Generalized Bures-Wasserstein Geometry for Positive Definite Matrices

Andi Han∗  Bamdev Mishra†  Pratik Jawanpuria†  Junbin Gao∗

Abstract

This paper proposes a generalized Bures-Wasserstein (BW) Riemannian geometry for the manifold of symmetric positive definite matrices. We explore the generalization of the BW geometry in three different ways: 1) by generalizing the Lyapunov operator in the metric, 2) by generalizing the orthogonal Procrustes distance, and 3) by generalizing the Wasserstein distance between the Gaussians. We show that they all lead to the same geometry. The proposed generalization is parameterized by a symmetric positive definite matrix \( M \) such that when \( M = I \), we recover the BW geometry. We derive expressions for the distance, geodesic, exponential/logarithm maps, Levi-Civita connection, and sectional curvature under the generalized BW geometry. We also present applications and experiments that illustrate the efficacy of the proposed geometry.

1 Introduction

Symmetric positive definite (SPD) matrices are fundamental in various fields of applications, such as machine learning, signal processing, computer vision, and medical imaging, where the object of interest is primarily modelled as a covariance/kernel matrix or a diffusion tensor [14, 19, 35, 41, 51].

The set of SPD matrices, denoted as \( \mathbb{S}_{++}^n \), is a convex subset of the Euclidean space \( \mathbb{R}^{n(n+1)/2} \). To measure the (dis)similarity between SPD matrices, one needs to assign a metric (a smooth inner product structure) on \( \mathbb{S}_{++}^n \), which yields a Riemannian manifold. Consequently, there exist a number of Riemannian metrics such as the Affine-Invariant [9, 41, 49], Log-Euclidean [5, 6], and Log-Cholesky [33] metrics, to name a few. Existing works also explore metrics induced from symmetric divergences [45], [46], [47].

Recently, the Bures-Wasserstein (BW) distance has gained popularity, especially in machine learning applications [10, 20, 36, 52]. It is defined as

\[
d_{bw}(X, Y) = \left( \text{tr}(X) + \text{tr}(Y) - 2 \text{tr}(X^{1/2}YX^{1/2})^{1/2} \right)^{1/2},
\]

where \( X \) and \( Y \) are SPD matrices and \( \text{tr}(X)^{1/2} \) denotes the trace of the matrix square root. It has been shown in [10, 36] that the BW distance induces a Riemannian metric and geometry on the manifold of SPD matrices. The BW metric between symmetric matrices \( U, V \) on \( T_X\mathbb{S}_{++}^n \) is defined as

\[
g_{bw}(U, V) = \frac{1}{2} \text{tr}(\mathcal{L}_X[U]V) = \frac{1}{2} \text{vec}(U)\top(X \otimes I + I \otimes X)^{-1} \text{vec}(V),
\]

∗University of Sydney (andi.han@sydney.edu.au, junbin.gao@sydney.edu.au).
†Microsoft India. (bamdevm@microsoft.com, pratik.jawanpuria@microsoft.com).
where the Lyapunov operator $\mathcal{L}_X[U]$ is defined as the solution of the matrix equation $X\mathcal{L}_X[U] + \mathcal{L}_X[U]X = U$ for $U \in S^n$ (which is the set of symmetric matrices of size $n \times n$). Here, $\text{vec}(U)$ and $\text{vec}(V)$ are the vectorization of matrices $U$ and $V$, respectively, and $\otimes$ denotes the Kronecker product.

The Bures-Wasserstein metric and distance have been employed in many areas, such as statistical optimal transport [10, 16], computer graphics [13, 14], neural sciences [18], and evolutionary biology [17], among others. It also connects to the theory of optimal transport and the $L_2$-Wasserstein distance between zero-centered Gaussian densities [10].

In this paper, we consider a natural extension of the BW metric by replacing the identity matrix in the Kronecker product sum in (2) with an arbitrary SPD matrix $M$, i.e., $X \otimes M + M \otimes X$, such that when $M = I$, it reduces to the BW metric. Note that the Affine-Invariant metric is given by $g_{ai}(U, V) = \text{vec}(U)^T (X \otimes X)^{-1} \text{vec}(V)$. Consequently, our proposed generalized BW metric coincides locally with the Affine-Invariant (AI) metric when $M = X$, i.e., around the neighbourhood of $X$. That is, the GBW metric bridges the gap between BW and (locally) AI metrics with different choices of $M$. Implications of this observation are discussed for log-determinant optimization later in Section 4.6.

As a contribution of the paper, we show that the proposed generalization of the BW metric, called the Generalized Bures-Wasserstein (GBW) metric, has connections with different existing theories. In particular, we show that generalizations from the metric, the Procrustes distance, and Wasserstein distance for Gaussians coincide. This is discussed in Section 2. In Section 3, we show that the manifold of SPD matrices equipped with the GBW metric has a smooth Riemannian manifold structure and we discuss the computations of various geometrical ingredients on the manifold. In particular, we explicitly derive expressions for geodesics, Exponential map, Logarithm map, sectional curvature, Levi-Civita connection, and barycenter computation. We discuss optimization aspects and applications of the GBW geometry in Section 4. Experiments in Section 5 illustrate the efficacy of the GBW geometry.

It should be highlighted that the results in the paper extend trivially to the Hermitian positive definite matrices.

## 2 Generalized Bures-Wasserstein (GBW) metric

The GBW metric that we introduce in this paper is parameterized by $M \in S^n_{++}$, i.e.,

$$g_{gbw}(U, V) = \langle U, V \rangle_{gbw} = \frac{1}{2} \text{tr}(\mathcal{L}_{X,M}[U]V) = \frac{1}{2} \text{vec}(U)^T (X \otimes M + M \otimes X)^{-1} \text{vec}(V),$$

(3)

where $\mathcal{L}_{X,M}[U]$ is the generalized Lyapunov operator, defined as the solution to the liner matrix equation $X\mathcal{L}_{X,M}[U] + M\mathcal{L}_{X,M}[U]X = U$. Similar to the special Lyapunov operator, the solution is symmetric given that $X, M \in S^n_{++}$ and $U \in S^n$.

As we show later in Section 3, the Riemannian distance associated with the GBW metric is derived as

$$d_{gbw}(X, Y) = \left( \text{tr}(M^{-1}X) + \text{tr}(M^{-1}Y) - 2\text{tr}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{1/2} \right)^{1/2},$$

(4)

which can be seen as the BW distance [11] between $M^{-1/2}XM^{-1/2}$ and $M^{-1/2}YM^{-1/2}$. It should be noted that

$$\text{tr}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{1/2} = \text{tr}(X^{1/2}YM^{-1}X^{1/2})^{1/2} = \text{tr}(M^{-1}YM^{-1}X)^{1/2}.$$
Below, we show that the same GBW (4) is realized under various contexts naturally. In those cases, the Euclidean norm, denoted by $\| \cdot \|_2$ is replaced with the more general Mahalanobis norm defined as $\| X \|_{M^{-1}} := \sqrt{\text{tr}(X^\top M^{-1} X)}$.

2.1 Orthogonal Procrustes problem

Any SPD matrix $X \in \mathbb{S}^{n}_{++}$ can be factorized as $X = PP^\top$ for $P \in M(n)$, the set of invertible matrices. This parameterization is invariant under the action of the orthogonal group $O(n)$. That is, for any $O \in O(n)$, $PO$ is also a valid parameterization. In [10], the BW distance is verified as the extreme solution of the orthogonal Procrustes problem where $P$ is set to be $X^{1/2}$, i.e., $d_{bw}(X, Y) = \min_{O \in O(n)} \| X^{1/2} - Y^{1/2}O \|_2$. We show in Proposition 1 that the GBW distance is obtained as the solution to the same orthogonal Procrustes problem in the Mahalanobis norm parameterized by $M^{-1}$.

Proposition 1. The GBW distance in (4) is realized as

$$d_{gbw}(X, Y) = \min_{O \in O(n)} \| X^{1/2} - Y^{1/2}O \|_{M^{-1}}.$$  

Proof. First we have

$$\min_{O \in O(n)} \| X^{1/2} - Y^{1/2}O \|_{M^{-1}}^2 = \text{tr}(M^{-1}X) + \text{tr}(M^{-1}Y) - 2 \max_{O \in O(n)} \text{tr}(M^{-1}X^{1/2}OY^{1/2}).$$

(5)

And the minimum of (5) is attained when $O$ is the orthogonal polar factor of $Y^{1/2}M^{-1}X^{1/2}$, which is $O = Y^{1/2}M^{-1}X^{1/2}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{-1/2}$, as proved in [10]. Substituting the expression of $O$ in (5) completes the proof.

2.2 Wasserstein distance and optimal transport

To demonstrate the connection of the GBW distance to the Wasserstein distance, we first show an analogue of [10, Theorem 2].

Proposition 2. Define $\tilde{F}(X, Y) = (X^{1/2}M^{-1}YM^{-1}X^{1/2})^{1/2}$. Then, for any $X, Y \in \mathbb{S}^n_{++}$,

1) $\tilde{F}(X, Y) = \min_{A \in \mathbb{S}_{++}^n} \frac{1}{2} \text{tr}(XA + M^{-1}YM^{-1}A^{-1})$.

2) $\tilde{F}(X, Y) = \min_{A \in \mathbb{S}_{++}^n} \sqrt{\text{tr}(XA)\text{tr}(M^{-1}YM^{-1}A^{-1})}$.

Proof. Following [10], the proof proceeds by analyzing the first-order stationary conditions, where we replace $Y$ with $M^{-1}YM^{-1}$.

The $L_2$-Wasserstein distance between two probability measures $\mu, \nu$ with finite second moments is

$$W^2(\mu, \nu) = \inf_{x \sim \mu, y \sim \nu} \mathbb{E}\|x - y\|_2^2 = \inf_{\gamma \sim \Gamma(\mu, \nu)} \int_{\mathbb{R}^n \times \mathbb{R}^n} \|x - y\|_2^2 d\gamma(x, y),$$

where $\Gamma(\mu, \nu)$ is the set of all probability measures with marginals $\mu, \nu$. It is a well known result that the $L_2$-Wasserstein distance between two zero-centered Gaussian distributions is equal to the BW distance between their covariance matrices [10] [12] [52]. The following proposition shows that the $L_2$-Wasserstein distance between such measures with respect to a Mahalanobis cost metric (which we term as generalized Wasserstein distance) coincides with the GBW distance in (4).
Proposition 3. Define the generalized Wasserstein distance as \( \bar{W}^2(\mu, \nu) := \inf_{x \sim \mu, y \sim \nu} E\|x - y\|_M^2 \), for any \( M^{-1} \in S_{++}^n \). Suppose \( \mu, \nu \) are two Gaussian measures with zero mean and covariances as \( X, Y \in S_{++}^n \) respectively. Then, we have \( \bar{W}^2(\mu, \nu) = d^2_{gbw}(X, Y) \).

Proof. We have \( X = E[xx^T] \) and \( Y = E[yy^T] \).
\[
\bar{W}^2(\mu, \nu) = \inf_{x \sim \mu, y \sim \nu} E\|x^TM^{-1}x + y^TM^{-1}y - 2x^TM^{-1}y\|_2
\]
\[
= \inf_{x \sim \mu, y \sim \nu} \text{tr}(M^{-1}X) + \text{tr}(M^{-1}Y) - 2\text{tr}(M^{-1}E[yx^T])
\]
\[
= \text{tr}(M^{-1}X) + \text{tr}(M^{-1}Y) - \sup_{K, \Sigma \succeq 0} 2\text{tr}(M^{-1}K^T),
\]
where \( K \) is the covariance between \( x, y \) such that the joint covariance matrix
\[
\Sigma = E\begin{bmatrix} xx^T & xy^T \\ yx^T & yy^T \end{bmatrix} = \begin{bmatrix} X & K \\ K^T & Y \end{bmatrix} \succeq 0.
\]
Two necessary and sufficient conditions for \( \Sigma \succeq 0 \) are (i) \( X \succeq KY^{-1}K^T \) and (ii) \( K = X^{1/2}CY^{1/2} \) for some contraction \( C \). Hence, \( \text{tr}(K) \leq \|X^{1/2}\|_2\|Y^{1/2}\|_2 = \sqrt{\text{tr}(X)\text{tr}(Y)} \). Also, for any \( A \in S_{++}^n \), the block matrix \( P = [A^{1/2} 0; 0 A^{−1/2}M^{-1}] \in M(2n) \). Then
\[
P\begin{bmatrix} X & K \\ K^T & Y \end{bmatrix}P^T = \begin{bmatrix} A^{1/2}XA^{1/2} & A^{1/2}KM^{-1}A^{-1/2} \\ A^{-1/2}M^{-1}K^TA^{1/2} & A^{-1/2}M^{-1}YM^{-1}A^{-1/2} \end{bmatrix} \succeq 0.
\]
This leads to
\[
\text{tr}(M^{-1}K^T) = \text{tr}(A^{−1/2}M^{−1}K^TA^{1/2})
\]
\[
\leq \sqrt{\text{tr}(A^{1/2}XA^{1/2})\text{tr}(A^{−1/2}M^{−1}YM^{−1}A^{−1/2})}
\]
\[
= \sqrt{\text{tr}(XA)\text{tr}(M^{−1}YM^{−1}A^{−1})).
\]
Hence,
\[
\max_{K: \Sigma \succeq 0} \text{tr}(M^{-1}K^T) = \min_{A \in S_{++}^n} \sqrt{\text{tr}(XA)\text{tr}(M^{−1}YM^{−1}A^{−1})} = \bar{F}(X, Y),
\]
and it follows \( \bar{W}^2(\mu, \nu) = \text{tr}(M^{-1}X) + \text{tr}(M^{-1}Y) - 2\text{tr}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{1/2} = d^2_{gbw}(X, Y) \). \( \square \)

Alternatively, the same distance is recovered by considering two scaled random Gaussian vector \( M^{−1/2}x, M^{−1/2}y \) under the Euclidean distance, i.e., \( d^2(X, Y) = \inf_{x \sim \mu, y \sim \nu} E\|M^{−1/2}x - M^{−1/2}y\|_2^2 \). Next, we derive the optimal transport plan as follows, where we denote \( A \# B \) as the matrix geometric mean under the Affine-Invariant metric, i.e., \( A \# B = A^{1/2}(A^{−1/2}BA^{−1/2})^{1/2}A^{1/2} = A(A^{−1}B)^{1/2} = (AB^{-1})^{1/2}B \).

