## Geometric data analysis

Lecture 5/7 – Riemannian metrics and geodesics

#### Jean Feydy HeKA team, Inria Paris, Inserm, Université Paris-Cité

#### Thursday, 9am-12pm - 7 lectures

#### Faculté de médecine, Hôpital Cochin, rooms 2001 + 2005

Validation: project + quizz

#### To mitigate the **curse of dimensionality**, we use:

- **Expert** knowledge: high-quality features.
- Relevant families of functions: kernels, convolutional networks.
- Relevant **neighborhood** structures: graphs.

Main challenge: **local** implementation  $\implies$  **global** understanding.

Produce guidelines and insights for practitioners.

## Large graphs are best understood as continuous objects [Pey11, EPW11]







Simple graph.

Manifold hypothesis.

Physical manifold.

## Long history in physics [Dat18, Bria, NWRC22]







The **Solar** system.

#### The **ideal gas** model.

#### Fluid simulation.

Lecture 5 – From discrete graphs to **continuous spaces**:

- The Poincaré disk.
- Local metrics and geodesics.

Lecture 6 – From discrete samples to continuous distributions:

- Duality: distributions and adversarial norms.
- Information geometry, kernels and optimal transport.

Lecture 7 – **Hardware** bottlenecks:

- Registers, parallel cores and compilers.
- Current trends.

#### Textbooks and introductions – in English:

- Poincaré and his disk Étienne Ghys, 2006.
- Hyperbolic geometry Cannon et al., 1997.
- Riemannian geometry: an introduction to curvature John M. Lee, 1997.
- Geometric data analaysis, beyond convolutions my PhD thesis, 2020.

#### **Lecture notes** available on my website – in French:

- Culture mathématique.
- Introduction à la géométrie riemannienne par l'étude des espaces de formes.

# The Poincaré disk

The Non-Euclidean World. – If geometrical space were a framework imposed on **each** of our representations considered **individually**, it would be **impossible** to represent to ourselves an image without this framework, and we should be quite **unable** to change our geometry.

But this is not the case; geometry is only the summary of the laws by which these images succeed each other.



There is nothing, therefore, to prevent us from imagining a **series of representations**, similar in every way to our ordinary representations, but succeeding one another according to laws which **differ** from those to which we are accustomed.

We may thus conceive that beings whose education has taken place in a medium in which those laws would be so different, might have **a very different geometry** from ours.



## Science and hypothesis – Henri Poincaré, 1902 [Nor]

Suppose, for example, a world **enclosed in a large sphere** and subject to the following laws:

• The temperature is not uniform;

it is **greatest at the centre**, and gradually decreases as we move towards the **circumference** of the sphere, where it is **absolute zero**.

#### The law of this temperature is as follows:

if R be the radius of the sphere, and r the distance of the point considered from the centre, the absolute temperature will be **proportional** to  $R^2 - r^2$ .



## Science and hypothesis – Henri Poincaré, 1902 [Nor]

 Further, I shall suppose that in this world all bodies have the same coefficient of dilatation, so that the linear dilatation of any body is proportional to its absolute temperature.

 Finally, I shall assume that a body transported from one point to another of different tem- perature is instantaneously in thermal equilibrium with its new environment.



## Science and hypothesis – Henri Poincaré, 1902 [Nor]

There is **nothing** in these hypotheses either **contradictory** or **unimaginable**. A moving object will become **smaller and smaller** as it approaches the **circumference** of the sphere.

Let us observe, in the first place, that although from the point of view of **our** ordinary geometry this world is **finite**, **to its inhabitants it will appear infinite**.

As they approach the surface of the sphere they become **colder**, and at the same time smaller and smaller. The steps they take are therefore also **smaller** and smaller, so that they can never reach the **boundary** of the sphere.



## The Poincaré metric is locally a Euclidean metric

With  $x^2 + y^2 < 1$ , we define:

$$\mathrm{d}\Big((x,y) \to (x,y) + (\mathrm{d} x,\mathrm{d} y)\Big) \ = \ 2 \ \frac{\sqrt{\mathrm{d} x^2 + \mathrm{d} y^2}}{1 - (x^2 + y^2)}$$

In other words:

$$\mathrm{d}^2 \Big( (x,y) \to (x,y) + (\mathrm{d} x,\mathrm{d} y) \Big) \ = \ 4 \ \frac{\mathrm{d} x^2 + \mathrm{d} y^2}{\big( 1 - (x^2 + y^2) \big)^2}$$

