On Procrustes Analysis in Hyperbolic Space

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Abstract—Congruent Procrustes analysis aims to find the best matching between two point sets through rotation, reflection and translation. We formulate the Procrustes problem for hyperbolic spaces, review the canonical definition of the center of point sets, and give a closed form solution for the optimal isometry for noise-free measurements. We also analyze the performance of the proposed method under measurement noise.

Index Terms—Hyperbolic geometry, Procrustes Analysis

I. INTRODUCTION

In Greek mythology, Procrustes was a robber who lived in Attica and deformed his victims to match the size of his bed. In 1962, Hurley and Catell used the story of Procrustes to describe a point set matching problem in Euclidean spaces [9], stated below.

Problem 1. Let \( \{z_n\}_{n=1}^N \) and \( \{z'_n\}_{n=1}^N \) be two point sets in \( \mathbb{R}^d \). The Procrustes problem asks to find a map \( \hat{T} \) that minimizes the sum of the mismatch norms, i.e.,

\[
\hat{T} = \arg \min_{T \in \mathcal{T}} \sum_{n=1}^N \|z_n - T(z'_n)\|_2^2,
\]

where \( \mathcal{T} \) is the set of rotation, reflection, translation, and uniform scaling maps and their compositions [9].

In computer vision, Procrustes analysis is of relevance in point cloud registration problems. The task of rigid registration is to find an isometry between two (or more) sets of points sampled from a 2 or 3 dimensional object. Point registration has applications in object recognition [13], medical imaging [6] and localization of mobile robotics [14]. In signal processing, Procrustes analysis often involved aligning shapes or point sets by a distance preserving bijection. Procrustes problems also naturally arise in distance geometry problems (DGPs) where one wants to find the location of a point set that best represents a given set of incomplete point distances, i.e.,

\[
z_1, \ldots, z_N \in \mathbb{R}^d : \|z_n - z_m\| = d_{mn}, \quad \forall (m, n) \in \mathcal{M}
\]

where \( \mathcal{M} \subseteq \{1, \ldots, N\}^2 \) and \( \{d_{mn} : (m, n) \in \mathcal{M}\} \) is the set of measured distances [10]. If a distance geometry problem has a solution, it is an orbit of the form

\[
O_Z = \left\{\{T(z_n)\}_{n=1}^N \mid \text{s.t. } T : \mathbb{R}^d \to \mathbb{R}^d \text{ is an isometry} \right\},
\]

where \( Z = \{z_n\}_{n=1}^N \) is a particular solution. In order to uniquely identify the correct solution from all the possible elements in the orbit \( O_Z \), we may be given the exact position of a subset of points, called anchors. We use Procrustes analysis to pick the correct solution by finding the best match between the anchors with their corresponding points in the orbit. This technique is commonly used in localization problems [4, 19].

Procrustes analysis can be performed in any metric space. In particular, hyperbolic Procrustes analysis is of great relevance due to the recent surge of interest in hyperbolic embeddings and machine learning [18, 13]. Furthermore, hyperbolic embeddings are closely connected to the study of hierarchical or tree-like data structures and hyperbolic Procrustes problem solutions may be used to align hierarchical data, e.g., ontologies [17, 5].

The goal of ontological studies is to find a (distance preserving) map between a fixed number of entities in two tree-like structures that are best aligned to each other (see Figure 1 for an illustration). For example, in ontology matching one aims to find correspondences between semantically related entities in heterogeneous ontologies with the goal of ontology merging, query response, or data translation [17].

In unsupervised matching problems, the first step in Procrustes-type analyses is to find the correspondence between two point clouds by using the iterative closest point algorithm [16]. Recently, Alvarez-Melis et al. cast the unsupervised hierarchy matching problem in hyperbolic space. Their proposed method jointly learns the “soft” correspondence and the alignment map characterized by a hyperbolic neural network.

In our work, we start with parametric isometries in the ‘Loid model of hyperbolic spaces. It is known that one can decompose any isometry into elementary isometries, e.g., hyperbolic translations and hyperbolic rotations (and reflections). In our setting, we aim to find a joint estimate for hyperbolic translation and rotation maps that best align two point sets.

To accomplish this task, we review the definition of the center of mass, or centroid, for a set of points in hyperbolic space. This enables us to subsequently “center” each set, and decouple the joint estimation problem into two steps: (1) translate the center of mass of each point set to the coordinate origin (of the Poincaré model), and (2) estimate the unknown rotation.