Proposition 4. Let \( x, y \in \mathbb{R}^n \) be random Gaussian vectors with zero mean and covariance matrices \( X, Y \in S_{++}^n \) respectively. The optimal transport plan from \( x \) to \( y \) under the Mahalanobis distance is \( T_{x \to y} = M(X^{−1} \# (M^{−1}YM^{−1})) \).

Proof. For any \( P \in M(n) \) as a transport plan,
\[
E\|M^{−1/2}x - PM^{−1/2}x\|_2^2
\]
\[
= \text{tr}(M^{-1}X) + \text{tr}(PM^{-1/2}XM^{-1/2}P^T) - 2\text{tr}(X^{1/2}M^{−1/2}PM^{−1/2}X^{1/2}).
\]
By comparing (6) to $d^2_{gbw}(X, Y)$, we set

$$X^{1/2}M^{-1/2}PM^{-1/2}X^{1/2} = (X^{1/2}M^{-1}YM^{-1}X^{1/2})^{1/2}$$

which gives an expression of $P$ as

$$P = M^{1/2}X^{-1/2}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{1/2}X^{-1/2}M^{1/2}$$

$$= M^{1/2}(X^{-1}#(M^{-1}YM^{-1}))M^{1/2}. \quad (7)$$

From this result, we have

$$\text{tr}(PM^{-1/2}XM^{-1/2}P)$$

$$= \text{tr}\left(M^{1/2}(X^{-1}#(M^{-1}YM^{-1}))X(X^{-1}#(M^{-1}YM^{-1}))M^{1/2}\right)$$

$$= \text{tr}\left(M^{1/2}X^{-1}(X^{-1}#(M^{-1}YM^{-1}))^{1/2}XX^{-1}(X^{-1}#(M^{-1}YM^{-1}))^{1/2}M^{1/2}\right)$$

$$= \text{tr}(M^{-1}Y),$$

where we use the property of matrix geometric mean. This suggests the definition of $P$ is the optimal transport map under the Euclidean distance. Combining (7) with (6) shows

$$\mathbb{E}\|M^{-1/2}x - M^{1/2}(X^{-1}#(M^{-1}YM^{-1}))x\|^2_2$$

$$= \mathbb{E}\|x - M(X^{-1}#(M^{-1}YM^{-1}))x\|^2_{M^{-1}}$$

$$= d^2_{gbw}(X, Y).$$

We can, therefore, define the transport plan as $T_{X \to Y} := M(X^{-1}#(M^{-1}YM^{-1}))$ and denote $y = T_{X \to Y} x$, which is a Gaussian random vector with covariance

$$T_{X \to Y}XT_{X \to Y}^\top = M(X^{-1}#(M^{-1}YM^{-1}))X(X^{-1}#(M^{-1}YM^{-1}))M = Y.$$ 

Thus, $\mathbb{E}\|x - y\|^2_{M^{-1}} = d^2_{gbw}(X, Y)$ where $y = T_{X \to Y}x$. From Proposition 3 we see $T_{X \to Y}$ is the optimal transport plan from $X$ to $Y$ under the Mahalanobis distance. \hfill $\Box$

### 3 Generalized Bures-Wasserstein Riemannian geometry

In this section, the geometry arising from the metric (3) is shown to have a Riemannian structure for a given $M \in \mathbb{S}^n_{++}$. The proposed Riemannian geometry is parameterized by $M$. We show the expressions of the Riemannian distance, geodesic, exponential/logarithm maps, Levi-Civita connection, sectional curvature as well as the geometric mean and barycenter. A summary of the results is presented in Table 1.

The general linear group $\text{GL}(n)$ is the set of invertible matrices with the group action of matrix multiplication. When endowed with a standard Euclidean inner product $\langle \cdot, \cdot \rangle_2$, the group becomes a Riemannian manifold, denoted as $\mathcal{M}_g$.

Similar to the BW geometry, the GBW Riemannian geometry, which we denote as $\mathcal{M}_{gbw}$, is pushed forward from the space of general linear group by a Riemannian submersion. First, recall that a smooth submersion is a smooth map $\pi : (\mathcal{M}, g) \to (\mathcal{N}, h)$ from Riemannian manifold $(\mathcal{M}, g)$ to $(\mathcal{N}, h)$ such that its differential $D\pi(x) : T_x\mathcal{M} \to T_{\pi(x)}\mathcal{N}$ is surjective for any $x \in \mathcal{M}$. Every
Table 1: Summary of expressions for the proposed generalized Bures-Wasserstein Riemannian geometry, which is parameterized by a symmetric positive definite matrix $M$.

| Metric          | Generalized Bures-Wasserstein Geometry |
|-----------------|----------------------------------------|
| Distance        | $d_{gbw}^2(X, Y) = \text{tr}(M^{-1}X) + \text{tr}(M^{-1}Y) - 2\text{tr}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{1/2}$ |
| Geodesic        | $\gamma(t) = ((1-t)X^{1/2} + tY^{1/2}O)((1-t)X^{1/2} + tY^{1/2}O)^\top$ with $O$ the orthogonal polar factor of $Y^{1/2}M^{-1}X^{1/2}$. |
| Exp             | $\exp_X(U) = X + U + ML_{X, M}[U]XL_{X, M}[U]M$ |
| Log             | $\log_X(Y) = M(M^{-1}XM^{-1}Y)^{1/2} + (YM^{-1}XM^{-1})^{1/2}M - 2X$ |
| Connection      | $\nabla_\xi \eta = D_\xi \eta + \{XL_{X, M}[\eta]ML_{X, M}[\xi]M + XL_{X, M}[\xi]ML_{X, M}[\eta]M\} - \{ML_{X, M}[\eta]\xi\} - \{ML_{X, M}[\xi]\eta\}$ |
| Min/Max Curvature | $K_{\min}(\pi(P)) = 0$, and $K_{\max}(\pi(P)) = \frac{3}{\sigma_i + \sigma_{i+1}^{-1}}$, where $\sigma_i$ is the $i$-th largest singular value of $P$, and $\pi(P) = M^{1/2}PP^\top M^{1/2}$. |

The tangent space $T_xM$ can be decomposed as $T_xM = V_x \oplus H_x = \text{Ker}(D\pi(x)) \oplus \text{Ker}(D\pi(x))^\perp$, where $\text{Ker}(f)$ denotes the kernel of a map and $\oplus$ is the direct sum. We respectively call $V_x, H_x$ as the vertical and horizontal subspaces. The map $\pi$ is called a Riemannian submersion if it is a smooth submersion and its differential restricted to the horizontal space, $D\pi(x) : H_x \to T_{\pi(x)}N$ is isometric for any $x \in M$, i.e. $g_x(u, v) = h_{\pi(x)}(D\pi(x)[u], D\pi(x)[v])$.

The following proposition introduces a Riemannian submersion from $M_{gl}$ to $M_{gbw}$.

**Proposition 5.** The map $\pi : M_{gl} \to M_{gbw}$ defined as $\pi(P) = M^{1/2}PP^\top M^{1/2}$ is a Riemannian submersion, for $P \in \text{GL}(n)$ and $M_{gbw}$ parameterized by $M \in S^n_{++}$ as in [3].

**Proof.** Note that the tangent space of $M_{gl}$, $T_P M_{gl}$, is the space of $\mathbb{R}^{n \times n}$. The differential of $\pi(P)$ in the direction $U \in \mathbb{R}^{n \times n}$ is given by $D\pi(P)[U] = M^{1/2}UP^\top M^{1/2} + M^{1/2}PU^\top M^{1/2}$. We can then derive the kernel of $D\pi(P)$ (vertical space $V_P$) and the orthogonal complement of the kernel (horizontal space $H_P$) as

$$\text{Ker}(D\pi(P)) = \{U : D\pi(P)[U] = 0\}
= \{U = M^{-1/2}KM^{-1/2}P^\top : K \text{ is skew-symmetric}\},$$

(8)

$$\text{Ker}(D\pi(P))^\perp = \{V : \text{tr}(V^\top M^{-1/2}KM^{-1/2}P^\top) = 0\}
= \{V = M^{1/2}SM^{1/2}P : S \in \mathbb{R}^n\}. $$

(9)

It is clear that $\pi$ is a smooth submersion. Now, we only need to verify that it also satisfies the isometry property. For any $S, H \in \mathbb{R}^n$, $M^{1/2}SM^{1/2}P, M^{1/2}HM^{1/2}P \in H_P$, and

$$D\pi(P)[M^{1/2}SM^{1/2}P] = MSM^{1/2}PP^\top M^{1/2} + M^{1/2}PP^\top M^{1/2}SM
= MS\pi(P) + \pi(P)SM$$

and

$$D\pi(P)[M^{1/2}HM^{1/2}P] = MHM^{1/2}PP^\top M^{1/2} + M^{1/2}PP^\top M^{1/2}HM
= MH\pi(P) + \pi(P)HM.$$
The inner product at \( \pi(P) \) is given by

\[
\langle D\pi(P)[M^{1/2}SM^{1/2}], D\pi(P)[M^{1/2}HM^{1/2}] \rangle_{gbw}
\]

\[
= \frac{1}{2} \text{tr}(L_{\pi(P)}M[D\pi(P)[M^{1/2}SM^{1/2}]D\pi(P)[M^{1/2}HM^{1/2}]])
\]

\[
= \frac{1}{2} \text{tr}(SMH\pi(P) + S\pi(P)HM) = \text{tr}(\pi(P)SMH),
\]

where the last equality is because \( S, M, H, \pi(P) \) are all symmetric. The inner product at \( P \) is given by

\[
\langle M^{1/2}SM^{1/2}, M^{1/2}HM^{1/2} \rangle_2 = \text{tr}(P^\top M^{1/2}SMHM^{1/2}P) = \text{tr}(\pi(P)SMH).
\]

This shows for any \( \bar{S}, \bar{H} \in H_p \), \( \langle \bar{S}, \bar{H} \rangle_2 = \langle D\pi(P)[\bar{S}], D\pi(P)[\bar{H}] \rangle_{gbw} \), thereby completing the proof.

### 3.1 Riemannian distance

Next, we derive the Riemannian distance on \( M_{gbw} \) in Proposition [6] as the pushforward of the Euclidean distance on \( M_{gl} \) by the Riemannian submersion \( \pi \). The following Theorem is used to show that the pushforward distance is indeed the Riemannian distance.

**Theorem 1** (Riemannian distance induced from Riemannian submersion [52, Theorem 4]). Consider \( \pi : (M, g) \to (N, h) \) as a Riemannian submersion. Let \( d_M \) be the Riemannian distance on \( (M, g) \) and the pushforward distance \( d_N(p, q) = \inf_{u \in \pi^{-1}(p), v \in \pi^{-1}(q)} d_M(u, v) \) is equal to the Riemannian distance.

**Proposition 6.** From Theorem [7], the Riemannian distance on \( M_{gbw} \) is derived as \( d_{gbw}(X, Y) = (\text{tr}(M^{-1}X) + \text{tr}(M^{-1}Y) - 2\text{tr}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{1/2})^{1/2} \).

**Proof.** From the definition of \( \pi \) and Theorem [1], we have for any \( X, Y \in S^n_+ \),

\[
\begin{align*}
    d_{gbw}^2(X, Y) &= \inf_{\Omega, R \in O(n)} d_{gl}^2(M^{-1/2}X^{1/2}\Omega, M^{-1/2}Y^{1/2}R) \\
    &= \inf_{\Omega, R \in O(n)} \|M^{-1/2}X^{1/2}\Omega - M^{-1/2}Y^{1/2}R\|_2 \\
    &= \text{tr}(M^{-1}X) + \text{tr}(M^{-1}Y) - 2 \sup_{\Omega, R \in O(n)} \text{tr}(M^{-1}X^{1/2}\Omega R^\top Y^{1/2}) \\
    &= \text{tr}(M^{-1}X) + \text{tr}(M^{-1}Y) - 2 \sup_{O \in O(n)} \text{tr}(M^{-1}X^{1/2}OY^{1/2}).
\end{align*}
\]

The supremum is attained when \( O = Y^{1/2}M^{-1}X^{1/2}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{-1/2} \) as in Proposition [1]. This completes the proof.

