{\mathcal{H}_A} \right)^{-1} (U) = \mathcal{L}_{AA^*}(U)A,$$

Let us push-forward the inner product from \mathcal{H}_A to $T_{AA^*}\text{Sym}^{++}(n)$.

From Eq. (69), we have

$$\begin{aligned} W_{AA^*}(U, V) &= \left\langle \left(d\sigma(A)|_{\mathcal{H}_A} \right)^{-1} (U), \left(d\sigma(A)|_{\mathcal{H}_A} \right)^{-1} (V) \right\rangle = \\ &= \langle \mathcal{L}_{AA^*}(U)A, \mathcal{L}_{AA^*}(V)A \rangle = \text{Tr} (\mathcal{L}_{AA^*}(U)AA^*\mathcal{L}_{AA^*}(V)). \end{aligned}$$

which depends on $AA^* = \Sigma$ only. ■

There is a tensorial form of Wasserstein Riemannian metric which is useful because it represents the bilinear form of the metric in the standard scalar product.

Proposition 4.3. *It holds*

$$(70) \quad W_{\Sigma}(U, V) = \frac{1}{2} \text{Tr} (\mathcal{L}_{\Sigma}(U)V) = \frac{1}{2} \langle \mathcal{L}_{\Sigma}(U), V \rangle \equiv \langle \mathcal{L}_{\Sigma}(U), V \rangle_2.$$

Proof. We have

$$(71) \quad \text{Tr} (\mathcal{L}_{\Sigma}(U) \Sigma \mathcal{L}_{\Sigma}(V)) = \text{Tr} (\mathcal{L}_{\Sigma}(V) \Sigma \mathcal{L}_{\Sigma}(U)) = \text{Tr} (\mathcal{L}_{\Sigma}(U) \mathcal{L}_{\Sigma}(V) \Sigma),$$

and, taking the semi-sum of the first and the last term of the previous equation, we have

$$(72) \quad W_{\Sigma}(U, V) = \frac{1}{2} \text{Tr} \{ \mathcal{L}_{\Sigma}(U) [\mathcal{L}_{\Sigma}(V) \Sigma + \Sigma \mathcal{L}_{\Sigma}(V)] \} = \frac{1}{2} \text{Tr} \{ \mathcal{L}_{\Sigma}(U)V \},$$

where the last line follows from Eq. (13). ■

We have seen that there is a metric geodesic for the Wasserstein distance, connecting a pair of matrices $\Sigma_1, \Sigma_2 \in \text{Sym}^{++}(n)$. We now show that the same curve is the Wasserstein Riemannian geodesic.

Recall that the symmetric matrix

$$(73) \quad T = \Sigma_1^{-1/2} (\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2})^{1/2} \Sigma_1^{-1/2} .$$

is the unique solution in $\text{Sym}^+(n)$ of the Riccati equation $T\Sigma_1 T = \Sigma_2$. Note further that

$$(74) \quad \det(T) = \det(\Sigma_2)^{1/2} \det(\Sigma_1)^{-1/2} > 0.$$

Proposition 4.4. *The parametric curve*

$$(75) \quad t \mapsto \Sigma(t) = ((1-t)I + tT)\Sigma_1((1-t)I + tT) \in \text{Sym}^{++}(n)$$

is the unique Wasserstein Riemannian geodesic from Σ_1 to Σ_2 .

Proof. Set $A_1 = \Sigma_1^{1/2}$ and $A_2 = T\Sigma_1^{1/2}$. We have

$$(76) \quad A_1, A_2 \in \mathcal{H}_{\Sigma_1^{1/2}}^{++} = \text{Sym}^{++}(n) \Sigma_1^{1/2}.$$

Actually, $A_1 = I\Sigma_1^{1/2}$ and $A_2 = T\Sigma_1^{1/2}$, with $I, T \in \text{Sym}^{++}(n)$.

Therefore the straight line from A_1 to A_2 ,

$$(77) \quad t \mapsto A(t) = (1-t)A_1 + tA_2 \in \mathcal{H}_{\Sigma_1^{1/2}}^{++}, \quad t \in [0, 1] ,$$

stays in $\mathcal{H}_{\Sigma_1^{1/2}}^{++}$. As a consequence, $t \mapsto A(t)A(t)^* = \Sigma(t)$ is a geodesic in the Wasserstein Riemannian metric connecting Σ_1 to $\Sigma_2 = A(1)A(1)^*$.

This way, we get the curve

$$(78) \quad t \mapsto \Sigma(t) = A(t)A(t)^* = (I + t(T - I))\Sigma_1(I + t(T - I)) \in \text{Sym}^{++}(n)$$

that agrees with Eq. (49). ■

Remark 4.5. The equivalence between Riemannian distance and Gini index (or Wasserstein distance) can be confirmed by computing the length in $\text{Sym}(n)$ of the the geodesic $t \mapsto A(t)$, $t \in [0, 1]$. As $\dot{A}(t) = (T - I)\Sigma_1^{1/2}$, we have

$$\begin{aligned} \|\dot{A}(t)\| &= \sqrt{\text{Tr}(\dot{A}(t)\dot{A}(t)^*)} = \sqrt{\text{Tr}((T - I)\Sigma_1(T - I))} = \\ &= \sqrt{(\text{Tr}(\Sigma_1) + \text{Tr}(\Sigma_2) - \text{Tr}(T\Sigma_1) - \text{Tr}(\Sigma_1 T))} = \\ &= \sqrt{\text{Tr}(\Sigma_1) + \text{Tr}(\Sigma_2) - \text{Tr}((\Sigma_2 \Sigma_1)^{1/2}) - \text{Tr}((\Sigma_1 \Sigma_2)^{1/2})} . \end{aligned}$$

In the last equality we have used Eq. (10) and Eq. (11).

5. Wasserstein Riemannian exponential. We aim now at reformulating Riemannian geodesic in terms of the exponential map. The purpose is that of writing the geodesic arc passing through a given point and having a given velocity at the point itself.

The velocity of the geodesic (75):

$$(79) \quad \dot{\Sigma}(t) = (T - I)\Sigma_1 + \Sigma_1(T - I) + 2t(T - I)\Sigma_1(T - I)$$

is affine in t . In particular, its initial velocity is

$$(80) \quad \dot{\Sigma}(0) = (T - I)\Sigma_1 + \Sigma_1(T - I).$$

By inverting Lyapunov equation (80), we get $T - I = \mathcal{L}_{\Sigma(0)}(\dot{\Sigma}(0))$. Therefore,

$$(81) \quad \begin{aligned} \Sigma(t) &= \Sigma(0) + t[(T - I)\Sigma(0) + \Sigma(0)(T - I)] + t^2(T - I)\Sigma(0)(T - I) \\ &= \Sigma(0) + t\dot{\Sigma}(0) + t^2\mathcal{L}_{\Sigma(0)}(\dot{\Sigma}(0))\Sigma(0)\mathcal{L}_{\Sigma(0)}(\dot{\Sigma}(0)). \end{aligned}$$

We are so led to the following definition (see [1, p. 101–102]).

Definition 5.1. For any $C \in \text{Sym}^{++}(n)$ and $V \in \text{Sym}(n) \simeq T_C \text{Sym}^{++}(n)$, the Wasserstein Riemannian exponential is

$$(82) \quad \text{Exp}_C(V) = C + V + \mathcal{L}_C(V)C\mathcal{L}_C(V) = (\mathcal{L}_C(V) + I)C(\mathcal{L}_C(V) + I),$$

Next proposition concerns properties of the Riemannian exponential.

Proposition 5.2. 1) All geodesics emanating from a point $C \in \text{Sym}^{++}(n)$ are of the form $\Sigma(t) = \text{Exp}_C(tV)$, with $t \in J_V$, where J_V is the open interval about the origin:

$$(83) \quad J_V = \{t \in \mathbb{R} : I + t\mathcal{L}_C(V) \in \text{Sym}^{++}(n)\}.$$

2) The map $V \mapsto \text{Exp}_C(V)$, restricted to the open set

$$(84) \quad \Theta = \{V \in \text{Sym}(n) : I + \mathcal{L}_C(V) \in \text{Sym}^{++}(n)\},$$

is a diffeomorphism of Θ into $\text{Sym}^{++}(n)$ with inverse

$$(85) \quad \text{Log}_C(B) = (BC)^{1/2} + (CB)^{1/2} - 2C;$$

3) The derivative of the Riemannian exponential is

$$(86) \quad d_X(V \mapsto \text{Exp}_C(V)) = X + \mathcal{L}_C(X)C\mathcal{L}_C(V) + \mathcal{L}_C(V)C\mathcal{L}_C(X).$$

Remark 5.3. Clearly, $0 \in J_V$. Moreover, the interval J_V is unbounded from the right, that is, it is of the kind $J_V = (\bar{t}, +\infty)$, provided $V \in \text{Sym}^+(n)$. Likewise, $J_V = (-\infty, \bar{t})$, if $V \in \text{Sym}^-(n)$.

Analogously, Θ is an open set containing the origin and so $V \mapsto \text{Exp}_C(V)$ is a local diffeomorphism around the origin.

Since the geodesics are not defined for all the values of the parameter $t \in \mathbb{R}$, we have that the Riemannian manifold $\text{Sym}^{++}(n)$ is *geodesically incomplete*. Of course this is not a surprising fact: $\text{Sym}^{++}(n)$ is not a complete metric space, and hence Hopf-Rinow theorem implies that it is not geodesically complete (see [11]).

Proof of Prop. 5.2. 1) Let

$$(87) \quad \Sigma(t) = \text{Exp}_C(tV) = C + tV + t^2 \mathcal{L}_C(V) C \mathcal{L}_C(V), \quad t \in J_V.$$

Clearly, $\Sigma(0) = C$, $\dot{\Sigma}(0) = V$. Pick a scalar $\bar{t} \in J_V$ and consider the two matrices $\Sigma(0)$ and $\Sigma(\bar{t})$ on the curve Σ . Introduce the new parametrization $\tilde{\Sigma}(\tau) = \Sigma(\tau\bar{t})$ so that $\tilde{\Sigma}(0) = \Sigma(0)$ and $\tilde{\Sigma}(1) = \Sigma(\bar{t})$. We have,

$$(88) \quad \tilde{\Sigma}(\tau) = C + \tau\bar{t}V + \tau^2\bar{t}^2 \mathcal{L}_C(V) C \mathcal{L}_C(V).$$

By the relation (13) and setting $T - I = \bar{t}\mathcal{L}_C(V)$, the equation above becomes

$$(89) \quad \tilde{\Sigma}(\tau) = C + \bar{t}\tau \mathcal{L}_C(V) C + \bar{t}\tau C \mathcal{L}_C(V) + \bar{t}^2 \tau^2 \mathcal{L}_C(V) C \mathcal{L}_C(V)$$

$$(90) \quad = C + \tau(T - I)C + \tau C(T - I) + \tau^2(T - I)C(T - I) = TCT$$

$$(91) \quad = [(1 - \tau)I + \tau T] C [(1 - \tau)I + \tau T].$$

On the other hand, $\bar{t} \in J_V$ implies that $T = I + \bar{t}\mathcal{L}_C(V) \in \text{Sym}^{++}(n)$. Moreover, $\tilde{\Sigma}(1) = TCT = T\tilde{\Sigma}(0)T$. In view of Eq. (75), the curve $\Sigma(t) = \text{Exp}_C(tV)$, with $t \in [0, \bar{t}]$ (or $[\bar{t}, 0]$) is a portion of the geodesic $\Sigma(t)$, $t \in J_V$.

