Classification with mixtures of curved Mahalanobis metrics

— or LMNN in Cayley-Klein geometries —

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Mahalanobis distances

- For $Q \succ 0$, a symmetric positive definite matrix like a covariance matrix, define **Mahalanobis distance**:

$$\boxed{D_Q(p,q) = \sqrt{(p-q)^\top Q(p-q)}}$$

  Metric distance (indiscernibles/symmetry/triangle inequality)
  Eg., $Q =$ *precision matrix* Σ^{-1}, where $\Sigma =$ *covariance matrix*

- Generalize Euclidean distance when $Q = I$: $D_I(p,q) = \|p-q\|$

- Mahalanobis distance interpreted as Euclidean distance after *Cholesky decomposition* $Q = L^\top L$ and **affine transformation** $x' \leftarrow L^\top x$:

$$\boxed{D_Q(p,q) = D_I(L^\top p, L^\top q) = \|p' - q'\|}$$

Generalizing Mahalanobis distances with Cayley-Klein projective geometries + Learning in Cayley-Klein spaces

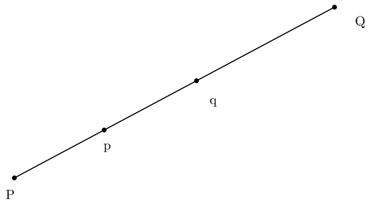
Cayley-Klein geometry: Projective geometry [7, 3]

- $\mathbb{RP}^d$: $(\lambda x, \lambda) \sim (x, 1)$
  homogeneous coordinates $x \mapsto \tilde{x} = (x, w = 1)$, and dehomogeneization by "perspective division" $\tilde{x} \mapsto \frac{x}{w}$

- **cross-ratio** measure is *invariant* by projectivity/homography/collineation:

$$(p, q; P, Q) = \frac{(p - P)(q - Q)}{(p - Q)(q - P)}$$

  where p, q, P, Q are collinear



Definition of Cayley-Klein geometries

A Cayley-Klein geometry is $\mathcal{K} = (\mathcal{F}, c_{\mathrm{dist}}, c_{\mathrm{angle}})$:

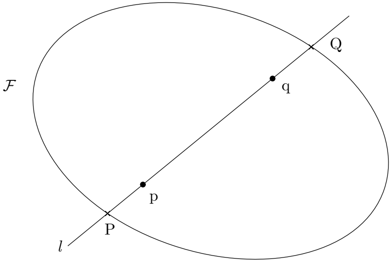
1. A fundamental conic: $\mathcal{F}$
2. A constant unit $c_{\mathrm{dist}} \in \mathbb{C}$ for measuring distances
3. A constant unit $c_{\mathrm{angle}} \in \mathbb{C}$ for measuring angles

See monograph [7]

Distance in Cayley-Klein geometries

$$\boxed{\mathrm{dist}(p, q) = c_{\mathrm{dist}} \ \mathrm{Log}((p, q; P, Q))}$$

where P and Q are intersection points of line $l = (pq)$ ($\tilde{l} = \tilde{p} \times \tilde{q}$ in 2D) with the conic.
Log is principal complex logarithm (modulo $2\pi i$)



Key properties of Cayley-Klein distances

- $\mathrm{dist}(p, p) = 0$ (law of indiscernibles)
- **Signed** distances : $\mathrm{dist}(p, q) = -\mathrm{dist}(q, p)$
- When p, q, r are collinear

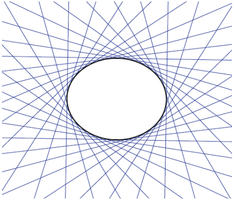
$$\boxed{\mathrm{dist}(p, q) = \mathrm{dist}(p, r) + \mathrm{dist}(r, q)}$$

Geodesics in Cayley-Klein geometries are **straight lines** (eventually clipped within the conic domain)