The next lemma studies the various expressions of the polar factor \( O \), which is used throughout the rest of the paper.

**Lemma 1.** Consider \( O \) as defined in the proof of Proposition [6], then

\[
O = Y^{1/2}(Y^{-1}MX^{-1}M)^{1/2}M^{-1}X^{1/2} = Y^{-1/2}(Y#(MX^{-1}M))M^{-1}X^{1/2}.
\]
Proof. From the definition of $O$,

$$
O = Y^{1/2}M^{-1}X^{1/2}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{-1/2}
= Y^{1/2}M^{-1}X^{1/2}(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{-1/2}X^{-1/2}MM^{-1}X^{1/2}
= Y^{1/2}(M^{-1}XM^{-1}Y)^{-1/2}M^{-1}X^{1/2}
= Y^{1/2}(Y^{-1}MX^{-1}M)^{1/2}M^{-1}X^{1/2},
= Y^{-1/2}Y*(MX^{-1}M)M^{-1}X^{1/2},
$$

(10)

where (10) can be proved as follows. Denote $C = (X^{1/2}M^{-1}YM^{-1}X^{1/2})^{-1/2}$ and we have

$$
I = CX^{1/2}M^{-1}YM^{-1}X^{1/2}C
= (M^{-1}X^{1/2}CX^{-1/2}M)M^{-1}XM^{-1}Y(M^{-1}X^{1/2}CX^{-1/2}M).
$$

Thus, $M^{-1}X^{1/2}CX^{-1/2}M = (M^{-1}XM^{-1}Y)^{-1/2}$.

Now we verify that the second-order approximation of the GBW distance recovers the proposed Riemannian metric in (9).

Proposition 7. The GBW distance is approximated as $d^2_{gbw}(X, X + \theta H) = \frac{\theta ^2}{2} \text{tr}(\mathcal{L}_{X,M}[H]H) + o(\theta ^2)$.

Proof. For $X \in S^n_+$ and $H \in S^n$ such that $X \pm H \in S^n_+$. Thus, for $\theta \in [-1, 1]$, $X + \theta H \in S^n_+$ and

$$
d^2_{gbw}(X, X + \theta H) = 2\text{tr}(M^{-1}X) + \theta \text{tr}(M^{-1}H)
- 2\text{tr}(X^{1/2}M^{-1}XM^{-1}X^{1/2} + \theta X^{1/2}M^{-1}HM^{-1}X^{1/2})^{1/2}
$$

The first-order derivative is

$$
\frac{d}{d\theta} d^2_{gbw}(X, X + \theta H)
= \text{tr}(M^{-1}H)
- 2\mathcal{L}_{X^{1/2}M^{-1}XM^{-1}X^{1/2}+\theta X^{1/2}M^{-1}HM^{-1}X^{1/2}}(X^{1/2}M^{-1}HM^{-1}X^{1/2})^{1/2}
= \text{tr}(M^{-1}H)
- (X^{1/2}M^{-1}XM^{-1}X^{1/2} + \theta X^{1/2}M^{-1}HM^{-1}X^{1/2})^{-1/2}X^{1/2}M^{-1}HM^{-1}X^{1/2},
$$

where we use the properties of standard Lyapunov operator, $D_V(X)^{1/2} = \mathcal{L}_{X^{1/2}}[V]$ and $\text{tr}(\mathcal{L}_X[U]) = \frac{1}{2} \text{tr}(X^{-1}U)$. Notice that

$$
\frac{d}{d\theta} d^2_{gbw}(X, X + \theta H)|_{\theta=0}
= \text{tr}(M^{-1}H) - \text{tr}(M^{-1}X^{1/2}(X^{1/2}M^{-1}XM^{-1}X^{1/2})^{-1/2}X^{1/2}M^{-1}H)
= \text{tr}(M^{-1}H) - \text{tr}\left((M^{-1}XM^{-1}X)^{-1/2}M^{-1}XM^{-1}H\right) = 0,
$$
Theorem 2

Thus, \( \frac{d^2}{d\theta^2} d_{gbw}^2(X, X + \theta H) \) is given by

\[
\frac{d^2}{d\theta^2} d_{gbw}^2(X, X + \theta H) = \text{tr}(d\frac{d}{d\theta}(X^{1/2}M^{-1}XM^{-1}X^{1/2} + \theta X^{1/2}M^{-1}HM^{-1}X^{1/2})^{-1/2} \times X^{1/2}M^{-1}HM^{-1}X^{1/2})
\]

Thus,

\[
\frac{d^2}{d\theta^2} d_{gbw}^2(X, X + \theta H)_{\theta=0} = \text{tr}(X^{1/2}M^{-1}XM^{-1}X^{1/2})^{-1/2} \mathcal{L}_{C^{1/2}} [X^{1/2}M^{-1}HM^{-1}X^{1/2}] \mathcal{C}^{-1/2} \times X^{1/2}M^{-1}HM^{-1}X^{1/2} \mathcal{C}^{-1/2}
\]

Notice, similarly from [10],

\[
(X^{1/2}M^{-1}XM^{-1}X^{1/2})^{1/2}X^{-1/2}M = X^{-1/2}M(X^{-1}MX^{-1})^{-1/2} = X^{1/2}, \text{ and } MX^{-1/2}(X^{1/2}M^{-1}XM^{-1}X^{1/2})^{1/2}X^{-1/2}M = X^{1/2}
\]

Let \( L := \mathcal{L}_{(X^{1/2}M^{-1}XM^{-1}X^{1/2})^{1/2}} [X^{1/2}M^{-1}HM^{-1}X^{1/2}] \). Then,

\[
H = MX^{-1/2}L(X^{1/2}M^{-1}XM^{-1}X^{1/2})^{1/2}X^{-1/2}M + MX^{-1/2}(X^{1/2}M^{-1}XM^{-1}X^{1/2})^{1/2}LX^{-1/2}M
\]

Thus, \( L_{X,M}[H] = X^{-1/2}LX^{-1/2} \) and \( \frac{d^2}{d\theta^2} d_{gbw}^2(X, X + \theta H)_{\theta=0} = \text{tr}(L_{X,M}[H]H) \). This completes the proof.

3.2 Riemannian geodesics, exponential map, and logarithm map

Next we derive the geodesic on the SPD manifold under the generalized BW metric [3]. To this end, we need the following well-known theorem.

**Theorem 2** (Geodesic induced from Riemannian submersion [10, 31, 51]). Consider \( \pi : (\mathcal{M}, g) \to (\mathcal{N}, h) \) as a Riemannian submersion. Let \( c \) be a geodesic on \( (\mathcal{M}, g) \) with \( c'(0) \) is horizontal. Then, we have
(1) $c'(t)$ is horizontal for all $t$.

(2) $\gamma := \pi \circ c$ is a geodesic on $(N, h)$ of the same length as $c$.

Based on Theorem 2 we show the geodesic in the proposition below.

**Proposition 8.** A geodesic on $M_{gbw}$ between any $X, Y \in S^n_{++}$ is given by $\gamma(t) = (\pi \circ c)(t)$, where $c(t) = (1 - t)M^{-1/2}X^{1/2} + tM^{-1/2}Y^{1/2}$. Here, $O$ is the orthogonal polar factor of $Y^{1/2}M^{-1}X^{1/2}$.

**Proof.** First, we see $\gamma(0) = X, \gamma(1) = Y$ and for $M, X, Y \in S^n_{++}$,

$$c(t) = ((1 - t)I + tM^{-1/2}Y^{-1/2}X^{-1/2}M^{-1/2})M^{-1/2}X^{1/2}$$

and hence, $c(t)$ lies entirely in $GL(n)$ for $t \in [0, 1]$ as it is closed under matrix multiplication. Also, $c(t)$ is a line segment, and thus, it is a valid geodesic on $M_{gl}$. Now, we need to show $c'(0)$ is horizontal. Indeed, we have

$$c'(0) = M^{-1/2}Y^{-1/2}O - M^{-1/2}X^{1/2}$$

$$= M^{1/2}(M^{-1}Y^{1/2}O - X^{1/2})$$

$$= M^{1/2}(M^{-1}Y^{-1/2}X^{-1/2}M - I)M^{-1}X^{1/2}$$

$$= M^{1/2}(M^{-1}Y(Y^{-1}MX^{-1}M)^{1/2}M^{-1} - M^{-1})M^{1/2}M^{-1/2}X^{1/2}$$

$$= M^{1/2}M^{-1}Y^{1/2}M^{-1/2}X^{1/2},$$

where $H := M^{-1}Y^{1/2}M^{-1}M^{-1} \in S^n$. Thus, from the definition of the horizontal space in [9], we have $c'(0) \in H_{M^{-1/2}X^{1/2}}$. This completes the proof. In addition, from Theorem 2 we can verify that the square of the Riemannian distance $\varrho_{gbw}$ is the same as the straight-line distance on $M_{gl}$, which is $\|M^{-1/2}X^{1/2} - M^{-1/2}Y^{1/2}\|^2 = tr(M^{-1}X) + tr(M^{-1}Y) - 2tr(X^{1/2}M^{-1}YM^{-1}X^{1/2})^{1/2}$. \[\square\]

The geodesic in Proposition 8 can be simplified as

$$\gamma(t) = \psi(t)\psi(t)^\top = ((1 - t)X^{1/2} + tY^{1/2})((1 - t)X^{1/2} + tY^{1/2}),$$

which coincides with the geodesic of the BW geometry except that $O$ is now the orthogonal polar factor of $Y^{1/2}M^{-1}X^{1/2}$ rather than $Y^{1/2}X^{1/2}$ as for BW. We can also rewrite the geodesic for GBW as

$$\gamma(t) = (1 - t)^2X + t^2Y + t(1 - t)\left(Y^{1/2}OX^{1/2} + X^{1/2}O^\top Y^{1/2}\right)$$

$$= (1 - t)^2X + t^2Y + t(1 - t)(Y^{1/2}(MX^{-1}M)^{-1}X + XM^{-1}(Y^{1/2}MX^{-1}M))$$

$$= (1 - t)^2X + t^2Y + t(1 - t)\left(YM^{-1}XM^{-1})^{1/2} + M(M^{-1}XM^{-1}Y)^{1/2}\right).$$

Next, we derive the exponential and logarithm maps in the following proposition.
Proposition 9. The Riemannian exponential map associated with the generalized BW metric is \( \Exp_X(tU) = X + tU + t^2M\L_{X,M}[U]X\L_{X,M}[U]M \). The neighbourhood \( \mathcal{X} := \{ M + tM\L_{X,M}[U]M \in S^n_+ \} \) is a totally normal neighbourhood where exponential map is a diffeomorphism with logarithm map \( \Log_X(Y) = M(M^{-1}XM^{-1}Y)^{1/2} + (YM^{-1}XM^{-1})^{1/2}M - 2X \).

Proof. We first simplify \((1 - t)X^{1/2} + tY^{1/2} = ((1 - t)I + tY^{1/2}UX^{-1/2})X^{1/2} = ((1 - t)M + tY#(MX^{-1}M))M^{-1}X^{1/2} \). With \( K := Y#(MX^{-1}M) \), we rewrite the geodesic as

\[ \gamma(t) = ((1 - t)X^{1/2} + tY^{1/2}O)((1 - t)X^{1/2} + tY^{1/2}O)^T = ((1 - t)M + tK)M^{-1}XM^{-1}((1 - t)M + tK) = X + tX(M^{-1}K - I) + t(KM^{-1} - I)X + t^2M(M^{-1}KM^{-1} - M^{-1})X(M^{-1}KM^{-1} - M^{-1})M. \]

The first-order derivative is

\[ \gamma'(0) = (K - M)M^{-1}X + XM^{-1}(K - M) = (KM^{-1} - I)X + X(M^{-1}K - I) = M(M^{-1}KM^{-1} - M^{-1})X + X(M^{-1}KM^{-1} - M^{-1})M. \]

Hence, \( \gamma(t) = X + t\gamma'(0) + t^2M\L_{X,M}[\gamma'(0)]X\L_{X,M}[\gamma'(0)]M \). The exponential map, therefore, is

\[ \Exp_X(tU) = X + tU + t^2M\L_{X,M}[U]X\L_{X,M}[U]M = (I + tM\L_{X,M}[U])X(I + t\L_{X,M}[U]M) = (M + tM\L_{X,M}[U]M)M^{-1}XM^{-1}(M + tM\L_{X,M}[U]M). \]

Note that \( \Exp_X(tU) \in S^n_+ \) if \( M + tM\L_{X,M}[U]M \in S^n_+ \).