2) By Eq. (82) we have the Riccati equation

$$(92) \quad \text{Exp}_C(V) = (I + \mathcal{L}_C(V))C(I + \mathcal{L}_C(V)) = B$$

which solution is

$$(93) \quad I + \mathcal{L}_C(V) = C^{-1/2}(C^{1/2}BC^{1/2})^{1/2}C^{-1/2} \quad \blacksquare$$

provided $I + \mathcal{L}_C(V) \in \text{Sym}^{++}(n)$. This is true for a sufficiently small neighborhood $\|V\| < r$ of the origin. The inversion of the operator $\mathcal{L}_C(\cdot)$ and Eq. (9) provide the desired formula for $\text{Log}_C(B)$.

3) The derivative follows from a simple bilinear computation.

6. Natural gradient. First, let us study the second order approximation of the matrix function in Eq. (2). For a given $\Sigma \in \text{Sym}^{++}(n)$, let $H \in \text{Sym}(n)$ such that $(\Sigma \pm H) \in \text{Sym}^{++}(n)$. It follows that $\Sigma + \theta H \in \text{Sym}^{++}(n)$ for all $\theta \in [-1, +1]$. Consider the divergence in Eq. (2) with $\mu_1 = \mu_2 = 0$, $\Sigma_1 = \Sigma$, $\Sigma_2 = \Sigma + \theta H$, and the parametric function

$$(94) \quad \theta \mapsto W^2(\Sigma, \Sigma + \theta H) = \text{Tr} \left(\Sigma + (\Sigma + \theta H) - 2 \left(\Sigma^{1/2}(\Sigma + \theta H)\Sigma^{1/2} \right)^{1/2} \right) = \\ 2 \text{Tr}(\Sigma) + \theta \text{Tr}(H) - 2 \text{Tr} \left(\left(\Sigma^2 + \theta \Sigma^{1/2} H \Sigma^{1/2} \right)^{1/2} \right).$$

The first derivative is computed using Eq. (15) and Eq. (18),

$$(95) \quad \frac{d}{d\theta} W^2(\Sigma, \Sigma + \theta H) = \text{Tr}(H) - 2 \text{Tr} \left(\mathcal{L}_{(\Sigma^2 + \theta \Sigma^{1/2} H \Sigma^{1/2})^{1/2}} \left[\Sigma^{1/2} H \Sigma^{1/2} \right] \right) = \\ \text{Tr}(H) - \text{Tr} \left(\left(\Sigma^2 + \theta \Sigma^{1/2} H \Sigma^{1/2} \right)^{-1/2} \left(\Sigma^{1/2} H \Sigma^{1/2} \right) \right).$$

We observe that

$$(96) \quad W^2(\Sigma, \Sigma + \theta H) \Big|_{\theta=0} = \frac{d}{d\theta} W^2(\Sigma, \Sigma + \theta H) \Big|_{\theta=0} = 0 ,$$

and proceed to the computation of the second derivative. We find, by derivation of the composed function, that

$$(97) \quad \frac{d^2}{d\theta^2} W^2(\Sigma, \Sigma + \theta H) = \text{Tr} \left(\left(\Sigma^2 + \theta \Sigma^{1/2} H \Sigma^{1/2} \right)^{-1/2} \mathcal{L}_{(\Sigma^2 + \theta \Sigma^{1/2} H \Sigma^{1/2})^{1/2}} \left[\Sigma^{1/2} H \Sigma^{1/2} \right] \left(\Sigma^2 + \theta \Sigma^{1/2} H \Sigma^{1/2} \right)^{-1/2} \left(\Sigma^{1/2} H \Sigma^{1/2} \right) \right) ,$$

so that

$$(98) \quad \frac{d^2}{d\theta^2} W^2(\Sigma, \Sigma + \theta H) \Big|_{\theta=0} = \text{Tr} \left(\Sigma^{-1} \mathcal{L}_{\Sigma} \left[\Sigma^{1/2} H \Sigma^{1/2} \right] \Sigma^{-1} \Sigma^{1/2} H \Sigma^{1/2} \right) = \text{Tr} \left(\Sigma^{-1/2} \mathcal{L}_{\Sigma} \left[\Sigma^{1/2} H \Sigma^{1/2} \right] \Sigma^{-1/2} H \right) = \text{Tr} \left(\mathcal{L}_{\Sigma} [H] H \right) ,$$

where we have used the Eq. (17). In conclusion we have shown that

$$(99) \quad W^2(\Sigma, \Sigma + \theta H) = \frac{\theta^2}{2} \text{Tr} \left(\mathcal{L}_{\Sigma} [H] H \right) + o(\theta^2) .$$

The equation above confirms that the form of the Riemannian metric associated to Wasserstein distance is the metric that has been introduced above. Moreover the solution of the problem

$$(100) \quad \begin{cases} \max f(X + H) - f(X) \\ \text{subject to} \\ W^2(X, X + H) = \varepsilon \text{ (small and fixed)} \end{cases}$$

allows to identify the direction of the maximal increase of the function f as the *natural gradient*, according to the name introduced by Amari [3] i.e., the Riemannian gradient as defined below.

The Riemannian gradient is the gradient with respect to the scalar product of the metric. We denote by ∇ the gradient with respect to the scalar product $\langle \cdot, \cdot \rangle_2$ and by grad the gradient with respect to the Riemannian metric. By Prop. 4.3 we now that $W_{\Sigma}(X, Y) = \langle \mathcal{L}_{\Sigma} [X], Y \rangle_2$, hence for each smooth scalar field ϕ we have

$$(101) \quad \text{grad} \phi(\Sigma) = \mathcal{L}_{\Sigma}^{-1}(\nabla \phi(\Sigma)) = \nabla \phi(\Sigma) \Sigma + \Sigma \nabla \phi(\Sigma) ,$$

where the second equality follows from Eq. (14). Conversely,

$$(102) \quad \mathcal{L}_{\Sigma} [\text{grad} \phi(\Sigma)] = \nabla \phi(\Sigma) .$$

The *gradient flow* of a smooth scalar field ϕ is the flow generated by the vector field $\gamma \mapsto (\gamma, -\text{grad } \phi(\gamma))$, that is, the flow of the differential equation

$$(103) \quad \dot{\gamma}(t) = -\text{grad } \phi(\gamma(t)) = -(\nabla \phi(\gamma(t))\gamma(t) + \gamma(t)\nabla \phi(\gamma(t))) .$$

We discuss below two relevant examples of gradient flow. With reference to the full Gaussian distribution, one considers smooth functions defined on $\mathbb{R}^n \times \text{Sym}^{++}(n)$. The first component of the gradient does not require a special gradient as the Riemannian structure is the Euclidean one. The full gradient will thus have two components:

$$(104) \quad \text{grad } \phi(\mu, \Sigma) = (\nabla_1 \phi(\mu, \Sigma), \text{grad}_2 \phi(\mu, \Sigma)) = (\nabla_1 \phi(\mu, \Sigma), \nabla_2 \phi(\mu, \Sigma)\Sigma + \Sigma \nabla_2 \phi(\mu, \Sigma)) .$$

The first example in Sec. 6.1 refers to the gradient flow of the mean value of an objective function $f: \mathbb{R}^n \rightarrow \mathbb{R}$. Its Euler scheme is used in optimization, see [1, Ch. 4] and [20]. In the second example in Sec. 6.2 we discuss the gradient flow of the entropy function of a centered Gaussian.

6.1. Relaxed function. We call *relaxation to the full Gaussian model* of the objective function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ the function

$$(105) \quad \phi(\mu, \Sigma) = \mathbb{E}[f(X)], \quad X \sim N_n(\mu, \Sigma) .$$

If we would include the Dirac measures in the Gaussian model, then $f(x) = \phi(x, 0)$ and the function ϕ would actually be an extension of the given function. However, we consider only $\Sigma \in \text{Sym}^{++}(n)$ in order to work with a function defined on our manifold.

There are two ways to calculate the expected value as a function of μ and Σ . Each of them leads to a peculiar expression of the natural gradient.

The first one arises from the relation

$$(106) \quad \phi(\mu, \Sigma) = \mathbb{E}\left[f(\Sigma^{1/2}Z + \mu)\right], \quad Z \sim N_n(0, I) .$$

which will lead to an equation for the gradient involving the derivatives of f . The second one uses

$$(107) \quad \phi(\mu, \Sigma) = \int f(x)(2\pi)^{-n/2} \det(\Sigma)^{-1/2} \exp\left(-\frac{1}{2}(x - \mu)^* \Sigma^{-1}(x - \mu)\right) dx .$$

In this second case the natural gradient will be achieved by an equation not involving the gradient of the function f . Both forms have their own field of application.

Let us start with Case (106). Under standard conditions regarding the derivation under the expectation sign, we have

$$(108) \quad \nabla_1 \phi(\mu, \Sigma) = \mathbb{E}\left[\nabla f(\Sigma^{1/2}Z + \mu)\right] = \mathbb{E}[\nabla f(X)] .$$

By means of (15), it is straightforward to calculate the derivative $d_U(\Sigma \mapsto \phi(\mu, \Sigma))$.