Fig. 1. Tree alignment in the Poincaré disk [21]. Hyperbolic Procrustes analysis aims to align two trees, depicted on the far left and far right figures. In steps (a) and (b) we center vertices in both trees, while in step (c) we estimate the unknown rotation map.
factor. While hyperbolic centering has been studied in the literature \([11]\), our Procrustes analysis framework is different from prior work in so far that it is similar to its Euclidean counterpart, and provides an optimal estimate for the unknown rotation factor, based on the weighted mean of pairwise inner products. Moreover, we prove a proof that our proposed method ensures the theoretically optimal isometry if the point sets match perfectly. We conclude the paper by giving numerical performance bounds for the task of matching noisy point sets.

Summary: Let \( \{x_n\}_{n \in [N]} \) and \( \{x_n'\}_{n \in [N]} \) be two sets of points in a hyperbolic space, related through an isometric map, i.e., \( x_n' = T(x_n) \), \( \forall n \in [N] \). Then,

\[
T = T_{m_o} \circ T_U \circ T_{-m_o}
\]

where \( m_o, m_n \in \mathbb{R}^d \) are the point sets’ centroids, \( T_b \) is the translation map by vector \( b \in \mathbb{R}^d \), and \( T_U \) is a rotation map by a unitary matrix \( U \in \mathbb{O}(d) \); see Section III-A. For noisy points, this isometry is suboptimal and can be fine-tuned via a gradient-based algorithm.

Notation. For \( N \in \mathbb{N} \), we let \( [N] = \{1, \ldots, N\} \). Depending on the context, \( x_1 \) can either be the first element of \( x \in \mathbb{R}^d \), or an indexed vector. We denote the set of orthogonal matrices as \( \mathbb{O}(d) = \{ R \in \mathbb{R}^{d \times d} \mid R^\top R = I \} \). For a function \( f \) and its inputs \( x_1, \ldots, x_N \), we write \( f(x) = \frac{1}{N} \sum_{n \in [N]} f(x_n) \). For a vector \( b \in \mathbb{R}^d \), we denote its \( \ell_2 \) norm as \( \|b\|_2 \).

II. 'LOID Model of Hyperbolic Space

Let \( x, x' \in \mathbb{R}^{d+1} \) with \( d \geq 1 \). The Lorentzian inner product between \( x \) and \( x' \) is defined as

\[
[x, x'] = x^\top H x' : H = \begin{pmatrix} -1 & 0^\top \\ 0 & I_d \end{pmatrix},
\]

where \( I_d \in \mathbb{R}^{d \times d} \) is the identity matrix. This is an indefinite inner product on \( \mathbb{R}^{d+1} \). The vector space \( \mathbb{R}^{d+1} \) equipped with the Lorentzian inner product is called a Lorentzian \( (d+1) \)-space. In a Lorentzian space, we can define notions similar to adjoint and unitary matrices in Euclidean spaces. The \( H \)-adjoint of the matrix \( R \), denoted by \( R^* \), is defined via

\[
[ R x, x' ] = [ x, R^* x' ], \quad \forall x, x' \in \mathbb{R}^{d+1},
\]

or simply as \( R^* = H^{-1} R^\top H \). An invertible matrix \( R \) is called \( H \)-unitary if \( R^* = R^{-1} \) [7].

The 'LOID model of \( d \)-dimensional hyperbolic space is a Riemannian manifold \( \mathbb{L}^d = (\mathbb{L}^d, (g_x)_x) \), where

\[
\mathbb{L}^d = \{ x \in \mathbb{R}^{d+1} \mid [x, x] = -1, x_1 > 0 \}
\]

and the Riemannian metric \( g_x : T_x \mathbb{L}^d \times T_x \mathbb{L}^d \to \mathbb{R} \) defined as \( g_x(u, v) = [u, v] \). The distance function in the 'LOID model is characterized by Lorentzian inner products as

\[
d(x, x') = \cosh(\langle [x, x'] \rangle), \quad \forall x, x' \in \mathbb{L}^d.
\]

A. Isometries

A map \( T : \mathbb{L}^d \to \mathbb{L}^d \) is an isometry if it is bijective and preserves distances, i.e. if

\[
d(x, x') = d(T(x), T(x')), \quad \forall x, x' \in \mathbb{L}^d.
\]

We can represent any hyperbolic isometry as a composition of two elementary maps that are parameterized by a \( d \)-dimensional vector and a \( d \times d \) unitary matrix, as described below.