Logarithm is transferring *multiplicative properties* of the cross-ratio to *additive properties* of Cayley-Klein distances.
When p, q, P, Q are collinear:
$(p, q; P, Q) = (p, r; P, Q) \cdot (r, q; P, Q)$

Dual conics

In projective geometry, *points* and *lines* are dual concepts



Dual parameterizations of the fundamental conic $\mathcal{F} = (A, A^{\Delta})$
Quadratic form $Q_A(x) = \tilde{x}^{\top} A \tilde{x}$

- primal conic = set of border points: $\mathcal{C}_A = \{\tilde{p} \ : \ Q_A(\tilde{p}) = 0\}$

- dual conic = set of tangent hyperplanes:
  $\mathcal{C}_A^* = \{\tilde{l} \ : \ Q_{A^{\Delta}}(\tilde{l}) = 0\}$

$A^{\Delta} = A^{-1}|A|$ is the **adjoint matrix**
Adjoint can be computed even when A is not invertible ($|A| = 0$)

Taxonomy

Signature of matrix = sign of eigenvalues of its eigen decomposition

Type	A	A^{Δ}	Conic
Elliptic	$(+,+,+)$	$(+,+,+)$	non-degenerate complex conic
Hyperbolic	$(+,+,-)$	$(+,+,-)$	non-degenerate real conic
Dual Euclidean	$(+,+,0)$	$(+,+,0)$	Two complex lines with a real intersection point
Dual Pseudo-euclidean	$(+,-,0)$	$(+,0,0)$	Two real lines with a double real intersection point Deux
Euclidean	$(+,0,0)$	$(+,+,0)$	Two complex points with a double real line passing through
Pseudo-euclidean	$(+,0,0)$	$(+,-,0)$	Two complex points with a double real line passing through
Galilean	$(+,0,0)$	$(+,0,0)$	Double real line with a real intersection point

Degenerate cases are obtained as limit of non-degenerate cases.

Measurements can be elliptic, hyperbolic or parabolic (degenerate case).

Real CK distances without cross-ratio expressions

For **real** Cayley-Klein measures, we choose the constants:

- Constants (κ is curvature):
  - Elliptic ($\kappa > 0$): $c_{\mathrm{dist}} = \frac{\kappa}{2i}$
  - Hyperbolic ($\kappa < 0$): $c_{\mathrm{dist}} = -\frac{\kappa}{2}$
- Bilinear form $S_{pq} = (p^\top, 1)^\top S(q, 1) = \tilde{p}^\top S \tilde{q}$
- Get rid of *cross-ratio* using:

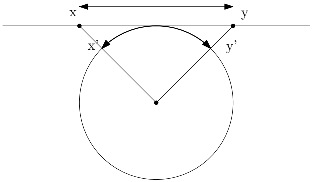
$$(p, q; P, Q) = \frac{S_{pq} + \sqrt{S_{pq}^2 - S_{pp}S_{qq}}}{S_{pq} - \sqrt{S_{pq}^2 - S_{pp}S_{qq}}}$$

Elliptic Cayley-Klein metric distance

$$d_E(p,q) = \frac{\kappa}{2i}\ \mathrm{Log}\left(\frac{S_{pq} + \sqrt{S_{pq}^2 - S_{pp}S_{qq}}}{S_{pq} - \sqrt{S_{pq}^2 - S_{pp}S_{qq}}}\right)$$

$$\boxed{d_E(p,q) = \kappa\ \arccos\left(\frac{S_{pq}}{\sqrt{S_{pp}S_{qq}}}\right)}$$

Notice that $d_E(p,q) < \kappa\pi$, domain $\mathbb{D}_S = \mathbb{R}^d$ in elliptic case.