This local Euclidean metric is the Riemannian metric:

$$\begin{split} \|(\mathrm{d}x,\mathrm{d}y)\|_{(x,y)}^2 \ &= \ \left\langle \left(\mathrm{d}x,\mathrm{d}y\right), \, g_{(x,y)}\left(\mathrm{d}x,\mathrm{d}y\right) \right\rangle \\ g_{(x,y)} \ &= \ \begin{pmatrix} 4/\big(1-(x^2+y^2)\big)^2 & 0 \\ 0 & 4/\big(1-(x^2+y^2)\big)^2 \end{pmatrix} \end{split}$$



## Length of curve

If  $\gamma:[0,1]\to B(0,1)$  is a smooth path, we define:

$$\ell(\gamma) = \int_0^1 \|\dot{\gamma}(t)\|_{\gamma(t)} \,\mathrm{d}t$$

For the **straight path**  $\gamma(t) = (t, 0)$ , we find:

$$\begin{split} \ell(\gamma) \;&=\; \int_0^1 \|(1,0)\|_{(t,0)} \,\mathrm{d}t \\ &=\; \int_0^1 \frac{2}{1-t^2} \,\mathrm{d}t \\ &=\; \int_0^1 \frac{2}{(1+t)(1-t)} \,\mathrm{d}t \;=\; +\infty \end{split}$$

The Poincaré disk is a universe in a nutshell.



## Tissot's indicatrix [Brib, Kü04]





Tissot's indicatrix at location (x, y) is a **unit ball** for the local metric. This ellipsoid allows us to **depict distortions** in cartography and fully describes a **Riemannian metric** on the 2D map.

Stereographic projections define bijections between the segment *I*, the half-circle *J* and the half-line *H*.

If we endow I with the Poincaré metric:

$$\|(\mathrm{d} x)\|_{(x)\in I} \,=\, 2\, \frac{\sqrt{\mathrm{d} x^2}}{1-x^2}\,,$$

then J and H are endowed with:

$$\|(\mathrm{d}x,\mathrm{d}z)\|_{(x,z)\in J} = \frac{\sqrt{\mathrm{d}x^2 + \mathrm{d}z^2}}{z}$$
$$\|(\mathrm{d}z)\|_{(z)\in H} = \frac{\sqrt{\mathrm{d}z^2}}{z}$$



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$$\|(\mathrm{d}z)\|_{(z)\in H} = \frac{\sqrt{\mathrm{d}z^2}}{z}$$



## Equivalent descriptions of the Poincaré disk

Stereographic projections define bijections between the disk *I*, the hemisphere *J* and the half-plane *H*.

If we endow I with the Poincaré metric:

$$\|(\mathrm{d} x,\mathrm{d} y)\|_{(x,y)\in I} \ = \ 2 \ \frac{\sqrt{\mathrm{d} x^2 + \mathrm{d} y^2}}{1 - (x^2 + y^2)} \ ,$$

$$\|(\mathrm{d}x,\mathrm{d}y,\mathrm{d}z)\|_{(x,y,z)\in J} = \frac{\sqrt{\mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2}}{z}$$
$$\|(\mathrm{d}y,\mathrm{d}z)\|_{(y,z)\in H} = \frac{\sqrt{\mathrm{d}y^2 + \mathrm{d}z^2}}{z}$$



## Tissot's indicatrix on the Poincaré disk, hemisphere and half-plane



## The discrete Poincaré grid





 $dy^2 + dz^2$ z

Octave grid based on a dyadic tree.

## **Geodesics on the Poincaré disk**

## Geodesics on the Poincaré grid



The green and red paths have the same length.



Going **up** is faster than travelling **sideways**.

If the source and target points belong to the **vertical axis** y = 0, the shortest path is **straight**:

$$\begin{split} \ell(y(t), z(t)) &= \int_0^1 \frac{\sqrt{\dot{y}(t)^2 + \dot{z}(t)^2}}{z(t)} \mathrm{d}t \\ &\leqslant \int_0^1 \frac{\sqrt{\dot{z}(t)^2}}{z(t)} \mathrm{d}t \\ &= \ell(0, z(t)) \,. \end{split}$$



Using our stereographic projections, the North pole (x, y, z) = (0, 0, +1) of the **hemisphere** corresponds to:

- the center (x, y) = (0, 0) of the **disk**,
- the point (y, z) = (0, +2) of the **half-plane**.



The vertical axis in the **half-plane** is equivalent to the **"Greenwich meridian"** in the **hemisphere**.

Since the Poincaré metric:

$$\|(\mathrm{d}x,\mathrm{d}y,\mathrm{d}z)\|_{(x,y,z)\in J} = \frac{\sqrt{\mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2}}{z}$$

is invariant by **rotations**:

 $(x,y,z)\mapsto \left(\cos(\theta)\,x,\sin(\theta)\,y,z\right),$ 

all great circles that pass through the North pole are also **geodesic curves**.