Fact 1. \([13]\) The function \( T : \mathbb{L}^d \to \mathbb{L}^d \) is an isometry if and only if it can be written as \( T(x) = R_U R_b x \), where

\[
R_U = \begin{pmatrix} 1 & 0^\top \\ 0 & U \end{pmatrix}, \quad R_b = \begin{pmatrix} \sqrt{1 + \|b\|_2^2} & b^\top \\ b & (I + bb^\top)^{1/2} \end{pmatrix}
\]

for a unitary matrix \( U \in \mathbb{O}(d) \) and a vector \( b \in \mathbb{R}^d \).

Fact 2. \([15]\) For noisy points, this isometry is suboptimal and can be fine-tuned via a gradient-based algorithm.

III. Procrustes Analysis

Euclidean (orthogonal) Procrustes analysis proceeds through two steps:

- Centering: moving the center of mass of both points set to the origin of Cartesian coordinates, and
- Finding the optimal rotation/reflection.

We proceed to review (and visualize) the definition of the center projection and its inverse.

Fact 1. \([14]\) The function \( T : \mathbb{L}^d \to \mathbb{L}^d \) is an isometry if and only if it can be written as \( T(x) = R_U R_b x \), where

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Definition 1. \([14]\) The projection operator \( P : \mathbb{L}^d \to \mathbb{R}^d \) and its inverse \( Q \) are defined as

\[
P\left( \begin{pmatrix} \sqrt{1 + \|z\|_2^2} \\ z \end{pmatrix} \right) = z, \quad Q(z) = \begin{pmatrix} \sqrt{1 + \|z\|_2^2} \\ z \end{pmatrix}.
\]

For brevity, we define \( P(X) = [P(x_1), \ldots, P(x_N)] \) where \( X = [x_1, \ldots, x_N] \in (\mathbb{L}^d)^N \). Similarly, we consider this extension for \( Q \) as well.

In Section III-A, we review the hyperbolic centering process \([11]\). In other words, we find a map \( T_b \) to move the center of
The main purpose of centering is to map each point set to new locations, i.e., centered point sets. Lemma 1 gives a simple method to estimate their joint unitary transformation. Now, let us consider the following noisy case,

\[ x_n = R_b R_U R_{e_n} x_n', \forall n \in [N] \]

where \( \epsilon_n \in \mathbb{R}^d \) is a translation noise for the point \( x_n' \). Let \( z_n = R_{e_n} x_n' \). Then we have \( R_{-m_z} z_n = R_V R_{-m_z} z_n \). The centroid \( m_z \) is related to \( m_{x'} + \epsilon \) for a \( \epsilon \in \mathbb{R}^d \). This leads to

\[ R_{-m_z} x_n = R_{V'} R_{e_n'} R_{-m_z} x_n', \forall n \in [N], \]

where \( R_{e_n'} = R_{-m_z} R_{e_n} R_{-m_{x'}}, V' \in O(d) \). If the translation noise of each point is sufficiently small, then \( R_{V'} R_{e_n} \approx R_{V} \), for a \( V' \in O(d) \).

### A. Hyperbolic Centering

In Euclidean Centering analysis, we have two point sets \( z_1, \ldots, z_N \) and \( z'_1, \ldots, z'_N \) that are related via a composition of rotation, reflection, and translation maps, i.e.,

\[ z_n = U z'_n + b \]

where \( U \in O(d) \) and \( b \in \mathbb{R}^d \). We extract translation invariant features by moving their point mass to \( 0 \in \mathbb{R}^d \), i.e.,

\[ z_n - z_n' = U(z_n' - z_n') \]

The main purpose of centering is to map each point set to new locations, \( z_n - z_n' \) and \( z_n' - z_n' \) that are invariant with respect to the unknown translation \( b \). Subsequently, we can estimate the unknown unitary matrix \( U \), and then the translation according to \( b = z_n' - U z_n' \).

In hyperbolic Procrustes analysis, we have

\[ x_n = R_b R_U x_n', \forall n \in [N] \]

where \( U \in O(d) \) and \( b \in \mathbb{R}^d \). In a similar way, we pre-process a point set to extract (hyperbolic) translation invariant locations, i.e., centered point sets. Lemma 1 gives a simple method to center a projected point set.

