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PERMUTATION-INVARIANT LOG-EUCLIDEAN GEOMETRIES ON FULL-RANK CORRELATION MATRICES *

YANN THANWERDAS[†]

Abstract. There is a growing interest in defining specific tools on correlation matrices which depart from those suited to SPD matrices. Several geometries have been defined on the open elliptope of full-rank correlation matrices: some are permutation-invariant, some others are log-Euclidean, i.e. diffeomorphic to a Euclidean space. In this work, we prove the existence of permutation-invariant log-Euclidean metrics by defining the families of off-log metrics and log-scaled metrics. Firstly, we prove that the recently introduced off-log bijection is a smooth diffeomorphism, allowing to pullback (permutation-invariant) inner products. We introduce the "cor-inverse" involution on the open elliptope which can be seen as analogous to the inversion of SPD matrices. We show that off-log metrics are not inverse-consistent. That is why secondly, we define the log-scaling smooth diffeomorphism between the open elliptope and the vector space of symmetric matrices with null row sums. This map is based on the congruence action of positive diagonal matrices on SPD matrices, more precisely on the existence and uniqueness of a "scaling", i.e. an SPD matrix with unit row sums within an orbit. Thanks to this multiplicative approach, log-scaled metrics are inverse-consistent. We provide the main Riemannian operations in closed form for the two families modulo the computation of the respective bijections.

Key words. SPD matrices, elliptope, correlation matrices, log-Euclidean metric, permutation-invariant, cor-inversion, off-log metric, log-scaled metric, quotient-affine metric

AMS subject classifications. 15B48, 15A63, 53B20, 53C22, 58D17, 53-08, 53A04, 62H20.

1. Introduction. In many domains such as Diffusion Tensor Imaging, Brain-Computer Interfaces, brain connectomes or radar signals, the data are time series which are often represented by their covariance matrices. They encode the dependence between the variables and the scale of intensity of these variables. Many Riemannian geometries were proposed to compute with covariance matrices with more natural tools that the Euclidean ones. The use of the affine-invariant metric was shown to outperform many results based on Euclidean metrics such as fiber reconstruction in DTI [36], movement classification in BCI [7] or detection of brain functional connectivity [43]. Shortly after, the log-Euclidean metric [5, 14] was shown to be a more efficient alternative to the affine-invariant metric with similar results. The Bures-Wasserstein metric was also proposed to deal with low-rank matrices since the two previous ones are only defined on the space $\operatorname{Sym}^+(n)$ of $\operatorname{Symmetric}$ Positive Definite (SPD) matrices. All these metrics belong to the wide families of kernel metrics [17] and $\operatorname{O}(n)$ -invariant metrics [41]. Non $\operatorname{O}(n)$ -invariant metrics were also proposed such as the Cholesky [45, 16], log-Euclidean-Cholesky [27] and log-Cholesky [28] metrics.

In the previously cited domains and in other domains such as electroencephalography [20], functional MRI [30, 43, 44], protein folding [6], finance and economics [3, 4, 32], genetics [12, 34], phylogenetic trees [15] or Gaussian graphical networks [26, 13], another possible and natural choice to represent the data instead of the covariance matrix is the correlation matrix. Correlation matrices forget about the scales of variables so they represent well the data when the scales are not relevant for the problem at hand. For example, in electroencephalography, two electrodes may be highly correlated with different intensities of signals. In single-cell analysis in genetics [29, 25], cells are sampled from a tissue and the goal is to identify types of different cells. For each cell i, the number of mRNA segments belonging to the gene

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[†]Université Côte d'Azur and Inria, Epione Project Team (yann.thanwerdas@inria.fr).

j is counted after a polymerase chain reaction (PCR). Thus the raw data are count matrices of size $n_{\rm cells} \times n_{\rm genes}$. An independent normalization of each row is usually applied to neglect effects related to the size of the cell: a big cell tends to have more mRNA segments than a smaller cell. Thus the correlation matrix of the count matrix is a relevant representation of the data.

However, the geometries of correlation matrices have been much less studied. Hence they are often considered as covariance matrices on which one can use the classical tools. Nevertheless, these tools are not adapted to correlation matrices, at least the O(n)-invariant ones. Indeed, firstly, the manifold of full-rank correlation matrices is not stable by the congruence action of the orthogonal group so this action has no sense for them. Secondly, it is not a totally geodesic submanifold for neither of the noted O(n)-invariant metrics on SPD matrices, except for the Euclidean metric. This motivates the study of intrinsic geometries of correlation matrices. Furthermore, when one uses classical metrics on SPD matrices, the scales of the variables and the correlations between the variables are completely mixed in the analysis while they may carry different information. While Euclidean metrics interpolate the trace monotonically and affine-invariant and log-Euclidean metrics interpolate the determinant monotonically, it was shown that such product metrics interpolate the correlation coefficient monotonically [40]. Thus, geometries of correlation matrices could also have a great impact on applications with covariance matrices since they would provide product metrics with one part on diagonal matrices and the other part on correlation matrices. It would thus allow to decouple the scales of the variables from the correlations between the variables.

Among the geometries proposed on correlation matrices, one involves a surjection from a product of spheres [37, 22]. It is an orbit space [1], this construction is quite analogous to the Bures-Wasserstein geometry of covariance matrices. However, to our knowledge, it has not been precisely described yet. A metric space structure called the Hilbert geometry relies on the convexity of the set [33]. Among the Riemannian structures, the recently introduced quotient-affine metric is obtained by taking the quotient of the affine-invariant metric under the congruence action of positive diagonal matri- $\operatorname{ces} \star : (\Delta, \Sigma) \in \operatorname{Diag}^+(n) \times \operatorname{Sym}^+(n) \longmapsto \Delta \Sigma \Delta \in \operatorname{Sym}^+(n)$ [11, 40]. Indeed, full-rank correlation matrices can be seen as the orbits of this action so the space $Cor^+(n)$ of such matrices is the quotient manifold $\operatorname{Sym}^+(n)/\operatorname{Diag}^+(n)$ and any invariant metric on $\operatorname{Sym}^+(n) \simeq \operatorname{Cor}^+(n) \times \operatorname{Diag}^+(n)$ descends to a Riemannian metric on $\operatorname{Cor}^+(n)$. These constructions have the common property to be invariant under permutations. It means that the statistical analysis is invariant under reordering the variables, which can be a relevant hypothesis when the order is arbitrary. When the order of the variables is meaningfully chosen depending on the application (e.g. for auto-correlation matrices), other Riemannian metrics that are not permutation-invariant can be considered. The metrics proposed in [42] provide a Hadamard structure or even a vector space structure, which are very convenient for computing with correlation matrices.

Given this short survey on geometries of correlation matrices, there is an obvious gap to fill in: does there exist permutation-invariant log-Euclidean metrics on the space $\operatorname{Cor}^+(n)$ of full-rank correlation matrices? By $\operatorname{log-Euclidean}$, we mean the pullback of an inner product on a vector space $\mathcal V$ by a smooth diffeomorphism referred to as a logarithm and denoted $\operatorname{Log}: \operatorname{Cor}^+(n) \longrightarrow \mathcal V$. Log-Euclidean metrics are particularly advantageous because they are flat and all the computations can be made in the diffeomorphic Euclidean space. Unfortunately, the image of the set of correlation matrices by the symmetric matrix logarithm $\operatorname{log}: \operatorname{Sym}^+(n) \longrightarrow \operatorname{Sym}(n)$ is not a vector space so one needs to define logarithms in a different way. On SPD

matrices, log-Euclidean metrics are inverse-consistent, which means that they give the same results on covariance matrices and on precision matrices. Invariance (under inversion, permutations, entry-wise scalings, orthogonal transformations, affine transformations, etc.) is a key property because it gives better control on modelling and data analysis. Indeed, if a metric is invariant, one can break the invariance in function of the problem at hand. For example, one may want to define an L^1 regularization on the precision matrix so that it is sparse. On the contrary, if a metric is not invariant, one has no clue on how differently covariance and precision matrices are treated. Invariance is also important because it makes the analysis independent from arbitrary choices, such as the order of variables in the case of a permutation-invariant metric.

In this work, we propose two approaches to define a logarithm. The first one is based on a recent bijective parametrization of full-rank correlation matrices by the space $\mathrm{LT}^0(n)$ of lower triangular matrices with null diagonal introduced by Archakov and Hansen [4]. The second one is entirely new. We rephrase their framework to present the two approaches in a similar way to facilitate the comparison between them and the comprehension of the second one by analogy with the first one. These two methods are respectively summarized in Tables 1.1 and 1.2 and explained below.

	Additive approach: off-log diffeomorphism	
Action	$+: \left\{ \begin{array}{ccc} \mathrm{Diag}(n) \times \mathrm{Sym}(n) & \longrightarrow & \mathrm{Sym}(n) \\ (D,S) & \longmapsto & D+S \end{array} \right.$	
Claim	$\forall S \in \operatorname{Sym}(n), \exists ! D := \mathcal{D}(S) \in \operatorname{Diag}(n) :$ $\exp(D+S) \in \operatorname{Cor}^+(n)$	
Status	Claim proved by Archakov and Hansen [4]	
Diagram	$\operatorname{Cor}^+(n)$ $\operatorname{Log=Off} \circ \operatorname{log} \nearrow \uparrow$	
	$\begin{array}{c} \operatorname{Log=Off \circ log} & \\ & \xrightarrow{\operatorname{Exp}} & \operatorname{exp} \circ (\mathcal{D} + \operatorname{Id}_{\operatorname{Sym}(n)}) \\ & \operatorname{Hol}(n) & \longrightarrow \operatorname{Sym}(n) & \xrightarrow{\mathcal{D}} \operatorname{Diag}(n) \end{array}$	
Outline	Section 2.1. Definition of \mathcal{D} Section 2.2. Definition of pullback metrics	

Table 1.1: Additive approach to define permutation-invariant log-Euclidean metrics on $\operatorname{Cor}^+(n)$, based on [4].

	Multiplicative approach: cor-exp diffeomorphism
Action	$\star : \left\{ \begin{array}{ccc} \operatorname{Diag}^{+}(n) \times \operatorname{Sym}^{+}(n) & \longrightarrow & \operatorname{Sym}^{+}(n) \\ (\Delta, \Sigma) & \longmapsto & \Delta \Sigma \Delta \end{array} \right.$
Claim	$\forall \Sigma \in \operatorname{Sym}^+(n), \exists ! \Delta := \mathcal{D}^*(\Sigma) \in \operatorname{Diag}^+(n) : \\ \log(\Delta \star \Sigma) \in \mathcal{V}^*$
Status	Claim proved for $\mathcal{V}^* = \text{Row}_0(n)$ in Section 3
Diagram	$\operatorname{Cor}^+(n) \operatorname{Sym}^+(n) \xrightarrow{\mathcal{D}^*} \operatorname{Diag}^+(n)$
	$\operatorname{Exp}^{\star} = \operatorname{Cor} \circ \operatorname{exp}^{\star} \bigvee^{\operatorname{log}} \circ (\mathcal{D}^{\star} \star \operatorname{Id}_{\operatorname{Sym}^{+}(n)})$
Outline	Section 3. Def. of \mathcal{D}^* (choice of appropriate \mathcal{V}^*) Section 4. Definition of pullback metrics

Table 1.2: Multiplicative approach to define permutation-invariant log-Euclidean metrics on $\operatorname{Cor}^+(n)$. This is new. The vector space \mathcal{V}^* is stable by permutations and satisfies $\operatorname{Sym}(n) = \mathcal{V}^* \oplus \operatorname{Diag}(n)$.

1.1. Results and organization of the paper. In the remainder of this section, we introduce the necessary notations and we explain our methodology based on Riemannian geometries of SPD matrices to define relevant Riemannian metrics on full-rank correlation matrices. In particular, we define the congruence action of signed permutations and a natural involution on the open elliptope called the cor-inversion, which allows to define a notion of inverse-consistency for Riemannian metrics.

In [4], Archakov and Hansen show the claim in Table 1.1, that is for all symmetric matrix S, there exists a unique diagonal matrix $D = \mathcal{D}(S)$ such that $\exp(D+S)$ is a full-rank correlation matrix. Thus it defines a surjective map $\pi: S \in \operatorname{Sym}(n) \longmapsto \exp \circ (\mathcal{D}(S) + S) \in \operatorname{Cor}^+(n)$ which is equivariant under permutations, and a bijective map $L \in \operatorname{LT}^0(n) \longmapsto \pi(L+L^\top) \in \operatorname{Cor}^+(n)$. We astutely replace the space $\operatorname{LT}^0(n)$ by the space $\mathcal{V} = \operatorname{Hol}(n)$ of symmetric matrices with null diagonal (which is of same dimension) so that the restriction $\operatorname{Exp} = \pi_{|\mathcal{V}|} : \mathcal{V} \longrightarrow \operatorname{Cor}^+(n)$ is also equivariant under permutations. Note that $\operatorname{Hol}(n)$ is actually the tangent space of $\operatorname{Cor}^+(n)$. Moreover, we trivially observe that π is invariant by the additive action of a diagonal matrix. Our contribution is to show that the bijection Exp is a smooth diffeomorphism, to define by pullback the family of off-log metrics and to provide all the Riemannian operations in closed form modulo the computation of \mathcal{D} . This additive approach is summarized in Table 1.1 and exposed in Section 2.

Our second approach consists in inverting the roles played by the vector spaces $\operatorname{Sym}(n) = \mathcal{V} \oplus \operatorname{Diag}(n)$ and the manifolds $\operatorname{Sym}^+(n) = \operatorname{Cor}^+(n) \times \operatorname{Diag}^+(n)$, as well as the matrix exponential and the matrix logarithm, and especially to replace the additive action of $\operatorname{Diag}(n)$ on $\operatorname{Sym}(n)$ by the congruence action $\star: (\Delta, \Sigma) \in \operatorname{Diag}^+(n) \times \operatorname{Sym}^+(n) \longmapsto \Delta \Sigma \Delta \in \operatorname{Sym}^+(n)$. In this work, we find a vector space \mathcal{V}^* such that for all $\Sigma \in \operatorname{Sym}^+(n)$, there exists a unique $\Delta = \mathcal{D}^*(\Sigma) \in \operatorname{Diag}^+(n)$ such that $\log(\Delta \Sigma \Delta) \in \mathcal{V}^*$. This allows to define the surjective map $\pi^*: \Sigma \in \operatorname{Sym}^+(n) \longmapsto \log(\mathcal{D}^*(\Sigma) \star \Sigma) \in \mathcal{V}^*$ and the bijective map $\operatorname{Log}^* = \pi_{|\operatorname{Cor}^+(n)} : \operatorname{Cor}^+(n) \longrightarrow \mathcal{V}^*$ which are equivariant under permutations. This multiplicative approach is summarized in Table 1.2 and exposed in Section 3. One major advantage of this multiplicative approach is that it intrinsically respects the structure of correlation matrices since $\operatorname{Cor}^+(n) = \operatorname{Sym}^+(n)/\operatorname{Diag}^+(n)$, contrarily to the additive approach. The main consequence is the compatibility with the inversion, i.e. $\pi^*(C^{-1}) = -\pi^*(C)$ for all $C \in \operatorname{Cor}^+(n)$.

