Hyperbolic Learning for Medical Imaging

Foundations on Non-Euclidean Geometry

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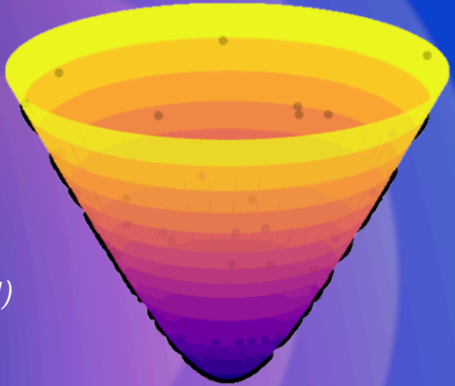


HyperMI

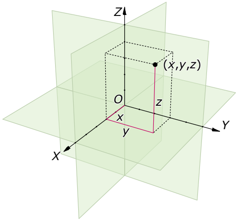
Website and material:

`https://hyperbolic-miccai.github.io`

Euclidean geometry

Humans perceive the world as three-dimensional Euclidean space.

Width, height, and depth are natural concepts.



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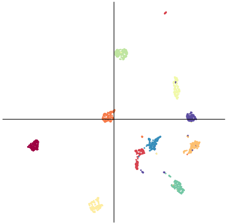
Computer linear algebra assumes Euclidean space.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}$$

Most Machine Learning is based on Euclidean space.



Spherical geometry

Some problems are naturally treated on the sphere.

Earth surface

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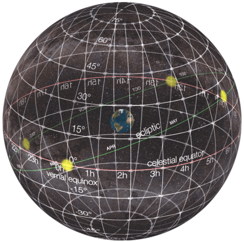
Celestial sphere



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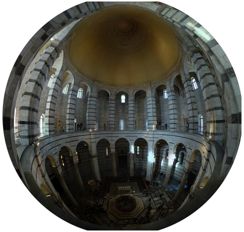
Fisheye camera



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More subtly, cosine distance is often used in embedding spaces.

Hyperbolic geometry

Hyperbolic geometry
is less common in nature...

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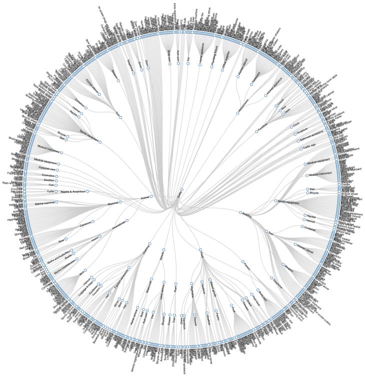
...but common in data!



[Schumann et al 2021]
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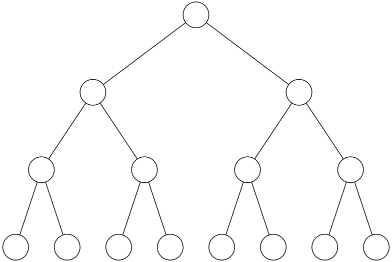
Hierarchies

Tree structures splitting at each level:



The number of leaves grows *exponentially* with the level.

This is often the structure of:

- Classification categories
- Images and their parts
- Words and their relations
- Tree graphs
- ...

Ubiquitous in Machine Learning!

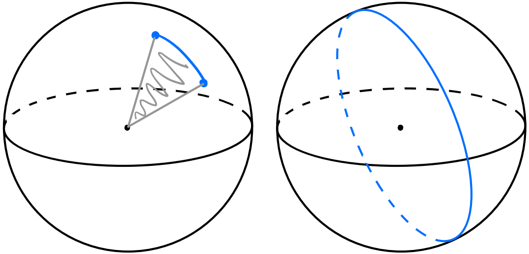
Program for 45 minutes

1. Motivation
2. Curvature
   - 2.1 Construction
   - 2.2 Properties
3. Hyperbolic geometry
   - 3.1 Lorentz hyperboloid model
   - 3.2 Poincaré ball model
   - 3.3 Isometries

Inspired by the tutorial on
Hyperbolic Representation Learning at ECCV 2022
by Mettes, Ghadimi Athig, Keller-Ressel, Gu, Yeung

Geodesics

Geodesics are shortest distance paths between points.
They are straight segments in the Euclidean plane, and great circle arcs on the sphere.

