Computing Hulls In Positive Definite Space*

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1 Introduction

There are many application areas where the basic objects of interest, rather than points in Euclidean space, are symmetric positive-definite $n \times n$ matrices (denoted by $\mathsf{P}(n)$). In diffusion tensor imaging [3], matrices in $\mathsf{P}(3)$ model the flow of water at each voxel of a brain scan. In mechanical engineering [7], stress tensors are modeled as elements of $\mathsf{P}(6)$. Kernel matrices in machine learning are elements of $\mathsf{P}(n)$ [12].

In these areas, a problem of great interest is the analysis [8, 9] of collections of such matrices (finding central points, clustering, doing regression). Since the geometry of $\mathsf{P}(n)$ is non-Euclidean, it is difficult to apply standard computational geometry tools.

The convex hull is fundamental to computational geometry. It can be used to manage the geometry of $\mathsf{P}(n)$, to find a center of a point set (via *convex hull peeling depth* [11, 2]), and capture extent properties of data sets like diameter, width, and bounding boxes (even in its approximate form [1]).

We introduce a generalization of the convex hull that can be computed (approximately) efficiently in $\mathsf{P}(2)$, is identical to the convex hull in Euclidean space, and always contains the convex hull in $\mathsf{P}(n)$. In the process, we also develop a generalized notion of *extent* [1] that might be of independent interest.

Convex Hulls in $\mathsf{P}(n)$. $\mathsf{P}(n)$ is an example of a proper $\mathrm{CAT}(0)$ space [6, II.10], and as such admits a well-defined notion of convexity, in which metric balls are convex. We can define the convex hull of a set of points as the smallest convex set that contains the points. This hull can be realized as the limit of an iterative procedure where we draw all geodesics between data points, add all the new points to the set, and repeat.

Lemma 1.1 ([5]). *If $X_0 = X$ and $X_{i+1} = \bigcup_{a,b \in X_i} [a, b]$, then $\mathcal{C}(X) = \bigcup_{i=0}^{\infty} X_i$.*

Berger [4] notes that it is unknown whether the convex hull of three points is in general closed, and the standing conjecture is that it is not. The above lemma bears this out, as it is an infinite union of closed sets, which in general is not closed. These facts present a significant barrier to the computation of convex hulls on general manifolds.

The *ball hull* of a set of points is the intersection of all (closed) metric balls containing the set. The ball hull has the advantage of being convex and closed. We provide an algorithm that computes an approximate ball hull.

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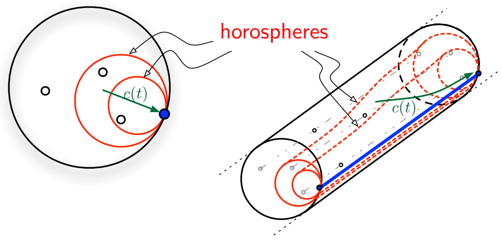


Figure 1: Left: projection of $X \subset \mathsf{P}(2)$ onto $\det(x) = 1$. Right: $X \subset \mathsf{P}(2)$. Two horospheres are drawn in both views.

2 Definitions

$\mathsf{P}(n)$ is the set of symmetric positive-definite real matrices. It is a Riemannian metric space with tangent space at point p equal to $\mathsf{S}(n)$, the vector space of symmetric matrices with inner product $\langle A, B \rangle_p = \mathrm{tr}(p^{-1}Ap^{-1}B)$. The exp map, $\exp_p : \mathsf{S}(n) \to \mathsf{P}(n)$ is defined $\exp_p(tA) = c(t) = p^{\frac{1}{2}} e^{p^{-\frac{1}{2}} tAp^{-\frac{1}{2}}} p^{\frac{1}{2}}$, where $c(t)$ is the geodesic with unit tangent A and $c(0) = p$. For simplicity, we often assume that $p = I$ so $\exp_I(tA) = e^{tA}$. The log map, $\log_p : \mathsf{P}(n) \to \mathsf{S}(n)$, indicates direction and distance and is the inverse of $\exp_p$. The metric $d(p, q) = \|\log_p(q)\| = \sqrt{\mathrm{tr}(\log(p^{-1}q)^2)}$.