Gnomonic projection $d_E(x,y) = \kappa \cdot \arccos\left(\langle x', y' \rangle\right)$

Hyperbolic Cayley-Klein distance

When $p, q \in \mathbb{D}_S := \{p : S_{pp} < 0\}$, the hyperbolic domain:

$$d_H(p,q) = -\frac{\kappa}{2}\log\left(\frac{S_{pq} + \sqrt{S_{pq}^2 - S_{pp}S_{qq}}}{S_{pq} - \sqrt{S_{pq}^2 - S_{pp}S_{qq}}}\right)$$

$$d_H(p,q) = -\kappa \, \mathrm{arctanh}\left(\sqrt{1 - \frac{S_{pp}S_{qq}}{S_{pq}^2}}\right)$$

$$\boxed{d_H(p,q) = -\kappa \, \mathrm{arccosh}\left(\frac{S_{pq}}{\sqrt{S_{pp}S_{qq}}}\right)}$$

with $\mathrm{arccosh}(x) = \log(x + \sqrt{x^2 - 1})$ and $\mathrm{arctanh}(x) = \frac{1}{2}\log\frac{1+x}{1-x}$.
Curvature $\kappa < 0$

Decomposition of the bilinear form [1]

Write $S = \begin{bmatrix} \Sigma & a \\ a^\top & b \end{bmatrix} = S_{\Sigma,a,b}$ with $\Sigma \succ 0$.

$$S_{p,q} = \tilde{p}^\top S \tilde{q} = p^\top \Sigma q + p^\top a + a^\top q + b$$

Let $\mu = -\Sigma^{-1} a \in \mathbb{R}^d$ ($a = -\Sigma\mu$) and $b = \mu^\top \Sigma \mu + \mathrm{sign}(\kappa)\frac{1}{\kappa^2}$

$$\kappa = \begin{cases} (b - \mu^\top \mu)^{-\frac{1}{2}} & b > \mu^\top \mu \\ -(\mu^\top \mu - b)^{-\frac{1}{2}} & b < \mu^\top \mu \end{cases}$$

Then the bilinear form writes as:

$$\boxed{S(p,q) = S_{\Sigma,\mu,\kappa}(p,q) = (p-\mu)^\top \Sigma (q-\mu) + \mathrm{sign}(\kappa)\frac{1}{\kappa^2}}$$

Curved Mahalanobis metric distances

We have [1]:

$$\boxed{\lim_{\kappa \to 0^+} D_{\Sigma,\mu,\kappa}(p,q) = \lim_{\kappa \to 0^-} D_{\Sigma,\mu,\kappa}(p,q) = D_\Sigma(p,q)}$$

Mahalanobis distance $D_\Sigma(p,q) = D_{\Sigma,0,0}(p,q)$

Thus hyperbolic/elliptic Cayley-Klein distances can be interpreted as **curved Mahalanobis distances**, or κ-Mahalanobis distances

When $S = \mathrm{diag}(1,1,...,1,-1)$, we recover the canonical hyperbolic distance [5] in Cayley-Klein model:

$$D_h(p,q) = \mathrm{arccosh}\left(\frac{1-\langle p,q\rangle}{\sqrt{1-\langle p,p\rangle}\sqrt{1-\langle q,q\rangle}}\right)$$

defined inside the interior of a unit ball.

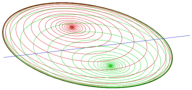
Cayley-Klein bisectors are affine

Bisector $\mathrm{Bi}(p, q)$:

$$\mathrm{Bi}(p,q) = \{x \in \mathbb{D}_S \ :\ \mathrm{dist}_S(p,x) = \mathrm{dist}_S(x,q)\}$$
$$\frac{S(p,x)}{\sqrt{S(p,p)}} = \frac{S(q,x)}{\sqrt{S(q,q)}}$$

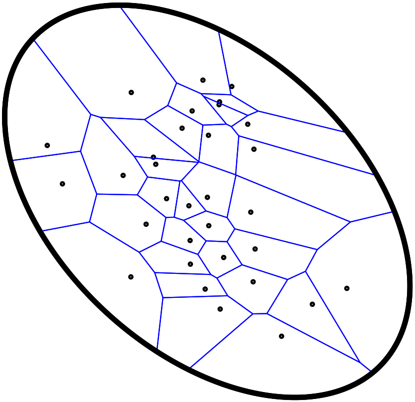
arccos and arccosh are monotonically increasing functions.