More precisely, we try to prove the claim with $\mathcal{V}^* = \operatorname{Hol}(n)$ and $\mathcal{V}^* = \operatorname{Row}_0(n)$, that are the vector spaces of symmetric matrices respectively with null diagonal and null row sums. With the first choice, we only manage to prove the existence. We actually prove that the uniqueness would imply the uniqueness of the Riemannian logarithm at identity of the quotient-affine metric mentioned above, which is an open problem. This is a secondary contribution that relates two problems on full-rank correlation matrices. In contrast, we prove the claim with $\mathcal{V}^* = \operatorname{Row}_0(n)$. Indeed, we show that $\exp(\operatorname{Row}_0(n)) = \operatorname{Row}_1^+(n)$, where $\operatorname{Row}_1^+(n)$ is the submanifold of SPD matrices with unit row sums. This reduces our question to the famous problem of scaling an SPD matrix to prescribed row sums by congruence of a positive diagonal matrix: for all SPD matrix Σ , does there exist a positive diagonal matrix $\Delta = \mathcal{D}^*(\Sigma)$ such that $\Delta \Sigma \Delta \in \operatorname{Row}_1^+(n)$. The answer is yes [31, 21] so the claim is true.

In Section 4, similarly to the additive approach, we prove that the bijection Log^* is a smooth diffeomorphism and we define by pushforward the family of log-scaled metrics. Contrarily to off-log metrics, they are inverse-consistent. We provide all the Riemannian operations in closed form modulo the computation of \mathcal{D}^* , that is the

computation of the scaling of an SPD matrix. We briefly discuss on the numerical method to compute the SPD scaling. We conclude in Section 5.

1.2. Notations.

1.2.1. Matrices. Tables 1.3 and 1.4 summarize our notations for matrix spaces. We also use the following constant and linear operators on vectors and matrices:

- $\cdot \mathbb{1} \in \mathbb{R}^n$ is the vector with all entries equal to 1;
- · diag : $\mathbb{R}^n \longrightarrow \text{Diag}(n)$ makes a diagonal matrix from a vector;
- \cdot sum : $\mathbb{R}^n \longrightarrow \mathbb{R}$ computes the sum of the entries of a vector;
- · Diag: $Mat(n) \longrightarrow Diag(n)$ extracts the diagonal matrix from a matrix;
- · Off: $Mat(n) \longrightarrow ker Diag substracts the diagonal matrix from a matrix;$
- · Sum : Mat $(n) \longrightarrow \mathbb{R}$ computes the sum of entries of a matrix;
- \cdot : $Mat(n) \times Mat(n) \longrightarrow Mat(n)$ computes the Schur (entry-wise) product of matrices.

Squared of size n	$Mat(n) = \{ M = [M_{ij}]_{1 \leqslant i,j \leqslant n} M_{ij} \in \mathbb{R} \}$
Skew-symmetric	$Skew(n) = \{ Y \in Mat(n) Y^{\top} = -Y \}$
Symmetric	$\operatorname{Sym}(n) = \{ X \in \operatorname{Mat}(n) X^{\top} = X \}$
Diagonal	$Diag(n) = \{Diag(X) X \in Mat(n)\}$
Symmetric hollow (null diagonal)	$Hol(n) = \{X \in Sym(n) Diag(X) = 0\}$
Symmetric null-row-sum	$Row_0(n) = \{X \in Sym(n) X\mathbb{1} = 0\}$

Table 1.3: Matrix vector spaces

Invertible	$\operatorname{GL}(n) = \{ A \in \operatorname{Mat}(n) \det(A) \neq 0 \}$
Orthogonal	$O(n) = \{ A \in GL(n) AA^{\top} = I_n \}$
Symmetric Positive Definite	$\operatorname{Sym}^+(n) = \{AA^\top A \in \operatorname{GL}(n)\}$
Positive diagonal	$\operatorname{Diag}^+(n) = \operatorname{Sym}^+(n) \cap \operatorname{Diag}(n)$
Full-rank correlation	$\operatorname{Cor}^+(n) = \{ C \in \operatorname{Sym}^+(n) \operatorname{Diag}(C) = I_n \}$
SPD unit-row-sum	$\operatorname{Row}_{\mathbb{1}}^{+}(n) = \{ \Sigma \in \operatorname{Sym}^{+}(n) \Sigma \mathbb{1} = \mathbb{1} \}$

Table 1.4: Matrix manifolds

We denote $\mathfrak{S}(n)$ the group of permutations σ as well as the group of permutation matrices $P_{\sigma} = [\delta_{i,\sigma(j)}]_{1 \leq i,j \leq n}$. We denote $\mathcal{D}^{\pm}(n) = \{\text{Diag}(\varepsilon_1,...,\varepsilon_n), \varepsilon \in \{-1,1\}^n\}$ the group of diagonal matrices with coefficients in $\{-1,1\}$. We denote $\mathfrak{S}^{\pm}(n) = \mathcal{D}^{\pm}(n)\mathfrak{S}(n)$ the group of signed permutation matrices.

We recall the definition of the matrix exponential map $\exp: M \in \operatorname{Mat}(n) \longrightarrow \sum_{k=0}^{+\infty} \frac{1}{k!} M^k \in \operatorname{GL}(n)$ which is a smooth map. Its restriction to symmetric matrices is a smooth diffeomorphism onto SPD matrices, $\exp: \operatorname{Sym}(n) \longrightarrow \operatorname{Sym}^+(n)$. The symmetric matrix logarithm is its smooth inverse, $\log: \operatorname{Sym}^+(n) \longrightarrow \operatorname{Sym}(n)$. The computation of exp, \log and their differentials is particularly simple modulo eigenvalue decomposition. Given $\Sigma = PDP^{\top} \in \operatorname{Sym}^+(n)$, $X = Q\Delta Q^{\top}$, $Y \in \operatorname{Sym}(n)$ where $P, Q \in \operatorname{O}(n)$, $D \in \operatorname{Diag}^+(n)$ and $\Delta \in \operatorname{Diag}(n)$:

(1.1)
$$\exp(X) = Q \exp(\Delta) Q^{\top},$$

(1.2)
$$\log(\Sigma) = P \log(D) P^{\top},$$

(1.3)
$$d_X \exp(Y) = Q\left([\exp^{[1]}(\delta_i, \delta_j)]_{1 \leqslant i, j \leqslant n} \bullet (Q^\top Y Q) \right) Q^\top,$$

$$(1.4) d_{\Sigma}\log(Y) = P\left([\log^{[1]}(d_i, d_j)]_{1 \leqslant i, j \leqslant n} \bullet (P^{\top}YP)\right) P^{\top},$$

where $f^{[1]}(x,y) = \begin{cases} \frac{f(x)-f(y)}{x-y} & \text{if} \quad x \neq y \\ f'(x) & \text{if} \quad x = y \end{cases}$ is the first divided difference of $f \in \{\exp, \log\}$ [9]. In other words, the maps $\exp, \log, d \exp, d \log$ are O(n)-equivariant, and therefore $\mathfrak{S}^{\pm}(n)$ -equivariant.

1.2.2. Correlation matrices. The manifold of full-rank correlation matrices is called the open elliptope. It it relatively open in Sym(n), i.e. open in $I_n + Hol(n)$.

The correlation coefficient between two random variables X_i and X_j is defined by $\operatorname{Cor}(X_i, X_j) = \frac{\operatorname{Cov}(X_i, X_j)}{\sqrt{\operatorname{Cov}(X_i, X_i)}\sqrt{\operatorname{Cov}(X_j, X_j)}}$ where $\operatorname{Cov}(X_i, X_j) = \mathbb{E}(X_i X_j) - \mathbb{E}(X_i) \mathbb{E}(X_j)$. Denoting C the correlation matrix and Σ the covariance matrix, the relation between the two is $C_{ij} = \frac{\Sigma_{ij}}{\sqrt{\Sigma_{ii}}\sqrt{\Sigma_{jj}}} = [\operatorname{Diag}(\Sigma)^{-1/2}]_{ii}\Sigma_{ij}[\operatorname{Diag}(\Sigma)^{-1/2}]_{jj}$, that is $C = \operatorname{Diag}(\Sigma)^{-1/2}\Sigma\operatorname{Diag}(\Sigma)^{-1/2}$.

This naturally defines a smooth submersion from SPD matrices to full-rank correlation matrices $\text{Cor}: \Sigma \in \text{Sym}^+(n) \longmapsto \text{Diag}(\Sigma)^{-1/2} \Sigma \text{Diag}(\Sigma)^{-1/2} \in \text{Cor}^+(n)$. Note that it reduces to the identity map on $\text{Cor}^+(n)$ so it is idempotent. Given $\Sigma \in \text{Sym}^+(n)$, $X \in \text{Sym}(n)$, denoting $\Delta = \text{Diag}(\Sigma)^{-1/2}$, its differential is:

(1.5)
$$d_{\Sigma}\operatorname{Cor}(X) = \Delta \left[X - \frac{1}{2}(\Delta^{2}\operatorname{Diag}(X)\Sigma + \Sigma\operatorname{Diag}(X)\Delta^{2}) \right] \Delta.$$

We introduce a notation for equicorrelation matrices $C(\rho) = (1-\rho)I_n + \rho\mathbb{1}\mathbb{1}^T \in \operatorname{Cor}^+(n)$ where $\rho \in (-\frac{1}{n-1},1)$. Given a correlation matrix $C \in \operatorname{Cor}^+(n)$, there exist partitions of n, i.e. sets $I = \{i_1, ..., i_p\}$ satisfying $i_1, ..., i_p \geqslant 1$ and $i_1 + \cdots + i_p = n$, partitioning the matrix C into equicorrelation diagonal blocks and constant off-diagonal blocks. The signature of C is the maximum I_C of such sets I with respect to the natural order on partitions of n. We say that C is a block equicorrelation matrix of signature I_C (see Table 1.5). For example, an equicorrelation matrix is a block equicorrelation matrix with signature $\{n\}$. The maps introduced in this paper preserve the signature.

$$C(\rho) = \begin{pmatrix} 1 & \rho & \cdots & \rho \\ \rho & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \rho \\ \rho & \dots & \rho & 1 \end{pmatrix} \begin{vmatrix} C(\rho_1) & \rho_{12} \mathbb{1} \mathbb{1}^\top & \cdots & \rho_{1p} \mathbb{1} \mathbb{1}^\top \\ \rho_{12} \mathbb{1} \mathbb{1}^\top & C(\rho_2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \rho_{p-1,p} \mathbb{1} \mathbb{1}^\top \\ \rho_{1p} \mathbb{1} \mathbb{1}^\top & \cdots & \rho_{p-1,p} \mathbb{1} \mathbb{1}^\top & C(\rho_p) \end{pmatrix}$$

Table 1.5: Equicorrelation and block equicorrelation matrices

1.3. From covariance matrices to correlation matrices. In this section, our goal is to transpose the principles underlying the definition of invariant Riemannian metrics on SPD matrices to principles that will guide us to define invariant Riemannian metrics on full-rank correlation matrices. We first recall the main results of existence of metrics on SPD matrices and their properties of invariance under congruence and inversion. Then, we prove that the biggest congruence action that can be defined on full-rank correlation matrices is the congruence action of signed permutation matrices. Afterwards, we show how the matrix inversion descends via the canonical submersion $\operatorname{Cor}: \Sigma \in \operatorname{Sym}^+(n) \longmapsto \operatorname{Diag}(\Sigma)^{-1/2} \Sigma \operatorname{Diag}(\Sigma)^{-1/2} \in \operatorname{Cor}^+(n)$ to a natural involution of full-rank correlation matrices, that we call the cor-inversion. Finally, we synthesize the natural mathematical questions opened by this elementary study and structuring the paper.

- **1.3.1.** Invariant Riemannian metrics on SPD matrices. We recall the definition of the congruence action $\star : (A, M) \in GL(n) \times Mat(n) \longmapsto AMA^{\top} \in Mat(n)$. Note that the manifold of SPD matrices is stable by this action: for all $A \in GL(n)$, for all $\Sigma \in Sym^+(n)$, $A\Sigma A^{\top} \in Sym^+(n)$. We recall the following theorems:
 - 1. There exist $\operatorname{GL}(n)$ -invariant (also called affine-invariant) inverse-consistent metrics on SPD matrices. More precisely, $\operatorname{GL}(n)$ -invariant metrics form a two-parameter family $(g^{\operatorname{AI}(\alpha,\beta)})$ defined by $g_{\Sigma}^{\operatorname{AI}(\alpha,\beta)}(X,X) = \alpha \operatorname{tr}(\Sigma^{-1}X\Sigma^{-1}X) + \beta \operatorname{tr}(\Sigma^{-1}X)^2$, for $\Sigma \in \operatorname{Sym}^+(n)$ and $X \in T_{\Sigma}\operatorname{Sym}^+(n)$, parameterized by $\alpha > 0$ and $\beta > -\frac{\alpha}{n}$ [35]. They are all inverse-consistent.
 - 2. There exist log-Euclidean O(n)-invariant inverse-consistent metrics on SPD matrices. An example of such metrics are the ones of the two-parameter family $(g^{LE(\alpha,\beta)})$ defined by $g_{\Sigma}^{LE(\alpha,\beta)}(X,X) = \alpha \operatorname{tr}(d_{\Sigma}\log(X)^2) + \beta \operatorname{tr}(\Sigma^{-1}X)^2$, for $\Sigma \in \operatorname{Sym}^+(n)$ and $X \in T_{\Sigma}\operatorname{Sym}^+(n)$, parameterized by $\alpha > 0$ and $\beta > -\frac{\alpha}{n}$ [5]. They are defined by pullback of O(n)-invariant inner products via the symmetric matrix logarithm $\log : \operatorname{Sym}^+(n) \longrightarrow \operatorname{Sym}(n)$ which is an O(n)-equivariant smooth diffeomorphism satisfying $\log(\Sigma^{-1}) = -\log(\Sigma)$.
 - 3. There does not exist any log-Euclidean GL(n)-invariant metric (for $n \ge 2$). Indeed, GL(n)-invariant metrics are curved [38] and log-Euclidean metrics are flat.

Therefore, it is natural to investigate how the congruence action and the inversion can be defined on full-rank correlation matrices.

1.3.2. Congruence action on full-rank correlation matrices. The manifold of full-rank correlation matrices $\operatorname{Cor}^+(n)$ is not stable by the congruence action. Therefore, what are the subgroups of $\operatorname{GL}(n)$ that stabilize this space? Note that if two subgroups G, G' stabilize $\operatorname{Cor}^+(n)$, then the subgroup $\langle G, G' \rangle$ generated by G and G' also stabilizes $\operatorname{Cor}^+(n)$. Hence, the question becomes: what is the biggest subgroup of $\operatorname{GL}(n)$ that stabilizes $\operatorname{Cor}^+(n)$. The following theorem gives the answer: the subgroup of signed permutation matrices $\mathfrak{S}^{\pm}(n)$.

THEOREM 1.1 (Congruence action on full-rank correlation matrices). The biggest subgroup G of GL(n) such that for all $A \in G$, for all $C \in Cor^+(n)$, $ACA^\top \in Cor^+(n)$ is $G = \mathfrak{S}^{\pm}(n)$.