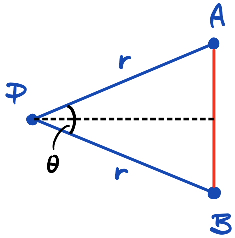


Euclidean distance between geodesics

An important characteristic of a geometry is the distance between geodesics at an angle θ, at a distance r from their intersection.

For the Euclidean plane

$$s_\theta = 2r\sin\frac{\theta}{2}.$$



Spherical distance between geodesics

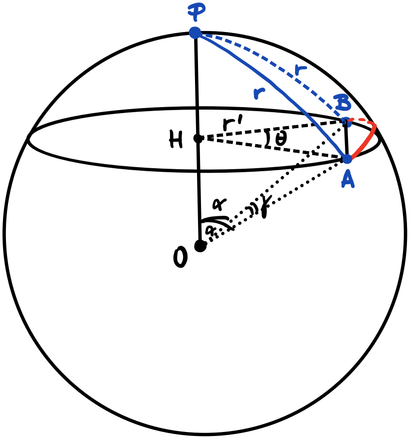
For the sphere

$$\alpha = \frac{r}{R}, \qquad r' = R \sin \alpha,$$

$$AB = 2r' \sin \frac{\theta}{2} = 2R \sin \frac{\gamma}{2},$$

$$\frac{\gamma}{2} = \sin^{-1}\left(\frac{r'}{R} \sin \frac{\theta}{2}\right),$$

$$s_\theta = R\gamma = 2R \sin^{-1}\left(\sin \frac{r}{R} \sin \frac{\theta}{2}\right).$$



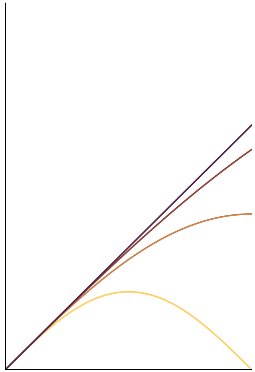
Volume element

In polar coordinates

$$\mathrm{d}s^2 = \mathrm{d}r^2 + [f(r)]^2 \mathrm{d}\theta^2 \quad \text{with} \quad f(r) = \left.\frac{\partial s_\theta}{\partial \theta}\right|_{\theta=0}.$$

- Euclidean $f(r) = r\cos\frac{\theta}{2}\Big|_{\theta=0} = r,$
- Spherical $f(r) = \left.\frac{R\cos\frac{\theta}{2}\sin\frac{r}{R}}{\sqrt{1-\sin^2\frac{\theta}{2}\sin^2\frac{r}{R}}}\right|_{\theta=0} = R\sin\frac{r}{R}.$

For $R \to +\infty$, spherical $\to$ Euclidean.



Negative curvature, imaginary radius

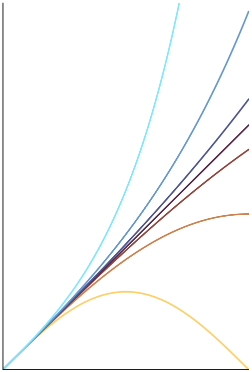
Define **curvature** as $\kappa := R^{-2}$.

$$f(r) = \frac{1}{\sqrt{\kappa}} \sin r\sqrt{\kappa}, \qquad \begin{cases} \text{Spherical} & \kappa > 0 \\ \text{Euclidean} & \kappa \to 0 \\ ? & \kappa < 0 \end{cases}.$$

Note $\kappa < 0$ means $R = i|R|$, rewrite

$$f(r) = -\frac{i}{\sqrt{-\kappa}} \sin\left(-ir\sqrt{-\kappa}\right) \qquad i\sin(ix) = \sinh x$$