$$\left\langle x, \sqrt{|S(p,p)|}\Sigma q - \sqrt{|S(q,q)|}\Sigma p \right\rangle + \sqrt{|S(p,p)|}(a^\top(q+x)+b) - \sqrt{|S(q,q)|}(a^\top(p+x)+b) = 0$$



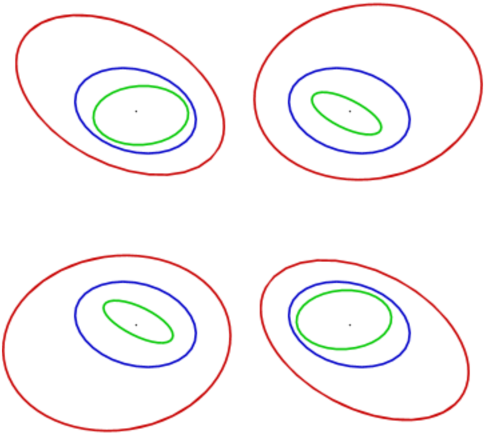
Hyperplanes (restricted to the domain)

Cayley-Klein Voronoi diagrams are affine



Can be computed from equivalent (clipped) power diagrams [2, 5]
https://www.youtube.com/watch?v=YHJLq3-RL58

Cayley-Klein balls



Blue: Mahalanobis Red: elliptic Green: Hyperbolic

Cayley-Klein balls have Mahalanobis ball shapes with displaced centers

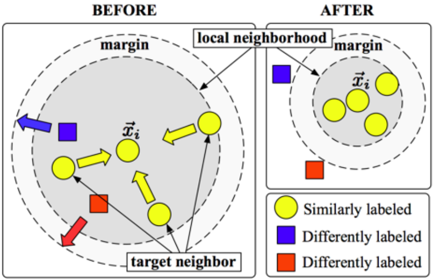
Learning curved Mahalanobis metrics

Large Margin Nearest Neighbors [8], LMNN

Learn Mahalanobis distance $M = L^\top L \succ 0$ for a given input data-set $\mathcal{P}$

- Distance of each point to its *target neighbors* shrink, $\epsilon_{\text{pull}}(L)$
$$\mathcal{S} = \{(x_i, x_j) \ : \ y_i = y_j \text{ and } x_j \in N(x_j)\}$$

- Keep a distance margin of each point to its *impostors*, $\epsilon_{\text{push}}(L)$
$$\mathcal{R} = \{(x_i, x_j, x_l) \ : \ (x_i, x_j) \in \mathcal{S} \text{ and } y_i \neq y_l\}$$



http://www.cs.cornell.edu/~kilian/code/lmnn/lmnn.html

LMNN: Cost function and optimization

Objective cost function [8]: convex and piecewise linear (SDP)

$$
\begin{aligned}
\epsilon_{\text{pull}}(L) &= \Sigma_{i,i\to j}\|L(x_i - x_j)\|^2, \\
\epsilon_{\text{push}}(L) &= \Sigma_{i,i\to j}\Sigma_j(1-y_{il})\left[1 + \|L(x_i - x_j)\|^2 - \|L(x_i - x_l)\|^2\right]_+, \\
\epsilon(L) &= (1-\mu)\epsilon_{\text{pull}}(L) + \mu\epsilon_{\text{push}}(L)
\end{aligned}
$$

$i \to j$: x_j is a target neighbor of x_i
$y_{il} = 1$ iff x_i and x_j have same label, $y_{il} = 0$ otherwise.
μ set by cross-validation