Proof. Let G be a subgroup of $\operatorname{GL}(n)$ such that for all $A \in G$, for all $C \in \operatorname{Cor}^+(n)$, $ACA^{\top} \in \operatorname{Cor}^+(n)$, i.e. $\operatorname{Diag}(ACA^{\top}) = I_n$, i.e. the columns of A^{\top} have unit C-norm. Thus, let us find the column vectors $x \in \mathbb{R}^n$ such that for all $C \in \operatorname{Cor}^+(n)$, $1 = x^{\top}Cx = \sum_{i,j} C_{ij}x_ix_j = \sum_{i=1}^n x_i^2 + 2\sum_{i < j} C_{ij}x_ix_j$. By deriving this expression with respect to C_{ij} , we find that for all $i, j \in [1, n]$, $x_ix_j = 0$. Therefore, $\sum_{i=1}^n x_i^2 = 1$. If $x_i \neq 0$, then for all $j \neq i$, $x_j = 0$ so $x_i^2 = 1$ and $x_i = \pm 1$. So $x = \pm e_i$, where $(e_1, ..., e_n)$ is the canonical basis of \mathbb{R}^n . Finally, since A^{\top} is invertible, it cannot have two proportional columns so A^{\top} is a signed permutation matrix and so does A. Conversely, $\mathfrak{S}^{\pm}(n)$ stabilizes $\operatorname{Cor}^+(n)$. So the biggest subgroup of $\operatorname{GL}(n)$ that stabilizes $\operatorname{Cor}^+(n)$ is $\mathfrak{S}^{\pm}(n)$.

Hence, it has a sense to look for permutation-invariant and signed-permutation-invariant metrics on full-rank correlation matrices.

1.3.3. Cor-inversion on full-rank correlation matrices. Since the matrix inversion is an important operation on SPD matrices, it is natural to ask if this involution descends to an involution of $\operatorname{Cor}^+(n)$ via the submersion $\operatorname{Cor}: \Sigma \in \operatorname{Sym}^+(n) \longmapsto \operatorname{Diag}(\Sigma)^{-1/2} \Sigma \operatorname{Diag}(\Sigma)^{-1/2}$.

More generally, given a surjective map $\pi: B \longrightarrow M$, what is a necessary and sufficient condition so that a map $F: B \longrightarrow B$ descends on M? That is, when does there exist a map $f: M \longrightarrow M$ such that $f \circ \pi = \pi \circ F$, or equivalently such that the following diagram commutes?

$$(1.6) B \xrightarrow{F} B \\ \downarrow_{\pi} \qquad \downarrow_{\pi} \\ M \xrightarrow{f} M$$

The first following lemma gives an answer to this question, the second one applies it to $B = \operatorname{Sym}^+(n)$, $M = \operatorname{Cor}^+(n)$, $\pi = \operatorname{Cor} : \operatorname{Sym}^+(n) \longrightarrow \operatorname{Cor}^+(n)$ and $F = \operatorname{inv} : \Sigma \in \operatorname{Sym}^+(n) \longmapsto \Sigma^{-1} \in \operatorname{Sym}^+(n)$.

LEMMA 1.2 (Descending a map via projection). Let $\pi: B \longrightarrow M$ be a surjective map between sets B and M. Let $F: B \longrightarrow B$ be a map.

- 1. There exists $f: M \longrightarrow M$ such that $f \circ \pi = \pi \circ F$ if and only if for all $p, q \in B$, if $\pi(p) = \pi(q)$, then $\pi(F(p)) = \pi(F(q))$. Moreover, f is unique.
- 2. In addition, f is injective if and only if for all $p, q \in B$, if $\pi(F(p)) = \pi(F(q))$, then $\pi(p) = \pi(q)$.
- 3. If in addition F is surjective, then f is surjective.
- Proof. 1. If there exists $f: M \longrightarrow M$ such that $f \circ \pi = \pi \circ F$, then for all $p, q \in B$, if $\pi(p) = \pi(q)$, then $\pi(F(q)) = f(\pi(p)) = f(\pi(q)) = \pi(F(q))$. Conversely, if for all $p, q \in B$, $\pi(p) = \pi(q) \Longrightarrow \pi(F(p)) = \pi(F(q))$, then for all $x \in B$, we can define $f(x) = \pi(F(p))$ where $p \in \pi^{-1}(x)$, which does not depend on the choice of p. If $g: M \longrightarrow M$ is such that $g \circ \pi = \pi \circ F$, then for all $x = \pi(p) \in M$, $g(x) = g(\pi(p)) = \pi(F(p)) = f(\pi(p)) = f(x)$ so g = f and f is unique.
- 2. If in addition for all $p, q \in B$, $\pi(F(p)) = \pi(F(q)) \Longrightarrow \pi(p) = \pi(q)$, let $x = \pi(p), y = \pi(q) \in M$ such that f(x) = f(y). Then $\pi(F(p)) = f(\pi(p)) = f(\pi(q)) = \pi(F(q))$ so $x = \pi(p) = \pi(q) = y$ and f is injective. Conversely, if in addition f is injective, then for all $p, q \in B$, if $\pi(F(p)) = \pi(F(q))$, then $f(\pi(p)) = f(\pi(q))$ so $\pi(p) = \pi(q)$.
- 3. If in addition F is surjective, then $\pi \circ F$ is surjective so for all $x \in M$, there exists $p \in B$ such that $x = \pi(F(p)) = f(\pi(p))$ so f is surjective.

LEMMA 1.3 (Compatibility between submersion Cor and inversion). Let $\pi = \text{Cor} : \text{Sym}^+(n) \longrightarrow \text{Cor}^+(n)$. The matrix inversion $F = \text{inv} : \Sigma \in \text{Sym}^+(n) \longmapsto \Sigma^{-1} \in \text{Sym}^+(n)$ satisfies all the hypotheses of Lemma 1.2. Therefore, inv descends to the bijective map $f = \mathcal{I} : C \in \text{Cor}^+(n) \longmapsto \text{Cor}(C^{-1}) \in \text{Cor}^+(n)$. This is represented on the following commuting diagram.

(1.7)
$$\operatorname{Sym}^{+}(n) \xrightarrow{\operatorname{inv}} \operatorname{Sym}^{+}(n)$$

$$\downarrow^{\operatorname{Cor}} \qquad \downarrow^{\operatorname{Cor}}$$

$$\operatorname{Cor}^{+}(n) \xrightarrow{\mathcal{I}} \operatorname{Cor}^{+}(n)$$

Proof. The matrix inversion is an involution so it is bijective. Moreover, for all $\Sigma, \Lambda \in \operatorname{Sym}^+(n)$, $\operatorname{Cor}(\Sigma) = \operatorname{Cor}(\Lambda)$ if and only if $\operatorname{Cor}(\Sigma^{-1}) = \operatorname{Cor}(\Lambda^{-1})$. So all the hypotheses of the previous lemma are satisfied. Thus, inv descends to the map $f: C \in \operatorname{Cor}^+(n) \longmapsto \operatorname{Cor}(C^{-1}) \in \operatorname{Cor}^+(n)$ because $C \in \operatorname{Cor}^{-1}(C)$.

This lemma supports the definition of the cor-inversion involution, which relates to partial correlations.

DEFINITION 1.4 (Cor-inversion). The cor-inversion is the smooth involution \mathcal{I} : $C \in \operatorname{Cor}^+(n) \longmapsto \operatorname{Cor}(C^{-1}) \in \operatorname{Cor}^+(n)$.

DEFINITION 1.5 (Partial correlation). Let $X_1, ..., X_n$ be n centered random variables on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Let $i, j \in [\![1, n]\!]$ be two distinct indices. Let $Z = (X_k)_{k \in [\![1, n]\!] \setminus \{i, j\}}$, $\beta_i = \operatorname{argmin}_{\beta \in \mathbb{R}^{n-1}} \mathbb{E}[(X_i - \beta^\top Z)^2]$ and $\beta_j = \operatorname{argmin}_{\beta \in \mathbb{R}^{n-1}} \mathbb{E}[(X_j - \beta^\top Z)^2]$. Let $R_i = X_i - \beta_i^\top Z$ and $R_j = X_j - \beta_j^\top Z$. The partial correlation coefficient Γ_{ij} between X_i and X_j given all others is defined as the correlation coefficient between R_i and R_j , namely $\Gamma_{ij} = \operatorname{Cor}(R_i, R_j) = \frac{\operatorname{Cov}(R_i, R_j)}{\sqrt{V(R_i)}\sqrt{V(R_j)}}$.

LEMMA 1.6 (Relation between partial correlations and cor-inversion). [26] Let $X_1, ..., X_n$ be n centered random variables. Let Σ be their covariance matrix. For all $i \neq j$, let Γ_{ij} be the partial correlation between X_i and X_j given all others. If Σ is invertible, then the correlation matrix $C = \text{Cor}(\Sigma) \in \text{Cor}^+(n)$ satisfies $\Gamma_{ij} = -[\mathcal{I}(C)]_{ij}$ for all $i \neq j$.

Proof. The proof of [26] assumes that $X = (X_1, ..., X_n)$ is a centered Gaussian vector. We give a more general proof in the Supplementary Material.

The bijective parametrization $C \mapsto \Gamma$ is used in the theory of stationary stochastic processes where the (potentially infinite and complex) matrices are Toeplitz. The set of partial correlation coefficients (along with the common variance) is considered as an alternative "represention of the second-order statistics" [10, Section II.B.5] of the process with respect to the traditional "auto-correlation" (or auto-covariance) function. This characterization is used in signal processing, especially in radar signal processing where the manifold of SPD Toeplitz matrices is traditionally endowed with the Poincaré polydisk geometry [8]. In Gaussian graphical networks, the partial correlation between two variables indicates the correlation between them conditionally to the other variables. Thus the partial correlations are the weights of the arrows in the network [26, 23, 13]. This approach is applied in many domains such as genomics [12, 34], brain connectomics [30, 44] and electroencephalography [20]. Hence the importance of partial correlations confirms that the cor-inversion is a relevant concept.

We consider the cor-inversion as analogous to the matrix inversion for SPD matrices inv: $\operatorname{Sym}^+(n) \longrightarrow \operatorname{Sym}^+(n)$. The cor-inversion commutes with signed permutations on full-rank correlation matrices as well as the inversion commutes with the congruence by $\operatorname{O}(n)$ on SPD matrices. Moreover, for all signature I, the space of block equicorrelation matrices of signature I is stable by the cor-inversion.

- 1.3.4. Does there exist invariant metrics on full-rank correlation matrices?. Now we have notions of congruence and inversion on full-rank correlation matrices, we can ask the following mathematical questions. On the manifold of full-rank correlation matrices $\operatorname{Cor}^+(n)$, does there exist Riemannian metrics which are:
 - 1. smooth, log-Euclidean, permutation-invariant?
 - 2. smooth, log-Euclidean, permutation-invariant, inverse-consistent?
 - 3. smooth, log-Euclidean, signed-permutation-invariant, inverse-consistent?

In this work, we solve the first two problems by explicitly building families of such metrics, based on previous works, mainly [4, 31]. The key result to ensure inverse-consistency is the following theorem.

Theorem 1.7 (Compatibility between the multiplicative approach and the corinversion). Let \mathcal{V}^* be a vector space stable by permutations and such that $\operatorname{Sym}(n) = \mathcal{V}^* \oplus \operatorname{Diag}(n)$. We assume that the claim in Table 1.1 is true, i.e. for all $C \in \operatorname{Cor}^+(n)$, there exists a unique $\Delta \in \operatorname{Diag}^+(n)$ such that $\log(\Delta C\Delta) \in \mathcal{V}^*$. This defines the inverse bijections $\operatorname{Log}^* : C \in \operatorname{Cor}^+(n) \longmapsto \log(\Delta C\Delta) \in \mathcal{V}^*$ and $\operatorname{Exp}^* = \operatorname{Cor} \circ \operatorname{exp} : \mathcal{V}^* \longrightarrow \operatorname{Cor}^+(n)$. Then, we automatically have $\operatorname{Log}^*(\mathcal{I}(C)) = -\operatorname{Log}^*(C)$, i.e. the following diagram commutes.

(1.8)
$$\operatorname{Cor}^{+}(n) \xrightarrow{\mathcal{I}} \operatorname{Cor}^{+}(n)$$

$$\downarrow^{\operatorname{Log}^{\star}} \qquad \downarrow^{\operatorname{Log}^{\star}}$$

$$\mathcal{V}^{\star} \xrightarrow{-\operatorname{Id}} \mathcal{V}^{\star}$$

Proof. Note that for all $\Sigma \in \operatorname{Sym}^+(n)$, we have $\operatorname{Cor}(\Sigma^{-1}) = \operatorname{Cor}(\operatorname{Cor}(\Sigma)^{-1})$. Indeed, if $\Sigma = DCD$ with $C = \operatorname{Cor}(\Sigma) \in \operatorname{Cor}^+(n)$, then we have $\operatorname{Cor}(\Sigma^{-1}) = \operatorname{Cor}(D^{-1}C^{-1}D^{-1}) = \operatorname{Cor}(C^{-1})$. Therefore, for all $X \in \mathcal{V}^*$ we have $\operatorname{Exp}^*(-X) = \operatorname{Cor}(\exp(-X)) = \operatorname{Cor}(\exp(X)^{-1}) = \operatorname{Cor}(\operatorname{Exp}^*(X)^{-1}) = \mathcal{I}(\operatorname{Exp}^*(X))$. Thus with $C = \operatorname{Exp}^*(X)$, we have $\operatorname{Log}^*(\mathcal{I}(X)) = -\operatorname{Log}^*(C)$.

Otherwise said, the multiplicative approach is automatically compatible with the cor-inversion. This is due to the use of the congruence action of positive diagonal matrices on SPD matrices instead of the additive action of diagonal matrices on symmetric matrices. Indeed, the former is intrinsically related to the definition of a correlation matrix. On the contrary, we can expect that the bijections built via the additive approach are not compatible with the cor-inversion in general.

Thus, if one finds a vector space \mathcal{V}^* satisfying the claim and if the bijections are smooth, the log-Euclidean metrics defined by pullback will automatically be inverse-consistent. This is quite satisfying for log-Euclidean metrics on full-rank correlation matrices in analogy with SPD matrices.

- 2. Permutation-invariant log-Euclidean metrics via the off-log diffeomorphism. In this section, we rephrase the framework of [4] (Section 2.1) to ease the comprehension of the next sections by analogy. In Section 2.2, we prove that the bijection they define, that we call the off-log bijection and that we denote Log: $\operatorname{Cor}^+(n) \longrightarrow \operatorname{Hol}(n)$, is actually a smooth diffeomorphism. It allows to pullback inner products on full-rank correlation matrices. Since the off-log diffeomorphism is equivariant under permutations, we give a characterization of permutation-invariant inner products on $\operatorname{Hol}(n)$ so that their pullbacks provide permutation-invariant log-Euclidean metrics on $\operatorname{Cor}^+(n)$. Then, we detail the Riemannian operations of these metrics. We prove that, as expected, the log-Euclidean metrics such defined are not inverse-consistent with respect to the cor-inversion. In Section 2.3, we simply recall the algorithm of [4] to compute the inverse diffeomorphism $\operatorname{Exp} = \operatorname{Log}^{-1}$, the speed of convergence and the complexity.
- **2.1. The off-log bijection.** Theorem 2.1 states that the claim in Table 1.1 is true. It allows to define the off-log bijection $\text{Log}: \text{Cor}^+(n) \longrightarrow \text{Hol}(n)$. Theorem 2.2 states some interesting properties of the off-log bijection. These results are due to Archakov and Hansen [4].