#### Lemma 1

Let \( x_1, x_2, \ldots, x_N \in L^d \). Then, we have

\[ \mathbb{P}(R_{-m_z} x_n) = 0 \]

where \( m_z \triangleq \frac{1}{\sqrt{-1}} \mathbb{P}(x_n') \).

In Proposition 1 we show that \( T_{-m_z} \) is the canonical translation map for centering the point set \( X \in (L^d)^N \).

#### Proposition 1

Let \( x_1, \ldots, x_N \) and \( x'_1, \ldots, x'_N \) in \( L^d \) such that

\[ x_n = R_b R_U x'_n, \forall n \in [N] \]

for \( b \in \mathbb{R}^d \) and \( U \in O(d) \). Then, \( R_{-m_z} x_n = R_V R_{-m_z} x_n' \) where \( R_V \) is a hyperbolic rotation matrix.

#### Proof

From Lemma 1 we have

\[ R_{-m_z} x_n = \begin{bmatrix} a_1 \\ 0 \end{bmatrix}, R_{-m_z} x_n' = \begin{bmatrix} a_2 \\ 0 \end{bmatrix} \]

for \( a_1, a_2 \in \mathbb{R} \). On the other hand, we can rewrite eq. 1 in the following form

\[ R_{-m_z} x_n = R'R_{-m_z} x_n', \forall n \in [N] \]

where \( R' = R_{-m_z} R_b R_U R_{m_z} \). Since \( R' \) is an \( H \)-unitary matrix, we can decompose it as \( R' = R_c R_V \) for some \( c \in \mathbb{R}^d \) and \( V \in O(d) \). Therefore, we have

\[ \begin{bmatrix} a_1 \\ 0 \end{bmatrix} = R_c R_V \begin{bmatrix} a_2 \\ 0 \end{bmatrix} \]

This gives \( c = 0 \).

The map \( T_{-m_z} \) not only centers a set of points, but also rotates them. This phenomena is rooted in the noncommutative property of hyperbolic translation or gyration. More clearly, for any two vectors \( b_1, b_2 \in \mathbb{R}^d \), we have

\[ R_{b_1} R_{b_2} = R_{V'} R_{b_2} R_{b_1} \]

for a specific unitary matrix \( V \in O(d) \) that accounts for the gyration factor; see the example in Figure 3 and the follow-up discussion in Section IV. This does not interfere with our analysis since any such rotation is absorbed in \( U \), and we can estimate their joint unitary transformation.

Now, let us consider the following noisy case,

\[ x_n = R_b R_U R_{e_n} x_n', \forall n \in [N] \]

where \( \epsilon_n \in \mathbb{R}^d \) is a translation noise for the point \( x_n' \). Let \( z_n = R_{e_n} x_n' \). Then we have \( R_{-m_z} z_n = R_V R_{-m_z} z_n \). The centroid \( m_z \) is related to \( m_{x'} + \epsilon \) for a \( \epsilon \in \mathbb{R}^d \). This leads to

\[ R_{-m_z} x_n = R_{V'} R_{e_n'} R_{-m_z} x_n', \forall n \in [N], \]

where \( R_{e_n'} = R_{-m_z} R_{e_n} R_{-m_{x'}} \). If the translation noise of each point is sufficiently small, then \( R_{V'} R_{e_n} \approx R_{V} \), for a \( V' \in O(d) \).

### B. Hyperbolic Rotation & Reflection

To estimate the unknown hyperbolic rotation, we consider minimizing a weighted discrepancy between the centered point sets. More precisely,

\[ \tilde{U} = \arg \min_{V' \in O(d)} \sum_{n \in [N]} w_n f(d(R_{-m_z} x_n, R_{V'} R_{-m_z} x_n')) \]

Fig. 2. Geometric illustration of \( P, Q, \) and stereographic projection \( h \).

mass of projected point sets to \( 0 \in \mathbb{R}^d \), i.e., \( \mathbb{P}(T_b(x_n)) = 0 \). Then, we show how this centering method helps simplify the hyperbolic Procrustes problem to a sub-problem similar to the famous (Euclidean) orthogonal Procrustes problem.
where \(d(x, x') = \cosh(-\sigma^\top H x')\), \(\{w_n\}_{n \in [N]}\) are positive weights, and \(f() = \cosh()\) is a monotonic function.