Note that ∇f is the column vector and so $\nabla^* f$ will be a row vector. We have

$$\begin{aligned} d_U \phi(\mu, \Sigma) &= \mathbb{E} \left[df(\Sigma^{1/2} Z + \mu) [\mathcal{L}_{\Sigma^{1/2}}(U) Z] \right] = \mathbb{E} \left[\nabla^* f(\Sigma^{1/2} Z + \mu) \mathcal{L}_{\Sigma^{1/2}}(U) Z \right] \\ &= \mathbb{E} \left[\text{Tr} \nabla^* f(\Sigma^{1/2} Z + \mu) \mathcal{L}_{\Sigma^{1/2}}(U) Z \right]. \end{aligned}$$

Under symmetrization (and setting $X = \Sigma^{1/2} Z + \mu$):

$$\begin{aligned} d_U \phi(\mu, \Sigma) &= \frac{1}{2} \mathbb{E} [\text{Tr} \mathcal{L}_{\Sigma^{1/2}}(U) (Z \nabla^* f(X) + \nabla f(X) Z)] \\ &= \langle U, \mathbb{E} ((Z \nabla^* f(X) + \nabla f(X) Z)) \rangle_{\Sigma^{1/2}} \\ &= \frac{1}{2} \mathbb{E} \text{Tr} \mathcal{L}_{\Sigma^{1/2}}(Z \nabla^* f(X) + \nabla f(X) Z) U \\ &= \langle \mathbb{E} \mathcal{L}_{\Sigma^{1/2}}(Z \nabla^* f(X) + \nabla f(X) Z), U \rangle_2. \end{aligned}$$

It follows that

$$(109) \quad \nabla_2 \phi(\mu, \Sigma) = \mathbb{E} \mathcal{L}_{\Sigma^{1/2}}(Z \nabla^* f(X) + \nabla f(X) Z).$$

Calculating the natural gradient:

$$\begin{aligned} \text{grad}_2 \phi(\mu, \Sigma) &= \Sigma \mathbb{E} \mathcal{L}_{\Sigma^{1/2}}(Z \nabla^* f(X) + \nabla f(X) Z) + \\ &\quad \mathbb{E} \mathcal{L}_{\Sigma^{1/2}}(Z \nabla^* f(X) + \nabla f(X) Z) \Sigma. \end{aligned}$$

If we set $\Xi = \mathbb{E} [Z \nabla^* f(X) + \nabla f(X) Z]$, the natural gradient admits the representation

$$(110) \quad \text{grad}_2 \phi(\mu, \Sigma) = \Sigma \mathcal{L}_{\Sigma^{1/2}}(\Xi) + \mathcal{L}_{\Sigma^{1/2}}(\Xi) \Sigma.$$

We move on to consider the second Case (107). Following the standard computation of the Fisher score and starting from the log-density $p(x; \mu, \Sigma)$ of $N_n(\mu, \Sigma)$, we have

$$(111) \quad \begin{aligned} \log p(x; \mu, \Sigma) &= -\frac{n}{2} \log 2\pi - \frac{1}{2} \log \det \Sigma - \frac{1}{2} (x - \mu)^* \Sigma^{-1} (x - \mu) \\ &= -\frac{n}{2} \log 2\pi - \frac{1}{2} \log \det \Sigma - \frac{1}{2} \text{Tr} (\Sigma^{-1} (x - \mu)(x - \mu)^*) . \end{aligned}$$

Denoting the partial derivative $d_u (\mu \mapsto \log p(x; \mu, \Sigma))$ as $d_u \log p(x; \mu, \Sigma)$, and $d_U (\Sigma \mapsto \log p(x; \mu, \Sigma))$ as $d_U \log p(x; \mu, \Sigma)$, we get:

$$\begin{aligned} d_u \log p(x; \mu, \Sigma) &= (x - \mu)^* \Sigma^{-1} u = \langle \Sigma^{-1} (x - \mu), u \rangle \\ d_U \log p(x; \mu, \Sigma) &= -\frac{1}{2} \text{Tr} (\Sigma^{-1} U) + \frac{1}{2} \text{Tr} (\Sigma^{-1} U \Sigma^{-1} (x - \mu)(x - \mu)^*) \\ &= \frac{1}{2} \langle \Sigma^{-1} (x - \mu)(x - \mu)^* \Sigma^{-1} - \Sigma^{-1}, U \rangle \\ &= \langle \Sigma^{-1} ((x - \mu)(x - \mu)^* - \Sigma) \Sigma^{-1}, U \rangle_2 \end{aligned}$$

So that

$$\begin{aligned} d_u \phi(\mu, \Sigma) &= \int f(x) d_u \log p(x; \mu, \Sigma) p(x; \mu; \Sigma) dx \\ &= \left\langle \Sigma^{-1} \int f(x)(x - \mu)p(x; \mu; \Sigma) dx, u \right\rangle \end{aligned}$$

and

$$\begin{aligned} d_U \phi(\mu, \Sigma) &= \int f(x) d_U \log p(x; \mu, \Sigma) p(x; \mu, \Sigma) dx \\ &= \left\langle \Sigma^{-1} \int f(x) ((x - \mu)(x - \mu)^* - \Sigma) p(x; \mu, \Sigma) dx \Sigma^{-1}, U \right\rangle_2. \end{aligned}$$

At last, thanks to (104), the natural gradient of $\phi(\mu, \Sigma)$ will be

$$\begin{aligned} \nabla_1 \phi(\mu, \Sigma) &= \Sigma^{-1} \int f(x)(x - \mu)p(x; \mu; \Sigma) dx \\ \text{grad}_2 \phi(\mu, \Sigma) &= \int f(x) ((x - \mu)(x - \mu)^* - \Sigma) p(x; \mu, \Sigma) dx \Sigma^{-1} \\ &\quad + \Sigma^{-1} \int f(x) ((x - \mu)(x - \mu)^* - \Sigma) p(x; \mu, \Sigma) dx. \end{aligned}$$

6.2. Entropy flow. The flow of entropy can be easily calculated by Eq. 111. We have

$$\begin{aligned} \mathcal{E}(\mu, \Sigma) &= - \int \log p(x; \mu, \Sigma) p(x; \mu, \Sigma) dx \\ &= \frac{n}{2} \log 2\pi + \frac{1}{2} \log \det \Sigma - \frac{1}{2} \text{Tr} (\Sigma^{-1} \Sigma) \\ &= \frac{n}{2} (\log 2\pi - 1) + \frac{1}{2} \log \det \Sigma. \end{aligned}$$

The entropy does not depend on μ so that $\nabla_1 \mathcal{E}(\mu, \Sigma) = 0$. Moreover (see [19, §8.3]) we know that $\nabla \mathcal{E}(\Sigma) = \Sigma^{-1}$, so that

$$(112) \quad \text{grad } \mathcal{E}(\Sigma) = (\Sigma^{-1} \Sigma + \Sigma \Sigma^{-1}) = 2I.$$

The entropic flow will be solution to the equations

$$(113) \quad \dot{\mu}(t) = 0, \quad \dot{\Sigma}(t) + 2I = 0,$$

that is

$$(114) \quad \mu(t) = \mu(0), \quad \Sigma(t) = \Sigma(0) - 2tI.$$

The integral curve is defined for all t such that $2t < \lambda_*$, λ_* being the minimum of the spectre of $\Sigma(0)$.

7. Second order geometry. Recall that $\text{Sym}^{++}(n)$ as an open set of the Hilbert space $\text{Sym}(n)$ endowed with the scalar product $\langle X, Y \rangle_2 = \frac{1}{2} \text{Tr}(XY)$. We have shown in Prop. 4.3 that the Wasserstein Riemannian metric W is expressed in terms of the scalar product of $\text{Sym}(n)$ by

$$(115) \quad W_\Sigma(X, Y) = \langle X, Y \rangle_\Sigma = \langle \mathcal{L}_\Sigma[X], Y \rangle_2 ,$$

for each $(\Sigma, X), (\Sigma, Y)$ in the trivial tangent bundle $T\text{Sym}^{++}(n) \simeq \text{Sym}^{++}(n) \times \text{Sym}(n)$. In the equation above, $\mathcal{L}: \text{Sym}^{++}(n) \mapsto L(\text{Sym}(n), \text{Sym}(n))$ is the operator defining the Wasserstein metric the standard scalar product.

In the trivial chart, a smooth vector field X is a smooth mapping $X: \text{Sym}^{++}(n) \rightarrow \text{Sym}(n)$. The action of the vector field X on the scalar field f that is, Xf , is expressed in the trivial chart by $d_X f$ that is, the scalar field whose value at point Σ is the derivative of f in the direction $X(\Sigma)$. Similarly, we denote by $d_Y X$ the vector field whose value at point Σ is the derivative at Σ of X in the direction $Y(\Sigma)$. The Lie bracket $[X, Y]$ of two smooth vector fields X, Y is expressed by $d_X Y - d_Y X$.

While we prefer to express our computation in matrix algebra, in some cases it is useful to use a vector basis. We discuss below a field of vector bases of particular interest for us.

The set of symmetric matrices

$$(116) \quad E^{p,q} = e_p e_q^* + e_q e_p^*, \quad p, q = 1, \dots, n ,$$

spans the vector space $\text{Sym}(n)$. There are repeated elements and a unique enumeration is given by the set A of parts on $\{1, \dots, n\}$ with 1 or 2 elements. This generating set is related to the product of matrices by the equation

$$(117) \quad E^{p,q} E^{r,s} + E^{r,s} E^{p,q} = \delta_{q,r} E^{p,s} + \delta_{q,s} E^{p,r} + \delta_{p,r} E^{q,s} + \delta_{p,s} E^{q,r} ,$$

where δ is the Kronecker symbol.

In particular, we can take the trace of the equation above to get

$$(118) \quad \langle E^{p,q}, E^{r,s} \rangle = \delta_{p,r} \delta_{q,s} + \delta_{p,s} \delta_{q,r} ,$$

which in turn implies

$$(119) \quad \langle E^{p,q}, E^{r,s} \rangle = \begin{cases} 0 & \text{if } \{p, q\} \neq \{r, s\}, \\ 1 & \text{if } \{p, q\} = \{r, s\} \text{ and } p \neq q, \\ 2 & \text{if } \{p, q\} = \{r, s\} \text{ and } p = q \end{cases}$$

We can select an orthogonal basis by canceling the repeated elements. In the sequel, we denote by $(E^\alpha)_{\alpha \in A}$ the vector basis above, properly normalized to obtain an orthonormal basis. We do not show the normalising constants in order to simplify the notation.

For each $\Sigma \in \text{Sym}^{++}(n)$ the sequence

$$(120) \quad \mathcal{E}^\alpha(\Sigma) = E^\alpha \Sigma + \Sigma E^\alpha, \quad \alpha \in A ,$$

is a vector basis of $\text{Sym}(n) \simeq T_\Sigma \text{Sym}^{++}(n)$ because it is the image of a vector basis under a linear mapping which is onto. We will call such a sequence of vector fields the (principal) *moving frame*. Notice the following properties: $\mathcal{E}^\alpha = d_{E^\alpha} \Sigma^2$; $\mathcal{L}_\Sigma [\mathcal{E}^\alpha(\Sigma)] = E^\alpha$; $\mathcal{E}^\alpha(I) = 2E^\alpha$.