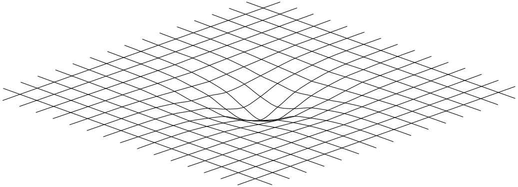
$$= \frac{1}{\sqrt{-\kappa}} \sinh\left(r\sqrt{-\kappa}\right). \qquad \sinh(x) = \frac{e^x - e^{-x}}{2}$$



The many faces of curvature

- **Intrinsic**: seen from within the space
  - Volume growth
  - Parallel postulate
  - Grid distortion
  - Parallel transport
  - Sum of internal angles
- **Extrinsic**: seen from a larger space
  - Principal curvatures
  - Gaussian curvature

- **Local**: at a given point in space
- **Global**: in a given region of space



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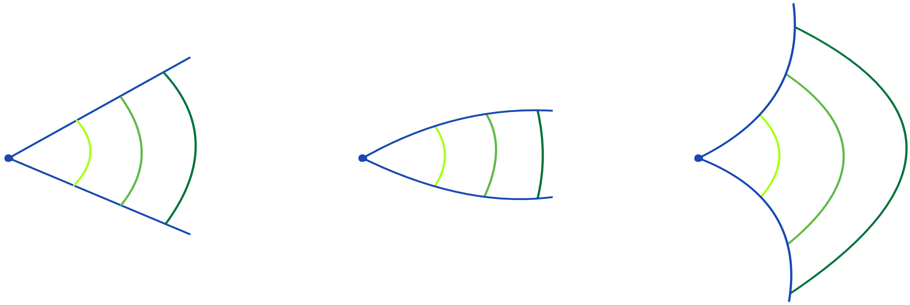
Space growth



$\kappa = 0$

polynomial

$$S_{n-1} = \Omega_n r^{n-1}$$

$\kappa > 0$

bounded

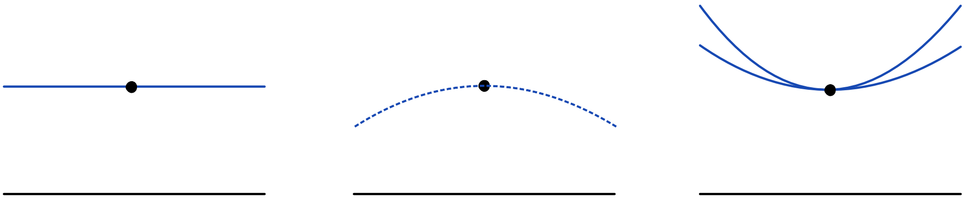
$$S^{+}_{n-1} = \Omega_n \left[R \sin \frac{r}{R} \right]^{n-1}$$

$\kappa < 0$

exponential

$$S^{-}_{n-1} = \Omega_n \left[|R| \sinh \frac{r}{|R|} \right]^{n-1}$$

Parallel postulate

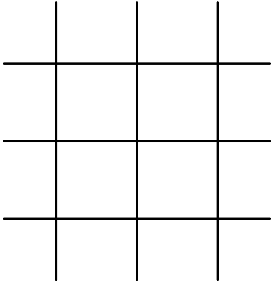


$\kappa = 0$ (one parallel)

$\kappa > 0$ (no parallel)

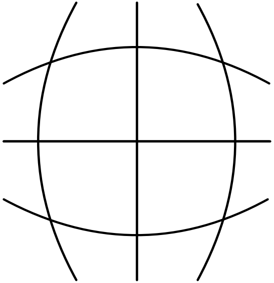
$\kappa < 0$ (many parallels)

Grid distortion



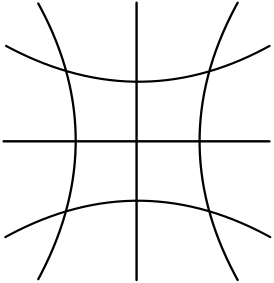
$\kappa = 0$

(flat)