**Proposition 2.** The optimal unitary matrix that solves \((5)\) equals \(\hat{U} = U_I U_0^\top\), where \(U_I U_0^\top\) is the singular value decomposition of \(P(R_m, x) W P(R_m, x')^\top\), and \(W = \text{diag}(w_1, \ldots, w_N)\).

**Proof.** We can simplify \((5)\) as follows:

\[
\hat{U} = \arg \max_{V \in \mathbb{O}(d)} \sum_{n \in [N]} \text{Tr} R_{m, x} x'_n w_n (R_{m, x} x'_n)^\top H R_V.
\]

From Fact 1, we know that \(R_V\) is only parameterized on its lower right block. The proof then follows from representing the sum in matrix form and invoking von Neumann’s trace inequality \([12]\).

**IV. Möbius Addition**

In the Poincaré model \((\mathbb{H}^d)\), the points reside in the \(d\)-dimensional Euclidean ball. The isometry between the 'Loid model and the Poincaré model \(h : \mathbb{L}^d \to \mathbb{H}^d\) is called the **stereographic projection** \([2]\). The distance between \(y, y' \in \mathbb{H}^d\) is given by \(d(y, y') = 2 \tan^{-1}((\|y - y'\|)/\|y\|))\) where \(\odot\) is Möbius addition — a noncommutative and nonassociative operator. **Gyration** measures the “deviation” of Möbius addition from commutativity, i.e., \(\text{gyr}(y, y') (y' \odot y) = y \odot y'\) \([20]\).

**Fact 3.** The maps \(h \circ R_U \circ h^{-1}\) and \(h \odot T_U \circ h^{-1}\) are isometries in the Poincaré model, and they can be written as

\[
h \circ T_U \circ h^{-1}(y) = U y, \quad h \odot T_b \circ h^{-1}(y) = b' \odot y
\]

where \(b' = h \odot Q(b), T_b \text{ and } T_U \text{ are defined in (2) and (3)}.\)

The translation isometry is a direct result of the Gyrotranslation theorem equality,

\[-(c \odot y) \odot c \odot y' = \text{gyr}[c, y] (-y \odot y'),\]

where \(c \in \mathbb{H}^d\) \([20]\). Therefore, left Möbius addition preserves the distances of point sets in the Poincaré model by (1) centering each point set, i.e., subtracting their center of mass from the left hand side of the Möbius addition, and (2) estimating the remaining rotation factor — a composition of gyrations and the initial unknown rotation between the two point sets.

**V. Numerical Analysis**

Let \(x_n = R^* R_{\epsilon_n} x'_n, \forall n \in [N]\) where \(R^*\) is an \(H\)-unitary matrix and \(\epsilon_1, \ldots, \epsilon_N\) is the set of translation noise samples.

We compute the following \(H\)-unitary operators to match the point sets \(X, X'\):

- **\(R_P\):** The matrix estimated by our proposed method;
- **\(R_{GD}\):** Let \(e(X, X) \triangleq \frac{1}{N^2} \sum_{n \in [N]} d(x_n, \tau_n)\) be the normalized discrepancy between \(X\) and \(\hat{X}\). The matrix \(R_{GD}\) is computed by an iterative gradient descent method: We initialize \(R_{GD} = I_{d \times d}\) and iterate the following steps:
  1. \(\hat{b} = -\alpha \frac{\partial}{\partial \hat{b}} e(X, R_{GD} X') \big|_{b = 0}\) for a small \(\alpha > 0\);
  2. \(\hat{U} = \arg \max_{U \in \mathbb{O}(d)} \sum_{n \in [N]} |x_n, R_U R_{GD} x'_n|\);
  3. Update \(R_{GD} \leftarrow R_U R_{GD};\)

**VI. Conclusion**

Inspired by its Euclidean counterpart, we introduced the Procrustes problem in hyperbolic spaces. We reviewed the (indefinite) Lorentzian inner product, and described how \(H\)-unitary matrices represent isometries in the 'Loid model of hyperbolic spaces. Using the parameterized decomposition of hyperbolic isometries in terms of hyperbolic rotation and translation, we showed that moving the center of mass to the origin gives point sets that are invariant to hyperbolic translation (for the case of no measurement noise). We then used the centered point sets to estimate the unknown rotation factor.

**VII. Acknowledgment**

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\footnote{Möbius gyrations hence keep the norm that they inherit from \(\mathbb{R}^d\) invariant, i.e., \(\|\text{gyr}(c, y)(-y \odot y')\| = \|-y \odot y'\|\) \([20]\).}
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