At a generic Σ , we can express each \mathcal{E}^α in the $(E^\beta)_\beta$'s orthonormal basis as

$$(121) \quad \mathcal{E}^\alpha(\Sigma) = \sum_{\beta} 2g_{\alpha,\beta}(\Sigma) E^\beta, \quad g_{\alpha,\beta}(\Sigma) = \text{Tr} \left(E^\alpha \Sigma E^\beta \right),$$

which is verified by right-multiplying by E^γ Eq. (120) and taking the trace of the resulting equation. As

$$(122) \quad W_\Sigma(\mathcal{E}^\alpha, \mathcal{E}^\beta) = \text{Tr} \left(\mathcal{L}_\Sigma [\mathcal{E}^\alpha(\Sigma)] \Sigma \mathcal{L}_\Sigma [\mathcal{E}^\beta(\Sigma)] \right) = \text{Tr} \left(E^\alpha \Sigma E^\beta \right),$$

the matrix $[g_{\alpha,\beta}]_{\alpha,\beta}$ is the expression of the Riemannian metric in the moving frame.

In fact, X, Y are vector fields expressed in the moving frame, $X = \sum_{\alpha} x_{\alpha} \mathcal{E}^{\alpha}$, $Y = \sum_{\beta} y_{\beta} \mathcal{E}^{\beta}$, then

$$(123) \quad W_\Sigma(X, Y) = \sum_{\alpha,\beta} x_{\alpha}(\Sigma) y_{\beta}(\Sigma) g_{\alpha,\beta}(\Sigma) = \text{Tr} \left(\left(\sum_{\alpha} x_{\alpha}(\Sigma) E^{\alpha} \right) \Sigma \left(\sum_{\beta} y_{\beta}(\Sigma) E^{\beta} \right) \right).$$

This expression of the scalar product is to be compared to that used in [27,].

Any vector field X has two representations, one with respect to the moving frame $(\mathcal{E}^\alpha)_\alpha$ and another one with respect to the basis $(E^\alpha)_\alpha$. The two representations are related to each other as follows. We have

$$(124) \quad X = \sum_{\alpha} x_{\alpha} \mathcal{E}^{\alpha} = \sum_{\alpha} x_{\alpha} \sum_{\beta} 2g_{\alpha,\beta} E^{\beta} = \sum_{\beta} \left(\sum_{\alpha} 2x_{\alpha} g_{\alpha,\beta} \right) E^{\beta},$$

so that

$$(125) \quad \langle X, E^\gamma \rangle_2 = \frac{1}{2} \text{Tr} (X E^\gamma) = \sum_{\beta} \left(\sum_{\alpha} x_{\alpha} g_{\alpha,\beta} \right) \text{Tr} (E^\beta E^\gamma) = \sum_{\alpha} x_{\alpha} g_{\alpha,\gamma},$$

hence, by applying the inverse matrix $[g^{\alpha,\beta}(\Sigma)] = [g_{\alpha,\beta}(\Sigma)]^{-1}$, we have

$$(126) \quad x_{\alpha} = \sum_{\gamma} g^{\alpha,\gamma} \langle X, E^\gamma \rangle_2.$$

For example, $\mathcal{L}_\Sigma [V] = \sum_{\alpha} \ell_{\Sigma}^{\alpha}(V) \mathcal{E}^{\alpha}(\Sigma)$, with

$$(127) \quad \ell_{\Sigma}^{\alpha}(V) = \sum_{\gamma} g^{\alpha,\gamma}(\Sigma) \langle \mathcal{L}_\Sigma [V], E^\gamma \rangle_2 = W_\Sigma(V, \sum_{\gamma} g^{\alpha,\gamma} E^\gamma).$$

The next example is related to the discussion of covariant derivatives to follow. Consider a third vector field $Z = \sum_{\gamma} z_{\gamma} \mathcal{E}^{\gamma}$. As the mapping $\Sigma \mapsto g_{\alpha,\beta}(\Sigma)$ is a restriction of a linear

mapping on $\text{Sym}(n)$, we have

$$(128) \quad d_Z W_\Sigma(X, Y) = \sum_{\alpha, \beta} (d_Z x_\alpha(\Sigma) y_\beta(\Sigma) + x_\alpha(\Sigma) d_Z y_\beta(\Sigma)) g_{\alpha, \beta}(\Sigma) + x_\alpha(\Sigma) y_\beta(\Sigma) \text{Tr} \left(E^\alpha Z(\Sigma) E^\beta \right) = \sum_{\alpha, \beta} (d_Z x_\alpha(\Sigma) y_\beta(\Sigma) + x_\alpha(\Sigma) d_Z y_\beta(\Sigma)) g_{\alpha, \beta}(\Sigma) + \sum_{\alpha, \beta, \gamma} x_\alpha(\Sigma) y_\beta(\Sigma) z_\gamma(\Sigma) \text{Tr} \left(E^\alpha \mathcal{E}^\gamma(\Sigma) E^\beta \right),$$

where $d_Z x_\alpha(\Sigma)$ and $d_Z y_\beta$ can be expanded with respect to the components z_γ of Z .

For couple of vector fields X, Y , we denote by $D_Y X$ the action of a *covariant derivative*, namely a bilinear operator satisfying, for each scalar field f ,

$$(CD1) \quad D_{fY} X = f D_Y X,$$

$$(CD2) \quad D_Y(fX) = d_Y f X + f D_Y X,$$

see e.g [11, Sect. 3] or [18, Ch. 8.4].

A convenient way to express a covariant derivative in the moving frame (120) is to define the *Christoffel symbols*

$$(129) \quad D_{\mathcal{E}^\alpha} \mathcal{E}^\beta = \sum_{\gamma} \Gamma_{\alpha, \beta}^{\gamma} \mathcal{E}^{\gamma},$$

For $X = \sum_{\alpha} x_{\alpha} \mathcal{E}^{\alpha}$, $Y = \sum_{\beta} y_{\beta} \mathcal{E}^{\beta}$, by using (CD1), (CD2), and Eq. (121), we obtain

$$(130) \quad D_X Y = \sum_{\alpha, \beta} x_{\alpha} D_{\mathcal{E}^{\alpha}} (y_{\beta} \mathcal{E}^{\beta}) = \sum_{\alpha, \beta} x_{\alpha} \left((d_{\mathcal{E}^{\alpha}} y_{\beta}) \mathcal{E}^{\beta} + y_{\beta} (D_{\mathcal{E}^{\alpha}} \mathcal{E}^{\beta}) \right) = \sum_{\alpha, \gamma} x_{\alpha} d_{\mathcal{E}^{\alpha}} y_{\gamma} \mathcal{E}^{\gamma} + \sum_{\alpha, \beta, \gamma} y_{\beta} \Gamma_{\alpha, \beta}^{\gamma} \mathcal{E}^{\gamma} = \sum_{\gamma} \sum_{\alpha, \beta} x_{\alpha} \left(d_{\mathcal{E}^{\alpha}} y_{\gamma} + y_{\beta} \Gamma_{\alpha, \beta}^{\gamma} \right) \mathcal{E}^{\gamma}.$$

The scalar product of $D_X Y$ with $Z = \sum_{\delta} z_{\delta} \mathcal{E}^{\delta}$ is

$$(131) \quad \langle D_X Y, Z \rangle_{\Sigma} = \sum_{\alpha, \beta, \gamma, \delta} x_{\alpha} \left(d_{\mathcal{E}^{\alpha}} y_{\gamma} + y_{\beta} \Gamma_{\alpha, \beta}^{\gamma} \right) g_{\delta, \gamma} z_{\delta}.$$

In Sec. 7.1 below we compute the Levi-Civita (covariant) derivative of a vector field, that is, the unique covariant derivative D that, for all vector fields X, Y, Z , is:

$$(LC1) \quad \text{compatible with the metric, } d_X W(Y, Z) = W(D_X Y, Z) + W(Y, D_X Z);$$

$$(LC2) \quad \text{torsion-free, } D_Y X - D_X Y = [X, Y] = d_Y X - d_X Y.$$

In Sec. 7.1.2 we compute the Riemannian parallel transport of vectors. In Sec. 7.2 we compute the Hessian of a scalar field.

All the computations are straightforward in matrix form. Lang [18, Ch. 8.4] in his statement MD3 provides an equation to compute the Levi-Civita derivative without actually introducing any base of the vector space of coordinates. In this formalism we use the Cristoffel symbol that is, minus the spray in Lang's language. This allow to write the the differential equation of the parallel transport without introducing a vector basis. Given the Levi-Civita derivative, the Riemannian Hessian of a scalar field f is given by the bi-linear operator $D_X d_Y f$. We provide too some of the expressions in the moving frame.

7.1. Levi-Civita derivative. In order to have a compact notation, it will be convenient to write the symmetrized of a matrix $A \in M(n)$ as $\{A\}_S = \frac{1}{2}(A + A^*)$. If either A or B is symmetric, then $\text{Tr}(\{A\}_S B) = \text{Tr}(AB)$. We denote by X, Y, Z smooth vector fields on $\text{Sym}^{++}(n)$. We shall use repeatedly the expression for the derivative of the vector field $\Sigma \mapsto \mathcal{L}_\Sigma[X]$. In view of Eq. 21 and our notation for the symmetrization, it holds

$$(132) \quad d_Y \mathcal{L}_\Sigma[X] = -2\mathcal{L}_\Sigma[\{\mathcal{L}_\Sigma[X]Y\}_S] .$$

Proposition 7.1. *The Levi-Civita derivative $D_X Y$ is implicitly defined by*

$$(133) \quad \begin{aligned} \langle D_X Y, Z \rangle_\Sigma = & \langle d_X Y, Z \rangle_\Sigma + \langle X, \{\mathcal{L}_\Sigma[Y]Z\}_S \rangle_\Sigma - \langle X, \{\mathcal{L}_\Sigma[Z]Y\}_S \rangle_\Sigma - \langle Y, \{\mathcal{L}_\Sigma[Z]X\}_S \rangle_\Sigma = \\ & \langle d_X Y, Z \rangle_\Sigma + \frac{1}{2} \text{Tr}(\mathcal{L}_\Sigma[X]Z\mathcal{L}_\Sigma[Y]) - \frac{1}{2} \text{Tr}(\mathcal{L}_\Sigma[X]Y\mathcal{L}_\Sigma[Z]) - \frac{1}{2} \text{Tr}(\mathcal{L}_\Sigma[Y]X\mathcal{L}_\Sigma[Z]) , \end{aligned}$$

while the Levi-Civita derivative itself is given by

$$(134) \quad D_X Y = d_X Y - \{\mathcal{L}_\Sigma[X]Y + \mathcal{L}_\Sigma[Y]X\}_S + \{\Sigma\mathcal{L}_\Sigma[X]\mathcal{L}_\Sigma[Y] + \Sigma\mathcal{L}_\Sigma[Y]\mathcal{L}_\Sigma[X]\}_S .$$