Given a geodesic ray $c(t) : \mathbb{R}^+ \to \mathsf{P}(n)$, a *Busemann function* $b_c : \mathsf{P}(n) \to \mathbb{R}$ is defined

$$b_c(p) = \lim_{t \to \infty} d(p, c(t)) - t.$$

A Busemann function is an example of a *horofunction* (see [6, II.8]). A *horoball* $B_r(h) \subset \mathsf{P}(n)$ is a sublevel set of a horofunction h, i.e. $B_r(h) = h^{-1}((-\infty, r])$. By [6, II.8], h is convex, so any sublevel set $B_r(h)$ is convex. A *horosphere* $S_r(h)$ is its boundary; i.e. $S_r(h) = h^{-1}(r)$. See Figure 1.

The *geodesic anisotropy* [10] of a point $p \in \mathsf{P}(n)$ measures disparity in its eigenvalues, and will be useful in our analysis. It is defined as $\mathrm{GA}(p) = d(\sqrt[n]{\det(p)} I, p) = \mathrm{tr}(\log(p/\sqrt[n]{\det(p)})^2)^{\frac{1}{2}}$.

Busemann functions in $\mathbb{R}^n$. As an illustration, we can easily compute the Busemann function in Euclidean space associated with a geodesic ray $c(t) = t\mathbf{u}$, where $\mathbf{u}$ is a unit vector. Since $\lim_{t \to \infty} \frac{1}{2t}(\|p - t\mathbf{u}\| + t) = 1$, $b_c(p) = \lim_{t \to \infty} \frac{1}{2t}(\|p - t\mathbf{u}\|^2 - t^2)$ and

$$b_c(p) = \lim_{t \to \infty} \frac{\|p\|^2}{2t} - \langle p, \mathbf{u} \rangle = - \langle p, \mathbf{u} \rangle .$$

Horospheres in Euclidean space are then just hyperplanes, and horoballs are halfspaces.

Busemann Functions in P(n) For geodesic $c(t) = e^{tA}$, where $A \in \mathrm{S}(n)$, the Busemann function $b_c : \mathrm{P}(n) \to \mathbb{R}$ is

$$b_c(p) = -\operatorname{tr}(A \log(\pi_c(p))),$$

where π_c is defined below [6, II.10].

There is a subgroup of $\mathrm{GL}(n)$, N_c (the *horospherical group*), that leaves the Busemann function b_c invariant [6, II.10]. That is, given $p \in \mathrm{P}(n)$, and $\nu \in N_c$, $b_c(\nu p \nu^T) = b_c(p)$. Let A be diagonal, where $A_{ii} > A_{jj}, \forall i \neq j$. Let $c(t) = e^{tA}$. Then $\nu \in N_c$ if and only if ν is a upper-triangular matrix with ones on the diagonal[1]. If $A \in S(n)$ is not sorted-diagonal, we may still use this characterization of N_c without loss of generality, since we may compute an appropriate diagonalization $A = QA'Q^T$, $QQ^T = I$, then apply the isometry $Q^T p Q$ to any element $p \in \mathrm{P}(n)$.

Let $A \in \mathrm{S}(n)$ and $c(t) = e^{tA}$ as above. If we consider all elements $f \in \mathrm{P}(n)$ that share eigenvectors Q with e^A, then $fe^A = e^A f$, and we call this space F_c, the *n-flat* containing c. If A is diagonal, $f \in F_c$ is diagonal, where the diagonal elements are positive [6, II.10]. Since we may assume that $Q \in \mathrm{SO}(n)$, every flat F_c corresponds to an element of $\mathrm{SO}(n)$. Moreover, since members of F_c commute, $\sqrt{\operatorname{tr}(\log(u^{-1}v)^2)} = \sqrt{\operatorname{tr}((\log(v) - \log(u))^2)}$ for all $u, v \in F_c$ so F_c is isometric to $\mathbb{R}^n$ with the Euclidean metric.

Given $p \in \mathrm{P}(n)$, there is a unique decomposition $p = \nu f \nu^T$ where $(\nu, f) \in N_c \times F_c$ [6, II.10]. Let $p \in \mathrm{P}(n)$ and $(\nu, f) \in N_c \times F_c$. If $p = \nu f \nu^T$, then define the *horospherical projection function* $\pi_c : \mathrm{P}(n) \to \mathrm{P}(n)$ as $\pi_c(p) = \nu^{-1} p \nu^{-T} = f$.