THEOREM 2.1 (Definition of \mathcal{D}). [4] For all $S \in \text{Sym}(n)$, there exists a unique $D \in \text{Diag}(n)$ such that $\exp(D+S) \in \text{Cor}^+(n)$. This allows to define:

· the surjective map $\mathcal{D}: S \in \operatorname{Sym}(n) \longmapsto D \in \operatorname{Diag}(n)$,

- the surjective map $\pi: S \in \operatorname{Sym}(n) \longmapsto \exp(\mathcal{D}(S) + S) \in \operatorname{Cor}^+(n)$ which is invariant under the additive group action $+: \operatorname{Diag}(n) \times \operatorname{Sym}(n) \longrightarrow \operatorname{Sym}(n)$,
- · the bijective map $\operatorname{Exp} = \pi_{|\operatorname{Hol}(n)} : \operatorname{Hol}(n) \longrightarrow \operatorname{Cor}^+(n)$ (note that $\pi = \operatorname{Exp} \circ \operatorname{Off}$),
- the smooth bijective inverse map $\text{Log} = \text{Exp}^{-1} = \text{Off} \circ \text{log} : \text{Cor}^+(n) \longrightarrow \text{Hol}(n)$ that we call the off-log bijection.

Theorem 2.2 (Properties of the off-log bijection). [4]

- 1. (Equivariance) Log and Exp are equivariant under permutations.
- 2. (Equicorrelation matrix) $\operatorname{Log}(C(\rho)) = \frac{1}{n} \ln \left(\frac{1 + (n-1)\rho}{1-\rho} \right) (\mathbb{1}\mathbb{1}^{\top} I_n)$ for all $\rho \in (-\frac{1}{n-1}, 1)$. In dimension n = 2, $\operatorname{Log}(C(\rho)) = \begin{bmatrix} 0 & F(\rho) \\ F(\rho) & 0 \end{bmatrix}$ where $F(\rho) = \frac{1}{2} \log(\frac{1+\rho}{1-\rho}) \in \mathbb{R}$ is the Fisher transformation of the correlation coefficient $\rho \in (-1, 1)$.
- (Block equicorrelation matrix) If C is a block equicorrelation matrix of signature I = {i₁,...,i_p}, then Log(C) is a block symmetric hollow matrix of signature I with multiples of 1_{ij} 1_{ij}[⊤] − I_{ij} on diagonal blocks and multiples of 1_{ij} 1_{ik} on off-diagonal blocks.
- 4. (Generalization) For all $\Delta \in \text{Diag}^+(n)$, for all $S \in \text{Sym}(n)$, there exists a unique $D \in \text{Diag}(n)$ such that $\text{Diag}(\exp(D+S)) = \Delta$.

Note that Theorem 2.1 is a particular case of Theorem 2.2 item 4 with $\Delta = I_n$. The result in dimension 2 was stated as a motivation in [4] to use the map Log = Off \circ log in higher dimensions since it gives in dimension 2 a well known transformation of the correlation coefficient. Interestingly, the same coefficient appears in dimension 2 for the quotient-affine metric [40].

By analogy with the symmetric matrix logarithm $\log : \operatorname{Sym}^+(n) \longrightarrow \operatorname{Sym}(n)$ satisfying $\log(\Sigma^{-1}) = -\log(\Sigma)$, one could expect that the off-log bijection $\operatorname{Log} : \operatorname{Cor}^+(n) \longrightarrow \operatorname{Hol}(n)$ "commutes with inversion", i.e. satisfies $\operatorname{Log}(\mathcal{I}(C)) = -\operatorname{Log}(C)$. We show that it is not the case as we argued in the introduction.

THEOREM 2.3 (Incompatibility between cor-inversion and off-log bijection). Let $n \ge 3$. There exists $C \in \operatorname{Cor}^+(n)$, such that $\operatorname{Log}(\mathcal{I}(C)) \ne -\operatorname{Log}(C)$. Otherwise said, the following diagram does not commute.

(2.1)
$$\operatorname{Cor}^{+}(n) \xrightarrow{\mathcal{I}} \operatorname{Cor}^{+}(n)$$

$$\downarrow^{\operatorname{Log}} \qquad \downarrow^{\operatorname{Log}}$$

$$\operatorname{Hol}(n) \xrightarrow{-\operatorname{Id}} \operatorname{Hol}(n)$$

Proof. It is easy to see it numerically. For a formal proof, one can look for a matrix $C \in \operatorname{Cor}^+(3)$ such that $\log(C)$ and $\log(\mathcal{I}(C))$ are easy to compute manually. We propose the following example with $x = \frac{1}{\sqrt{7}}$: $C = \begin{bmatrix} 1 & x - x \\ x & 1 & 0 \\ -x & 0 & 1 \end{bmatrix} = PDP^\top$ with $P = \frac{1}{2} \begin{bmatrix} 0 & \sqrt{2} & \sqrt{2} \\ \sqrt{2} & 1 & -1 \\ \sqrt{2} & -1 & 1 \end{bmatrix}$ and $D = \operatorname{diag}(1, 1 + \frac{\sqrt{2}}{\sqrt{7}}, 1 - \frac{\sqrt{2}}{\sqrt{7}})$. Then $\mathcal{I}(C) = \begin{bmatrix} 1 & -a & a \\ -a & 1 & -a^2 \\ a & -a^2 & 1 \end{bmatrix} = Q\Delta Q^\top$

with
$$a = \frac{x}{\sqrt{1-x^2}} = \frac{1}{\sqrt{6}}$$
, $Q = \frac{1}{\sqrt{14}} \begin{bmatrix} 0 & \sqrt{6} & 2\sqrt{2} \\ \sqrt{7} & -2 & \sqrt{3} \end{bmatrix}$ and $\Delta = \frac{1}{6} \operatorname{diag}(5, 10, 3)$. Thus:

$$[\operatorname{Log}(C) + \operatorname{Log}(\mathcal{I}(C))]_{12} = [\operatorname{log}(C) + \operatorname{log}(\mathcal{I}(C))]_{12}$$

$$= [P \operatorname{log}(D)P^{\top} + Q \operatorname{log}(\Delta)P^{\top}]_{12}$$

$$= \sum_{k=1}^{3} (\ln(D_{kk})P_{1k}P_{2k} + \ln(\Delta_{kk})Q_{1k}Q_{2k})$$

$$= \frac{1}{2\sqrt{2}} \ln\left(\frac{\sqrt{7} + \sqrt{2}}{\sqrt{7} - \sqrt{2}}\right) + \frac{\sqrt{6}}{7} \ln\left(\frac{3}{10}\right) > 0.$$

For $n \ge 4$, it suffices to take the block diagonal matrix $\operatorname{Diag}(C, I_{n-3})$.

This incompatibility is one of the justifications of the multiplicative approach that we present in Section 3. Still, this bijection $Log : Cor^+(n) \longrightarrow Hol(n)$ remains a very nice tool that allows to define permutation-invariant log-Euclidean metrics on full-rank correlation matrices. Let us show this.

2.2. Permutation-invariant pullback metrics via the off-log diffeomorphism. This section is part of our contributions. We prove that the off-log bijection $\text{Log}: \text{Cor}^+(n) \longrightarrow \text{Hol}(n)$ is actually a smooth diffeomorphism (Section 2.2.1), which is essential to define smooth Riemannian metrics by pullback. Then we characterize all permutation-invariant inner products on Hol(n) (Section 2.2.2) and we pull them back to permutation-invariant log-Euclidean metrics on $\text{Cor}^+(n)$ (Section 2.2.3).

2.2.1. The off-log bijection is a smooth diffeomorphism.

THEOREM 2.4 (Log = Off \circ log is a smooth diffeomorphism). The off-log bijection Log: $\operatorname{Cor}^+(n) \longrightarrow \operatorname{Hol}(n)$ is a smooth diffeomorphism. We give the differentials of Log and Exp in function of the differentials of the symmetric matrix logarithm and exponential maps log and exp. For all $C \in \operatorname{Cor}^+(n)$ and $S, X, Y \in \operatorname{Hol}(n)$, we define $H^0 \in \operatorname{Sym}^+(n)$ by $H^0_{il} = \sum_{j,k} P_{ij} P_{ik} P_{lj} P_{lk} \exp^{(1)}(\delta_j, \delta_k)$, where $P \in \operatorname{O}(n)$ and $\Delta = \operatorname{diag}(\delta_1, ..., \delta_n) \in \operatorname{Diag}(n)$ are such that $S + \mathcal{D}(S) = P\Delta P^{\top}$. Then:

(2.2)
$$d_C \operatorname{Log}(X) = \operatorname{Off}(d_C \operatorname{log}(X)),$$

(2.3)
$$d_S \mathcal{D}(Y) = -\operatorname{diag}((H^0)^{-1}\operatorname{Diag}(d_{S+\mathcal{D}(S)}\exp(Y))\mathbb{1}),$$

(2.4)
$$d_S \operatorname{Exp}(Y) = d_{S+\mathcal{D}(S)} \exp(Y + d_S \mathcal{D}(Y)).$$

Proof. It suffices to show that \mathcal{D} is smooth. We use the implicit function theorem with the smooth map $\Phi: (S,D) \in \operatorname{Sym}(n) \times \operatorname{Diag}(n) \longmapsto \operatorname{Diag}(\exp(D+S)) - I_n \in \operatorname{Diag}(n)$ which is such that $D = \mathcal{D}(S)$ if and only if $\Phi(S,D) = 0$. We want to show that for $(S,D) \in \Phi^{-1}(0)$, the differential of $\Phi_S: D \in \operatorname{Diag}(n) \longmapsto \Phi(S,D) \in \operatorname{Diag}(n)$ is invertible. It is proved in the Appendix of [4] that H^0 is the Jacobian matrix of Φ_S at $\mathcal{D}(S)$ and that $H^0 \in \operatorname{Sym}^+(n)$. This proves that $d_{\mathcal{D}(S)}\Phi_S$ is invertible. Hence, the implicit function $\mathcal{D}: \operatorname{Sym}(n) \longrightarrow \operatorname{Diag}(n)$ is smooth so $\pi = \exp \circ (\mathcal{D} + \operatorname{Id}_{\operatorname{Sym}(n)}): \operatorname{Sym}(n) \longrightarrow \operatorname{Cor}^+(n)$ is smooth. Then $\operatorname{Exp} = \pi_{|\operatorname{Hol}(n)}: \operatorname{Hol}(n) \longrightarrow \operatorname{Cor}^+(n)$ is smooth and Log is a smooth diffeomorphism.

Since Log = Off \circ log and Off is linear, the differential of Log is clear. The differential of Exp = $\exp \circ (\operatorname{Id}_{\operatorname{Hol}(n)} + \mathcal{D}_{|\operatorname{Hol}(n)})$ is also clear in function of the differential of \mathcal{D} . Let us compute the differential of \mathcal{D} . Let $S \in \operatorname{Sym}(n)$, $C = \operatorname{Exp}(S) \in \operatorname{Cor}^+(n)$,

$$\begin{split} D, \Delta \in \operatorname{Diag}(n), \, X \in \operatorname{Hol}(n) \text{ and } Y &= d_C \operatorname{Log}(X) \in \operatorname{Hol}(n). \\ 0 &= d_{(S, \mathcal{D}(S))} \Phi(Y, d_S \mathcal{D}(Y)) = \operatorname{Diag}(d_{S + \mathcal{D}(S)} \exp(d_S \mathcal{D}(Y) + Y)) \\ - \operatorname{Diag}(d_{S + \mathcal{D}(S)} \exp(Y)) &= \operatorname{Diag}(d_{S + \mathcal{D}(S)} \exp(d_S \mathcal{D}(Y))) \\ &= \operatorname{Diag}(P d_\Delta \exp(P^\top d_S \mathcal{D}(Y) P) P^\top) \\ [-\operatorname{Diag}(d_{S + \mathcal{D}(S)} \exp(Y)) \mathbb{1}]_i &= \sum_{l=1}^n \sum_{j,k} P_{ij} P_{ik} P_{lj} P_{lk} \exp^{(1)}(\delta_j, \delta_k) [d_S \mathcal{D}(Y)]_l \\ &= [H^0 d_S \mathcal{D}(Y) \mathbb{1}]_i \\ d_S \mathcal{D}(Y) &= -\operatorname{diag}((H^0)^{-1} d_{S + \mathcal{D}(S)} \exp(Y) \mathbb{1}) \end{split}$$

2.2.2. Permutation-invariant inner products on Hol(n)**.** The characterization of permutation-invariant inner products on Hol(n) can be found in [39, Example 3.8].

Theorem 2.5 (Permutation-invariant inner products on $\operatorname{Hol}(n)$). [39] For $n \geqslant 4$, permutation-invariant inner products on $\operatorname{Hol}(n)$ are the symmetric bilinear forms associated to the following positive definite quadratic forms defined for $X \in \operatorname{Hol}(n)$:

(2.5)
$$q(X) = \alpha \operatorname{tr}(X^2) + \beta \operatorname{Sum}(X^2) + \gamma \operatorname{Sum}(X)^2$$

with $\alpha > 0$, $2\alpha + (n-2)\beta > 0$ and $\alpha + (n-1)(\beta + n\gamma) > 0$. For n=3, the permutation-invariant inner products have the same form with $\alpha = 0$, i.e. $q(X) = \beta \operatorname{Sum}(X^2) + \gamma \operatorname{Sum}(X)^2$ with $\beta > 0$ and $\beta + 3\gamma > 0$. For n=2, they have the same form with $\alpha = \beta = 0$, i.e. $q(X) = \gamma \operatorname{Sum}(X)^2$ with $\gamma > 0$.

2.2.3. Pullback metrics via the off-log diffeomorphism.

DEFINITION 2.6 (Off-log metrics). An off-log metric on $\operatorname{Cor}^+(n)$ is the pullback metric of a permutation-invariant inner product characterized by a quadratic form q as in Theorem 2.5. For all $C \in \operatorname{Cor}^+(n)$ and $X \in T_C \operatorname{Cor}^+(n) = \operatorname{Hol}(n)$, it writes $g_C(X,X) = q(d_C \operatorname{Log}(X))$ where $d_C \operatorname{Log}(X) = \operatorname{Off}(d_C \operatorname{log}(X))$.

THEOREM 2.7 (Riemannian operations of off-log metrics). We consider an off-log metric characterized by the quadratic form q. Let $C, C', C_1, ..., C_k \in \text{Cor}^+(n)$, $X \in \text{Hol}(n)$. The Riemannian operations of this metric are summarized in Table 2.1.