Proof. In our case, Eq. MD3 of [18, p. 205] becomes

$$(135) \quad \begin{aligned} 2 \langle D_X Y, \mathcal{L}_\Sigma[Z] \rangle_2 = & 2 \langle d_X Y, \mathcal{L}_\Sigma[Z] \rangle_2 + \langle Y, d_X \mathcal{L}_\Sigma[Z] \rangle_2 + \langle X, d_Y \mathcal{L}_\Sigma[Z] \rangle_2 - \langle X, d_Z \mathcal{L}_\Sigma[Y] \rangle_2 . \end{aligned}$$

By Eq. (21) we have

$$(136) \quad \langle Y, d_X \mathcal{L}_\Sigma[Z] \rangle_2 = -2 \langle Y, \mathcal{L}_\Sigma[\{\mathcal{L}_\Sigma[Z]X\}_S] \rangle_2 = -2 \langle Y, \{\mathcal{L}_\Sigma[Z]X\}_S \rangle_\Sigma ,$$

and, analogously,

$$(137) \quad \langle X, d_Y \mathcal{L}_\Sigma[Z] \rangle_2 = -2 \langle X, \{\mathcal{L}_\Sigma[Z]Y\}_S \rangle_\Sigma , \quad \langle X, d_Z \mathcal{L}_\Sigma[Y] \rangle_2 = -2 \langle X, \{\mathcal{L}_\Sigma[Y]Z\}_S \rangle_\Sigma .$$

This way, Eq. (135) becomes the first part of Eq. (133).

The second part of Eq. (133) are then easily obtained. For instance,

$$(138) \quad \langle X, \{\mathcal{L}_\Sigma[Z]\}_S \rangle_\Sigma = \frac{1}{2} \text{Tr}(\mathcal{L}_\Sigma[X]\{Z\mathcal{L}_\Sigma[Y]\}_S) = \frac{1}{2} \text{Tr}(\mathcal{L}_\Sigma[X]Z\mathcal{L}_\Sigma[Y]) .$$

Regarding the explicit formula of the Levi-Civita derivative (134), observe that

$$(139) \quad \begin{aligned} \frac{1}{2} \text{Tr}(\mathcal{L}_\Sigma[X]Z\mathcal{L}_\Sigma[Y]) = & \frac{1}{2} \text{Tr}(\mathcal{L}_\Sigma[Y]\mathcal{L}_\Sigma[X]Z) = \frac{1}{2} \text{Tr}(\{\mathcal{L}_\Sigma[X]\mathcal{L}_\Sigma[Y]\}_S Z) = \\ & \frac{1}{2} \text{Tr}(\mathcal{L}_\Sigma[\{\mathcal{L}_\Sigma[X]\mathcal{L}_\Sigma[Y]\}_S \Sigma + \Sigma\{\mathcal{L}_\Sigma[X]\mathcal{L}_\Sigma[Y]\}_S Z) = \\ & \langle \{\mathcal{L}_\Sigma[X]\mathcal{L}_\Sigma[Y]\}_S \Sigma + \Sigma\{\mathcal{L}_\Sigma[X]\mathcal{L}_\Sigma[Y]\}_S, Z \rangle_\Sigma = \\ & \langle \{\Sigma\mathcal{L}_\Sigma[X]\mathcal{L}_\Sigma[Y]\}_S + \{\Sigma\mathcal{L}_\Sigma[Y]\mathcal{L}_\Sigma[X]\}_S, Z \rangle_\Sigma = \\ & \langle \{\Sigma\mathcal{L}_\Sigma[X]\mathcal{L}_\Sigma[Y] + \Sigma\mathcal{L}_\Sigma[Y]\mathcal{L}_\Sigma[X]\}_S, Z \rangle_\Sigma . \end{aligned}$$

Moreover,

$$(140) \quad \frac{1}{2} \operatorname{Tr}(\mathcal{L}_\Sigma[X] Y \mathcal{L}_\Sigma[Z]) + \frac{1}{2} \operatorname{Tr}(\mathcal{L}_\Sigma[Y] X \mathcal{L}_\Sigma[Z]) = \\ \frac{1}{2} \operatorname{Tr}(\{\mathcal{L}_\Sigma[X] Y + \mathcal{L}_\Sigma[Y] X\}_S \mathcal{L}_\Sigma[Z]) = \langle \{\mathcal{L}_\Sigma[X] Y + \mathcal{L}_\Sigma[Y] X\}_S, Z \rangle_\Sigma .$$

Therefore, Eq. (133) can be written as

$$(141) \quad \langle D_X Y, Z \rangle_\Sigma = \\ \langle d_X Y - \{\mathcal{L}_\Sigma[X] Y + \mathcal{L}_\Sigma[Y] X\}_S + \{\Sigma \mathcal{L}_\Sigma[X] \mathcal{L}_\Sigma[Y] + \Sigma \mathcal{L}_\Sigma[Y] \mathcal{L}_\Sigma[X]\}_S, Z \rangle_\Sigma ,$$

and the desired result obtains.

The equation we have used for computing the Levi-Civita derivative is proved in the given reference. However, in order to have a self-contained presentation, we proceed by checking Eq. (133) against conditions (LC1) and (LC2). In fact, we have

$$(142) \quad \langle D_X Y, Z \rangle_\Sigma + \langle Y, D_X Z \rangle_\Sigma = \langle d_X Y, Z \rangle_\Sigma + \langle Y, d_X Z \rangle_\Sigma - \operatorname{Tr}(\mathcal{L}_\Sigma[Y] X \mathcal{L}_\Sigma[Z]) .$$

On the other hand, if we compute the derivative of $W(Y, Z)$ at Σ , we obtain

$$(143) \quad d_X \langle Y, Z \rangle_\Sigma = d_X \operatorname{Tr}(\mathcal{L}_\Sigma[Y] \Sigma \mathcal{L}_\Sigma[Z]) = \\ \operatorname{Tr}(d_X \mathcal{L}_\Sigma[Y] \Sigma \mathcal{L}_\Sigma[Z]) + \operatorname{Tr}(\mathcal{L}_\Sigma[Y] \Sigma d_X \mathcal{L}_\Sigma[Z]) + \operatorname{Tr}(\mathcal{L}_\Sigma[Y] X \mathcal{L}_\Sigma[Z]) .$$

Since

$$(144) \quad d_X \mathcal{L}_\Sigma[Y] = \mathcal{L}_\Sigma[d_X Y] - 2 \mathcal{L}_\Sigma[\{\mathcal{L}_\Sigma[Y]\}_S X] ,$$

we have

$$(145) \quad \operatorname{Tr}(d_X \mathcal{L}_\Sigma[Y] \Sigma \mathcal{L}_\Sigma[Z]) = \langle d_X Y, Z \rangle_\Sigma - 2 \langle \{\mathcal{L}_\Sigma[Y] X\}_S, Z \rangle_\Sigma = \\ \langle d_X Y, Z \rangle_\Sigma - \operatorname{Tr}(\{\mathcal{L}_\Sigma[Y] X\}_S \mathcal{L}_\Sigma[Z]) = \langle d_X Y, Z \rangle_\Sigma - \operatorname{Tr}(\mathcal{L}_\Sigma[Y] X \mathcal{L}_\Sigma[Z]) ,$$

and, in a similar way, we can write

$$(146) \quad \operatorname{Tr}(\mathcal{L}_\Sigma[Y] \Sigma d_X \mathcal{L}_\Sigma[Z]) \langle Y, d_X Z \rangle_\Sigma - \operatorname{Tr}(\mathcal{L}_\Sigma[Z] X \mathcal{L}_\Sigma[Y]) .$$

Substitution of the equations above in Eq. (143) proves (LS1).

Condition (LS2), is checked by

$$(147) \quad \langle D_X Y - D_Y X, Z \rangle_\Sigma = \langle d_X Y - d_Y X, Z \rangle_\Sigma = \langle [Y, X], Z \rangle_\Sigma . \quad \blacksquare$$

7.1.1. Levi-Civita derivative in the moving frame. Let us express the Levi-Civita derivative in the moving frame (120). Consider the vector field $X(\Sigma) = \mathcal{E}^\alpha(\Sigma) = E^\alpha\Sigma + \Sigma E^\alpha$ and the vector field $Y(\Sigma) = \mathcal{E}^\beta(\Sigma) = E^\beta\Sigma + \Sigma E^\beta$. By Eq. (134), we have

$$(148) \quad D_{\mathcal{E}^\alpha} \mathcal{E}^\beta = d_{\mathcal{E}^\alpha} \mathcal{E}^\beta - \left\{ \mathcal{L}_\Sigma [\mathcal{E}^\alpha] \mathcal{E}^\beta + \mathcal{L}_\Sigma [\mathcal{E}^\beta] \mathcal{E}^\alpha \right\}_S + \left\{ \Sigma \mathcal{L}_\Sigma [\mathcal{E}^\alpha] \mathcal{L}_\Sigma [\mathcal{E}^\beta] + \Sigma \mathcal{L}_\Sigma [\mathcal{E}^\beta] \mathcal{L}_\Sigma [\mathcal{E}^\alpha] \right\}_S .$$

We are going to compute one by one the three terms in the equation above.