Optimize by gradient descent: $\epsilon(L_{t+1}) = \epsilon(L_t) - \gamma\frac{\partial\epsilon(L_t)}{\partial L}$

$$
\frac{\partial\epsilon}{\partial L} = (1-\mu)\Sigma_{i,i\to j}C_{ij} + \mu\Sigma_{(i,j,l)\in\mathcal{R}_t}(C_{ij} - C_{il})
$$

where $C_{ij} = (x_i - x_j)^\top(x_i - x_j)$

Easy, no projection mechanism like for Mahalanobis Metric for Clustering (MMC) [9]

Elliptic Cayley-Klein LMNN [1], CVPR 2015

$$\epsilon(L) = (1-\mu)\sum_{i,i\to j} d_E(x_i,x_j) + \mu \sum_{i,i\to j}\sum_{l}(1-y_{il})\zeta_{ijl}$$

with $\zeta_{ijl} = [1 + d_E(x_i,x_j) - d_E(x_i,x_l)]_+$ (hinge loss)

$$\frac{\partial \epsilon(L)}{\partial L} = (1-\mu)\sum_{i,i\to j}\frac{\partial d_E(x_i,x_j)}{\partial L} + \mu \sum_{i,i\to j}\sum_{l}(1-y_{il})\frac{\partial \zeta_{ijl}}{\partial L}$$

$$C_{ij} = (x_i^\top, 1)^\top (x_j^\top, 1)$$

$$\frac{\partial d_E(x_i,x_j)}{\partial L} = \frac{k}{\sqrt{S_{ii}S_{jj} - S_{ij}^2}} L\left(\frac{S_{ij}}{S_{ii}}C_{ii} + \frac{S_{ij}}{S_{jj}}C_{jj} - (C_{ij} + C_{ji})\right)$$

$$\frac{\partial \zeta_{ijl}}{\partial L} = \begin{cases} \frac{\partial d_E(x_i,x_j)}{\partial L} - \frac{\partial d_E(x_i,x_l)}{\partial L}, & \text{if } \zeta_{ijl} \geq 0, \\ 0, & \text{otherwise.} \end{cases}$$

Hyperbolic Cayley-Klein LMNN (new case)

To ensure S keeps correct signature $(1, d, 0)$ during the LMNN gradient descent, we decompose $S = L^\top D L$ (with $L \succ 0$) and perform a gradient descent on L with the following gradient:

$$\boxed{\frac{\partial d_H(x_i, x_j)}{\partial L} = \frac{k}{\sqrt{S_{ij}^2 - S_{ii}S_{jj}}} DL \left(\frac{S_{ij}}{S_{ii}} C_{ii} + \frac{S_{ij}}{S_{jj}} C_{jj} - (C_{ij} + C_{ji}) \right)}$$

Recall two difficulties of hyperbolic case compared to elliptic case:

- Hyperbolic Cayley-Klein distance may be very large (unbounded vs. $< \kappa\pi$ for elliptic case)
- Data-set should be contained inside the compact domain $\mathbb{D}_S$

HCK-LMNN: Initialization and learning rate

- Initialize $L = \begin{pmatrix} L' & \\ & 1 \end{pmatrix}$ and D so that $\mathcal{P} \in \mathbb{D}_S$ with $\Sigma^{-1} = L'^\top L'$ (eg., precision matrix of $\mathcal{P}$).

$$D = \begin{pmatrix} -1 & & & \\ & \ddots & & \\ & & -1 & \\ & & & \kappa \ \max_x \|L'x\|^2 \end{pmatrix}$$

  with $\kappa > 1$.

- At iteration t, it may happen that $\mathcal{P} \notin \mathbb{D}_{S_t}$ since we do not know the optimal learning rate γ. When this happens, we reduce $\gamma \leftarrow \frac{\gamma}{2}$, otherwise we let $\gamma \leftarrow 1.01\gamma$.