$\kappa > 0$

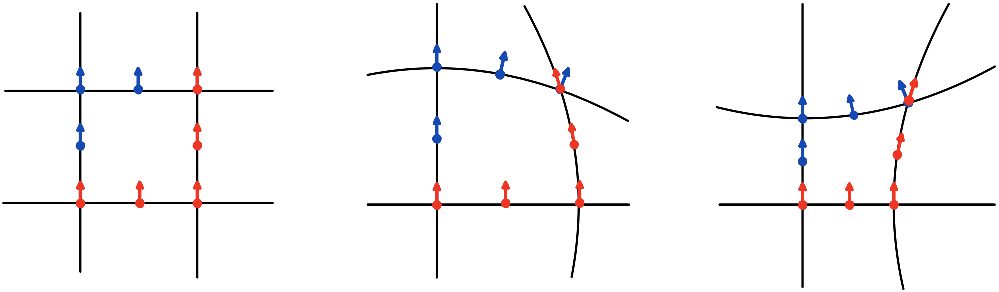
(barrel)



$\kappa < 0$

(pincushion)

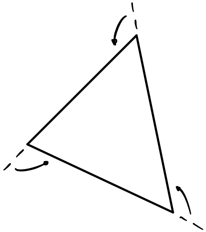
Parallel transport



$\kappa = 0$ $\kappa > 0$ $\kappa < 0$

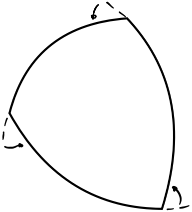
Triangles

Sum of internal angles



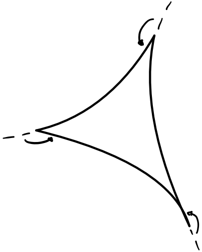
$\kappa = 0$

$\sum_i \alpha_i = \pi$



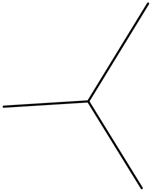
$\kappa > 0$

$\sum_i \alpha_i > \pi$



$\kappa < 0$

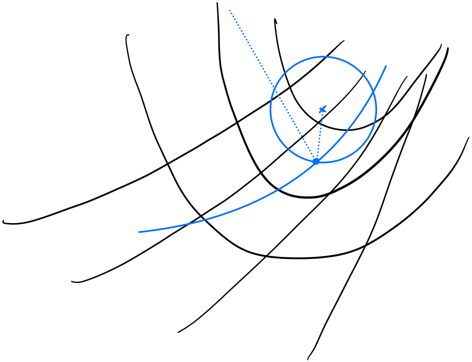
$\sum_i \alpha_i < \pi$



$\kappa \to -\infty$

$\sum_i \alpha_i = 0$

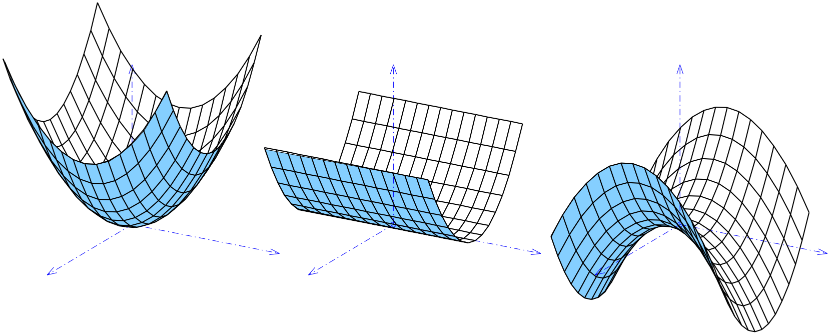
Principal curvatures



Principal curvatures are defined by the minimum and maximum radius of the circles that locally approximate a (hyper-)surface.

Gaussian curvature

Gaussian curvature is the determinant of extrinsic curvatures,
it coincides with intrinsic curvature.