The first term in Eq. (148) is

$$(149) \quad d_{\mathcal{E}^\alpha} \mathcal{E}^\beta = d_{(E^\alpha\Sigma + \Sigma E^\alpha)} (E^\beta\Sigma + \Sigma E^\beta) = E^\beta (E^\alpha\Sigma + \Sigma E^\alpha) + (E^\alpha\Sigma + \Sigma E^\alpha) E^\beta = E^\beta E^\alpha\Sigma + E^\beta\Sigma E^\alpha + E^\alpha\Sigma E^\beta + \Sigma E^\alpha E^\beta .$$

The second one is

$$(150) \quad - \left\{ \mathcal{L}_\Sigma [\mathcal{E}^\alpha] \mathcal{E}^\beta + \mathcal{L}_\Sigma [\mathcal{E}^\beta] \mathcal{E}^\alpha \right\}_S = - \left\{ E^\alpha (E^\beta\Sigma + \Sigma E^\beta) + E^\beta (E^\alpha\Sigma + \Sigma E^\alpha) \right\}_S = - \left\{ E^\alpha E^\beta\Sigma + E^\alpha\Sigma E^\beta + E^\beta E^\alpha\Sigma + E^\beta\Sigma E^\alpha \right\}_S = - \frac{1}{2} \left(E^\alpha E^\beta\Sigma + E^\beta E^\alpha\Sigma + \Sigma E^\beta E^\alpha + \Sigma E^\alpha E^\beta \right) - \left(E^\alpha\Sigma E^\beta + E^\beta\Sigma E^\alpha \right) .$$

The sum is

$$(151) \quad \frac{1}{2} \left(E^\beta E^\alpha\Sigma + \Sigma E^\alpha E^\beta \right) - \frac{1}{2} \left(E^\alpha E^\beta\Sigma + \Sigma E^\beta E^\alpha \right) .$$

The third term is

$$(152) \quad \left\{ \Sigma \mathcal{L}_\Sigma [\mathcal{E}^\alpha] \mathcal{L}_\Sigma [\mathcal{E}^\beta] + \Sigma \mathcal{L}_\Sigma [\mathcal{E}^\beta] \mathcal{L}_\Sigma [\mathcal{E}^\alpha] \right\}_S = \left\{ \Sigma E^\alpha E^\beta + \Sigma E^\beta E^\alpha \right\}_S = \frac{1}{2} \left(\Sigma E^\alpha E^\beta + \Sigma E^\beta E^\alpha + E^\beta E^\alpha\Sigma + E^\alpha E^\beta\Sigma \right) .$$

In conclusion,

$$(153) \quad D_{\mathcal{E}^\alpha} \mathcal{E}^\beta = E^\beta E^\alpha\Sigma + \Sigma E^\alpha E^\beta .$$

The computation of the Christoffel symbols $\sum_\gamma \Gamma_{\alpha,\beta}^\sigma \mathcal{E}^\gamma = D_{\mathcal{E}^\alpha} \mathcal{E}^\beta$ would require the solution of the equations

$$(154) \quad E^\beta E^\alpha\Sigma + \Sigma E^\alpha E^\beta = \sum_\gamma \Gamma_{\alpha,\beta}^\gamma(\Sigma) (E^\gamma\Sigma + \Sigma E^\gamma) .$$

We do not do that here.

Instead, let us take now $X = x_\alpha \mathcal{E}^\alpha$ and $Y = y_\beta \mathcal{E}^\beta$. From the properties (CD1) and (CD2), we have

$$(155) \quad D_{(x_\alpha \mathcal{E}^\alpha)}(y_\beta \mathcal{E}^\beta) = x_\alpha D_{E^\alpha}(y_\beta E^\beta) = x_\alpha \left(d_{E^\alpha} y_\beta E^\beta + y_\beta D_{E^\alpha} E^\beta \right) = \\ x_\alpha d_{E^\alpha} y_\beta E^\beta + x_\alpha y_\beta \left(E^\beta E^\alpha \Sigma + \Sigma E^\alpha E^\beta \right) .$$

Finally, for general X and Y ,

$$(156) \quad D_X Y = \sum_{\alpha, \beta} x_\alpha d_{E^\alpha} y_\beta E^\beta + \sum_{\alpha, \beta} x_\alpha y_\beta \left(E^\beta E^\alpha \Sigma + \Sigma E^\alpha E^\beta \right) .$$

7.1.2. Parallel transport. The expression of the Levi-Civita derivative in Eq. (133) can be re-written as

$$(157) \quad \langle D_X Y, Z \rangle_\Sigma = \langle d_X Y, Z \rangle_\Sigma + \langle \Gamma(\Sigma; X, Y), Z \rangle_\Sigma ,$$

where $\Gamma(\Sigma; \cdot, \cdot)$ is the symmetric tensor field defined by

$$(158) \quad \langle \Gamma(\Sigma; X, Y), Z \rangle_\Sigma = \\ \frac{1}{2} \text{Tr} (\mathcal{L}_\Sigma [X] Z \mathcal{L}_\Sigma [Y]) - \frac{1}{2} \text{Tr} (\mathcal{L}_\Sigma [X] Y \mathcal{L}_\Sigma [Z]) - \frac{1}{2} \text{Tr} (\mathcal{L}_\Sigma [Y] X \mathcal{L}_\Sigma [Z]) = \\ \frac{1}{2} \text{Tr} (\mathcal{L}_\Sigma [Y] \mathcal{L}_\Sigma [X] Z) - \frac{1}{2} \text{Tr} ((\mathcal{L}_\Sigma [X] Y + \mathcal{L}_\Sigma [Y] X) \mathcal{L}_\Sigma [Z]) = \\ \frac{1}{2} \text{Tr} (\mathcal{L}_\Sigma [Y] \mathcal{L}_\Sigma [X] (\mathcal{L}_\Sigma [Z] \Sigma + \Sigma \mathcal{L}_\Sigma [Z])) - \frac{1}{2} \text{Tr} ((\mathcal{L}_\Sigma [X] Y + \mathcal{L}_\Sigma [Y] X) \mathcal{L}_\Sigma [Z]) = \\ \frac{1}{2} \text{Tr} ((\Sigma \mathcal{L}_\Sigma [Y] \mathcal{L}_\Sigma [X] + \mathcal{L}_\Sigma [Y] \mathcal{L}_\Sigma [X] \Sigma - \mathcal{L}_\Sigma [X] Y - \mathcal{L}_\Sigma [Y] X) \mathcal{L}_\Sigma [Z]) = \\ \langle \{ \Sigma \mathcal{L}_\Sigma [Y] \mathcal{L}_\Sigma [X] + \mathcal{L}_\Sigma [Y] \mathcal{L}_\Sigma [X] \Sigma - \mathcal{L}_\Sigma [X] Y - \mathcal{L}_\Sigma [Y] X \}_S, Z \rangle_\Sigma .$$

We have

$$(159) \quad \Gamma(\Sigma; X, Y) = \{ \Sigma \mathcal{L}_\Sigma [Y] \mathcal{L}_\Sigma [X] + \mathcal{L}_\Sigma [Y] \mathcal{L}_\Sigma [X] \Sigma - \mathcal{L}_\Sigma [X] Y - \mathcal{L}_\Sigma [Y] X \}_S ,$$

and, on the diagonal,

$$(160) \quad \Gamma(\Sigma; X, X) = \Sigma \mathcal{L}_\Sigma [X] \mathcal{L}_\Sigma [X] + \mathcal{L}_\Sigma [X] \mathcal{L}_\Sigma [X] \Sigma - \mathcal{L}_\Sigma [X] X - X \mathcal{L}_\Sigma [X] .$$

$\Gamma(\Sigma; X, Y)$ is the expression in the trivial chart of the Christoffel symbol of the Levi-Civita derivative as in [17]. In [18], $-\Gamma$ is called the spray of the Levi-Civita derivative. Given the Christoffel symbol, we can write the linear differential equation of the parallel transport along a curve $t \mapsto \Sigma(t)$ as

$$(161) \quad \begin{cases} \dot{U}_V(t) + \Gamma(\Sigma(t); \dot{\Sigma}(t), U_V(t)) = 0 , \\ U_V(0) = V , \end{cases}$$

see [18, VIII, §3 and §4]. Recall that the parallel transport for the Levi-Civita derivative is isometric.

We do not discuss here the representation in the moving frame of Eq. (161). We limit ourselves to mention that the action of the Christoffel symbol on vector fields expressed in the moving frame can be computed from

$$\begin{aligned}
(162) \quad \Gamma(\Sigma; \mathcal{E}^\alpha, \mathcal{E}^\beta) = & \\
& \left\{ \Sigma \mathcal{L}_\Sigma [\mathcal{E}^\beta] \mathcal{L}_\Sigma [\mathcal{E}^\alpha] + \mathcal{L}_\Sigma [\mathcal{E}^\beta] \mathcal{L}_\Sigma [\mathcal{E}^\alpha] \Sigma - \mathcal{L}_\Sigma [\mathcal{E}^\alpha] \mathcal{E}^\beta - \mathcal{L}_\Sigma [\mathcal{E}^\beta] \mathcal{E}^\alpha \right\}_S = \\
& \left\{ \Sigma E^\beta E^\alpha + E^\beta E^\alpha \Sigma - E^\alpha (E^\beta \Sigma + \Sigma E^\beta) - E^\beta (E^\alpha \Sigma + \Sigma E^\alpha) \right\}_S = \\
& \left\{ \Sigma E^\beta E^\alpha + E^\beta E^\alpha \Sigma - E^\alpha E^\beta \Sigma - E^\alpha \Sigma E^\beta - E^\beta E^\alpha \Sigma - E^\beta \Sigma E^\alpha \right\}_S = \\
& \quad - (E^\alpha \Sigma E^\beta + E^\beta \Sigma E^\alpha) .
\end{aligned}$$

7.2. Riemannian Hessian. According to [1, Def. 5.5.1] and [11, p. 141], the Riemannian Hessian of a smooth scalar field $\phi: \text{Sym}^{++}(n) \rightarrow \mathbb{R}$, is the Levi-Civita covariant derivative of $\text{grad } \phi$, namely, for each vector field X , it is the vector field $\text{Hess}_X \phi$ whose value at Σ is

$$(163) \quad \text{Hess}_X \phi(\Sigma) = D_X(\text{grad } \phi)(\Sigma) = D_X(\nabla \phi(\Sigma) \Sigma + \Sigma \nabla \phi(\Sigma)) .$$

The associated symmetric bilinear form is (see [1, Proposition 5.5.3])

$$(164) \quad \text{Hess } \phi(\Sigma)(X, Y) = \langle D_X(\text{grad } \phi)(\Sigma), Y \rangle_\Sigma .$$

It is enough to compute the diagonal of the symmetric form, hence we let $X = Z = V$ in the second part of Eq. (133) to obtain

$$\begin{aligned}
\text{Hess } \phi(\Sigma)(V, V) = & \langle d_V Y, V \rangle_\Sigma + \\
& \frac{1}{2} \text{Tr} [\mathcal{L}_\Sigma(V) V \mathcal{L}_\Sigma(Y)] - \frac{1}{2} \text{Tr} [\mathcal{L}_\Sigma(V) Y \mathcal{L}_\Sigma(V)] - \frac{1}{2} \text{Tr} [\mathcal{L}_\Sigma(V) V \mathcal{L}_\Sigma(Y)] = \\
& \langle d_V Y, V \rangle_\Sigma - \frac{1}{2} \text{Tr} [\mathcal{L}_\Sigma(V) Y \mathcal{L}_\Sigma(V)] ,
\end{aligned}$$

where $Y = \text{grad } \phi(\Sigma)$. After plugging $Y = \text{grad } \phi(\Sigma) = \Sigma \nabla \phi(\Sigma) + \nabla \phi(\Sigma) \Sigma$ into it, we get easily

$$\begin{aligned}
(165) \quad \text{Hess } \phi(\Sigma)(V, V) = & \\
& \langle \nabla_V^2 \phi(\Sigma) \Sigma + \Sigma \nabla_V^2 \phi(\Sigma), V \rangle_\Sigma + \text{Tr} [\nabla \phi(\Sigma) V \mathcal{L}_\Sigma(V)] - \text{Tr} [\mathcal{L}_\Sigma(V) \nabla \phi(\Sigma) \Sigma \mathcal{L}_\Sigma(V)] .
\end{aligned}$$

Plugging $V = \mathcal{L}_\Sigma[V] \Sigma + \Sigma \mathcal{L}_\Sigma[V]$ into the second term of the RHS, we have at last

$$(166) \quad \text{Hess } \phi(\Sigma)(V, V) = \langle \nabla_V^2 \phi(\Sigma) \Sigma + \Sigma \nabla_V^2 \phi(\Sigma), V \rangle_\Sigma + \text{Tr} [\nabla \phi(\Sigma) \mathcal{L}_\Sigma(V) \Sigma \mathcal{L}_\Sigma(V)] .$$

Relation (166) substantiates the following important property that links the Hessian to the derivative along a geodesic (see the proof of Proposition 5.5.4 of [1]).