To derive the logarithm map, let \( Y = \Exp_X(U) \). We first have

\[ M + M\L_{X,M}[U]M \]

\[ = (M^{-1}XM^{-1})^{-1/2} \left( (M^{-1}XM^{-1})^{1/2}Y(M^{-1}XM^{-1})^{1/2} \right)^{1/2} (M^{-1}XM^{-1})^{-1/2}. \]

and

\[ \L_{X,M}[U] = -M^{-1} + M^{-1}(M^{-1}XM^{-1})^{-1/2} \times \left( (M^{-1}XM^{-1})^{1/2}Y(M^{-1}XM^{-1})^{1/2} \right)^{1/2} (M^{-1}XM^{-1})^{-1/2}M^{-1} \]

Hence, let \( S_M := ((M^{-1}XM^{-1})^{1/2}Y(M^{-1}XM^{-1})^{1/2})^{1/2} \). Then,

\[ U = X\L_{X,M}[U]M + M\L_{X,M}[U]X = 2\{XM^{-1}(M^{-1}XM^{-1})^{-1/2}S_M(M^{-1}XM^{-1})^{-1/2}\}_S - 2X = 2\{MM^{-1}(M^{-1}XM^{-1})^{1/2}S_M(M^{-1}XM^{-1})^{-1/2}\}_S - 2X = M(M^{-1}XM^{-1}Y)^{1/2} + (YM^{-1}XM^{-1})^{1/2}M - 2X, \]

where we denote \( \{A\}_S := (A + A^\top)/2 \), for \( A \in \mathbb{R}^{n \times n} \). This completes the proof. \( \square \)
3.3 Levi-Civita connection

The Levi-Civita connection (or Levi-Civita derivative) of a vector field on a manifold $\mathcal{M}$ is the unique covariant derivative that satisfies (1) torsion-free property, i.e., $\nabla_\xi \eta - \nabla_\eta \xi = D_\xi \eta - D_\eta \xi = [\xi, \eta]$ and (2) metric compatibility, i.e., $\nabla_\xi (\eta, \zeta)_\mathcal{M} = (\nabla_\eta \xi)_\mathcal{M} + (\eta, \nabla_\xi \zeta)_\mathcal{M}$, for any vector fields $\xi, \eta, \zeta$.

Proposition 10. The Levi-Civita connection with the GBW geometry is given by

$$\nabla_\xi \eta = \nabla_\xi \eta + \left\{ \mathcal{L}_X \mathcal{M}[\eta] \mathcal{M} \mathcal{L}_X \mathcal{M}[\xi] \mathcal{M} + \mathcal{X} \mathcal{L}_X \mathcal{M}[\xi] \mathcal{M} \mathcal{L}_X \mathcal{M}[\eta] \mathcal{M} \right\}_S$$

Proof. The Levi-Civita connection can be derived by applying [29 MD.3]. For any vector fields $\xi, \eta, \zeta$ on $\mathcal{M}_{gbw}$, it satisfies for any $X \in \mathcal{M}_{gbw}$,

$$\langle \nabla_\xi \eta, \mathcal{L}_X \mathcal{M}[\xi] \rangle_2$$

$$= \langle \mathcal{D}_\xi \eta, \mathcal{L}_X \mathcal{M}[\xi] \rangle_2 + \frac{1}{2} \langle \mathcal{D}_\xi \mathcal{L}_X \mathcal{M}[\xi], \mathcal{L}_X \mathcal{M}[\eta] \rangle_2 + \frac{1}{2} \langle \mathcal{L}_X \mathcal{M}[\xi], \mathcal{D}_\xi \mathcal{L}_X \mathcal{M}[\eta] \rangle_2 - \frac{1}{2} \langle \mathcal{D}_\xi \mathcal{L}_X \mathcal{M}[\eta], \xi \rangle_2 - \frac{1}{2} \langle \mathcal{D}_\xi \mathcal{L}_X \mathcal{M}[\eta], \xi \rangle_2$$

The second term of (13) is rewritten as

$$\frac{1}{2} \langle \mathcal{L}_X \mathcal{M}[\eta], \mathcal{L}_X \mathcal{M}[\xi], \mathcal{M} \mathcal{L}_X \mathcal{M}[\eta] \rangle_2$$

$$= \frac{1}{2} \langle \mathcal{L}_X \mathcal{M} \mathcal{L}_X \mathcal{M}[\xi], \mathcal{M} \mathcal{L}_X \mathcal{M}[\eta] \rangle_2$$

$$= \frac{1}{2} \langle \mathcal{L}_X \mathcal{M} \mathcal{L}_X \mathcal{M}[\xi], \mathcal{M} \mathcal{L}_X \mathcal{M}[\eta] \rangle_2$$

Similarly,

$$\frac{1}{2} \langle \mathcal{L}_X \mathcal{M}[\xi], \mathcal{L}_X \mathcal{M}[\xi], \mathcal{M} \mathcal{L}_X \mathcal{M}[\eta] \rangle_2 + \langle \mathcal{L}_X \mathcal{M}[\xi], \mathcal{M} \mathcal{L}_X \mathcal{M}[\eta] \rangle_2$$

Applying the results in (14), (15), and (16) in (13), the proof is complete.

3.4 Sectional curvature

Let $\mathcal{X}(\mathcal{M})$ be the space of vector fields on the Riemannian manifold $(\mathcal{M}, g)$. The curvature tensor $R$ is defined for any $X, Y, Z \in \mathcal{X}(\mathcal{M})$, $R(X, Y)Z := \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X, Y]} Z$, where $[X, Y] = XY - YX$ is the Lie bracket and $\nabla$ is the Levi-Civita connection. At point $p$, $R_p$ defines
For any \( T_p \mathcal{M}_{gl} \), it can be projected onto the vertical and horizontal spaces defined in Proposition 5, i.e., \( U = U^V + U^H \), where

\[
U^H = M^{1/2}L_{M,M}^{1/2}P^T M^{1/2}[M^{1/2}(U^T + PU^T)M^{1/2}] M^{1/2}P,
\]

\[
U^V = M^{-1/2}L_{M^{-1},M^{1/2}PP^T M^{1/2}}^{-1}M^{-1/2}(UP^{-1} - P^{-T} U^T)M^{-1/2}P^{-T}.
\]

**Proof.** Based on Proposition 5, for \( U \in T_p \mathcal{M}_{gl} \), it can be decomposed as \( U = U^V + U^H = M^{-1/2}K M^{-1/2}P^{-T} + M^{1/2}S M^{1/2}P \), for \( K \) skew-symmetric and \( S \) symmetric. From the decomposition, \( U^T = -P^{-1}K M^{-1/2}K^{-1/2} + P^{-1} M^{1/2}S M^{1/2} \). Thus, we have

\[
M^{1/2}(U^T + PU^T)M^{1/2} = SM^{1/2}P^T M^{1/2} + M^{1/2}PP^T M^{1/2}.
\]

Hence, \( S = L_{M,M}^{1/2}PP^T M^{1/2}[M^{1/2}(U^T + PU^T)M^{1/2}] \). Similarly, we also have

\[
M^{-1/2}(UP^{-1} - P^{-T} U^T)M^{-1/2} = M^{-1/2}K M^{-1/2}P^{-T} P^{-1} M^{-1/2} + M^{-1/2}P^{-T} P^{-1} M^{-1/2}K M^{-1/2}
\]

Thus, \( K = L_{M^{-1},M^{1/2}PP^T M^{1/2}}^{-1}[M^{-1/2}(UP^{-1} - P^{-T} U^T)M^{-1/2}] \), which is clearly skew-symmetric given that \( UP^{-1} - P^{-1} U^T \) is skew-symmetric. \( \square \)

The sectional curvature of \( \mathcal{M}_{gbw} \) is given as a corollary of Theorem 3.
Proposition 11. Let $U, V \in \mathcal{X}(\mathcal{M}_{glb})$ be two (independent) vector fields. The respective horizontal lifts are given by $\tilde{U}(P) = M^{1/2}S_U H^{1/2}P$, for $P \in \mathcal{M}_{gl}$, where $S_U = \mathcal{L}_{M, \pi(P)}[U(\pi(P))]$ and similarly for $\tilde{V}$. Suppose $\tilde{U}(P), \tilde{V}(P)$ are orthonormal on $H_P \mathcal{M}_{gl}$. Then, the sectional curvature of the subspace spanned by $U(\pi(P)), V(\pi(P))$ is

$$K(U(\pi(P)), V(\pi(P))) = \sum_{i,j} 3C_{ij}^{2} \left( \sigma_i^{2} + \sigma_i^{-1} \sigma_j^{2} \right)$$

where $C = V^T(\tilde{V}(P)^T \tilde{U}(P) - \tilde{U}(P)^T \tilde{V}(P))V$ and the singular value decomposition gives $P = U \Sigma V^T$ with $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n)$, $\sigma_1 \geq \cdots \geq \sigma_n$.

Proof. To start, it is clear $\tilde{U}(P) \in H_P$ according to the definition of the horizontal space in Proposition 5. Also, we have

$$D\pi(P)[\tilde{U}(P)] = M \mathcal{L}_{M, \pi(P)}[U(\pi(P))][M^{1/2}PP^T M^{1/2} + M^{1/2}PP^T M^{1/2} \mathcal{L}_{M, \pi(P)}[U(\pi(P))] M$$

$$= U(\pi(P)), \quad \forall P \in \mathcal{M}_{gl}.$$

This suggests $\tilde{U} \in \mathcal{X}(\mathcal{M}_{gl})$ is indeed a horizontal lift of $U \in \mathcal{X}(\mathcal{M}_{gbw})$. Next we compute the sectional curvature following Theorem 3.

First, we derive an expression for the Lie bracket. For any two horizontal tangent vectors $\tilde{U}(P), \tilde{V}(P)$, they can be written as $\tilde{U}(P) = M^{1/2}S_U H^{1/2}P$ and $\tilde{V}(P) = M^{1/2}S_V H^{1/2}P$, for arbitrary symmetric matrices $S_U, S_V$. Therefore,

$$[\tilde{U}, \tilde{V}](P)$$

$$= D\tilde{V}(P)[\tilde{U}(P)] - D\tilde{U}(P)[\tilde{V}(P)]$$

$$= M^{1/2}DS_U [\tilde{U}(P)]M^{1/2}P + M^{1/2}S_V H^{1/2}P - M^{1/2}DS_U [\tilde{V}(P)]M^{1/2}P$$

$$- M^{1/2}S_U H^{1/2}P.$$

From Lemma 5 to project the result onto the vertical space, we need to first evaluate

$$M^{-1/2}(([\tilde{U}, \tilde{V}](P))P^{-1} - P^{-T}([\tilde{U}, \tilde{V}](P))^T)M^{-1/2}$$

$$= DS_U [\tilde{U}(P)] + S_V MS_U - DS_U [\tilde{V}(P)] - S_U MS_V - DS_U [\tilde{U}(P)] - S_U MS_V$$

$$+ DS_U [\tilde{V}(P)] + S_V MS_U$$

$$= 2(S_V MS_U - S_U MS_V),$$

and the vertical projection is

$$([\tilde{U}, \tilde{V}](P))^V = M^{-1/2} \mathcal{L}_{M^{-1}, \pi(P)^{-1}}[2S_V MS_U - 2S_U MS_V]M^{-1/2}P^{-T}.$$

To study the trace norm of the vertical projection, we denote

$$L := \mathcal{L}_{M^{-1}, \pi(P)^{-1}}[2S_V MS_U - 2S_U MS_V].$$
Then, from the definition of generalized Lyapunov operator,

\[ \begin{align*}
P^\top M^{-1/2}LM^{-1/2}P^\top + P^{-1}M^{-1/2}LM^{-1/2}P \\
= 2P^\top M^{1/2}(S_V MS_U - S_U MS_V)M^{1/2}P \\
= 2\tilde{V}(P)^\top \tilde{U}(P) - 2\tilde{U}(P)^\top \tilde{V}(P).
\end{align*} \]

Now, consider the singular value decomposition of \( P = U\Sigma V^\top \) with the singular values sorted decreasingly. Denote \( C := V^\top (\tilde{V}(P)^\top \tilde{U}(P) - \tilde{U}(P)^\top \tilde{V}(P))V \). This yields

\[ 2C = \Sigma U^\top M^{-1/2}LM^{-1/2}U\Sigma^{-1} + \Sigma^{-1}U^\top M^{-1/2}LM^{-1/2}U\Sigma. \tag{18} \]

Denote \( \tilde{L} := U^\top M^{-1/2}LM^{-1/2}U \). Result \( \text{(18)} \) indicates \( (\sigma_i\sigma_j^{-1} + \sigma_i^{-1}\sigma_j)\tilde{L}_{ij} = 2C_{ij} \). Hence, \( M^{-1/2}LM^{-1/2} = U\tilde{L}U^\top \) and

\[ \|(\tilde{U}, \tilde{V})(P)\|^2_2 = \|U\tilde{L}U^\top P^\top\|^2_2 = \|U\Sigma^{-1}V\|^2_2 = \|\tilde{L}\Sigma^{-1}\|_2^2 = \sum_{i,j} \frac{4C_{ij}^2}{\sigma_i^2(\sigma_i\sigma_j^{-1} + \sigma_i^{-1}\sigma_j)^2}. \]

Based on Theorem \( \text{[3]} \), the proof is complete by noticing \( \mathcal{M}_{gl} \) has zero curvature and choosing orthonormal tangent vectors \( \tilde{U}(P), \tilde{V}(P) \) without loss of generality.

We now compute the bounds for the sectional curvature following \( \text{[37]} \). We need the following lemma, which bounds the skew operation of matrix product.

**Lemma 3** (Lemma 2 in \( \text{[37]} \)). For arbitrary matrices \( A, B \in \mathbb{R}^{n \times n} \) with \( \|A\|_2 = \|B\|_2 = 1 \), we have \( \|A^\top B - B^\top A\|_2^2 \leq 2 \).