Exponential map	$\operatorname{Exp}_{C}(X) = \operatorname{Exp}(\operatorname{Log}(C) + d_{C}\operatorname{Log}(X)))$
Logarithm map	$Log_C(C') = d_{Log(C)} Exp(Log(C') - Log(C))$
Geodesic	$\gamma(t) = \operatorname{Exp}((1-t)\operatorname{Log}(C) + t\operatorname{Log}(C'))$
Squared distance	$d(C, C')^2 = q(\operatorname{Log}(C') - \operatorname{Log}(C))$
Fréchet mean	$\bar{C} = \operatorname{Exp}(\frac{1}{k} \sum_{i=1}^{k} \operatorname{Log}(C_i))$
Curvature	R = 0
Parallel transport	$\Pi_{C \to C'} X = (d_{C'} \operatorname{Log})^{-1} (d_C \operatorname{Log}(X))$

Table 2.1: Riemannian operations of off-log metrics

In particular, the off-log metrics with $q(X) = \alpha \operatorname{tr}(X^2)$ are signed-permutation-invariant.

Beware that the Riemannian exponential and logarithm maps only coincide with the diffeomorphisms $\operatorname{Exp}:\operatorname{Hol}(n)\longrightarrow\operatorname{Cor}^+(n)$ and $\operatorname{Log}:\operatorname{Cor}^+(n)\longrightarrow\operatorname{Hol}(n)$ at $C=I_n$ introduced in Theorem 2.1. They differ from the symmetric matrix diffeomorphisms $\operatorname{exp}:\operatorname{Sym}(n)\longrightarrow\operatorname{Sym}^+(n)$ and $\operatorname{log}:\operatorname{Sym}^+(n)\longrightarrow\operatorname{Sym}(n)$.

Therefore, the off-log diffeomorphism provides a closed-form distance between two full-rank correlation matrices (modulo the computation of a symmetric matrix logarithm, i.e. modulo an eigenvalue decomposition). Moreover, all the other Riemannian operations can be computed in closed form modulo the computation of Exp, i.e. the computation of \mathcal{D} . We recall that Archakov and Hansen [4] defined an algorithm to compute $\mathcal{D}(S)$ for $S \in \operatorname{Sym}(n)$ by defining the following sequence: $D_0 = 0$ and $D_{k+1} = \varphi_S(D_k)$ where $\varphi_S : D \in \operatorname{Diag}(n) \longmapsto D - \log(\operatorname{Diag}(\exp(D+S))) \in \operatorname{Diag}(n)$ is an L-contractant map (with $L \in [0,1)$). Therefore, the convergence is linear: $\|D_{k+1} - \mathcal{D}(S)\| \le L\|D_k - \mathcal{D}(S)\|$.

In this section, we recalled the main facts on the off-log parametrization introduced in [4] and we transformed it as a geometric tool to introduce log-Euclidean metrics on full-rank correlation matrices. We also formalized this tool in terms of invariance under a group action and we showed that off-log metrics are not inverse-consistent. In the next sections, we rely on this formalization to introduce the family of log-scaled metrics which are permutation-invariant, log-Euclidean and inverse-consistent.

- 3. The log-scaling bijection. In this section, we examine two versions of the following conjecture: for all $\Sigma \in \operatorname{Sym}^+(n)$, there exists a unique $\Delta \in \operatorname{Diag}^+(n)$ such that $\log(\Delta\Sigma\Delta) \in \mathcal{V}^*$. This conjecture depends on \mathcal{V}^* , which is a vector space stable by permutations satisfying $\operatorname{Sym}(n) = \mathcal{V}^* \oplus \operatorname{Diag}(n)$. In Section 3.1, we relate the conjecture with $\mathcal{V}^* = \operatorname{Hol}(n)$ to the problem of the quotient-affine logarithm [11, 40]. We prove the existence and we explain why the uniqueness remains difficult to prove. In Section 3.2, we explain why $\mathcal{V}^* = \operatorname{Row}_0(n)$ is a good candidate for the conjecture to be true and in Section 3.3, we prove the conjecture thanks to a result known as the existence and uniqueness of the scaling of SPD matrices [31, 21]. In Section 3.4, we give the properties of our new Euclideanization called the log-scaling bijection.
- **3.1.** Is the conjecture true with $\mathcal{V}^* = \text{Hol}(n)$?. Before relating the conjecture with $\mathcal{V}^* = \text{Hol}(n)$ to the problem of existence and uniqueness of the Riemannian logarithm at I_n of the quotient-affine metric, we recall the conjecture and the definition of the quotient-affine metric.

Conjecture 3.1 (The result is true with $\mathcal{V}^* = \operatorname{Hol}(n)$). For all $\Sigma \in \operatorname{Sym}^+(n)$, there exists a unique matrix $\Delta \in \operatorname{Diag}^+(n)$ such that $\log(\Delta \Sigma \Delta) \in \operatorname{Hol}(n)$.

DEFINITION 3.2 (Quotient-affine metric). The quotient-affine metric on $\operatorname{Cor}^+(n)$ is the quotient metric of the affine-invariant metric on $\operatorname{Sym}^+(n)$ by the congruence action of $\operatorname{Diag}^+(n)$ [11]. At I_n , the horizontal space is $\mathcal{H}_{I_n}^{\operatorname{QA}} = \operatorname{Hol}(n)$, the quotient-affine metric writes $g_{I_n}^{\operatorname{QA}}(X,X) = \operatorname{tr}(X^2)$ and the exponential map writes $\operatorname{Exp}_{I_n}^{\operatorname{QA}}(X) = \operatorname{Cor}(\exp(X))$ for all $X \in \operatorname{Hol}(n)$ [40].

THEOREM 3.3 (Existence and equivalence of conjectures). We define the smooth map $f: \Delta \in \text{Diag}^+(n) \longmapsto d^{\text{AI}}(I_n, \Delta C \Delta)^2 = \text{tr}(\log(\Delta C \Delta)^2)$. It gives the affine-invariant squared distance between I_n and all points of the fiber $\text{Cor}^{-1}(C) = \{\Delta C \Delta \in \text{Sym}^+(n) | \Delta \in \text{Diag}^+(n) \}$.

- 1. The smooth map f has a global minimizer.
- 2. For all $\Sigma \in \operatorname{Sym}^+(n)$, there exists $\Delta \in \operatorname{Diag}^+(n)$ such that $\log(\Delta \Sigma \Delta) \in$

Hol(n).

- 3. The following conjectures are equivalent for all $C \in \operatorname{Cor}^+(n)$.
 - (i) There exists a unique $\Delta \in \operatorname{Diag}^+(n)$ such that $\log(\Delta C\Delta) \in \operatorname{Hol}(n)$ (Conjecture 3.1).
 - (ii) There exists a unique $X \in \text{Hol}(n)$ such that $\text{Exp}_{I_n}^{QA}(X) = C$.
 - (iii) There exists a unique local minimizer of the smooth map f, which is actually the global minimizer ensured by statement 1.
- 4. The previous conjectures imply the uniqueness of the quotient-affine logarithm at I_n .
- *Proof.* 1. The smooth map f has a global minimizer because it is coercive [40, cf. HAL version].
- Hence, there exists Δ ∈ Diag⁺(n) such that f(Δ) = min f. In other words, ΔCΔ is "in optimal position" to I_n [18, Definition 2.3]. Thus [18, Theorem 2.4], the geodesic from I_n to ΔCΔ is horizontal, i.e. Log^{AI}_{In}(ΔCΔ) ∈ ℋ^{QA}_{In}, i.e. log(ΔCΔ) = Hol(n). For Σ = Diag(Σ)^{1/2} C Diag(Σ)^{1/2}, it suffices to take ΔDiag(Σ)^{-1/2} ∈ Diag⁺(n).
 Since Exp^{QA}_{In} = Cor ∘ exp, we clearly have (i) ⇐⇒ (ii) because X = log(ΔCΔ)
- 3. Since $\operatorname{Exp}_{I_n}^{QA} = \operatorname{Coro} \exp$, we clearly have (i) \iff (ii) because $X = \log(\Delta C\Delta)$ and $\Delta = \operatorname{Diag}(\exp(X))^{1/2}$. To prove (i) \iff (iii), let us compute the differential and the Hessian of f. Let $\Delta \in \operatorname{Diag}^+(n)$ and $D, D' \in \operatorname{Diag}(n)$. We denote $E = D\Delta^{-1} \in \operatorname{Diag}(n)$ and $A = \Delta C\Delta = PBP^{\top} \in \operatorname{Sym}^+(n)$ with $P \in \operatorname{O}(n)$ and $B \in \operatorname{Diag}^+(n)$. We define $L_{il} = \sum_{j,k} P_{ij} P_{ik} P_{lj} P_{lk} \log^{[1]}(b_j, b_k) (b_j + b_k)$. Then, L is a principal submatrix of $(P \otimes P)\mathbb{B}(P \otimes P)^{\top} \in \operatorname{Sym}^+(n)$ with $\mathbb{B} \in \operatorname{Diag}^+(n)$ defined by $\mathbb{B}_{(n-1)j+k,(n-1)j+k} = \log^{[1]}(b_j,b_k)(b_j + b_k)$, so $L \in \operatorname{Sym}^+(n)$.

$$d_{\Delta}f(D) = 2\operatorname{tr}(\log(\Delta C\Delta) d_{\Delta C\Delta} \log((DC\Delta + \Delta CD)))$$

$$= 2\operatorname{tr}(\log(A) d_A \log(EA + AE^{\top}))$$

$$= 2\operatorname{tr}(\log(B) d_B \log(P^{\top}EPB + BP^{\top}E^{\top}P))$$

$$= 2\operatorname{tr}(\log(B)B^{-1}(P^{\top}EPB + BP^{\top}E^{\top}P))$$

$$= 4\operatorname{tr}(\log(A)E) = 4\operatorname{tr}(\log(\Delta C\Delta)D\Delta^{-1}),$$

$$\begin{split} d_{\Delta}f &= 0 \Longleftrightarrow \operatorname{Diag}(\log(\Delta C \Delta)) = 0 \Longleftrightarrow \log(\Delta C \Delta) \in \operatorname{Hol}(n), \\ H_{\Delta}f(D,D') &= 4\operatorname{tr}(d_A \log(EA + AE^{\top})D'\Delta^{-1} - \log(A)D'\Delta^{-1}D\Delta^{-1}) \\ &= 4\operatorname{tr}(d_B \log(P^{\top}EPB + BP^{\top}EP)P^{\top}D'\Delta^{-1}P - \operatorname{Diag}(\log(\Delta C \Delta))\Delta^{-2}DD') \\ &= 4\sum_{i,j,k,l} \log^{[1]}(b_j,b_k)P_{ij}P_{ik}\delta_i^{-1}d_i(b_j+b_k)P_{lj}P_{lk}\delta_l^{-1}d_l' - 4\operatorname{tr}(\operatorname{Diag}(\log(\Delta C \Delta))\Delta^{-2}DD') \\ &= 4\operatorname{tr}(L\Delta^{-2}DD' - \operatorname{Diag}(\log(\Delta C \Delta))\Delta^{-2}DD'), \\ H_{\Delta}f(D,D) &= 4\operatorname{tr}((L - \operatorname{Diag}(\log(\Delta C \Delta)))\Delta^{-2}D^2). \end{split}$$

Hence, if $\Delta \in \operatorname{Diag}^+(n)$ is such that $\log(\Delta C\Delta) \in \operatorname{Hol}(n)$, then the Hessian of f at Δ is $4L \in \operatorname{Sym}^+(n)$ so f has a local minimum at Δ . Thus, if proposition (iii) is true, then Δ has to be the global minimizer so it is unique. Conversely, if f has a local minimum at $\Delta \in \operatorname{Diag}^+(n)$, then $d_{\Delta}f = 0$ so $\log(\Delta C\Delta) \in \operatorname{Hol}(n)$. Thus, if proposition (i) is true, then Δ is unique. Therefore, assertions (i) and (iii) are equivalent.

4. A quotient-affine logarithm of $C \in \operatorname{Cor}^+(n)$ at I_n is a tangent vector $X \in \operatorname{Hol}(n)$ of minimal length such that $\operatorname{Exp}_{I_n}^{\operatorname{QA}}(X) = \operatorname{Cor}(\exp(X)) = C$. Otherwise said, it is a tangent vector $X = \log(\Delta C \Delta)$ where Δ minimizes $f(\Delta) = \operatorname{tr}(X^2) = \|X\|^2$. Thus the uniqueness in the conjectures of statement 3 imply the uniqueness of the quotient-affine logarithm at I_n .

Otherwise said, Conjecture 3.1 is stronger than the conjecture stating the uniqueness of the quotient-affine logarithm at I_n . On the one hand, this could provide a new path to prove the latter. However, Conjecture 3.1 seems difficult to prove because the manifold $\exp(\text{Hol}(n))$ is hard to describe in terms of properties on the coefficients of the matrices. Thus it is difficult to determine whether its intersection with the fiber $\text{Diag}^+(n)\star\Sigma=\text{Cor}^{-1}(\text{Cor}(\Sigma))$ is reduced to one point or not. On the other hand, this could also help to show that Conjecture 3.1 is false. Indeed, the quotient-affine metric has both positive and negative curvature so the quotient-affine logarithm might not be unique. Hence, this seems to be a difficult problem.

3.2. Why $\mathcal{V}^* = \operatorname{Row}_0(n)$ seems to be a better choice. Nevertheless, another interesting decomposition of symmetric matrices where each subspace is stable by permutations is given by $\operatorname{Sym}(n) = \operatorname{Row}_0(n) \oplus \operatorname{Diag}(n)$, where $\operatorname{Row}_0(n) = \{S \in \operatorname{Sym}(n) | S\mathbb{1} = 0\}$ is the vector space of symmetric matrices with null row sum. That is why we propose to examine $\mathcal{V}^* = \operatorname{Row}_0(n)$. In the following theorem, we show that $\exp(\operatorname{Row}_0(n))$ has a nice form.

THEOREM 3.4 (exp : $\operatorname{Row}_0(n) \longrightarrow \operatorname{Row}_1^+(n)$ is a smooth diffeomorphism). The symmetric matrix logarithm is a smooth diffeomorphism from $\operatorname{Row}_1^+(n) = \{\Sigma \in \operatorname{Sym}^+(n) | \Sigma \mathbb{1} = \mathbb{1}\}$ onto $\operatorname{Row}_0(n) = \{S \in \operatorname{Sym}(n) | S\mathbb{1} = 0\}$.

Proof. It is clear that $\exp(\operatorname{Row}_0(n)) \subset \operatorname{Row}_1^+(n)$ since if $S \in \operatorname{Row}_0(n)$, then $\exp(S)\mathbbm{1} = \sum_{k=0}^\infty \frac{1}{k!} S^k \mathbbm{1} = \mathbbm{1}$. Conversely, let $\Sigma \in \operatorname{Row}_1^+(n)$. Then the Lagrange polynomial $P(X) = \sum_{\lambda \in \operatorname{eig}(\Sigma)} \log(\lambda) \prod_{\mu \in \operatorname{eig}(\Sigma), \mu \neq \lambda} \frac{X+1-\mu}{\lambda-\mu}$ satisfies $P(\Sigma - I_n) = \log \Sigma$. Since $1 \in \operatorname{eig}(\Sigma)$, $P(0) = \log(1) + \sum_{\lambda \neq 1} \log(\lambda) \frac{1-1}{\lambda-1} \prod_{\mu \neq \lambda, 1} \frac{1-\mu}{\lambda-\mu} = 0$. Hence $\log(\Sigma)\mathbbm{1} = P(\Sigma - I_n)\mathbbm{1} = P(0)\mathbbm{1} = 0$. So $\log(\operatorname{Row}_1^+(n)) \subset \operatorname{Row}_0(n)$. Finally, $\operatorname{Row}_1^+(n) = \exp(\operatorname{Row}_0(n))$ so $\log : \operatorname{Row}_1^+(n) \longrightarrow \operatorname{Row}_0(n)$ is a smooth diffeomorphism.