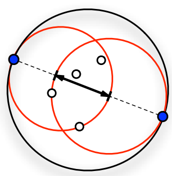
3 Ball Hulls

For a subset $X \subset \mathrm{P}(n)$, the *ball hull* $\mathcal{B}(X)$ is the intersection of all horoballs that also contain X:

$$\mathcal{B}(X) = \bigcap_{b_c, r} B_r(b_c), \; X \subset B_r(b_c).$$

We know that any horoball is convex. Because the ball hull is the intersection of convex sets, it is itself convex (and therefore $\mathcal{C}(X) \subseteq \mathcal{B}(X)$).

Since measuring width by recording the distance between two parallel planes does not have a direct analogue in $\mathrm{P}(n)$, we propose the use of *horoextents*. Let $c(t) = e^{tA}$ be a geodesic ray, and $X \subset \mathrm{P}(n)$. The *horoextent* $E_c(X)$ with respect to c is defined as:



horoextent

$$E_c(X) = \left| \max_{x \in X} b_c(x) + \max_{x \in X} b_{-c}(x) \right|$$

where $-c$ is understood to mean $e^{t(-A)}$ (the ray pointing opposite c)[2]. Observe that for any c, $E_c(X) = E_c(\mathcal{C}(X)) = E_c(\mathcal{B}(X))$.

[1] For simplicity, we consider only those rays with unique diagonal entries, but this definition may be extended to those with multiplicity.

[2] While $-A$ and A share eigenvectors, the eigenvalues of $-A$ will be sorted opposite to those of A, so the projections π_c and π_{-c} will be different.

4 Algorithm for ε-Ball Hull

An intersection of horoballs is called a *ε-ball hull* ($\mathcal{B}_\varepsilon(X)$) if for all geodesic rays c, $|E_c(\mathcal{B}_\varepsilon(X)) - E_c(X)| \leq \varepsilon$.

Lemma 4.1. *For any horosphere $S_r(b_c)$, there is a hyperplane $H_r \subset \log(F_c) \subset S(n)$ such that $\log(\pi_c(S_r(b_c))) = H_r$.*

Lemma 4.2 (Lipschitz condition on P(2))**.** *Given a point $p \in P(2)$, a rotation matrix Q corresponding to an angle of $\theta/2$, geodesics $c(t) = e^{tA}$ and $c'(t) = e^{tQAQ^T}$,*

$$b_c(p) - b_{c'}(p) \leq |\theta| \cdot 2\sqrt{2} \sinh\left(\mathrm{GA}(p)/\sqrt{2}\right).$$

Algorithm. For $X \subset \mathrm{P}(2)$ we can construct $\mathcal{B}_\varepsilon(X)$ as follows. Let $g_X = \max_{p \in X} \mathrm{GA}(p)$. We place a grid G_ε on $\mathrm{SO}(2)$ so that for any $\theta' \in \mathrm{SO}(2)$, there is another $\theta \in G_\varepsilon$ such that $|\theta - \theta'| \leq (\varepsilon/2)/(2\sqrt{2}\sinh(g_X/\sqrt{2}))$. For each c corresponding to $\theta \in G_\varepsilon$, we consider $\pi_c(X)$, the projection of X into the 2-flat F_c. Within F_c, we construct a convex hull of $\pi_c(X)$, and return the horoball associated with each hyperplane passing through each facet of the convex hull, as in Lemma 4.1. Since between elements of G_ε, the points of $\pi_c(X)$ do not change the values of their horofunctions by more than $\varepsilon/2$ (by Lemma 4.2), the extents do not change by more than ε, and the returned set of horoballs is a $\mathcal{B}_\varepsilon(X)$.

Theorem 4.1. *For a set $X \subset P(2)$ of size N, we can construct an $\mathcal{B}_\varepsilon(X)$ of size $O((\sinh(g_X)/\varepsilon)N)$ in time $O((\sinh(g_X)/\varepsilon)N \log N)$.*

This can be improved by using an ε-kernel [1] on $\pi_c(X)$.

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