Proposition 7.2. *Let $\phi : \text{Sym}^{++}(n) \rightarrow \mathbb{R}$ be a smooth scalar field and define*

$$(167) \quad \varphi(t) = \phi(\exp_{\Sigma}(tV)) .$$

It holds

$$(168) \quad \ddot{\varphi}(0) = \text{Hess } \phi(\Sigma)(V, V) .$$

Proof. By Proposition 5.2

$$(169) \quad \Sigma(t) = \text{Exp}_{\Sigma}(tV) = \Sigma + tV + t^2 \mathcal{L}_{\Sigma}(V) \Sigma \mathcal{L}_{\Sigma}(V)$$

where $\Sigma(0) = \Sigma$ and $\dot{\Sigma}(0) = V$. Hence $\dot{\varphi}(t) = \langle \nabla \phi(\Sigma(t)), \dot{\Sigma}(t) \rangle_2$, and

$$(170) \quad \ddot{\varphi}(t) = \langle \nabla^2 \phi(\Sigma(t))[\dot{\Sigma}(t)], \dot{\Sigma}(t) \rangle_2 + \langle \nabla \phi(\Sigma(t)), \ddot{\Sigma}(t) \rangle_2 .$$

At $t = 0$,

$$(171) \quad \ddot{\varphi}(0) = \langle \nabla^2 \phi(\Sigma)[V], V \rangle_2 + 2 \langle \nabla \phi(\Sigma), \mathcal{L}_{\Sigma}(V) \Sigma \mathcal{L}_{\Sigma}(V) \rangle_2 .$$

In view of Eq. (166),

$$(172) \quad \text{Hess } \phi(\Sigma)(V, V) = \langle \nabla_V^2 \phi(\Sigma), V \rangle_2 + 2 \langle \nabla \phi(\Sigma), \mathcal{L}_{\Sigma}(V) \Sigma \mathcal{L}_{\Sigma}(V) \rangle = \ddot{\varphi}(0) .$$

■

8. Discussion. The present paper is intended to be an introduction to a research project in progress. It contains both a review of the literature and novel results. The issue of a comparison between Fisher and Wasserstein metric is not discussed as it is, for example, in Chevallier et al. [10].

It is the Authors' plan to investigate the following developments and applications.

1. Push-back of the geometry with the mapping $\text{Sym}(n) \ni A \mapsto e^A \in \text{Sym}^{++}(n)$.
2. Computation of the curvature tensor.
3. Numerical solution and simulation methods for the relevant equation of the geometry namely: geodesic, parallel transport, Hessian.
4. Linear optimization method using the natural gradient as direction of increase using the Riemannian exponential as a retraction. Cf. [1] and in Amari monograph [4].
5. Second order optimization method with the Riemannian Hessian and the Riemannian exponential. Cf. [1] and [4].
6. Diffusions on $\text{Sym}^{++}(n)$ with the method of J. Armstrong and D. Brigo [6].
7. Sub-manifold of the correlation matrices i.e. with diagonal elements all equal 1. In this case, the tangent space at each point is the space of symmetric matrices with zero diagonal.
8. Sub-manifold of trace 1 matrices. This application possibly requires the generalization to Complex Gaussians see e.g., Fassino et al. [13], and Hermitian matrices as in Bhatia et al. [8].

9. Sub-manifold of the concentration matrices with a given sparsity pattern. In this case the Wasserstein distance interpretation is not available but see the Bhatia interpretation of the distance [8].

REFERENCES

- [1] P.-A. ABSIL, R. MAHONY, AND R. SEPULCHRE, *Optimization algorithms on matrix manifolds*, Princeton University Press, 2008. With a foreword by Paul Van Dooren.
- [2] C. D. ALIPRANTIS AND K. C. BORDER, *Infinite dimensional analysis*, Springer, Berlin, third ed., 2006. A hitchhiker's guide.
- [3] S.-I. AMARI, *Natural gradient works efficiently in learning*, *Neural Computation*, 10 (1998), pp. 251–276, <https://doi.org/10.1162/089976698300017746>, <http://dx.doi.org/10.1162/089976698300017746>.
- [4] S.-I. AMARI, *Information geometry and its applications*, vol. 194 of Applied Mathematical Sciences, Springer, [Tokyo], 2016, <https://doi.org/10.1007/978-4-431-55978-8>.
- [5] T. W. ANDERSON, *An introduction to multivariate statistical analysis*, Wiley Series in Probability and Statistics, Wiley-Interscience [John Wiley & Sons], Hoboken, NJ, third ed., 2003.
- [6] J. ARMSTRONG AND D. BRIGO, *Coordinate-free Stochastic Differential Equations as Jets*. arXiv:1602.03931, Feb. 2016.
- [7] R. BHATIA, *Positive definite matrices*, Princeton Series in Applied Mathematics, Princeton University Press, Princeton, NJ, 2007.
- [8] R. BHATIA, T. JAIN, AND Y. LIM, *On the Bures-Wasserstein distance between positive definite matrices*. arXiv:1712.01504, Dec. 2017.
- [9] Y. BRENIER, *Polar factorization and monotone rearrangement of vector-valued functions*, *Comm. Pure Appl. Math.*, 44 (1991), pp. 375–417, <https://doi.org/10.1002/cpa.3160440402>.
- [10] E. CHEVALLIER, E. KALUNGA, AND J. ANGULO, *Kernel density estimation on spaces of Gaussian distributions and symmetric positive definite matrices*, *SIAM J. Imaging Sci.*, 10 (2017), pp. 191–215, <https://doi.org/10.1137/15M1053566>.
- [11] M. P. DO CARMO, *Riemannian geometry*, Mathematics: Theory & Applications, Birkhuser Boston Inc., 1992. Translated from the second Portuguese edition by Francis Flaherty.
- [12] D. C. DOWSON AND B. V. LANDAU, *The Fréchet distance between multivariate normal distributions*, *J. Multivariate Anal.*, 12 (1982), pp. 450–455, [https://doi.org/10.1016/0047-259X\(82\)90077-X](https://doi.org/10.1016/0047-259X(82)90077-X), [http://dx.doi.org/10.1016/0047-259X\(82\)90077-X](http://dx.doi.org/10.1016/0047-259X(82)90077-X).
- [13] C. FASSINO, G. PISTONE, E. RICCOMAGNO, AND M. P. ROGANTIN, *Moments of the multivariate Gaussian complex random variable*. arXiv:170809622, Aug. 2017.
- [14] M. GELBRICH, *On a formula for the L^2 Wasserstein metric between measures on Euclidean and Hilbert spaces*, *Math. Nachr.*, 147 (1990), pp. 185–203, <https://doi.org/10.1002/mana.19901470121>.
- [15] C. R. GIVENS AND R. M. SHORTT, *A class of Wasserstein metrics for probability distributions*, *Michigan Math. J.*, 31 (1984), pp. 231–240, <https://doi.org/10.1307/mmj/1029003026>.
- [16] P. R. HALMOS, *Finite-dimensional vector spaces*, The University Series in Undergraduate Mathematics, D. Van Nostrand Co., Inc., Princeton-Toronto-New York-London, 1958. 2nd ed.
- [17] W. P. A. KLINGENBERG, *Riemannian geometry*, vol. 1 of De Gruyter Studies in Mathematics, Walter de Gruyter & Co., Berlin, second ed., 1995, <https://doi.org/10.1515/9783110905120>.
- [18] S. LANG, *Differential and Riemannian manifolds*, vol. 160 of Graduate Texts in Mathematics, Springer-Verlag, third ed., 1995.
- [19] J. R. MAGNUS AND H. NEUDECKER, *Matrix differential calculus with applications in statistics and econometrics*, Wiley Series in Probability and Statistics, John Wiley & Sons, Ltd., Chichester, 1999. Revised reprint of the 1988 original.
- [20] L. MALAGÒ AND G. PISTONE, *Combinatorial optimization with information geometry: Newton method*, *Entropy*, 16 (2014), pp. 4260–4289.
- [21] O. L. MANGASARIAN AND S. FROMOVITZ, *The Fritz John necessary optimality conditions in the presence of equality and inequality constraints*, *J. Math. Anal. Appl.*, 17 (1967), pp. 37–47, [https://doi.org/10.1016/0022-247X\(67\)90163-1](https://doi.org/10.1016/0022-247X(67)90163-1).

- [22] R. J. McCANN, *Polar factorization of maps on Riemannian manifolds*, *Geom. Funct. Anal.*, 11 (2001), pp. 589–608, <https://doi.org/10.1007/PL00001679>.
- [23] I. OLKIN AND F. PUKELSHEIM, *The distance between two random vectors with given dispersion matrices*, *Linear Algebra Appl.*, 48 (1982), pp. 257–263, [https://doi.org/10.1016/0024-3795\(82\)90112-4](https://doi.org/10.1016/0024-3795(82)90112-4).
- [24] F. OTTO, *The geometry of dissipative evolution equations: the porous medium equation*, *Comm. Partial Differential Equations*, 26 (2001), pp. 101–174, <https://doi.org/10.1081/PDE-100002243>.
- [25] A. PAPADOPOULOS, *Metric spaces, convexity and non-positive curvature*, vol. 6 of IRMA Lectures in Mathematics and Theoretical Physics, European Mathematical Society (EMS), Zürich, second ed., 2014, <https://doi.org/10.4171/132>.
- [26] V. SIMONCINI, *Computational methods for linear matrix equations*, *SIAM Rev.*, 58 (2016), pp. 377–441, <https://doi.org/10.1137/130912839>.
- [27] A. TAKATSU, *Wasserstein Geometry of Gaussian measures*, *Osaka J. Math.*, 48 (2011), pp. 1005–1026.
- [28] E. L. WACHSPRESS, *Trail to a Lyapunov equation solver*, *Comput. Math. Appl.*, 55 (2008), pp. 1653–1659, <https://doi.org/10.1016/j.camwa.2007.04.048>.