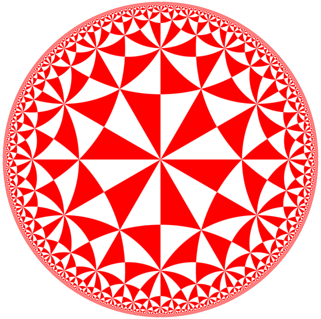


$\kappa > 0$ $\kappa = 0$ $\kappa < 0$

Definition and history

Hyperbolic space is the space of **constant negative curvature**.

- Developed in the 19th century by Gauss, Lobachevsky, and Bolyai.
- Is the geometry of Einstein's theory of special relativity.
- Inspired artworks by Maurits C. Escher.



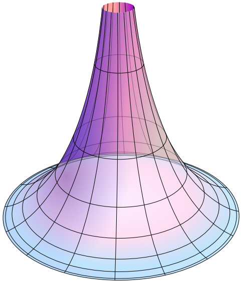
Hilbert's theorem

Bad piece of news:

> *There is no way to completely represent*
> *the hyperbolic space of dimension 2*
> *in the Euclidean space of dimension 3.*
>
> [Hilbert (1901)]

The best we can do is the *tractroid*,
but this is singular at the equator.

This is why we have to resort to *models*.



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Models of hyperbolic geometry

- Hyperboloid or Lorentz model
- Poincaré disk/ball
- Beltrami–Klein model
- Poincaré half-plane
- ...

All *equivalent*, but depending on the operation some may be more *convenient*.

A *conformal* model is one that preserves angles.

Minkowski space

Euclidean space $\mathbb{R}^n$ with an additional dimension

$$x = (x_0, x_1, \ldots, x_n) = (x_0, \vec{x})$$

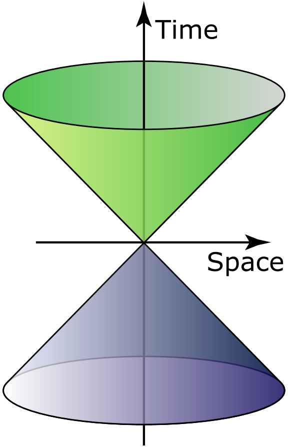
x_0 and $\vec{x}$ are called *time* and *space* components

Introduce the pseudo-scalar product

$$\begin{aligned} \langle x, y \rangle_{\mathcal{L}} &= x_0 y_0 - (x_1 y_1 + \cdots + x_n y_n) \\ &= x_0 y_0 - \vec{x} \cdot \vec{y}. \end{aligned}$$

This is not positive definite!

Example: $x^2 = 0$ when $x_0^2 = x_1^2 + x_2^2$



Lorentz hyperboloid model

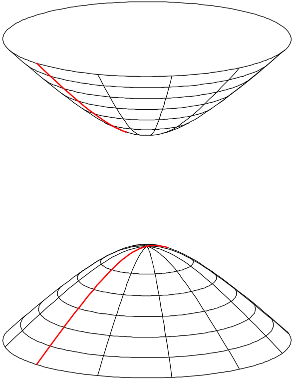
The Lorentz hyperboloid model is the manifold

$$x^2 = x_0^2 - \vec{x}^2 = -1/\kappa \quad \text{with} \quad x_0 > 0,$$

so x_0 is fully determined by $\vec{x}$

$$x_0 = \sqrt{\vec{x}^2 - 1/\kappa}.$$

A definition of distance is needed.



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Distance in the sphere

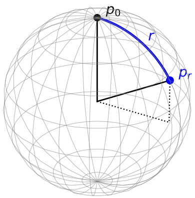
Rewriting a distance r as a scalar product extends it to the whole space.