Curved Mahalanobis learning: Results

Experimental results on some UCI data-sets

k	Data-set	elliptic	Hyperbolic	Mahalanobis
1	wine	**0.989**	0.865	0.984
	vowel	**0.832**	0.797	0.827
	balance	**0.924**	0.891	0.846
	pima	**0.726**	0.706	0.709
3	wine	0.983	0.871	**0.984**
	vowel	**0.828**	0.782	0.827
	balance	**0.917**	0.911	0.846
	pima	0.706	0.695	**0.709**
5	wine	0.983		**0.984**
	vowel	0.826	0.805	**0.827**
	balance	**0.907**	0.895	0.846
	pima	**0.714**	0.712	0.709
11	wine	**0.994**	0.983	0.984
	vowel	**0.839**	0.767	0.827
	balance	0.874	**0.897**	0.846
	pima	**0.713**	0.698	0.709

For classification, enough to consider $\kappa \in \{-1, 0, +1\}$

Spectral decomposition and fast proximity queries

- Avoid to compute d_E or d_H for arbitrary S
- Apply *spectral decomposition* (elliptic case $S = L^\top L$, or hyperbolic case $S = L^\top DL$) and perform coordinate changes so that we consider the canonical metric distances:

$$
\begin{aligned}
d_E(x', y') &= \arccos\left(\frac{\langle x', y'\rangle}{\|x'\|\|y'\|}\right), \\
d_H(x', y') &= \mathrm{arccosh}\left(\frac{1 - \langle x', y'\rangle}{\sqrt{1 - \langle x', x'\rangle}\sqrt{1 - \langle y', y'\rangle}}\right)
\end{aligned}
$$

- Proximity query: Eg, Vantage Point Tree data-structures [10, 6] (with metric pruning).

Mixed curved Mahalanobis distance

$$d(x,y) = \alpha d_E(x,y) + (1-\alpha) d_H(x,y)$$

1. Sum of Riemannian metric distances is metric ("blending" positive with negative constant curvatures)
2. Mixed of bounded distance (elliptic CK) with unbounded distance (hyperbolic CK), hyperparameter tuning α

Datasets	Mahalanobis	elliptic	Hyperbolic	Mixed	α	$\beta = (1-\alpha)$
Wine	**0.993**	0.984	0.893	0.986	0.741	0.259
Sonar	0.733	0.788	0.640	**0.802**	0.794	0.206
Balance	0.846	0.910	0.904	**0.920**	0.440	0.560
Pima	0.709	0.712	0.699	**0.720**	0.584	0.416
Vowel	0.827	0.825	0.816	**0.841**	0.407	0.593

Although mixed CK distance is a Riemannian metric distance, it is **not of constant curvature**.

Conclusion

Contributions and perspectives

- Study of Cayley-Klein elliptic/hyperbolic geometries: Affine bisector, Voronoi diagrams from (clipped) power diagrams, Cayley-Klein balls (Mahalanobis shapes with displaced centers), etc.
- Classification with Large Margin Nearest Neighbor (LMNN) in Cayley-Klein elliptic/hyperbolic geometries (hyperbolic geometry: compact domain & unbounded distance)
- Experiments on mixed Cayley-Klein distances

Ongoing work:
Extensions of Cayley-Klein geometries to Machine Learning

Thank you!

https://www.lix.polytechnique.fr/~nielsen/CayleyKlein/

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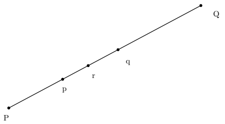
Overview

Properties of the cross-ratio

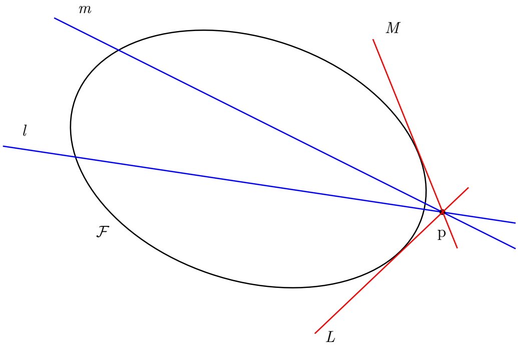
- $(p, p; P, P) = 1$
- $(p, q; Q, P) = \frac{1}{(p,q;P,Q)}$
- $(p, q; P, Q) = (p, r; P, Q) \cdot (r, q; P, Q)$ when r is collinear with p, q, P, Q