**Proposition 12.** Under the same settings as Proposition \( \text{[11]} \), the minimum sectional curvature is zero and the maximum is \( 3/(\sigma_n^2 + \sigma_{n-1}^2) \), which is achieved for \( \tilde{U}(P) = M^{1/2}S_U M^{1/2}P, \tilde{V}(P) = M^{1/2}S_V M^{1/2}P \), where

\[ \begin{align*}
S_U &= \frac{M^{-1/2}U\Sigma^{-1}(E_{(n-1,n-1)} - E_{(n,n)})\Sigma^{-1}U^\top M^{-1/2}}{2\sqrt{\sigma_n^2 + \sigma_{n-1}^2}}, \\
S_V &= \frac{M^{-1/2}U\Sigma^{-1}E_{(n,n-1)}\Sigma^{-1}U^\top M^{-1/2}}{\sqrt{\sigma_n^2 + \sigma_{n-1}^2}}
\end{align*} \]

with \( E_{(i,j)} = e_ie_j^\top + e_je_i^\top, e_i \in \mathbb{R}^n \) as the \( i \)-th standard basis vector.

**Proof.** It is clear when \( C = 0 \), the sectional curvature is zero, which happens when for example, \( S_U = M^{-1}, S_V = S \) for arbitrary symmetric \( S \). This holds even when \( \tilde{U}(P), \tilde{V}(P) \) are not orthonormal.

Also, we have

\[ K(U(\pi(P)), V(\pi(P))) = \sum_{i,j} \frac{3C_{ij}^2}{\sigma_i^2(\sigma_i\sigma_j^{-1} + \sigma_i^{-1}\sigma_j)^2} = \sum_{i,j} \frac{3\sigma_i^2C_{ij}^2}{(\sigma_i^2 + \sigma_j^2)^2} = 3\sum_{i>j} (\sigma_i^2 + \sigma_j^2)C_{ij}^2 = \sum_{i>j} \frac{3C_{ij}^2}{\sigma_i^2 + \sigma_j^2} \]

\[ \leq \frac{3}{2(\sigma_n^2 + \sigma_{n-1}^2)}\|C\|_2^2 \leq \frac{3}{\sigma_n^2 + \sigma_{n-1}^2}, \]

15
where we notice $C$ is skew-symmetric and apply Lemma 3. To verify the choice of $\tilde{U}(P), \tilde{V}(P)$ that achieves the maximum curvature, we first see

$$
\text{tr}(\tilde{U}(P)\top \tilde{V}(P)) = \frac{\text{tr}(\Sigma^{-2}(E_{(n-1,n-1)} - E_{(n,n)})E_{(n,n-1)})}{2(\sigma_n^2 + \sigma_{n-1}^2)} = \frac{\text{tr}(\Sigma^{-2}(e_n e_n\top - e_n e_{n-1}\top))}{\sigma_n^2 + \sigma_{n-1}^2} = 0,
$$

$$
\text{tr}(\tilde{U}(P)\top \tilde{U}(P)) = \text{tr}(\tilde{V}(P)\top \tilde{V}(P)) = \frac{\text{tr}(\Sigma^{-2}(e_n e_n\top + e_{n-1} e_{n-1}\top))}{\sigma_n^2 + \sigma_{n-1}^2} = 1
$$

which shows $\tilde{U}(P), \tilde{V}(P)$ are orthonormal.

Also, we have

$$
C = V\top (\tilde{V}(P)\top \tilde{U}(P) - \tilde{U}(P)\top \tilde{V}(P)) V
= \frac{E_{(n,n-1)} \Sigma^{-2}(E_{(n-1,n-1)} - E_{(n,n)}) - (E_{(n-1,n-1)} - E_{(n,n)}) \Sigma^{-2} E_{(n,n-1)}}{2(\sigma_n^2 + \sigma_{n-1}^2)}
= e_n e_{n-1}\top - e_{n-1} e_n\top.
$$

This leads to the maximum sectional curvature as $
\sum_{i>j} \frac{3C_{ij}^2}{\sigma_i^2 + \sigma_j^2} = \frac{3}{\sigma_n^2 + \sigma_{n-1}^2}.
$

The minimum and maximum curvature for the generalized BW geometry derived here generalize the results in [37]. Although sharing the minimum curvature with the BW geometry, the maximum curvature is affected by the choice of $M$ from the definition of Riemannian submersion $\pi$.

### 3.5 Geometric mean and barycenter

The geometric mean between symmetric positive definite matrices $X$ and $Y$ under the GBW geometry is the mid-point $\gamma(1/2)$ on the geodesic $\gamma$ that connects $X$ to $Y$. Following the notation in [10], we denote the interpolation of the generalized BW geodesic as $X \star_t Y := \gamma(t)$ derived in Proposition 8.

We show an operator inequality between the interpolation on GBW and convex combination on the Euclidean space.

**Proposition 13.** For any $X, Y \in S^{n}_{++}$, we have $X \star_t Y \preceq (1-t)X + tY$, for $t \in [0,1]$, where $\preceq$ denotes the Löwner partial order.
Proof. From the expression of GBW geodesic, we have

\[
\gamma(t) = (1-t)^2 X + t^2 Y + t(1-t) \left( (YM^{-1}XM^{-1})^{1/2}M + M(\gamma^{1/2})X \right)
\]

\[
= (1-t)^2 X + t^2 Y + t(1-t) \left( Y^{1/2}(YM^{-1}XM^{-1})^{1/2}Y^{1/2} - Y^{-1/2}M 
\right.
\]

\[
+ MY^{-1/2}(YM^{-1}XM^{-1}Y^{1/2})/2Y^{1/2}
\]

\[
= MY^{-1/2} \left( (1-t)^2(Y^{1/2}M^{-1}X^{1/2}Y^{1/2}) + t^2(Y^{1/2}M^{-1}YM^{-1}Y^{1/2}) - t(1-t)(YM^{-1}XM^{-1}Y^{1/2})^2Y^{1/2}M
\right)
\]

\[
= MY^{-1/2} \left( (1-t)(Y^{1/2}M^{-1}X^{1/2}Y^{1/2}) + t(1-t)(YM^{-1}YM^{-1}Y^{1/2}) - Y^{-1/2}M
\right)
\]

where the second equality follows from the property of geometric mean \((AB)^{1/2} = A(B^{-1}B)^{1/2} = A^{1/2}(B^{1/2}B^{-1}B^{1/2})^{1/2}A^{1/2} \). 

An immediate result from this proposition is that \( \log \det (X + tY) \leq \log \det ((1-t)X + tY) \). This has implication in the application of Diffusion Tensor Imaging, where the larger determinant of interpolation of SPD matrices indicates the larger diffusion, known as the swelling effect, which is physically undesirable \([5,41]\). Although we later show in Proposition 15 that under the GBW geometry, the swelling effect still exists unlike the AI or LE geometry, the level of adverse effect is smaller compared to Euclidean metric based on this proposition.

The GBW barycenter considers the following minimization problem:

\[
\min_{A \in S_{+}^n} F(A) := \sum_{l=1}^{N} w_l d_{gbw}^2(X_t, A),
\]

with \( \sum_{l=1}^{N} w_l = 1 \). This is an extension of the Wasserstein barycenter of Gaussian measures \([2,10]\). Denote the minimizer as \( A(X_{1:N}, w) := \arg \min_{A \in S_{+}^n} F(A) \). We can show, from matrix theory, that the minimizer is unique and is the solution to a specific nonlinear matrix equation. This generalizes the results in \([10]\).

**Theorem 4.** The function \( F(A) \) is strictly convex in the convex cone of \( S_{+}^n \), which admits a unique GBW barycenter \( A(X_{1:N}, w) \). The barycenter is the solution to the equation

\[
A^{1/2}M^{-1}A^{1/2} = \sum_{l=1}^{N} w_l (A^{1/2}M^{-1}X_lM^{-1}A^{1/2})^{1/2}.
\]

Proof. First we see

\[
F(A) = \sum_{l=1}^{N} w_l \text{tr}(M^{-1}X_l) + \sum_{l=1}^{N} w_l \text{tr}(M^{-1}A - 2\text{tr}(X_l^{1/2}M^{-1}AM^{-1}X_l^{1/2})^{1/2}).
\]
Thus to show strict convexity of \( F(A) \), we only need to show

\[
S(A) = \text{tr}(X_t^{1/2}M^{-1}A M^{-1}X_t^{1/2})^{1/2}
\]

is strictly concave. This is true because \( \text{tr}(X)^{1/2} \) is strictly concave. See proof in [10, 7].

By first-order stationarity, we need to find the derivative of \( F(A) \). First we write \( S(A) = \text{tr}(h \circ \phi)(A) \), where \( h(A) = A^{1/2} \) and \( \phi(A) = X_t^{1/2}M^{-1}A M^{-1}X_t^{1/2} \). Recall that \( D h(X)[U] = L_{X^{1/2}}[U] \) by the derivative of the inverse function law [36, 10]. Thus by chain rule,

\[
DS(A)[U] = \text{tr}
\left(
(Dh(\phi(A)) \circ D\phi(A))[U]
\right)
\]

\[
= \text{tr}
\left(
L_{X^{1/2}M^{-1}A M^{-1}X_t^{1/2}}[X_t^{1/2}M^{-1}U M^{-1}X_t^{1/2}]
\right)
\]

\[
= \frac{1}{2} \text{tr}
\left(
M^{-1}X_t^{1/2}(X_t^{1/2}M^{-1}A M^{-1}X_t^{1/2})^{-1/2}X_t^{1/2}M^{-1}U
\right)
\]

\[
= \frac{1}{2} \text{tr}
\left(
(A^{-1}M X_t^{-1}M)^{1/2}M^{-1}X_t M^{-1}U
\right)
\]

\[
= \frac{1}{2} \text{tr}
\left(
(A^{-1}#(M^{-1}X_t M^{-1}))U
\right),
\]

where the second equality follows from \( \text{tr}(L_X[U]) = \frac{1}{2} \text{tr}(X^{-1}L_X[U]X + L_X[U]) = \frac{1}{2} \text{tr}(X^{-1}U) \) and the third equality is due to (11).

Hence, \( DF(A)[U] = \sum_t w_t \text{tr}(M^{-1}U - A^{-1} #(M^{-1}X_t M^{-1})U) \). From the first-order optimality of the convex function \( F(A) \), i.e. \( DF(A)[U] = 0 \) for all \( U \), the unique minimizer \( A(X_{1:N}, w) \) satisfies \( M^{-1} = \sum_{t=1}^{N} w_t A^{-1} #(M^{-1}X_t M^{-1}) \), which is equivalent to \( A^{1/2}M^{-1}A^{1/2} = \sum_{t=1}^{N} w_t (A^{1/2}M^{-1}X_t M^{-1}A^{1/2})^{1/2} \).

Next we show how to compute the barycenter by a fixed point iteration similar in [10, 4]. Define

\[
K(A) := MA^{-1/2} \left( \sum_{t=1}^{N} w_t (A^{1/2}M^{-1}X_t M^{-1}A^{1/2})^{1/2} A^{-1/2} M \right)
\]

and perform the iteration update by \( A_{t+1} = K(A_t) \). We can show this update converges to \( A(X_{1:N}, w) \), formalized in the following Theorem.

**Theorem 5.** Initialize \( A_0 \in S_{++}^n \) randomly and consider the update \( A_{t+1} = K(A_t) \). Then \( \lim_{t \to \infty} A_t = A(X_{1:N}, w) \).

**Proof.** First by convexity of the matrix square,

\[
K(A) \leq MA^{-1/2} \left( \sum_{t=1}^{N} w_t A^{1/2}M^{-1}X_t M^{-1}A^{1/2} \right) A^{-1/2} M \leq \sum_{t=1}^{N} X_t.
\]

Hence, \( K(A) \) is bounded in \( S_{++}^n \). Also, we claim \( F(A_{t+1}) \leq F(A_t) \), where \( F(A) \) is the objective function defined in (19). To see this, first we recall from Proposition 1, the optimal transport map between two zero-mean Gaussians is \( T_{X \to Y} = M(X^{-1} #(M^{-1}YM^{-1})) \) with \( X, Y \) the respective
covariance matrices. Now suppose \(a \in \mathbb{R}^n\) is a random Gaussian vector with mean zero and covariance \(A\) and define \(x_t = T_A \to x_t\ a\). From Proposition 4, \(x_t\) is Gaussian distributed with covariance \(X_t\) and

\[
F(A) = \sum_{l=1}^{N} w_l \, d_{gbw}^2(A, X_t) = \sum_{l=1}^{N} w_l \, \mathbb{E}\|a - x_l\|_M^2.
\]

In addition, we verify that \(T_A \to K(A) = \sum_{l=1}^{N} w_l T_A \to x_l\). That is,

\[
T_A \to K(A) = M(A^{-1}\#(M^{-1}K(A)M^{-1}))
\]

\[
= M\left(A^{-1}\#\left(A^{-1/2}(\sum_{l=1}^{N} w_l (A^{1/2}M^{-1}X_lM^{-1}A^{1/2})^{1/2})A^{-1/2}\right)\right)
\]

\[
= M\left(A^{-1/2}(\sum_{l=1}^{N} w_l (A^{1/2}M^{-1}X_lM^{-1}A^{1/2})A^{-1/2}\right)\]

\[
= \sum_{l=1}^{N} w_l M\left(A^{-1/2}(A^{1/2}M^{-1}X_lM^{-1}A^{1/2})A^{-1/2}\right) = \sum_{l=1}^{N} w_l T_A \to x_l.
\]