For the n-dimensional sphere within $\mathbb{R}^{n+1}$, choose a meridian from the north pole

$$p_r = \begin{pmatrix} R\cos\left(\frac{r}{R}\right) \\ \hat{v} R \sin\left(\frac{r}{R}\right) \end{pmatrix}, \quad p_0 = \begin{pmatrix} R \\ \vec{0} \end{pmatrix},$$

$$\langle p_0, p_r \rangle = R^2 \cos\left(\frac{r}{R}\right),$$

$$r = R\cos^{-1}\left(\frac{\langle p_0, p_r \rangle}{R^2}\right).$$

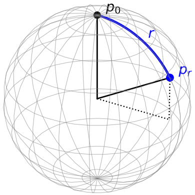


Distance in the sphere

Rewriting a distance r as a scalar product extends it to the whole space.

For the n-dimensional sphere within $\mathbb{R}^{n+1}$,
choose a meridian from the north pole

$$p_r = \begin{pmatrix} \frac{1}{\sqrt{\kappa}} \cos(r\sqrt{\kappa}) \\ \frac{\hat{v}}{\sqrt{\kappa}} \sin(r\sqrt{\kappa}) \end{pmatrix}, \quad p_0 = \begin{pmatrix} \frac{1}{\sqrt{\kappa}} \\ \vec{0} \end{pmatrix},$$



$$\langle p_0, p_r \rangle = \frac{1}{\kappa} \cos(r\sqrt{\kappa}),$$

$$r = \frac{1}{\sqrt{\kappa}} \cos^{-1}(\kappa \langle p_0, p_r \rangle).$$

Distance in the Lorentz hyperboloid

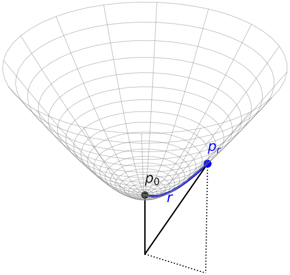
Rewriting a distance r as a scalar product extends it to the whole space.

For the n-dimensional Lorentz hyperboloid in $(1, n)$ Minkowski space

$$p_r = \begin{pmatrix} \frac{1}{\sqrt{-\kappa}} \cosh\left(r\sqrt{-\kappa}\right) \\ \frac{\hat{v}}{\sqrt{-\kappa}} \sinh\left(r\sqrt{-\kappa}\right) \end{pmatrix}, \; p_0 = \begin{pmatrix} \frac{1}{\sqrt{-\kappa}} \\ \vec{0} \end{pmatrix},$$

$$\langle p_0, p_r \rangle_{\mathcal{L}} = \frac{1}{-\kappa} \cosh\left(r\sqrt{-\kappa}\right),$$

$$r = \frac{1}{\sqrt{-\kappa}} \cosh^{-1}\left(-\kappa \langle p_0, p_r \rangle_{\mathcal{L}}\right).$$



Exponential map

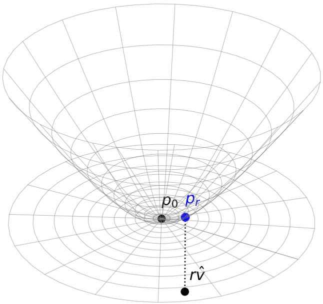
Let $v = (0, \hat{v})$.
$\langle p_0, v \rangle_{\mathcal{L}} = 0$ so v is in the tangent space $\mathrm{T}_{p_0} \sim \mathbb{R}^n$.

A geodesic at a point p_0 in the direction v

$$p_r = \exp_{p_0}(r, v) = \cosh\left(r\sqrt{-\kappa}\right) p_0 + \sinh\left(r\sqrt{-\kappa}\right) \frac{v}{\sqrt{-\kappa}},$$

is the intersection of a plane with the hyperboloid.

This is the **exponential map** that lifts points from the tangent space to the hyperboloid.
The inverse **logarithmic map** projects points from the hyperboloid to the tangent space.



From Lorentz hyperboloid to Poincaré disk

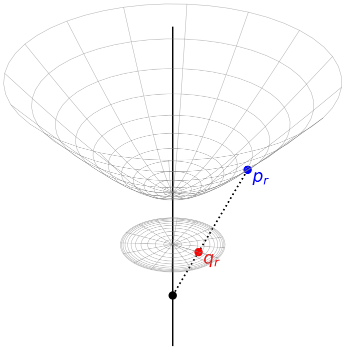
The **Poincaré disk** is a scaled projection of the Lorentz hyperboloid to the $x_0 = 0$ plane via the point $(-1/\sqrt{-\kappa}, \vec{0})$, and vice versa.

