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 $P(n)$). In diffusion tensor imaging [3], matrices in $P(3)$ model the flow of water at each voxel of a brain scan. In mechanical engineering [7], stress tensors are modeled as elements of $P(6)$. Kernel matrices in machine learning are elements of $P(n)$ [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 $P(n)$ 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 $P(n)$, 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 $P(2)$, identical to the convex hull in Euclidean space, and always contains the convex hull in $P(n)$. In the process, we also develop a generalized notion of extent [1] that might be of independent interest.

Convex Hulls in $P(n)$. $P(n)$ is an example of a proper 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 the new points to the convex hull of the current set, and repeat.

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

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

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*This research was supported in part by NSF grants 0937060 (sub-award CIF-32) and SGER-0841185.
Busemann Functions in $P(n)$ For geodesic $c(t) = e^{tA}$, where $A \in S(n)$, the Busemann function $b_c : P(n) \to \mathbb{R}$ is

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

where $\pi_c$ is defined below [6, II.10].

There is a subgroup of $\text{GL}(n)$, $N_c$ (the horospherical group), that leaves the Busemann function $b_c$ invariant [6, II.10]. That is, given $p \in P(n)$, and $\nu \in N_c$, $b_c(\nu p\nu^T) = b_c(p)$. Let $A$ be diagonal, then $A_i > A_j$, $\forall i \neq j$. Let $c(t) = e^{tA}$. Then $\nu \in N_c$ if and only if $\nu$ is an upper-triangular matrix with ones on the diagonal.

For all elements $\pi_c$ of $SO(n)$, it is understood to mean $e^{\nu \pi_c f}$ (the ray pointing opposite $c^2$). Observe that for any $c$, $E_c(x) = E_c(\pi_c(x)) = E_c(\pi_c(B(X)))$.

The horofunction $E_c(X)$ with respect to $c$ is defined as:

$$E_c(X) = \max_{x \in X} b_c(x) = \max_{x \in X} b_{-c}(x),$$

where $-c$ is understood to mean $e^{c(-A)}$ (the ray pointing opposite $c$).

## 4 Algorithm for $\varepsilon$-Ball Hull

An intersection of horoballs is called a $\varepsilon$-ball hull ($B_\varepsilon(X)$) if for all geodesic rays $c$, $|E_c(B_\varepsilon(X)) - E_c(X)| \leq \varepsilon$. Let $b_c(p) = b_{-c}(p) \leq |\varepsilon| \cdot 2\sqrt{2} \sinh \left( \frac{\text{GA}(p)}{\sqrt{2}} \right).

### Lemma 4.1

For any horosphere $S_c(b_c)$, there is a hyperplane $H_c \subset \log(F_c) \subset S(n)$ such that $\log(\pi_c(S_c(b_c))) = H_c$.

### Lemma 4.2

(Lipschitz condition on $P(2)$). Given a point $p \in P(2)$, a rotation matrix $Q \in SO(n)$ corresponding to an angle of $\theta/2$, geodesics $c(t) = e^{tA}$ and $c(t) = e^{t\sqrt{Q}AQ^T}$,

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

**Algorithm.** For $X \subset P(2)$ we can construct $B_\varepsilon(X)$ as follows. Let $g_X = \max_{p \in X} \text{GA}(p)$. We place a grid $G_x$ on $SO(2)$ so that for any $\theta \in SO(2)$, there is another $\theta \in G_x$ such that $|\theta - \theta| \leq (\varepsilon/2) \cdot (2\sqrt{2} \sinh(g_X/\sqrt{2}))$. For each $c$ corresponding to $\theta \in G_x$, 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 $G_x$, 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 $\varepsilon$, and the returned set of horoballs is a $B_\varepsilon(X)$.

**Theorem 4.1.** For a set $X \subset P(2)$ of size $N$, we can construct an $\varepsilon$-ball hull 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 $\varepsilon$-kernel [1] on $\pi_c(X)$.

### References