Denote \(\bar{x} := \sum_{l=1}^{N} w_l x_l\). Then

\[
d_{gbw}^2(A, K(A)) = \mathbb{E}\|a - T_A \to K(A) a\|_M^2 = \mathbb{E}\|a - \sum_{l=1}^{N} w_l x_l\|_M^2 = \mathbb{E}\|a - \bar{x}\|_M^2.
\]

Notice \(\bar{x} = T_A \to K(A) a\) is also a zero-mean Gaussian random vector with covariance \(K(A)\). It follows that \(d_{gbw}^2(K(A), X_t) \leq \mathbb{E}\|\bar{x} - x_l\|_M^2\). Next recall the variance formula for Euclidean random vector, i.e. \(\text{Var}(y) = \mathbb{E}\|y - \mathbb{E}[y]\|^2 = \mathbb{E}\|y\|^2 - \|\mathbb{E}[y]\|^2 = \mathbb{E}\|x - y\|^2 - \|x - \mathbb{E}[y]\|^2\), for arbitrary \(x\). The analogue under Mahalanobis distance and finite average also holds, i.e.,

\[
\sum_{l=1}^{N} w_l\|x_l - \bar{x}\|_M^2 = \sum_{l=1}^{N} w_l\|a - x_l\|_M^2 - \|a - \bar{x}\|_M^2.
\]

Finally, based on these results, we have

\[
F(K(A)) = \sum_{l=1}^{N} w_l d_{gbw}^2(K(A), X_t) \leq \sum_{l=1}^{N} w_l \mathbb{E}\|\bar{x} - x_l\|_M^2
\]

\[
= \sum_{l=1}^{N} w_l \mathbb{E}\|a - x_l\|_M^2 - \mathbb{E}\|a - \bar{x}\|_M^2
\]

\[
\leq F(A) - d_{gbw}^2(A, K(A)).
\]

This suggests \(F(K(A)) \leq F(A)\) and hence together with the boundedness of \(K(A)\), the sequence \(A_t\) converges. In the limit, we shall observe \(F(K(A_t)) = F(A_t)\) when \(t \to \infty\) and thus \(d^2(A, K(A)) = 0\). From the definition of \(K(A)\) and the optimality condition, we conclude the limit point is \(A(X_{1:N}, w)\).

4 Applications of the GBW geometry

In this section, we discuss a number of applications where the proposed generalized BW geometry may be employed.
4.1 Riemannian optimization over the GBW geometry

Learning over SPD matrices usually concerns optimizing an objective function with respect to the parameter, which is constrained to be SPD. Riemannian optimization is an elegant approach that converts the constrained optimization into an unconstrained problem on manifolds \([1, 12]\). Among the metrics for the SPD matrices, the Affine-Invariant metric is seemingly the most popular choice for Riemannian optimization due to its efficiency and convergence guarantees. Recently, however, in \([20]\), the Bures-Wasserstein metric is shown to be a promising alternative for various learning problems. Below, we provide the Riemannian optimization ingredients for the GBW geometry.

Given a function \(f : \mathcal{M} \to \mathbb{R}\), the Riemannian gradient at \(x \in \mathcal{M}\), denoted by \(\nabla f(x)\), is the unique tangent vector satisfying \((\nabla f(x), u)_x = D_u f(x)\), for any \(u \in T_x \mathcal{M}\). \(D_u f(x)\) is the directional derivative. Riemannian Hessian at \(x\), \(\text{Hess}_f(x) : T_x \mathcal{M} \to T_x \mathcal{M}\) is defined as the Levi-Civita derivative of the Riemannian gradient, i.e., \(\nabla^2 f(x)\). We note that with the expressions for the Riemannian gradient (and Hessian), we can implement various Riemannian first-order (and second-order) optimization methods for different problems, e.g., using toolboxes like Manopt \([13]\) and Pymanopt \([50]\).

**Proposition 14.** The Riemannian gradient and Hessian of a real-valued function \(f : \mathcal{M}_{gbw} \to \mathbb{R}\) is given by

\[
\begin{align*}
\nabla f(X) &= 2X \nabla f(X) M + 2M \nabla f(X) X, \\
\text{Hess}_f(X)[U] &= 4\{M \nabla^2 f(X) [U] X\} + 2\{M \nabla f(X) U\} X \\
&\quad + 4\{X \{\nabla f(X) M \mathcal{L}_{X,M}[U]\} S M\} - \{M \mathcal{L}_{X,M}[U] \nabla f(X)\} S.
\end{align*}
\]

**Proof.** For the Riemannian gradient, we require

\[
\text{tr}(\nabla f(X) V) = \frac{1}{2} \text{tr}(\mathcal{L}_{X,M}[\nabla f(X)] V)
\]

for any \(V \in T_X \mathcal{M}_{gbw}\). Thus, we have \(\nabla f(X) = \mathcal{L}_{X,M}^{-1}[2\nabla f(X)] = 2X \nabla f(X) M + 2M \nabla f(X) X\).

For the Riemannian Hessian, we have for any \(U \in T_X \mathcal{M}\)

\[
\begin{align*}
\text{Hess}_f(X)[U] &= \nabla U \nabla f(X) \\
&= DU \nabla f(X) - \{M \mathcal{L}_{X,M}[\nabla f(X)] U\} S - \{M \mathcal{L}_{X,M}[U] \nabla f(X)\} S \\
&\quad + \{X \mathcal{L}_{X,M}[\nabla f(X)] M \mathcal{L}_{X,M}[U]\} M + X \mathcal{L}_{X,M}[U] M \mathcal{L}_{X,M}[\nabla f(X)] M S \\
&= DU \nabla f(X) + \{4X \{\nabla f(X) M \mathcal{L}_{X,M}[U]\} S M\} - 2M \nabla f(X) U S \\
&\quad - \{M \mathcal{L}_{X,M}[U] \nabla f(X)\} S,
\end{align*}
\]

where we use \(\mathcal{L}_{X,M}[UXM + UX] = U\). Now we compute \(DU \nabla f(X)\), which is

\[
\begin{align*}
DU \nabla f(X) &= 2DU (X \nabla f(X) M + M \nabla f(X) X) \\
&= 2U \nabla f(X) M + 2X \nabla^2 f(X) [U] M + 2M \nabla^2 f(X) [U] X + 2M \nabla f(X) U \\
&= 4\{M \nabla f(X) U\} S + 4\{M \nabla^2 f(X) [U] X\} S.
\end{align*}
\]

Combining \(21\) with \(20\) completes the proof. \hfill \Box
4.2 Geodesic convexity

Geodesic convexity is a generalization of standard convexity in the Euclidean space. It plays a crucial role in Riemannian optimization problems, where for geodesic convex problems, the convergence rates have been shown to be superior in many cases [48, 54, 34]. Consequently, geodesic convexity has been exploited to develop better algorithms for machine learning applications such as Gaussian mixture models [24] and metric learning [53]. Recently, geodesic convexity has allowed to develop provably accelerated algorithms on manifolds [3]. Below, we show some interesting classes of objective functions for SPD matrices that are geodesic convex under the GBW geometry.

A geodesic convex set \( X \subseteq \mathcal{M} \) requires, for any \( x, y \in X \), the distance minimizing geodesic \( \gamma \) connecting the two points lie entirely in the set. A function \( f : X \rightarrow \mathbb{R} \) is called geodesic convex if, for any \( x, y \in X \), it satisfies that, for all \( t \in [0, 1] \), \( f(\gamma(t)) \leq (1 - t)f(x) + tf(y) \).

**Proposition 15.** Suppose \( A \in \mathbb{S}^n_+ \), the set of \( n \times n \) semi-definite matrices, and let \( \lambda^j : \mathbb{S}^n_+ \rightarrow \mathbb{R}^n_+ \) be the eigenvalue map that is decreasingly sorted and \( h : \mathbb{R}^+ \rightarrow \mathbb{R} \) be a monotonically increasing and convex function.

Then the following functions \( f_1(X) = \text{tr}(XA) \), \( f_2(X) = \text{tr}(XAX) \), \( f_3(X) = -\log \det(X) \), \( f_4(X) = \sum_{j=1}^k h(\lambda^j_j(X)) \), \( k \in [1, n] \), are geodesic convex under the GBW geometry for any choice of \( M \).

**Proof.** To prove geodesic convexity for \( f_1, f_2 \), we require a second-order characterization of geodesic convexity. That is, a twice continuously differentiable function \( f \) is geodesic convex if \( \frac{d^2f(\gamma(t))}{dt^2} \geq 0 \) for all \( t \in [0, 1] \). Now recall from Proposition 8 and the simplification in (12), the geodesic for GBW shares the same form as BW except for the value of polar factor \( U \). Nevertheless, the non-negativity of second-order derivatives does not depend on the choice of \( U \) according to the proof of Proposition 1 in [20]. Hence, we can follow the exact proof to show \( f_1 \) and \( f_2 \) are geodesic convex on the GBW geometry.

For \( f_3 \), we have

\[
\log \det(\gamma(t)) = 2\log \det((1 - t)X^{1/2} + tY^{1/2}U) \\
= 2\log \det(((1 - t)M + tY^{1/2}UX^{-1/2}M)M^{-1}X^{1/2}) \\
\geq 2(1 - t)\log \det(M) + 2t\log \det(Y^{1/2}UX^{-1/2}M) + 2\log \det(M^{-1}) \\
+ 2\log \det(X^{1/2}) \\
= 2t\log \det(Y^{1/2}) - 2t\log \det(X^{1/2}) + 2\log \det(X^{1/2}) \\
= (1 - t)\log \det(X) + t\log \det(Y),
\]

where the first inequality is due to the concavity of log-det on SPD matrices and from Lemma 1, we see \( Y^{1/2}UX^{-1/2}M \succeq 0 \).

Finally for \( f_4 \), the geodesic convexity simply follows from the result of \( X \ast_t Y \succeq (1 - t)X + tY \) in Proposition 13 and Theorem 2.3 in [48].

4.3 Robust generalized Bures-Wasserstein distance

The relationship between the Bures-Wasserstein distance and the \( L_2 \)-Wasserstein distance between zero-centered Gaussians has been well-studied in [10, 52]. In Section 2.2, we discuss the latter’s
relationship with the GBW distance. In this section, we show that a variant of the GBW distance is related to a class of ‘max-min’ robust $L_2$-Wasserstein distance between zero-centered Gaussians.

In [23, 40], a projection robust Wasserstein distance is considered in order to mitigate the exponentially growing sample complexity to compute the Wasserstein distance. That is, for two $n$-dimensional measures $\mu, \nu$, the aim is to seek for a projection matrix $W \in \mathbb{R}^{n \times d}$ $(d < n)$, which gives

$$
\mathcal{P}_d(\mu, \nu) = \sup_{W:W^\top W = I} \inf_{\gamma \sim \Gamma(\mu, \nu)} \int \|W(x - y)\|^2 d\gamma(x, y).
$$

When $\mu$ and $\nu$ are zero-centered Gaussians with covariance matrices $X$ and $Y$, respectively, this reduces to

$$
\mathcal{P}_d(\mu = \mathcal{N}(0, X), \nu = \mathcal{N}(0, Y)) = 
$$

based on Proposition 3. The term $\text{tr}(X^{1/2}YY^{1/2})$ is also compactly written as $\text{tr}(W^\top X WW^\top Y WW^\top X^{1/2})^{1/2}$. If $W^*$ is an optimal solution of (22), then we also have the following equivalence:

$$
\mathcal{P}_d(\mu = \mathcal{N}(0, X), \nu = \mathcal{N}(0, Y)) = d_{\text{rgbw}}^2(X, Y) = \max_{M^{-1} \in C} d_{\text{gbw}}^2(X, Y)
$$

for a closed convex set $C \subseteq S_n^{++}$. We emphasize the maximization of $S$ over the set $C$. It follows from (22) & (23) that the projection robust Wasserstein distance for zero-centered Gaussians is a particular case of the robust GBW distance. Below we show that (23) is a distance metric.

**Proposition 16.** The robust GBW distance defined in (23) in the set $C \subseteq S_n^{++}$ is a distance metric.

**Proof.** From (23), we see $d_{\text{rgbw}}^2(X, Y) \geq 0$ and is clearly symmetric. The triangle inequality also easily follows as shown below. Let

$$
S^* = \arg \max_{S \in C} d_{\text{gbw}}^2(X, Y).
$$

Therefore, from (24), we have

$$
d_{\text{rgbw}}(X, Y) = d_{\text{gbw}}(X, Y) \quad \text{for} \quad S^*
$$

$$
\leq d_{\text{gbw}}(X, Z) + d_{\text{gbw}}(Z, Y) \quad \text{for} \quad S^* \text{ as GBW is a distance}
$$

$$
\leq (\max_{S_1 \in C} d_{\text{gbw}}(X, Z) \quad \text{for} \quad S_1) + (\max_{S_2 \in C} d_{\text{gbw}}(Z, Y) \quad \text{for} \quad S_2)
$$

$$
= d_{\text{rgbw}}(X, Z) + d_{\text{rgbw}}(Z, Y),
$$

where $X, Y,$ and $Z$ are SPD matrices. Finally, the identity of indiscernibles property is satisfied as the robust GBW distance is based on the GBW distance (which itself satisfies the property). This completes the proof.
Additionally, the robust GBW distance (23) is invariant to affine transformations of input SPD matrices provided the set $C$ is closed under affine transformations, i.e., $PSP^\top \in C$ for $P \in M(n)$. This is because

\[
d^2_{rgbw}(P^\top XP, P^\top YP) = \max_{S \in C} \text{tr}(SP^\top XP + SP^\top YP - 2(SP^\top YPSP^\top XP)^{1/2})
\]

When the set $C$ is either the full space $S^{n}_{++}$ or $S^{n}_{+}$, the closure is trivially satisfied. Another example is the set $C = \{S \in S^{n}_{++} : 0 \preceq S \preceq I\}$ for which the robust BW distance in $C$ is invariant to restricted affine transformations that belong to the set $D = \{P \in M(n) : PP^\top \succeq I\}$. To see this, suppose that $d^2_{rgbw}(X, Y)$ is achieved at $S^* \in C$, then for any $W \in D$, $P^{-1}SP^{-1} \in C$, which is the maximizer for $d^2_{rgbw}(P^\top XP, P^\top YP)$.