Measuring angles in Cayley-Klein geometries

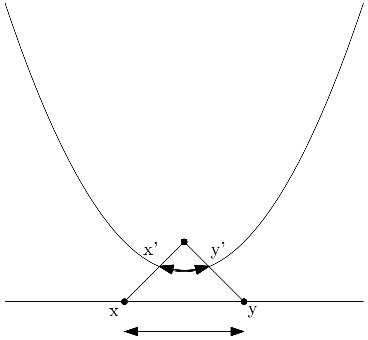
$$\mathrm{angle}(l, m) = c_{\mathrm{angle}} \log((l, m; L, M))$$

where L and M are tangent lines to A passing through the intersection point p ($p = l \times m$ in 2D) of l m.



Interpretation of hyperbolic Cayley-Klein distance

$$d_H(x, y) = \kappa \,\mathrm{arccosh}\left(\prec x', y' \succ\right)$$



Cayley-Klein Voronoi diagrams from (clipped) power diagrams

$$c_i = \frac{\Sigma p_i + a}{2\sqrt{S_{p_i p_i}}}$$

$$r_i^2 = \frac{\|\Sigma p_i + a\|^2}{4 S_{p_i p_i}} + \frac{a^\top p_i + b}{\sqrt{S_{p_i p_i}}}$$

Cayley-Klein balls have Mahalanobis ball shapes

Elliptic Cayley-Klein ball case:

$$\begin{aligned} \Sigma' &= \tilde{r}^2 \Sigma - a a^\top \\ c' &= \Sigma'^{-1}(b' a' - \tilde{r}^2 a) \\ r'^2 &= b'^2 - \tilde{r}^2 b + \langle c', c' \rangle_{\Sigma'} \end{aligned} \qquad \text{with} \qquad \begin{aligned} \tilde{r} &= \sqrt{S_{c,c}} \cos(r) \\ a' &= \Sigma c + a \\ b' &= a^\top c + b \end{aligned}$$

Cayley-Klein balls have Mahalanobis ball shapes

Hyperbolic Cayley-Klein ball case:

$$\begin{aligned} \Sigma' &= aa^\top - \tilde{r}^2\Sigma \\ c' &= \Sigma'^{-1}(\tilde{r}^2 a - b'a') \\ r'^2 &= \tilde{r}^2 b - b'^2 + \langle c', c' \rangle_{\Sigma'} \end{aligned} \quad \text{with} \quad \begin{aligned} \tilde{r} &= \sqrt{S_{c,c}}\cosh(r) \\ a' &= \Sigma c + a \\ b' &= a^\top c + b \end{aligned}$$

... and drawing a Mahalanobis ball amounts to draw a Euclidean ball after affine transformation $x' \leftarrow L^\top x$.

Spectral decomposition and signature

- Eigenvalue decomposition: $S = O\Lambda O^\top$.

$$\Lambda = \mathrm{diag}(\Lambda_{1,1}, \ldots, \Lambda_{d+1,d+1})$$

- Canonical decomposition: $S = OD^{\frac{1}{2}} \begin{bmatrix} I & 0 \\ 0 & \lambda \end{bmatrix} D^{\frac{1}{2}} O^\top$, where $\lambda = \in \{-1, 1\}$ and O= orthogonal matrix ($O^{-1} = O^\top$)

- Diagonal matrix D has all positive values, with $D_{i,i} = \Lambda_{i,i}$ and $D_{d+1,d+1} = |\Lambda_{d+1,d+1}|$