9. Appendix.

9.1. Proof of Proposition 3.1. A symmetric matrix $\Sigma \in \text{Sym}(2n)$ is non-negative definite if, and only if, it is of the form $\Sigma = SS^*$, with $S \in M(2n)$. In our case, given the block structure of Σ in (42), we can write

$$(173) \quad \begin{bmatrix} \Sigma_1 & K \\ K^* & \Sigma_2 \end{bmatrix} = \begin{bmatrix} A \\ B \end{bmatrix} \begin{bmatrix} A^* & B^* \end{bmatrix} = \begin{bmatrix} AA^* & AB^* \\ BA^* & BB^* \end{bmatrix},$$

where A and B are two matrices in $M(n \times 2n)$.

Therefore, problem (42) becomes

$$(174) \quad \begin{cases} \alpha(\Sigma_1, \Sigma_2) = \max_{A, B \in M(n \times 2n)} 2 \text{Tr}(AB^*) \\ \text{subject to} \\ \Sigma_1 = AA^*, \quad \Sigma_2 = BB^* \end{cases}$$

We have already observed that the optimum exists, so the necessary conditions of Lagrange theorem allows us to characterize this optimum. However, the two constraints $\Sigma_1 = AA^*$ and $\Sigma_2 = BB^*$ are not necessarily regular at every point (i.e., the Jacobian of the transformation may fail to be of full rank at some point), so we must take into account that the optimum could be an irregular point. To this purpose, as a customary, we shall adopt Fritz John first-order formulation for the Lagrangian (see [21]).

We shall initially assume that both Σ_1 and Σ_2 are non-singular.

Let then $(\nu_0, \Lambda, \Gamma) \in \{0, 1\} \times \text{Sym}(n) \times \text{Sym}(n)$, with $(\nu_0, \Lambda, \Gamma) \neq (0, 0, 0)$, where the symmetric matrices Λ and Γ are the Lagrange multipliers. The Lagrangian function will be

$$\begin{aligned} L &= 2\nu_0 \text{Tr}(AB^*) - \text{Tr}(\Lambda AA^*) - \text{Tr}(\Gamma BB^*) \\ &= 2\nu_0 \text{Tr}(AB^*) - \text{Tr}(A^* \Lambda A) - \text{Tr}(B^* \Gamma B) \end{aligned}$$

The critical points of L lead to the following first order conditions

$$(175) \quad \begin{cases} \nu_0 B = \Lambda A, & \nu_0 A = \Gamma B \\ \Sigma_1 = AA^*, & \Sigma_2 = BB^* \end{cases}.$$

In the case $\nu_0 = 1$, i.e., the case of stationary regular points, Eq. (175) becomes

$$(176) \quad \begin{cases} B = \Lambda A, & A = \Gamma B \\ \Sigma_1 = AA^*, & \Sigma_2 = BB^* \end{cases},$$

which in turn implies

$$(177) \quad \begin{cases} \Lambda \Sigma_1 \Lambda = \Sigma_2 \\ \Gamma \Sigma_2 \Gamma = \Sigma_1 \end{cases}, \quad \Lambda, \Gamma \in \text{Sym}(n)$$

and further

$$(178) \quad K = \Sigma_1 \Lambda = \Gamma \Sigma_2.$$

Of course, Eq.s (177) could be more general than Eq.s (176) and thus possibly contain undesirable solutions. In this light, we establish the following facts, in which both matrices Σ_1 and Σ_2 must be nonsingular. Notice that in this case Eq.s (177) imply that both Λ and Γ are nonsingular as well.

Claim 1: If (Γ, Λ) is a solution to (177) and $\Lambda^{-1} = \Gamma$, then the couple (Γ, Λ) are Lagrange multipliers of Problem (42).

Actually, let $\Sigma_1 = AA^*$, $A \in M(n \times 2n)$ be any representation of the matrix Σ_1 . Define $B = \Lambda A$ so that $A = \Lambda^{-1}B = \Gamma B$. Moreover

$$(179) \quad BB^* = \Lambda AA^* \Lambda = \Lambda \Sigma_1 \Lambda = \Sigma_2 ,$$

and so (Λ, Γ) are multipliers associated with the feasible point (A, B) .

Claim 2: The set of solutions to (177), such that $\Gamma^{-1} = \Lambda$, is not empty. In particular, there is a unique pair $(\tilde{\Lambda}, \tilde{\Gamma})$ where both $\tilde{\Lambda}$ and $\tilde{\Gamma}$ are positive definite.

We have already observed that Eq.s (177) imply that Λ and Γ are nonsingular. Moreover, we have $\Gamma^{-1}\Sigma_1\Gamma^{-1} = \Sigma_2$. Recalling that Riccati's equation has one and only one solution in the class of positive definite matrices, then $X = \Lambda = \Gamma^{-1}$.

Now we proceed to study the solutions to $\Lambda\Sigma_1\Lambda = \Sigma_2$ and we shall show that Eq (177) has infinitely many solutions. In correspondence to each one Λ , the value of the objective function will be given by $2 \operatorname{Tr}(K) = 2 \operatorname{Tr}(\Sigma_1\Lambda)$. Therefore, we must select the matrix Λ such that $\operatorname{Tr}(\Sigma_1\Lambda)$ be maximized.

Following [12], we define

$$(180) \quad R = \Sigma_1^{1/2} \Lambda \Sigma_1^{1/2} \in \operatorname{Sym}(n) ,$$

so that, in view of (177), we have

$$(181) \quad R^2 = \Sigma_1^{1/2} \Lambda \Sigma_1^{1/2} \Sigma_1^{1/2} \Lambda \Sigma_1^{1/2} = \Sigma_1^{1/2} \Lambda \Sigma_1 \Lambda \Sigma_1^{1/2} = \Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \in \operatorname{Sym}^+(n) .$$

Moreover,

$$(182) \quad \operatorname{Tr}(R) = \operatorname{Tr}\left(\Sigma_1^{1/2} \Lambda \Sigma_1^{1/2}\right) = \operatorname{Tr}\left(\Sigma_1^{1/2} \Sigma_1^{1/2} \Lambda\right) = \operatorname{Tr}(\Sigma_1 \Lambda) = \operatorname{Tr}(K) .$$

Eq. (181) shows that, though the Lagrangian can have many rest points (i.e., many solutions Λ) the matrix $R^2 = \Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \in \operatorname{Sym}^+(n)$ remains constant. Not so the value of the objective function $\operatorname{Tr}(K) = \operatorname{Tr}(R)$ which depends on R (i.e., on Λ).

Let

$$(183) \quad R^2 = \sum_k \lambda_k E_k$$

denote the spectral decomposition of R^2 , then the solutions to R will be

$$(184) \quad R = \sum_k \varepsilon_k \lambda_k^{1/2} E_k$$

with $\varepsilon_k = \pm 1$. Hence $\text{Tr}(K) = \text{Tr}(R)$ will be maximized whenever $\varepsilon_k \equiv 1$ and so $R \in \text{Sym}^+(n)$. Clearly the objective function will be minimized if $\varepsilon_k \equiv -1$. From now on the proof of the min statement follows similarly.

It follows that the maximum of the trace occurs at

$$(185) \quad R = \left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2},$$

namely $\Lambda = \Sigma_1^{-1/2} \left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2} \Sigma_1^{-1/2}$. Thanks to Claims 1-2 this matrix is a multiplier of the Lagrangian and so we would have

$$(186) \quad \alpha(\Sigma_1, \Sigma_2) = 2\text{Tr} \left(\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2} \right)^{1/2},$$

as long as the optimum is attained at a regular point. In fact, to complete the proof, we must still examine the case $\nu_0 = 0$, for which Eq. (175) becomes

$$(187) \quad \Lambda A = 0, \quad \Gamma B = 0.$$

It follows

$$\begin{aligned} \Lambda \Sigma_1 &= \Lambda A A^* = 0 \\ \Gamma \Sigma_2 &= \Gamma B B^* = 0, \end{aligned}$$

and consequently $\Lambda = \Gamma = 0$. Therefore there is no irregular point, provided Σ_1 and Σ_2 are not singular matrices. So we have proved the relation (186) under the above assumptions.

Last step will be that of extending our result when the matrices Σ_1 and Σ_2 are not both nonsingular.

Given the two matrices $\Sigma_1, \Sigma_2 \in \text{Sym}^+(n)$, set

$$(188) \quad \Sigma_1(\varepsilon) = \Sigma_1 + \varepsilon I_n \quad \text{and} \quad \Sigma_2(\varepsilon) = \Sigma_2 + \varepsilon I_n, \quad \text{with } \varepsilon \in [0, 1].$$

If $\varepsilon > 0$, then

$$(189) \quad \det(\Sigma_i + \varepsilon I) = \prod_{j=1}^n (\lambda_{i,j} + \varepsilon) > 0, \quad i = 1, 2.$$

where $\lambda_{i,j}$, $j = 1, \dots, n$ is a set of eigenvalues of Σ_i , $i = 1, 2$. Let us consider the parametric programming problem

$$(190) \quad \begin{cases} \alpha(\Sigma_1(\varepsilon), \Sigma_2(\varepsilon)) = \max_{K \in \mathcal{M}(n)} 2 \operatorname{Tr}(K) \\ \text{subject to} \\ \begin{bmatrix} \Sigma_1(\varepsilon) & K \\ K^* & \Sigma_2(\varepsilon) \end{bmatrix} \in \operatorname{Sym}^+(2n) \end{cases}$$

Observe that the feasible region is contained in a compact set independent of $\varepsilon \in [0, 1]$ because of the bound (36).

Now the continuity of the optimal value $\varepsilon \mapsto \alpha(\Sigma_1(\varepsilon), \Sigma_2(\varepsilon))$ follows easily from Berge maximum theorem, see for instance [2, Th. 17.31]. Hence

$$(191) \quad \alpha(\Sigma_1, \Sigma_2) = \lim_{\varepsilon \rightarrow 0} \alpha(\Sigma_1(\varepsilon), \Sigma_2(\varepsilon)) = 2 \operatorname{Tr} \left((\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2})^{1/2} \right)$$

and the assertion is proved for any $\Sigma_1, \Sigma_2 \in \operatorname{Sym}^+(n)$.