Hence, the question becomes: for all $\Sigma \in \operatorname{Sym}^+(n)$, does there exist a unique $\Delta \in \operatorname{Diag}^+(n)$ such that $\Delta \Sigma \Delta \in \operatorname{Row}_1^+(n)$? The answer is yes [31, 21], let us explain why.

3.3. The conjecture is true with $\mathcal{V}^* = \operatorname{Row}_0(n)$. We recall that we denote $\star : \operatorname{Diag}^+(n) \times \operatorname{Sym}^+(n) \longrightarrow \operatorname{Sym}^+(n)$ the congruence action of positive diagonal matrices on SPD matrices.

THEOREM 3.5 (Definition of \mathcal{D}^*). For all $\Sigma \in \operatorname{Sym}^+(n)$, there exists a unique $\Delta \in \operatorname{Diag}^+(n)$ such that $\Delta \Sigma \Delta \in \operatorname{Row}^+_1(n)$ [31, 21] or equivalently $\log(\Delta \Sigma \Delta) \in \operatorname{Row}_0(n)$ by Theorem 3.4. This allows to define:

- the surjective map $\mathcal{D}^*: \Sigma \in \operatorname{Sym}^+(n) \longmapsto \Delta \in \operatorname{Diag}^+(n)$,
- the surjective map $\pi^* : \Sigma \in \operatorname{Sym}^+(n) \longmapsto \log(\mathcal{D}^*(\Sigma) * \Sigma) \in \operatorname{Row}_0(n)$ which is invariant under the congruence group action of $\operatorname{Diag}^+(n)$ on $\operatorname{Sym}^+(n)$,
- the bijective map $\operatorname{Log}^* = \pi_{|\operatorname{Cor}^+(n)}^* : \operatorname{Cor}^+(n) \longrightarrow \operatorname{Row}_0(n)$ that we call the log-scaling (note that $\pi^* = \operatorname{Log}^* \circ \operatorname{Cor}$),
- · the smooth bijective inverse map $\operatorname{Exp}^* = (\operatorname{Log}^*)^{-1} = \operatorname{Cor} \circ \exp : \operatorname{Row}_0(n) \longrightarrow \operatorname{Cor}^+(n)$.

Proof. The existence and uniqueness are due to [31], the uniqueness has been proved differently later in [21].

- The map \mathcal{D}^* is surjective because $\mathcal{D}^*(\Delta^{-2}) = \Delta$ for all $\Delta \in \text{Diag}^+(n)$.
- The map π^* is surjective because if $S \in \text{Row}_0(n)$, then $\pi^*(\exp(S)) = S$.
- · The map $\operatorname{Log}^{\star}$ is surjective because $\operatorname{Log}^{\star}(\operatorname{Cor}(\exp(S))) = S$ and injective because if $C, C' \in \operatorname{Cor}^+(n)$ are such that $\operatorname{Log}^*(C) = \operatorname{Log}^*(C')$, then $\mathcal{D}^*(C) \star$ $C = \mathcal{D}^{\star}(C') \star C'$ so $C = \operatorname{Cor}(\mathcal{D}^{\star}(C) \star C) = \operatorname{Cor}(\mathcal{D}^{\star}(C') \star C') = C'$.
- · We just showed that $(\text{Log}^*)^{-1} = \text{Cor} \circ \exp \text{ so } \text{Exp}^* = (\text{Log}^*)^{-1}$ is bijective and smooth.
- **3.4.** Properties of the log-scaling bijection. Let us give properties of the log-scaling bijection Log* that are analogous to the properties of the off-log bijection Log introduced in Section 2.

Theorem 3.6 (Properties of the log-scaling bijection).

- 1. (Equivariance) Log* and Exp* are equivariant under permutations.
- 2. (Equicorrelation) $\operatorname{Log}^{\star}(C(\rho)) = \frac{1}{n} \ln \left(\frac{1 + (n-1)\rho}{1-\rho} \right) (\mathbb{1}\mathbb{1}^{\top} nI_n)$ for all $\rho \in$ $(-\frac{1}{n-1},1)$. In dimension n=2, $\operatorname{Log}^{\star}(C(\rho))=\begin{pmatrix} -F(\rho) & F(\rho) \\ F(\rho) & -F(\rho) \end{pmatrix}$ where $F(\rho) = \frac{1}{2} \log(\frac{1+\rho}{1-\rho}) \in \mathbb{R}$ is the Fisher transformation of the correlation coefficient $\rho \in (-1,1)$.
- 3. (Block equicorrelation matrix) If C is a block equicorrelation matrix of signature $I = \{i_1, ..., i_p\}$, then $Log^*(C)$ is a block symmetric matrix with null row sum of signature I with diagonal blocks of the form $(\alpha_j - \beta_j)I_{i_j} + \beta_j \mathbb{1}_{i_j} \mathbb{1}_{i_j}$ and off-diagonal blocks of the form $\beta_{jk} \mathbb{1}_{i_j} \mathbb{1}_{i_k}^\top$.
- 4. (Generalization) For all $x \in (\mathbb{R}^+)^n$, for all $\Sigma \in \operatorname{Sym}^+(n)$, there exists a unique $\Delta \in \text{Diag}^+(n)$ such that $\log(\Delta \Sigma \Delta)x = 0$.
- 1. For all $\Sigma \in \operatorname{Sym}^+(n)$, $D \in \operatorname{Diag}^+(n)$ and $\sigma \in \mathfrak{S}(n)$, we have Proof. $D\Sigma D\mathbb{1} = \mathbb{1}$ if and only if $P_{\sigma}DP_{\sigma}^{\top}P_{\sigma}\Sigma P_{\sigma}^{\top}P_{\sigma}DP_{\sigma}^{\top}\mathbb{1} = \mathbb{1}$, so $\mathcal{D}^{\star}(P_{\sigma}\Sigma P_{\sigma}^{\top}) = \mathbb{1}$ $P_{\sigma}\mathcal{D}^{\star}(\Sigma)P_{\sigma}^{\top}$. This proves that \mathcal{D}^{\star} is equivariant under permutations, and so do Log* and Exp*.
- 2. Let $C=C(\rho)$. The result is clear for $\rho=0$ so we assume that $\rho\neq 0$. One easily checks that $\Delta=\sqrt{a}I_n$ with $a=\frac{1}{1+(n-1)\rho}$ satisfies $\Sigma:=\Delta C\Delta=aC=$ $(a-b)I_n + b\mathbb{1}\mathbb{1}^\top \in \text{Row}_{\mathbb{1}}^+(n) \text{ with } b = a\rho = \frac{\rho}{1 + (n-1)\rho}. \text{ Indeed, } a + (n-1)b = 1.$ Since $\log(\Sigma)$ is a polynomial in Σ , there exists $(\alpha, \beta) \in \mathbb{R}^2$ such that $\log(\Sigma) =$ $(\alpha - \beta)I_n + \beta \mathbb{1}\mathbb{1}^{\top}$ and $\alpha + (n-1)\beta = 0$. Moreover, $\operatorname{eig}(\Sigma) = \{1; a-b\}$ with $a-b \neq 1$ and $\operatorname{eig}(\log(\Sigma)) = \{0; \alpha-\beta\}$ so $\alpha-\beta = \ln(a-b) = -\ln\left(\frac{1+(n-1)\rho}{1-\rho}\right)$. Therefore, $n\beta = -(\alpha - \beta) = \ln\left(\frac{1 + (n-1)\rho}{1-\rho}\right)$ and: $\operatorname{Log}^{\star}(C) = (\alpha - \beta)I_n + \beta \mathbb{1}\mathbb{1}^{\top} = \beta(\mathbb{1}\mathbb{1}^{\top} - nI_n) = \frac{1}{n}\ln\left(\frac{1 + (n-1)\rho}{1-\rho}\right)(\mathbb{1}\mathbb{1}^{\top} - nI_n).$

$$\operatorname{Log}^{\star}(C) = (\alpha - \beta)I_n + \beta \mathbb{1}\mathbb{1}^{\top} = \beta(\mathbb{1}\mathbb{1}^{\top} - nI_n) = \frac{1}{n} \ln \left(\frac{1 + (n - 1)\rho}{1 - \rho} \right) (\mathbb{1}\mathbb{1}^{\top} - nI_n).$$

- 3. If C is a block equicorrelation matrix of signature $I = \{i_1, ..., i_p\}$, it is clear that the matrix Δ is a block diagonal matrix of signature I with scalar blocks because the sums of all the rows belonging to the same interval $[i_i + 1; i_{i+1}]$ are equal. The matrix product preserves the signature and the form of the blocks so the logarithm as well.
- 4. Similarly to Theorem 3.4, one can prove that given $x \in (\mathbb{R}^+)^n$, the map $\exp: \{S \in \operatorname{Sym}(n) | Sx = 0\} \longrightarrow \{\Sigma \in \operatorname{Sym}^+(n) | \Sigma x = x\} \text{ is a smooth }$ diffeomorphism. We denote $X = \operatorname{diag}(x) \in \operatorname{Diag}^+(n)$. Therefore, for all $\Delta \in \operatorname{Diag}^+(n), \log(\Delta \Sigma \Delta)x = 0$ if and only if $\Delta \Sigma \Delta x = x$ if and only if

 $X\Delta\Sigma\Delta X\mathbb{1} = X^2\mathbb{1}$ if and only if $X\Delta \in \text{Diag}^+(n)$ scales Σ onto an SPD matrix with row sums prescribed by $X^2\mathbb{1}$. Thus the existence and uniqueness are ensured by [31].

The log-scaling bijection has an additional property: it is compatible with the cor-inversion. It is a corollary of Theorem 1.7, the key reason being the use of the congruence action of positive diagonal matrices instead of the additive action of diagonal matrices.

THEOREM 3.7 (Compatibility between inversion and log-scaling bijection). For all $C \in \text{Cor}^+(n)$, $\text{Log}^*(\mathcal{I}(C)) = -\text{Log}^*(C)$. Otherwise said, the following diagram commutes.

(3.1)
$$\operatorname{Cor}^{+}(n) \xrightarrow{\mathcal{I}} \operatorname{Cor}^{+}(n)$$

$$\downarrow^{\operatorname{Log}^{\star}} \qquad \downarrow^{\operatorname{Log}^{\star}}$$

$$\operatorname{Row}_{0}(n) \xrightarrow{-\operatorname{Id}} \operatorname{Row}_{0}(n)$$

3.5. Numerical computation of \mathcal{D}^* . Several algorithms exist to compute the scaling of a matrix to prescribed row sums since it is an important research topic in different scientific communities from linear algebra to probability theory. In general, scaling a matrix $\Sigma \in \operatorname{Mat}(n)$ to $\mu \in \mathbb{R}^n$ means finding positive diagonal matrices $D_1, D_2 \in \operatorname{Diag}(n)$ such that $D_1 \Sigma D_2 \mathbb{1} = \mu$. The reader may refer to [21, 19, 2] for surveys on theoretical results and algorithms.

Following the proof of [31], given $\Sigma \in \operatorname{Sym}^+(n)$, $D = \mathcal{D}^*(\Sigma)$ if and only if D minimizes the strictly convex map $F : D \in \operatorname{Diag}^+(n) \longmapsto \frac{1}{2}\mathbb{1}^\top D^\top \Sigma D\mathbb{1} - \operatorname{tr}(\log(D)) \in \mathbb{R}$. The author warmly thanks Pierre-Antoine Absil for this bright observation.

Indeed, the gradient of F at $D \in \operatorname{Diag}^+(n)$ is $\nabla_D F = \Sigma D\mathbb{1} - D^{-1}\mathbb{1}$ and the Hessian of F at D is $H_D F = \Sigma + D^{-2}$. F is coercive and strictly convex so it has a unique minimum D satisfying $\nabla_D F = 0$, that is $D\Sigma D\mathbb{1} = \mathbb{1}$, that is $D = \mathcal{D}^*(\Sigma)$. F is even strongly convex since $H_D F \succcurlyeq \min \operatorname{sp}(\Sigma) I_n$, and self-concordant since the derivative at 0 of the map $t \longmapsto H_{D+t\Delta} F = \Sigma + (D+t\Delta)^{-2}$ is $-2D^{-3}\Delta$ for all $\Delta \in \operatorname{Diag}(n)$ and:

$$2D^{-2} \leq 2(\Sigma + D^{-2}) = 2H_D F,$$

$$\forall i, d_i^{-1} |\delta_i| \leq (\operatorname{tr}(D^{-2}\Delta^2))^{1/2} \leq (\operatorname{tr}(\Delta \Sigma \Delta + D^{-2}\Delta^2))^{1/2} = (\operatorname{tr}(\Delta (H_D F)\Delta))^{1/2},$$
so $2D^{-3} |\Delta| \leq 2(\operatorname{tr}(\Delta (H_D F)\Delta))^{1/2} H_D F.$

Therefore, the numerical computation could also be performed via Newton's method by computing the unique zero of the function $f: x \in (\mathbb{R}^+)^n \longmapsto \Sigma x - \frac{1}{x}$, where $\frac{1}{x} = (\frac{1}{x_1}, ..., \frac{1}{x_n})$. Each step of Newton's method requires to solve a symmetric system, which has complexity $\frac{n^3}{2} + \mathrm{O}(n^2)$ via the Cholesky decomposition. Since the convergence is asymptotically quadratic, only a few steps are necessary to get a good precision.

As a comparison, the computation of the symmetric matrix logarithm requires one eigenvalue decomposition. This can be computed via the QR algorithm after putting the matrix under Hessenberg form, which has complexity $\frac{4n^3}{3} + O(n^2)$. So computing the log-scaling costs roughly twice more than computing the logarithm.

In this section, we proved the existence in the conjecture with $\mathcal{V}^* = \operatorname{Hol}(n)$ and we proved the conjecture for $\mathcal{V}^* = \operatorname{Row}_0(n)$. This provides a bijective map $\operatorname{Log}^* : \operatorname{Cor}^+(n) \longrightarrow \operatorname{Row}_0(n)$ called the log-scaling bijection.

4. Permutation-invariant log-Euclidean metrics via the log-scaling bijection. In this section, we use the log-scaling bijection to define log-Euclidean metrics on $\operatorname{Cor}^+(n)$. More precisely, in Section 4.1, we prove that the log-scaling bijection is a smooth diffeomorphism. In Section 4.2, we characterize all permutation-invariant inner products on $\operatorname{Row}_0(n)$. In Section 4.3, we define permutation-invariant log-Euclidean metrics by pullback and we give their geometric properties.