### 4.4 Geometry-aware principal component analysis (PCA)

Geometry-aware principal component analysis (PCA) for SPD matrices extends the classical PCA to manifolds by maximizing the deviation from the reduced SPD matrices to the reduced barycenter $[23, 22, 27]$. Using the BW distance, the PCA objective is formulated naturally as the GBW distance between matrices, where $M^{-1}$ is parameterized as $WW^\top$ with $W \in \mathbb{R}^{n \times d}$. Consequently, the objective function is

\[
\max_{M^{-1} = WW^\top, W^\top W = I} \sum_{i=1}^{N} d^2_{gbw}(X_i, \bar{X})
\]

\[
= \max_{W : W^\top W = I} \sum_{i=1}^{N} d^2_{bw}(W^\top X_i W, W^\top \bar{X} W)
\]

\[
= \max_{W : W^\top W = I} \sum_{i=1}^{N} (\text{tr}(W^\top X_i W) + \text{tr}(W^\top \bar{X} W) - 2\text{tr}(W^\top X_i WW^\top \bar{X} W)^{1/2})
\]

for samples $X_i \in S^{n}_{++}, i = 1, \ldots, N$, where $\bar{X} = \arg\min \sum_{i=1}^{N} d^2_{bw}(X_i, C)$ is the barycenter in the original space. $\bar{X}$ can be computed via the fixed point iteration algorithm (Theorem 5) by setting $M = I$. The constraint of column orthonormality on $W$, i.e., $W^\top W = I$, ensures that $W$ projects the covariance matrices onto a $d$-dimensional space. In many practical scenarios, $d$ is often chosen to be much less than $n$, i.e., $d \ll n$.

### 4.5 Metric learning

The problem of metric learning amounts to learning a suitable Mahalanobis (symmetric positive, and possibly, semi-definite) matrix from pairs of similarity and dissimilarity information, e.g., in a classification task $[15, 53, 21, 19, 22, 26, 27]$. A particular formulation of interest is based on the objective function proposed in $[21]$. Specifically, given a set of data-target pairs $\{X_i, t_i\}, X_i \in S^{n}_{++}$ and $t_i$ categorical, we define the class adjacency
Table 2: Riemannian optimization ingredients for the Affine-Invariant and Generalized Bures-Wasserstein (with \( M = X \)) geometries for log-determinant optimization.

|                      | Affine-Invariant | Generalized Bures-Wasserstein (with \( M = X \)) |
|----------------------|-----------------|-----------------------------------------------|
| \( \text{Exp} \)    | \( \text{Exp}_X(U) = X^{1/2} \exp(X^{-1}U)X^{1/2} \) | \( \text{Exp}_X(U) = X + U + \frac{1}{2}UX^{-1}U \) |
| \( \text{Grad} \)   | \( \text{grad}(f(X)) = XCX - X \) | \( \text{grad}(f(X)) = 4XCX - 4X \) |
| \( \text{Hess} \)   | \( \text{Hess}(f(X))[U] = 2U + \{UCX\}_S \) | \( \text{Hess}(f(X))[U] = 2U + 2\{UCX\}_S \) |

matrix \( A_{ij} = 1 \) if sample \( i, j \) are from the same class (i.e., \( t_i = t_j \)) and \( A_{ij} = -1 \) otherwise. To this end, the objective function is given as

\[
\min_{S \succeq 0} \sum_{i,j}^N \log(1 + \exp(A_{ij}(\text{tr}(SX_i) + \text{tr}(SX_j) - 2\text{tr}(X_i^{1/2}SX_jS^{1/2}X_i^{1/2})^{1/2}))). \tag{25}
\]

It should be emphasized that the objective function in (25) is formulated by directly making use of the BW distance in the objective function of [21]. However, from the definition of the GBW distance 4 between \( X_i \) and \( X_j \) and by taking \( M^{-1} = S \), we observe that the problem (25) may be equivalently rewritten as

\[
\min_{S \succeq 0} \sum_{i,j}^N \log(1 + \exp(A_{ij}d^2_{gbw}(X_i, X_j))).
\]

This suggests that the GBW geometry naturally captures the metric learning properties of the space.

Note that \( S \) can be arbitrary semi-definite matrix and one usually parameterizes \( S = WW^\top \), where \( W \) is a matrix of size \( n \times d \). Similar to Section 4.4, the choice for \( d \) is motivated by computational considerations and is usually \( d \ll n \).

4.6 Log-determinant Riemannian optimization

Log-determinant or log-det optimization is common in statistical machine learning, such as density estimation, with an objective concerning \( \min_{X \in S_n^{++}} f(X) = -\log \det(X) \). From the analysis in [20], optimization with the BW geometry is less well-conditioned compared to the AI geometry. This is because the Euclidean Hessian is \( \nabla^2 f(X)[U] = X^{-1}UX^{-1} \), which leads to the Riemannian Hessian at optimality as \( \text{Hess}_{ai}f(X^*)[U] = U \) for the AI geometry and \( \text{Hess}_{bw}f(X^*)[U] = 4\{(X^*)^{-1}U\}_S \) for the BW geometry. This suggests, under the BW geometry, the condition number of Hessian at optimality depends on the solution \( X^* \), while no dependence on \( X^* \) under the AI geometry. Consequently, the BW geometry leads to a poor performance in log-det optimization as highlighted in [20].

Here, we show how the GBW geometry helps to address this issue. Specifically, with the GBW geometry, we see from Proposition 14 that by choosing \( M = X^* \), the Riemannian Hessian is \( \text{Hess}_{gbw}f(X^*)[U] = U \), which becomes well-conditioned (around the optimal solution). This provides the motivation for a choice of \( M \). As the optimal solution \( X^* \) is unknown in optimization problems, choice of \( M \) is not trivial. In practice, one may choose \( M = X \) dynamically at every or after a few iterations. This strategy corresponds to modifying the GBW geometry dynamically with iterations.
To show how properly selected $\mathbf{M}$ can help improve the convergence of with the BW geometry, we consider the problem

$$\min_{\mathbf{X} \in \mathbb{S}^n_+} f(\mathbf{X}) = -\log \det(\mathbf{X}) + \text{tr}(\mathbf{C}\mathbf{X}),$$

(26)

where $\mathbf{C} \in \mathbb{S}^n_+$ is a given SPD matrix. The Euclidean gradient $\nabla f(\mathbf{X}) = -\mathbf{X}^{-1} + \mathbf{C}$ and the Euclidean Hessian $\nabla^2 f(\mathbf{X})[\mathbf{U}] = \mathbf{X}^{-1}\mathbf{UX}^{-1}$. From Proposition 15 this problem is geodesic convex with the optimal solution $\mathbf{X}^* = \mathbf{C}^{-1}$.

Choosing $\mathbf{M} = \mathbf{X}$ and following derivations in Section 4.1, the expressions for the exponential map, Riemannian gradient, and Hessian under the GBW geometry are shown in Table 2, where we also draw comparisons to the AI geometry. We see that the choice of $\mathbf{M} = \mathbf{X}$ allows GBW to locally approximate the AI geometry up to some constants. The gradient expressions are the same (up to a scaling which is immaterial). However, the differences appear in the Hessian and exponential map expressions. For example, the AI exponential map $\mathbf{X}^{1/2} \exp(\mathbf{X}^{-1}\mathbf{U})\mathbf{X}^{1/2}$ can approximate by second-order terms as $\mathbf{X} + \mathbf{U} + \frac{1}{2}\mathbf{UX}^{-1}\mathbf{U}$. This is different from the GBW exponential map, which is $\mathbf{X} + \mathbf{U} + \frac{1}{4}\mathbf{UX}^{-1}\mathbf{U}$, up to an additional term $\frac{1}{4}\mathbf{UX}^{-1}\mathbf{U}$. Similarly, there is a difference of the term $\{\mathbf{UCX}\}$ in the Hessian expression. Overall, the similarity of optimization ingredients help GBW (with $\mathbf{M} = \mathbf{X}$) perform as similar as the AI geometry, which helps to resolve the poor performance of BW for log-det optimization problems as observed in [20].

5 Experiments

In this section, we perform experiments showing the benefit of the GBW geometry. The algorithms are implemented in Matlab using the Manopt toolbox [13]. The codes are available at https://github.com/andyjm3/GBW.

5.1 Results on log-determinant Riemannian optimization

We show experiments on the problem (26). For creating problem instances, we follow the same settings as in [20] and consider two instances where the condition number of $\mathbf{X}^*$ is 10 (well-conditioned) and 1000 (ill-conditioned). $\mathbf{C}$ is then obtained as $(\mathbf{X}^*)^{-1}$.

To compare the convergence performance of optimization methods under the AI, LE, BW, and GBW (with $\mathbf{M} = \mathbf{X}$) geometries, we implement the Riemannian trust region (a second-order solver) with the considered geometries [1, 12]. To measure convergence, we use the distance to (theoretical) optimal solution, i.e., $\|\mathbf{X}_t - \mathbf{X}^*\|_2$. We plot this distance against the cumulative inner iterations that the trust region method takes to solve a particular trust region sub-problem at every iteration. The inner iterations are a good measure to show convergence of trust region algorithms [1, Chapter 7].

From Figures 1(a) & 1(b), we observe the faster convergence with the GBW geometry compared to other geometries regardless of the condition number. In contrast, the BW geometry performs poorly in log-determinant optimization problems as pointed out in [20]. Thus, the GBW geometry effectively resolves the convergence issues with the BW geometry for such settings. Based on our discussion in Section 4.6 we see that GBW with $\mathbf{M} = \mathbf{X}$ performs similar to the AI geometry. Empirically, it proves the argument that the GBW geometry effectively bridges the gap between BW and AI geometries for optimization problems.
We also consider the problem of Gaussian mixture model (GMM) [23], i.e.,

$$L = \sum_{i=1}^{N} \log \left( \sum_{j=1}^{K} \omega_j p_{N}(x_i; \Sigma_j) \right),$$

where $x_i \in \mathbb{R}^n$, $i = 1, \ldots, N$ are samples with $K$ Gaussian components, with reformulated Gaussian density $p_{N}(x; \Sigma) = (2\pi)^{-d/2} \det(\Sigma)^{-1/2} \exp(-\frac{1}{2} x^\top \Sigma x)$. From Proposition 15, it follows that the GMM objective (27) is geodesic convex under the GBW geometry.

For experiments, we consider four datasets: iris, kmeansdata from https://au.mathworks.com/help/stats/sample-data-sets.html and balance, phoneme from https://sci2s.ugr.es/keel/datasets.php. For comparisons, we implement the Riemannian stochastic gradient descent method [11] as it is widely used in GMM problems [24]. The batch size is set to 50 and we use a decaying stepsize for all the geometries following [20]. For the GBW case, we set $M = X$ at every iteration. Without access to the optimal solution, the convergence is measured in terms of the Euclidean gradient norm $\| \Sigma_t \nabla L(\Sigma_t) \|_2$ for comparability across geometries. Figures 1(c)-(f) show convergence along with the best selected initial stepsize. We again observe that convergence under the GBW geometry is competitive and clearly outperforms the BW geometry based algorithm.
Table 3: Summary statistics for MNIST, ETH, YTC datasets

|        | SPD samples | SPD Dim | # Class |
|--------|-------------|---------|---------|
| MNIST  | 835         | 100     | 10      |
| ETH    | 80          | 100     | 8       |
| YTC    | 194         | 100     | 9       |

Table 4: Geometry-aware PCA average classification accuracy (%). GBW allows lower dimensional projection with accuracy comparable to that in the original dimension.

|        | AI | LE | BW | GBW $d = 5$ | $d = 10$ | $d = 30$ | $d = 50$ | $d = 70$ | $d = 90$ |
|--------|----|----|----|-------------|---------|---------|---------|---------|---------|
| MNIST  | 100| 100| 100| 99.33       | 100     | 100     | 100     | 100     | 100     |
| ETH    | 76.25 | 84.50 | 87.75 | 80.75       | 84.75   | 86.75   | 88.00   | 87.75   | 87.75   |
| YTC    | 74.70 | 79.00 | 76.40 | 60.60       | 72.40   | 76.50   | 76.00   | 76.30   | 76.40   |

5.2 Results on geometry-aware PCA

For the application of geometry-aware PCA, we consider two vision tasks, i.e., image set classification and video-based face recognition. Following the pre-processing steps in [22, 27], we treat each vectorized image (or video frame) as a sample in the set and compute the sample covariance to represent the entire image set (or a video). The task is to classify each image set or video represented by a covariance SPD matrix.