Setting $x_0 = 0$ in the linear combination gives

$$p_{r,\lambda} = \lambda p_r + (1-\lambda)\begin{pmatrix} -1/\sqrt{-\kappa} \\ \vec{0} \end{pmatrix}$$

$$= \frac{1}{\sqrt{-\kappa}}\begin{pmatrix} \lambda \cosh\left(r\sqrt{-\kappa}\right) - (1-\lambda) \\ \hat{v}\lambda \sinh\left(r\sqrt{-\kappa}\right) \end{pmatrix} \stackrel{!}{=} \frac{1}{\sqrt{-\kappa}}\begin{pmatrix} 0 \\ \vec{q} \end{pmatrix},$$

so $\lambda = \left[\cosh\left(r\sqrt{-\kappa}\right) - 1\right]^{-1}$.



Poincaré disk algebra

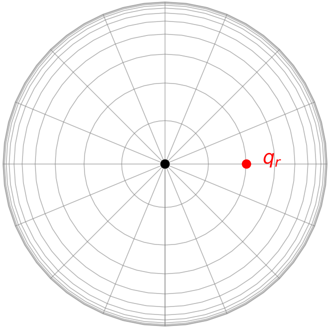
The point at distance r from the origin in direction $\hat{v}$ is then

$$\vec{q} = \hat{v}\frac{\sinh\left(r\sqrt{-\kappa}\right)}{\cosh\left(r\sqrt{-\kappa}\right)-1} = \hat{v}\tanh\frac{r\sqrt{-\kappa}}{2},$$

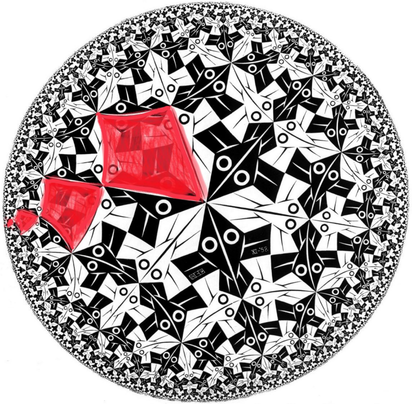
which gives $|\vec{q}| < 1$, a disk/ball without shell.

The distance between two points in the Poincaré model is given by

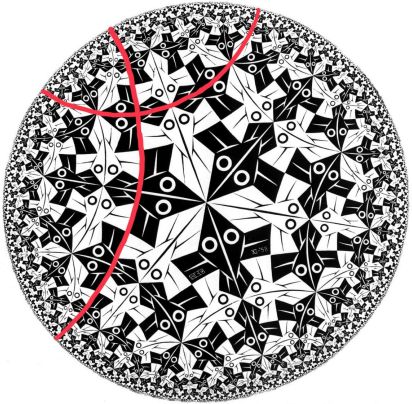
$$d(\vec{p},\vec{q}) = \frac{1}{\sqrt{-\kappa}}\cosh^{-1}\left(1+\frac{2|\vec{p}-\vec{q}|^2}{(1-|\vec{p}|^2)(1-|\vec{q}|^2)}\right).$$



Poincaré disk graphics



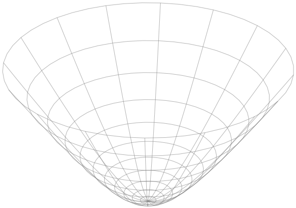
Areas and distances
appear smaller at the boundary.

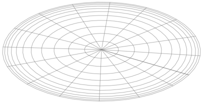


Geodesics are arcs of circles that
meet the boundary at right angles.

Origins

The Lorentz hyperboloid and Poincaré disk/ball have circular symmetry.