4.1. The cor-exp bijection is a smooth diffeomorphism.

THEOREM 4.1 (Exp* = Cor \circ exp is a smooth diffeomorphism). The log-scaling bijection $\operatorname{Log}^{\star}: \operatorname{Cor}^{+}(n) \longrightarrow \operatorname{Row}_{0}(n)$ is a smooth diffeomorphism. We give the differentials of $\operatorname{Log}^{\star}$ and $\operatorname{Exp}^{\star}$ in function of the differentials of the symmetric matrix logarithm and exponential maps log and exp . For all $C \in \operatorname{Cor}^{+}(n)$, $S, Y \in \operatorname{Row}_{0}(n)$ and $X \in \operatorname{Hol}(n)$ such that $\Sigma = \mathcal{D}^{\star}(C) \star C = \exp(S)$:

$$(4.1)$$

$$d_S \operatorname{Exp}^{\star}(Y) = \Delta^{-1} \left[d_S \exp(Y) - \frac{1}{2} (\Delta^{-2} \operatorname{Diag}(d_S \exp(Y)) \Sigma + \Sigma \operatorname{Diag}(d_S \exp(Y)) \Delta^{-2}) \right] \Delta^{-1},$$

$$(4.2)$$

$$d_C \operatorname{Log}^{\star}(X) = d_{\Sigma} \log \left(\Delta X \Delta + \frac{1}{2} (X^0 \Sigma + \Sigma X^0) \right),$$

where
$$\Delta = \operatorname{Diag}(\Sigma)^{1/2}$$
 and $X^0 = -2\operatorname{diag}((I_n + \Sigma)^{-1}\Delta X\Delta\mathbb{1}).$

Proof. It suffices to show that \mathcal{D}^* is smooth. We apply the implicit function theorem to the smooth function $\Phi^*: (\Sigma, \Delta) \in \operatorname{Sym}^+(n) \times \operatorname{Diag}^+(n) \longmapsto \Delta \Sigma \Delta \mathbb{1} - \mathbb{1} \in (\mathbb{R}^+)^n$ which satisfies $\Delta = \mathcal{D}^*(\Sigma)$ if and only if $\Phi^*(\Sigma, \Delta) = 0$. Let us prove that for all $(\Sigma, \Delta) \in (\Phi^*)^{-1}(0)$, the differential of the partial function $\Phi^*_{\Sigma}: \Delta \in \operatorname{Diag}^+(n) \longmapsto \Phi^*(\Sigma, \Delta) \in (\mathbb{R}^+)^n$ is invertible. In the direction $D \in T_\Delta \operatorname{Diag}^+(n) = \operatorname{Diag}(n)$:

$$\begin{split} d_{\Delta}\Phi_{\Sigma}^{\star}(D) &= D\Sigma\Delta\mathbb{1} + \Delta\Sigma D\mathbb{1} \\ &= D\Delta^{-1}\mathbb{1} + \Delta\Sigma D\mathbb{1} \\ &= \Delta(\Delta^{-2} + \Sigma)D\mathbb{1}. \end{split}$$

Since $\Delta(\Delta^{-2} + \Sigma) \in GL(n)$, the differential is invertible so \mathcal{D}^* is smooth.

Since $\operatorname{Exp}^* = \operatorname{Cor} \circ \operatorname{exp}$, we have $d_S \operatorname{Exp}^*(Y) = d_\Sigma \operatorname{Cor} (d_S \operatorname{exp}(Y))$ with $\Sigma = \operatorname{exp}(S)$. Using $d_\Sigma \operatorname{Cor}(Z) = \Delta^{-1} \left[Z - \frac{1}{2} (\Delta^{-2} \operatorname{Diag}(Z) \Sigma + \Sigma \operatorname{Diag}(Z) \Delta^{-2}) \right] \Delta^{-1}$ with $\Delta = \operatorname{Diag}(\Sigma)^{1/2}$ and $Z = d_S \operatorname{exp}(Y) \in T_\Sigma \operatorname{Row}_1^+(n) = \operatorname{Row}_0(n)$, we get the expected result. Now we want to invert the relation $X = d_S \operatorname{Exp}^*(Y)$ to get $Y = d_C \operatorname{Log}^*(X)$. We use the intermediate matrices $\Sigma \in \operatorname{Row}_1^+(n)$ and $Z \in \operatorname{Row}_0(n)$ and the relations $X = d_\Sigma \operatorname{Cor}(Z)$ and $Y = d_\Sigma \operatorname{log}(Z)$.

$$\begin{split} \Delta X \Delta &= Z - \frac{1}{2} (\Delta^{-2} \mathrm{Diag}(Z) \Sigma + \Sigma \mathrm{Diag}(Z) \Delta^{-2}), \\ \Delta X \Delta \mathbb{1} &= -\frac{1}{2} (\Delta^{-2} \mathrm{Diag}(Z) \Sigma \mathbb{1} + \Sigma \mathrm{Diag}(Z) \Delta^{-2} \mathbb{1}) \\ &= -\frac{1}{2} (I_n + \Sigma) \Delta^{-2} \mathrm{Diag}(Z) \mathbb{1}, \\ \Delta^{-2} \mathrm{Diag}(Z) \mathbb{1} &= -2 (I_n + \Sigma)^{-1} \Delta X \Delta \mathbb{1}, \\ \Delta^{-2} \mathrm{Diag}(Z) &= X^0, \\ Z &= \Delta X \Delta + \frac{1}{2} (X^0 \Sigma + \Sigma X^0), \end{split}$$

which allows to conclude with $d_{\Sigma} \operatorname{Log}^{*}(X) = Y = d_{\Sigma} \log(Z)$.

4.2. Permutation-invariant inner products on $Row_0(n)$.

THEOREM 4.2 (Permutation-invariant inner products on $Row_0(n)$). For $n \ge 4$, permutation-invariant inner products on $Row_0(n)$ are the symmetric bilinear forms associated to the following positive definite quadratic forms q^* defined for $Y \in Row_0(n)$:

(4.3)
$$q^{\star}(Y) = \alpha \operatorname{tr}(Y^2) + \delta \operatorname{tr}(\operatorname{Diag}(Y)^2) + \zeta \operatorname{tr}(Y)^2,$$

with $\alpha > 0$, $n\alpha + (n-2)\delta > 0$ and $n\alpha + (n-1)(\delta + n\zeta) > 0$. For n=3, the permutation-invariant inner products have the same form with $\alpha = 0$. For n=2, they have the same form with $\alpha = \delta = 0$.

Proof. We rely on the characterization of permutation-invariant inner products on $\operatorname{Hol}(n)$ and on the equivariant isomorphism $\Theta: \left\{ \begin{array}{ll} \operatorname{Hol}(n) & \longrightarrow & \operatorname{Row}_0(n) \\ X & \longmapsto & Y = AXA^\top \end{array} \right.$ with $A = I_n - \frac{1}{n}\mathbbm{1}\mathbbm{1}^\top$ found in [24], whose inverse isomorphism is given by $X = \Theta^{-1}(Y) = Y - (\mu\mathbbm{1}^\top + \mathbbm{1}\mu^\top)$ with $\mu = \frac{1}{2}\operatorname{Diag}(Y)\mathbbm{1}$. Indeed, let $q^\star: \operatorname{Row}_0(n) \longrightarrow \mathbbm{1}$ be a permutation-invariant quadratic form. Then q^\star is positive definite if and only if $q^\star \circ \Theta: \operatorname{Hol}(n) \longrightarrow \mathbbm{1}$ is a permutation-invariant positive definite quadratic form on $\operatorname{Hol}(n)$. Hence, by Theorem 2.5, q^\star is of the form $q^\star(Y) = \alpha\operatorname{tr}(\Theta^{-1}(Y)^2) + \beta\operatorname{Sum}(\Theta^{-1}(Y)^2) + \gamma\operatorname{Sum}(\Theta^{-1}(Y))^2$ with $\min(\alpha, 2\alpha + (n-2)\beta, \alpha + (n-1)(\beta + n\gamma)) > 0$. We compute X^2 with $X = \Theta^{-1}(Y)$, and the three terms:

$$\begin{split} X^2 &= Y^2 + \frac{1}{2} \mathrm{tr}(Y) (\mu \mathbb{1}^\top + \mathbb{1} \mu^\top) + n \mu \mu^\top + \|\mu\|^2 \mathbb{1} \mathbb{1}^\top - Y \mu \mathbb{1}^\top - \mathbb{1} \mu^\top Y, \\ \mathrm{tr}(X^2) &= \mathrm{tr}(Y^2) + \frac{1}{2} \mathrm{tr}(Y)^2 + \frac{n}{2} \mathrm{tr}(\mathrm{Diag}(Y)^2), \\ \mathrm{Sum}(X^2) &= \frac{n}{2} \mathrm{tr}(Y)^2 + \frac{n}{4} \mathrm{tr}(Y)^2 + \frac{n^2}{4} \mathrm{tr}(\mathrm{Diag}(Y)^2), \\ \mathrm{Sum}(X) &= -n \, \mathrm{tr}(Y), \\ \mathrm{Sum}(X)^2 &= n^2 \mathrm{tr}(Y)^2. \end{split}$$

Hence $g(Y,Y) = \alpha \operatorname{tr}(Y^2) + \delta \operatorname{tr}(\operatorname{Diag}(Y)^2) + \zeta \operatorname{tr}(Y)^2$ with $\delta = \frac{n}{2}(\alpha + \frac{n}{2}\beta)$ and $\zeta = \frac{\alpha}{2} + \frac{3n}{4}\beta + n^2\gamma$. The inverse relations between coefficients are $\beta = \frac{4^2}{n^2}\delta - \frac{2}{n}\alpha$ and $\gamma = \frac{1}{n^2}(\zeta - \frac{3}{n}\delta + \alpha)$. Thus $2\alpha + (n-2)\beta = \frac{4}{n^2}(n\alpha + (n-2)\delta)$ and $\alpha + (n-1)(\beta + n\gamma) = \frac{1}{n^2}(n\alpha + (n-1)(\delta + n\zeta))$, which gives the expected positivity condition.

4.3. Pullback metrics via the log-scaling diffeomorphism.

DEFINITION 4.3 (Log-scaled metrics). A log-scaled metric on $\operatorname{Cor}^+(n)$ is the pull-back metric of a permutation-invariant inner product characterized by a quadratic form q^* as in Theorem 4.2. For all $C \in \operatorname{Cor}^+(n)$ and $X \in T_C \operatorname{Cor}^+(n) = \operatorname{Hol}(n)$, it writes $g_C^*(X,X) = q^*(d_C \operatorname{Log}^*(X))$ where $d_C \operatorname{Log}^*(X) = d_C \operatorname{log}(X + \frac{1}{2}(X^0C + CX^0))$ with $X^0 = -2\operatorname{diag}((I_n + C)^{-1}X\mathbb{1})$.

THEOREM 4.4 (Riemannian operations of log-scaled metrics). We consider a log-scaled metric characterized by the quadratic form q^* . Let $C, C', C_1, ..., C_n \in \text{Cor}^+(n)$, $X \in \text{Row}_0(n)$. The Riemannian operations of this metric are summarized in Table 4.1. Moreover, the metric is permutation-invariant and inverse-consistent, i.e. it is invariant under the pullback by the cor-inversion $\mathcal{I}: \text{Cor}^+(n) \longrightarrow \text{Cor}^+(n)$.

Beware not to confuse the Riemannian maps $\operatorname{Exp}_C^{\star}: T_C\operatorname{Cor}^+(n) = \operatorname{Hol}(n) \longrightarrow \operatorname{Cor}^+(n)$ and $\operatorname{Log}_C^{\star}: \operatorname{Cor}^+(n) \longrightarrow T_C\operatorname{Cor}^+(n) = \operatorname{Hol}(n)$ with the smooth diffeomorphisms $\operatorname{Exp}^{\star}: \operatorname{Row}_0(n) \longrightarrow \operatorname{Cor}^+(n)$ and $\operatorname{Log}^{\star}: \operatorname{Cor}^+(n) \longrightarrow \operatorname{Row}_0(n)$.

Exponential map	$\operatorname{Exp}_{C}^{\star}(X) = \operatorname{Exp}^{\star}(\operatorname{Log}^{\star}(C) + d_{C}\operatorname{Log}^{\star}(X)))$
Logarithm map	$\log_C^*(C') = d_{\text{Log}^*(C)} \text{Exp}^*(\text{Log}^*(C') - \text{Log}^*(C))$
Geodesic	$\gamma^*(t) = \operatorname{Exp}^*((1-t)\operatorname{Log}^*(C) + t\operatorname{Log}^*(C'))$
Squared distance	$d^{\star}(C, C')^{2} = q^{\star}(\operatorname{Log}^{\star}(C') - \operatorname{Log}^{\star}(C))$
Fréchet mean	$\bar{C}^* = \operatorname{Exp}^*(\frac{1}{k} \sum_{i=1}^k \operatorname{Log}^*(C_i))$
Curvature	$R^{\star} = 0$
Parallel transport	$\Pi_{C \to C'}^{\star} X = (d_{C'} \operatorname{Log}^{\star})^{-1} (d_C \operatorname{Log}^{\star}(X))$

Table 4.1: Riemannian operations of log-scaled metrics

As for the off-log metrics, all the Riemannian operations can be computed in closed form modulo the computation of Log^* , i.e. the computation of \mathcal{D}^* , i.e. the computation of the scaling of an SPD matrix.

Since one motivation behind the off-log bijection in [4] was the closed form expression in dimension 2 (cf. Theorem 2.2, item 2), it seems important to note the following result.

Theorem 4.5 (Coincidence of the metrics in dimension 2). In dimension 2, up to a positive scaling factor, the quotient-affine metric, the off-log metric and the log-scaled metric coincide. We recall that the Fisher transformation is the increasing map

$$F: \rho \in (-1,1) \longmapsto \frac{1}{2} \ln(\frac{1+\rho}{1-\rho}) \in \mathbb{R}^+$$
. Let $C = C(\rho)$ and $X = \begin{pmatrix} 0 & x \\ x & 0 \end{pmatrix}$ with $\rho \in (-1,1)$ and $x \in \mathbb{R}$. Then:

- 1. (Metric) $g_C(X,X) = \frac{x^2}{(1-\rho^2)^2}$ (up to a scaling factor $\alpha > 0$),
- 2. (Geodesic) $\gamma(t) = C(\rho(t))$ where $\rho(t) = \frac{\rho_1 \cosh(\lambda t) + \sinh(\lambda t)}{\rho_1 \sinh(\lambda t) + \cosh(\lambda t)}$ with $\lambda = F(\rho_2) F(\rho_1)$ is monotonic (increasing if $\rho_1 < \rho_2$, decreasing if $\rho_1 > \rho_2$, constant if $\rho_1 = \rho_2$),
- 3. (Distance) $d(C_1, C_2) = |\lambda| = |F(\rho_2) F(\rho_1)|$ (up to a scaling factor $\sqrt{\alpha}$).

Proof. It suffices to use the 2nd statement of Theorems 2.2 and 3.6 and the formulae of distances of the off-log metric and the log-scaled metric. For the former, $d(C_1, C_2) = q(F(\rho_2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - F(\rho_1) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}) \propto \lambda^2$ and similarly for the ladder. Up to a multiplicative constant, these distances are equal to the quotient-affine distance in dimension 2 [40]. Therefore, the Riemannian metrics coincide up to a constant and the geodesics coincide. The formulae can be found in [42].