Three real-world datasets are considered, including the MNIST handwritten digits (MNIST) [30], ETH-80 object (ETH) [32], and YouTube Celebrities (YTC) [28] datasets. To process MNIST dataset, we use 42,000 training samples, and, for each class, we partition the samples into subgroups randomly, each containing 50 images. Then for each subgroup, the covariance matrix is computed. ETH dataset contains image sets of 8 objects, each with 10 subclasses. The 80 subgroups are processed accordingly. YTC is a collection of low-resolution videos of celebrities. Due to the sparsity of the dataset, we only consider 9 persons with video number greater than 15. All images or video frames are resized to $10 \times 10$ and the SPD matrix generated as the covariance is of size $100 \times 100$. The statistics of all the considered datasets are in Table 3.

We follow Section 4.4 to find the transformation matrix $W \in \mathbb{R}^{n \times d}$. To validate the effectiveness of dimensionality reduction under the GBW geometry, we perform nearest neighbour classification on the reduced data matrix $W^T X_i W$, $i = 1, \ldots, N$. The reduced dimension $d$ is a hyperparameter, and we, therefore, present classification accuracy with $d = \{5, 10, 30, 50, 70, 90\}$. Given that the sample size may be small for some classes, for each class, we take 50% as the training set and the rest as the test set. Such a random splitting is repeated ten times and we report the average accuracy in Table 4 where we also report results with AI and LE distances as benchmarks. We use the Riemannian trust region method to solve the maximization problem in Section 4.4.

We see that the classification performance under various choices of $d$ does not largely degrade and may even be enhanced, which suggests the global properties of SPD samples can be well-preserved.
even with a lower-dimensional representation. This also suggests that GBW is a better modeling approach than BW for the geometric PCA problem.

6 Conclusion

In this paper, we propose a Riemannian geometry that generalizes the recently introduced Bures-Wasserstein geometry for SPD matrices. This generalized geometry has natural connections to the orthogonal Procrustes problem as well as to the optimal transport theory, and still possesses many interesting properties of the Bures-Wasserstein geometry (which is a special case). The new geometry is shown to be parameterized by an arbitrary SPD matrix $M$. This offers necessary flexibility in applications. Experiments showed that learning of $M$ (or its inverse $M^{-1}$) leads to better modeling in various applications.

As future research, we intend to investigate how learning of $M$ improves convergence of algorithms and whether this leads to a principled preconditioning approach for problems with SPD matrices under the GBW geometry.

Existing works already formalize a family of metrics unifying Bures-Wasserstein and Log-Euclidean [38], as well as Affine-Invariant (AI) and Log-Euclidean [49] metrics. An interesting research direction would be to consider unification of all three and whether the GBW generalization offers additional insights for this. This is especially relevant given our analysis for log-determinant optimization, where we find similarity of optimization ingredients for AI and GBW (with a particular choice of $M$).

References

[1] P.-A. Absil, R. Mahony, and R. Sepulchre. Optimization algorithms on matrix manifolds. Princeton University Press, 2008.

[2] Martial Agueh and Guillaume Carlier. Barycenters in the Wasserstein space. SIAM Journal on Mathematical Analysis, 43(2):904–924, 2011.

[3] Kwangjun Ahn and Suvrit Sra. From Nesterov’s estimate sequence to Riemannian acceleration. In Conference on Learning Theory, 2020.

[4] Pedro C Álvarez-Esteban, E Del Barrio, JA Cuesta-Albertos, and C Matrán. A fixed-point approach to barycenters in Wasserstein space. Journal of Mathematical Analysis and Applications, 441(2):744–762, 2016.

[5] Vincent Arsigny, Pierre Fillard, Xavier Pennec, and Nicholas Ayache. Log-Euclidean metrics for fast and simple calculus on diffusion tensors. Magnetic Resonance in Medicine: An Official Journal of the International Society for Magnetic Resonance in Medicine, 56(2):411–421, 2006.

[6] Vincent Arsigny, Pierre Fillard, Xavier Pennec, and Nicholas Ayache. Geometric means in a novel vector space structure on symmetric positive-definite matrices. SIAM Journal on Matrix Analysis and Applications, 29(1):328–347, 2007.

[7] Richard Bellman. Some inequalities for the square root of a positive definite matrix. Linear Algebra and its applications, 1(3):321–324, 1968.
[8] Arthur L Besse. *Einstein manifolds*. Springer Science & Business Media, 2007.

[9] Rajendra Bhatia. *Positive definite matrices*. Princeton university press, 2009.

[10] Rajendra Bhatia, Tanvi Jain, and Yongdo Lim. On the Bures-Wasserstein distance between positive definite matrices. *Expositiones Mathematicae*, 37(2):165–191, 2019.

[11] Silvere Bonnabel. Stochastic gradient descent on riemannian manifolds. *IEEE Transactions on Automatic Control*, 58(9):2217–2229, 2013.

[12] N. Boumal. *An introduction to optimization on smooth manifolds*. Available online, Aug, 2020.

[13] N. Boumal, B. Mishra, P.-A. Absil, and R. Sepulchre. Manopt, a Matlab toolbox for optimization on manifolds. *Journal of Machine Learning Research*, 15(1):1455–1459, 2014.

[14] Daniel A Brooks, Olivier Schwander, Frédéric Barbaresco, Jean-Yves Schneider, and Matthieu Cord. Exploring complex time-series representations for Riemannian machine learning of radar data. In *IEEE International Conference on Acoustics, Speech and Signal Processing*, 2019.

[15] Jason V Davis, Brian Kulis, Prateek Jain, Suvrit Sra, and Inderjit S Dhillon. Information-theoretic metric learning. In *International Conference on Machine learning*, 2007.

[16] Eustasio Del Barrio, Juan Antonio Cuesta-Albertos, Carlos Matrán, and Agustín Mayo-Iscar. Robust clustering tools based on optimal transportation. *Statistics and Computing*, 29(1):139–160, 2019.

[17] Pinar Demetci, Rebecca Santorella, Bjorn Sandstede, William Stafford Noble, and Ritambhara Singh. Gromov-wasserstein optimal transport to align single-cell multi-omics data. *BioRxiv*, 2020.

[18] Alexandre Gramfort, Gabriel Peyré, and Marco Cuturi. Fast optimal transport averaging of neuroimaging data. In *International Conference on Information Processing in Medical Imaging*, 2015.

[19] Matthieu Guillaumin, Jakob Verbeek, and Cordelia Schmid. Is that you? metric learning approaches for face identification. In *International Conference on Computer Vision*, 2009.

[20] Andi Han, Bamdev Mishra, Pratik Jawanpuria, and Junbin Gao. On Riemannian optimization over positive definite matrices with the Bures-Wasserstein geometry. In *Advances in Neural Information Processing Systems*, 2021.

[21] Mehrtash Harandi, Mathieu Salzmann, and Richard Hartley. Joint dimensionality reduction and metric learning: A geometric take. In *International Conference on Machine Learning*, 2017.

[22] Mehrtash T Harandi, Mathieu Salzmann, and Richard Hartley. From manifold to manifold: Geometry-aware dimensionality reduction for SPD matrices. In *European Conference on Computer Vision*, 2014.

[23] Inbal Horev, Florian Yger, and Masashi Sugiyama. Geometry-aware principal component analysis for symmetric positive definite matrices. In *Asian Conference on Machine Learning*, 2016.
[24] Reshad Hosseini and Suvrit Sra. An alternative to EM for Gaussian mixture models: batch and stochastic Riemannian optimization. *Mathematical Programming*, 181(1):187–223, 2020.

[25] Minhui Huang, Shiqian Ma, and Lifeng Lai. Projection robust Wasserstein barycenters. In *International Conference on Machine Learning*, 2021.

[26] Zhiwu Huang, Ruiping Wang, Xianqiu Li, Wenxian Liu, Shiguang Shan, Luc Van Gool, and Xilin Chen. Geometry-aware similarity learning on SPD manifolds for visual recognition. *IEEE Transactions on Circuits and Systems for Video Technology*, 28(10):2513–2523, 2017.

[27] Zhiwu Huang, Ruiping Wang, Shiguang Shan, Xianqiu Li, and Xilin Chen. Log-Euclidean metric learning on symmetric positive definite manifold with application to image set classification. In *International Conference on Machine Learning*, 2015.

[28] Minyoung Kim, Sanjiv Kumar, Vladimir Pavlovic, and Henry Rowley. Face tracking and recognition with visual constraints in real-world videos. In *Conference on Computer Vision and Pattern Recognition*, 2008.

[29] Serge Lang. *Differential and Riemannian manifolds*. Springer Science & Business Media, 2012.

[30] Yann LeCun, Léon Bottou, Yoshua Bengio, and Patrick Haffner. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.

[31] John M Lee. *Introduction to Riemannian manifolds*. Springer, 2018.

[32] Bastian Leibe and Bernt Schiele. Analyzing appearance and contour based methods for object categorization. In *Conference on Computer Vision and Pattern Recognition*, 2003.

[33] Zhenhua Lin. Riemannian geometry of symmetric positive definite matrices via cholesky decomposition. *SIAM Journal on Matrix Analysis and Applications*, 40(4):1353–1370, 2019.

[34] Yuanyuan Liu, Fanhua Shang, James Cheng, Hong Cheng, and Licheng Jiao. Accelerated first-order methods for geodesically convex optimization on riemannian manifolds. In *Advances in Neural Information Processing Systems*, 2017.

[35] Sridhar Mahadevan, Bamdev Mishra, and Shalini Ghosh. A unified framework for domain adaptation using metric learning on manifolds. In *European Conference on Machine Learning and Knowledge Discovery in Databases*, 2019.

[36] Luigi Malagò, Luigi Montrucchio, and Giovanni Pistone. Wasserstein Riemannian geometry of Gaussian densities. *Information Geometry*, 1(2):137–179, 2018.

[37] Estelle Massart, Julien M Hendrickx, and P-A Absil. Curvature of the manifold of fixed-rank positive-semidefinite matrices endowed with the Bures-Wasserstein metric. In *International Conference on Geometric Science of Information*, 2019.

[38] Hà Quang Minh. A unified formulation for the Bures-Wasserstein and Log-Euclidean/Log-Hilbert-Schmidt distances between positive definite operators. In *International Conference on Geometric Science of Information*, 2019.
[39] Barrett O’Neill. The fundamental equations of a submersion. *Michigan Mathematical Journal*, 13(4):459–469, 1966.

[40] François-Pierre Paty and Marco Cuturi. Subspace robust Wasserstein distances. In *International Conference on Machine Learning*, 2019.

[41] Xavier Pennec, Pierre Fillard, and Nicholas Ayache. A Riemannian framework for tensor computing. *International Journal of computer vision*, 66(1):41–66, 2006.

[42] G. Peyré and M. Cuturi. Computational optimal transport. *Foundations and Trends in Machine Learning*, 11(5-6):355–607, 2019.

[43] Julien Rabin, Gabriel Peyré, Julie Delon, and Marc Bernot. Wasserstein barycenter and its application to texture mixing. In *International Conference on Scale Space and Variational Methods in Computer Vision*, 2011.

[44] Justin Solomon, Fernando De Goes, Gabriel Peyré, Marco Cuturi, Adrian Butscher, Andy Nguyen, Tao Du, and Leonidas Guibas. Convolutional wasserstein distances: Efficient optimal transportation on geometric domains. *ACM Transactions on Graphics*, 34(4):1–11, 2015.

[45] Suvery Sra. A new metric on the manifold of kernel matrices with application to matrix geometric means. *Advances in Neural Information Processing Systems*, 2012.

[46] Suvery Sra. Positive definite matrices and the S-divergence. *Proceedings of the American Mathematical Society*, 144(7):2787–2797, 2016.

[47] Suvery Sra. Metrics induced by jensen-shannon and related divergences on positive definite matrices. *Linear Algebra and its Applications*, 616:125–138, 2021.

[48] Suvery Sra and Reshad Hosseini. Conic geometric optimization on the manifold of positive definite matrices. *SIAM Journal on Optimization*, 25(1):713–739, 2015.

[49] Yann Thanwerdas and Xavier Pennec. Is affine-invariance well defined on SPD matrices? a principled continuum of metrics. In *International Conference on Geometric Science of Information*, 2019.

[50] J. Townsend, N. Koep, and S. Weichwald. Pymanopt: A python toolbox for optimization on manifolds using automatic differentiation. *Journal of Machine Learning Research*, 17(137):1–5, 2016.

[51] Koji Tsuda, Gunnar Rätsch, and Manfred K. Warmuth. Matrix exponentiated gradient updates for on-line learning and Bregman projection. *Journal of Machine Learning Research*, 6(34):995–1018, 2005.

[52] Jesse van Oostrum. Bures-Wasserstein geometry. *arXiv:2001.08056*, 2020.

[53] Pourya Zadeh, Reshad Hosseini, and Suvery Sra. Geometric mean metric learning. In *International Conference on Machine Learning*, 2016.

[54] Hongyi Zhang and Suvery Sra. First-order methods for geodesically convex optimization. In *Conference on Learning Theory*, 2016.