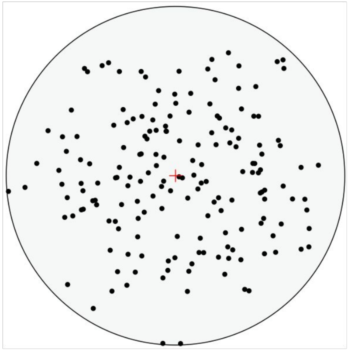


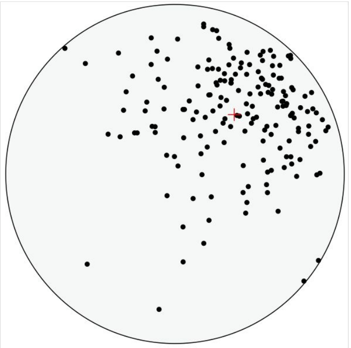
All points in the hyperbolic manifold have the same properties.

The origins are only special with respect to the coordinate system!

Hyperbolic isometries

A **hyperbolic translation** τ_x moves 0 to x keeping all pairwise distances constant.
Other names: Lorentz boost, Möbius transformation, gyrovectorspace addition





Formulas for hyperbolic translations

Lorentz hyperboloid (Lorentz boost)

$$\tau_x(y) = \Lambda_x y \quad \text{where} \quad \Lambda_x = \begin{pmatrix} x_0 & \vec{x}^T \\ \vec{x} & \sqrt{\mathbb{I} + \vec{x}\vec{x}^T} \end{pmatrix}. \tag{1}$$

Poincaré ball (gyrovectorspace addition)

$$\tau_{\vec{p}}(\vec{q}) = \vec{p} \oplus \vec{q} = \frac{(1 - |\vec{p}|^2)\vec{q} + (1 + 2\vec{p} \cdot \vec{q} + |\vec{q}|^2)\vec{p}}{1 + 2\vec{p} \cdot \vec{q} + |\vec{p}|^2|\vec{q}|^2}.$$

Note $\vec{p} \oplus \vec{q} \neq \vec{q} \oplus \vec{p}$.

Gyrovectorspace calculus

Gyrovectorspace addition:

$$\vec{p} \oplus \vec{q} = \frac{(1 - |\vec{p}|^2)\vec{q} + (1 + 2\vec{p} \cdot \vec{q} + |\vec{q}|^2)\vec{p}}{1 + 2\vec{p} \cdot \vec{q} + |\vec{p}|^2 |\vec{q}|^2}.$$

Gyrovectorspace product with scalar:

$$r \otimes \vec{p} = \vec{p} \otimes r = \tanh\left(r \tanh^{-1} |\vec{p}|\right) \frac{\vec{p}}{|\vec{p}|}.$$

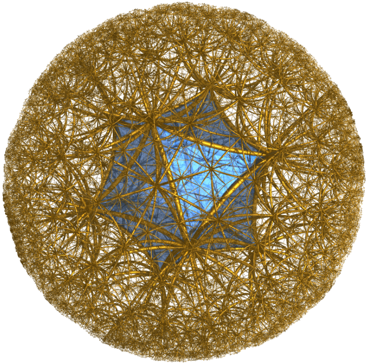
Geodesic arc from $\vec{p}$ to $\vec{q}$:

$$\lambda(t) = \vec{p} \oplus ([(-\vec{p}) \oplus \vec{q}] \otimes t), \quad t \in [0, 1].$$

This is similar to the Euclidean formula $\lambda(t) = \vec{p} + (\vec{q} - \vec{p})t$.

Summary

- Hyperbolic space can describe **hierarchical data** thanks to **exponential growth** with distance.
- **Curvature** is the concept underlying space growth, grid distortion, and parallel transport.
- **Hyperbolic space** is defined by **constant negative curvature**. It ccorresponds to a sphere of imaginary radius.
- The **Lorentz hyperboloid** and **Poincaré ball** are hyperbolic space models with different but equivalent **formulas**.



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