We showed in this section that the log-scaling bijection is a smooth diffeomorphism. Thus, it provides a family of permutation-invariant and inverse-consistent log-Euclidean metrics by pulling back permutation-invariant inner products on $\operatorname{Row}_0(n)$. Hence, the Riemannian operations are trivial. As shown in Table 4.1, they are known in closed form modulo the computation of $\operatorname{Log}^*: \operatorname{Cor}^+(n) \longrightarrow \operatorname{Row}_0(n)$ or equivalently the computation of $\mathcal{D}^*: \operatorname{Sym}^+(n) \longrightarrow \operatorname{Diag}^+(n)$, which can be computed efficiently via Newton's method.

5. Conclusion. We introduced two families of permutation-invariant log-Euclidean metrics on full-rank correlation matrices. The first family was built via the off-log diffeomorphism whose algebraic properties were introduced in [4]. The second family was built via the log-scaling diffeomorphism thanks to the result on the scaling of symmetric matrices [31]. In addition, the log-scaled metrics are inverse-consistent

contrarily to the off-log metrics. These metrics allow to compute with correlation matrices very efficiently since they are flat and the main Riemannian operations are known in closed form modulo the computation of the maps \mathcal{D} and \mathcal{D}^* , which can be done very efficiently.

These permutation-invariant log-Euclidean metrics fill a gap in the study of Riemannian metrics on the open elliptope since they gather the invariance under permutations satisfied by several existing structures [22, 33, 11, 40] and the log-Euclidean geometry of some others [42]. More generally, we tried to introduce a comprehensive formalism on full-rank correlation matrices in terms of stability under the action of permutations and under the cor-inverse involution. This systematic approach allowed to satisfy intrinsically the requirement of inverse-consistency in the construction of log-Euclidean metrics. We hope that this presentation will help to manipulate correlation matrices as easily as we work with SPD matrices. This approach could also help define appropriate geometries of block equi-correlation matrices of a given signature.

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REFERENCES

- [1] D. ALEKSEEVSKY, A. KRIEGL, M. LOSIK, AND P. W. MICHOR, The Riemannian geometry of orbit spaces. The metric, geodesics, and integrable systems, Publicationes Mathematicae, 62 (2001), pp. 1–30.
- [2] Z. Allen-Zhu, Y. Li, R. Oliveira, and A. Wigderson, Much faster algorithms for matrix scaling, in 2017 IEEE 58th Annual Symposium on Foundations of Computer Science (FOCS), Los Alamitos, CA, USA, oct 2017, IEEE Computer Society, pp. 890–901, https://doi.org/10.1109/FOCS.2017.87, https://doi.ieeecomputersociety.org/10.1109/FOCS.2017.87
- I. ARCHAKOV AND P. R. HANSEN, A Canonical Representation of Block Matrices with Applications to Covariance and Correlation Matrices, arXiv:2012.02698 [econ, q-fin, stat], (2020), http://arxiv.org/abs/2012.02698 (accessed 2021-07-07). arXiv: 2012.02698.
- I. Archakov and P. R. Hansen, A New Parametrization of Correlation Matrices, Econometrica, 89 (2021), pp. 1699–1715, https://doi.org/10.3982/ECTA16910, https://onlinelibrary.wiley.com/doi/abs/10.3982/ECTA16910.
- [5] V. ARSIGNY, P. FILLARD, X. PENNEC, AND N. AYACHE, Log-Euclidean metrics for fast and simple calculus on diffusion tensors, Magnetic Resonance in Medicine, 56 (2006), pp. 411– 421, https://doi.org/10.1002/mrm.20965, https://hal.inria.fr/inria-00502678.
- [6] C. Baldassi, M. Zamparo, C. Feinauer, A. Procaccini, R. Zecchina, M. Weigt, and A. Pagnani, Fast and accurate multivariate gaussian modeling of protein families: predicting residue contacts and protein-interaction partners, PloS one, 9 (2014), p. e92721.
- [7] A. BARACHANT, S. BONNET, M. CONGEDO, AND C. JUTTEN, Classification of covariance matrices using a Riemannian-based kernel for BCI applications, Neurocomputing, 112 (2013), pp. 172–178, https://doi.org/10.1016/j.neucom.2012.12.039, https://hal.archives-ouvertes.fr/hal-00820475.
- [8] F. BARBARESCO, Information Geometry of Covariance Matrix: Cartan-Siegel Homogeneous Bounded Domains, Mostow/Berger Fibration and Fréchet Median, in Matrix Information Geometry, F. Nielsen and R. Bhatia, eds., Springer, Berlin, Heidelberg, 2013, pp. 199–255, https://doi.org/10.1007/978-3-642-30232-9_9, https://doi.org/10.1007/978-3-642-30232-9_9.

- [9] R. Bhatia, Matrix Analysis, vol. 169 of Graduate Texts in Mathematics, Springer New York, New York, NY, 1997, https://doi.org/10.1007/978-1-4612-0653-8, http://link.springer.com/10.1007/978-1-4612-0653-8.
- [10] J. P. Burg, Maximum Entropy Spectral Analysis, PhD thesis, Stanford University, 1975.
- [11] P. DAVID AND W. Gu, A Riemannian structure for correlation matrices, Operators and Matrices, 13 (2019), pp. 607–627.
- [12] A. DE LA FUENTE, N. BING, I. HOESCHELE, AND P. MENDES, Discovery of meaningful associations in genomic data using partial correlation coefficients, Bioinformatics, 20 (2004), pp. 3565-3574, https://doi.org/10.1093/bioinformatics/bth445, https://doi.org/10.1093/bioinformatics/bth445.
- [13] S. EPSKAMP AND E. I. FRIED, A tutorial on regularized partial correlation networks, Psychological Methods, 23 (2018), pp. 617–634, https://doi.org/10.1037/met0000167. Place: US Publisher: American Psychological Association.
- [14] P. FILLARD, X. PENNEC, V. ARSIGNY, AND N. AYACHE, Clinical DT-MRI estimation, smoothing, and fiber tracking with log-Euclidean metrics., IEEE Transactions on Medical Imaging, 26 (2007), pp. 1472–82, https://doi.org/10.1109/TMI.2007.899173, https://hal.inria. fr/inria-00502645.
- [15] M. K. Garba, T. M. W. Nye, J. Lueg, and S. F. Huckemann, Information geometry for phylogenetic trees, Journal of Mathematical Biology, 82 (2021), pp. 1–39, https://doi.org/ 10.1007/s00285-021-01553-x, https://doi.org/10.1007/s00285-021-01553-x.
- [16] I. GRUBIŠIĆ AND R. PIETERSZ, Efficient rank reduction of correlation matrices, Linear Algebra and its Applications, 422 (2007), pp. 629–653, https://doi.org/https://doi.org/10.1016/j. laa.2006.11.024, https://www.sciencedirect.com/science/article/pii/S0024379506005222.
- [17] F. HIAI AND D. Petz, Riemannian metrics on positive definite matrices related to means, Linear Algebra and its Applications, 430 (2009), pp. 3105–3130, https://doi.org/https://doi.org/10.1016/j.laa.2009.01.025, https://www.sciencedirect.com/science/article/pii/S0024379509000767.
- [18] S. HUCKEMANN, T. HOTZ, AND A. MUNK, Intrinsic shape analysis: Geodesic PCA for Riemannian manifolds modulo isometric Lie group actions, Statistica Sinica, 20 (2010), pp. 1–58.
- [19] M. IDEL, A review of matrix scaling and Sinkhorn's normal form for matrices and positive maps, 2016, https://arxiv.org/abs/1609.06349.
- [20] M. Jalili and M. G. Knyazeva, Constructing brain functional networks from eeg: partial and unpartial correlations, Journal of integrative neuroscience, 10 (2011), pp. 213–232.
- [21] C. R. Johnson and R. Reams, Scaling of symmetric matrices by positive diagonal congruence, Linear and Multilinear Algebra, 57 (2009), pp. 123–140, https://doi.org/10.1080/03081080600872327, http://www.tandfonline.com/doi/abs/10.1080/03081080600872327.
- [22] A. N. KERCHEVAL, On Rebonato and Jäckel's parametrization method for finding nearest correlation matrices, International Journal of Pure and Applied Mathematics, 45 (2008), pp. 383–390.
- [23] D. Koller and N. Friedman, Probabilistic graphical models: principles and techniques, Adaptive computation and machine learning, MIT Press, Cambridge, MA, 2009.
- [24] H. Kurata and R. B. Bapat, Moore-Penrose inverse of a hollow symmetric matrix and a predistance matrix, Special Matrices, 4 (2016), https://doi.org/doi:10.1515/spma-2016-0028, https://doi.org/10.1515/spma-2016-0028.
- [25] D. LÄHNEMANN, J. KÖSTER, E. SZCZUREK, D. J. McCARTHY, S. C. HICKS, M. D. ROBINSON, C. A. VALLEJOS, K. R. CAMPBELL, N. BEERENWINKEL, A. MAHFOUZ, ET AL., Eleven grand challenges in single-cell data science, Genome biology, 21 (2020), pp. 1–35.
- [26] S. L. LAURITZEN, Graphical Models, Oxford Statistical Science Series, Oxford University Press, Oxford, New York, May 1996.
- [27] P. LI, Q. WANG, H. ZENG, AND L. ZHANG, Local Log-Euclidean Multivariate Gaussian Descriptor and Its Application to Image Classification, IEEE Transactions on Pattern Analysis and Machine Intelligence, 39 (2017), pp. 803–817, https://doi.org/10.1109/TPAMI.2016. 2560816.
- [28] Z. Lin, Riemannian Geometry of Symmetric Positive Definite Matrices via Cholesky Decomposition, SIAM Journal on Matrix Analysis and Applications, 40 (2019), pp. 1353–1370, https://doi.org/10.1137/18M1221084, https://epubs.siam.org/doi/10.1137/18M1221084.
- [29] M. D. LUECKEN AND F. J. THEIS, Current best practices in single-cell rna-seq analysis: a tutorial, Molecular systems biology, 15 (2019), p. e8746.
- [30] G. MARRELEC, A. KRAINIK, H. DUFFAU, M. PÉLÉGRINI-ISSAC, S. LEHÉRICY, J. DOYON, AND H. BENALI, Partial correlation for functional brain interactivity investigation in functional MRI, NeuroImage, 32 (2006), pp. 228–237, https://doi.org/10.1016/j.neuroimage.2005.12. 057

- [31] A. W. MARSHALL AND I. OLKIN, Scaling of matrices to achieve specified row and column sums, Numerische Mathematik, 12 (1968), pp. 83–90, https://doi.org/10.1007/BF02170999, https://doi.org/10.1007/BF02170999.
- [32] G. MARTI, V. GOUBET, AND F. NIELSEN, cCorrGAN: Conditional Correlation GAN for Learning Empirical Conditional Distributions in the Elliptope, in Geometric Science of Information, F. Nielsen and F. Barbaresco, eds., Lecture Notes in Computer Science, Cham, 2021, Springer International Publishing, pp. 613–620, https://doi.org/10.1007/ 978-3-030-80209-7_66.
- [33] F. Nielsen and K. Sun, Clustering in Hilbert's Projective Geometry: The Case Studies of the Probability Simplex and the Elliptope of Correlation Matrices, in Geometric Structures of Information, F. Nielsen, ed., Springer International Publishing, Cham, 2019, pp. 297–331, https://doi.org/10.1007/978-3-030-02520-5_11, https://doi.org/10.1007/978-3-030-02520-5_11.
- [34] J. Peng, P. Wang, N. Zhou, and J. Zhu, Partial Correlation Estimation by Joint Sparse Regression Models, Journal of the American Statistical Association, 104 (2009), pp. 735– 746, https://doi.org/10.1198/jasa.2009.0126, https://www.ncbi.nlm.nih.gov/pmc/articles/ PMC2770199/.
- [35] X. Pennec, Statistical Computing on Manifolds: From Riemannian Geometry to Computational Anatomy, in Emerging Trends in Visual Computing: LIX Fall Colloquium, ETVC 2008, Palaiseau, France, November 18-20, 2008. Revised Invited Papers, vol. 5416 of Lecture Notes in Computer Science, Springer, Berlin, Heidelberg, 2009, pp. 347–386, https://doi.org/10.1007/978-3-642-00826-9_16, https://doi.org/10.1007/978-3-642-00826-9_16.
- [36] X. Pennec, P. Fillard, and N. Ayache, A Riemannian Framework for Tensor Computing, International Journal of Computer Vision, 66 (2006), pp. 41–66, https://doi.org/10.1007/s11263-005-3222-z, https://doi.org/10.1007/s11263-005-3222-z.
- [37] R. REBONATO AND P. JAECKEL, The most general methodology to create a valid correlation matrix for risk management and option pricing purposes, Journal of Risk, 2 (2001), pp. 17– 27, https://doi.org/10.2139/ssrn.1969689.
- [38] L. T. SKOVGAARD, A Riemannian Geometry of the Multivariate Normal Model, Scandinavian Journal of Statistics, 11 (1984), pp. 211–223, http://www.jstor.org/stable/4615960.
- [39] Y. Thanwerdas, Riemannian and stratified geometries of covariance and correlation matrices, PhD thesis, Université Côte d'Azur and Inria, 2022.
- [40] Y. Thanwerdas and X. Pennec, Geodesics and Curvature of the Quotient-Affine Metrics on Full-Rank Correlation Matrices, in Proceedings of GSI 2021 - 5th conference on Geometric Science of Information, vol. 12829 of Lecture Notes in Computer Science, Paris, France, July 2021, Springer International Publishing, pp. 93–102, https://hal.archives-ouvertes.fr/hal-03157992.
- [41] Y. THANWERDAS AND X. PENNEC, O(n)-invariant Riemannian metrics on SPD matrices. Preprint, Sept. 2022, https://hal.archives-ouvertes.fr/hal-03338601.
- [42] Y. Thanwerdas and X. Pennec, Theoretically and computationally convenient geometries on full-rank correlation matrices. Preprint, Jan. 2022, https://hal.archives-ouvertes.fr/hal-03527072.
- [43] G. VAROQUAUX, F. BARONNET, A. KLEINSCHMIDT, P. FILLARD, AND B. THIRION, Detection of brain functional-connectivity difference in post-stroke patients using group-level covariance modeling, in Medical Image Computing and Computer Added Intervention, D. Shen, A. Frangi, and G. Szekely, eds., Lecture Notes in Computer Science, Beijing, China, Sept. 2010, Tianzi Jiang, Springer, pp. 200–208, https://doi.org/10.1007/978-3-642-15705-9-25, https://hal.inria.fr/inria-00512417.
- [44] Y. Wang, J. Kang, P. B. Kemmer, and Y. Guo, An efficient and reliable statistical method for estimating functional connectivity in large scale brain networks using partial correlation, Frontiers in neuroscience, 10 (2016), p. 123.
- [45] Z. WANG, B. C. VEMURI, Y. CHEN, AND T. H. MARECI, A constrained variational principle for direct estimation and smoothing of the diffusion tensor field from complex dwi, IEEE Transactions on Medical Imaging, 23 (2004), pp. 930–939, https://doi.org/10.1109/TMI. 2004.831218.