The vertical axis in the **half-plane** is equivalent to the **"Greenwich meridian"** in the **hemisphere**.

Since the Poincaré metric:

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## Meridians on the three Poincaré models







Diameters.

Meridians.

 $\begin{array}{l} \mbox{Half-circles that pass} \\ \mbox{through } (y,z) = (0,+2) \,. \end{array} \end{array}$ 

**Half-circles** that are perpendicular to the horizontal axis **are all geodesics**.

This is because the Poincaré metric:

$$\|(\mathrm{d} y,\mathrm{d} z)\|_{(y,z)\in H}\,=\,\frac{\sqrt{\mathrm{d} y^2+\mathrm{d} z^2}}{z}$$

is invariant by **horizontal translations**:

 $(y,z)\mapsto (y+\Delta y,z)$ 

and **scalings** with a positive constant a > 0:

 $(y,z)\mapsto (ay,az)$  .



## Geodesics on the Poincaré grid, half-plane and disk







Up-and-down paths.

Half-circles and vertical lines.

Orthogonal circles and diameters.

#### A continuous tree



Circle Limit IV by **M.C. Escher**: a **regular** tiling of the Poincaré disk.



The Cayley graph of  $SL_2(\mathbb{Z})$ is to the **Poincaré** disk what a regular grid is to the **Euclidean** plane. 31

#### We should **remember** that:

- A **Riemannian** metric is a smooth field of Euclidean norms. It is equivalent to **Tissot's indicatrix** in cartography.
- **Convenient** way of defining arbitrary geometries: the Poincaré disk is a continuous tree.
- **Changes of coordinates** are key to eloquent proofs. Don't get stuck on one parameterization.
- **Discrete** ↔ **Continuous** analogies go both ways.

## Riemannian geometry, in practice

## A convenient way of working with surfaces





#### As a surface **embedded in 3D**.

The torus as a **flat 2D square**.

## A convenient way of working with surfaces





Geodesics on the donut.

The torus as a **curved 2D square**.

## Mathematical objects [AFPA06, KSA19]





**Covariance matrices:** geodesics for the **Euclidean**, affine-invariant and log-Euclidean metrics. **3D rotations**: geodesics for the Lie group structure.

#### Probability distributions - see Lecture 6! [PC18]





Gaussians + Wasserstein metric = Euclidean. Gaussians + relative **entropy** = **Poincaré**.

#### Shape metrics - remember Lecture 1!





The **plane** of triangle shapes.

The **sphere** of triangle shapes.

## Shape metrics [KMP07]



Geodesics in spaces of elephants and skeletons.

## Shape metrics [vRESH16]



Barycentric interpolation in a space of hands.

## Network architectures are "projections" from parameter space to function space



Standard gradient descent on the parameters Riemannian gradient descent on the network. Core idea behind the natural gradient, neural tangent kernels, (Wasserstein) gradient flows...

## Graph and point cloud embeddings [SDSGR18, NK17]



ven-Toed Unsulate Ungulate Odd-Toed Ungulate

Embedding a **tree** in the Poincaré disk.

WordNet mammals subtree

UMAP (Uniform **Manifold** Approximation and Projections) also works with Riemannian metrics. If  $H(q,p) = \frac{1}{2} \langle p, g_q^{-1}p \rangle$  denotes the **Hamiltonian** for the Riemannian metric  $g_q$ , we can show that **paths** q(t) that **minimize length** locally and travel at **constant speed** follow a **coupled Ordinary Differential Equation** with a **momentum** vector p(t):

$$\begin{cases} \dot{q}(t) = + \frac{\partial H}{\partial p}(q(t), p(t)) & \text{follow the velocity } v(t) = g_{q(t)}^{-1} p(t). \\ \dot{p}(t) = - \frac{\partial H}{\partial q}(q(t), p(t)) & \text{steer the momentum to stay on a geodesic path.} \end{cases}$$

Geodesic paths are fully determined by:

- the starting **position** q(t = 0),
- the starting momentum  $p(t=0) \iff$  the velocity  $\dot{q}(t=0) = g_{q(t=0)}p(t=0).$

## The exponential map [Chr10, Rok08]







From the 1D line to the **circle**.

From the 2D plane to the **sphere**.

Azimuthal equidistant projection.

 $\exp_{q_0}(p_0) \text{ denotes the solution } q(t=1) \text{ of the geodesic equation}$  with initial condition  $q(t=0)=q_0$ ,  $p(t=0)=p_0$ .

## Computing geodesics from A to B – three main scenarios

#### 1. The metric has a lot of structure – closed formulas:

- Just like the Poincaré disk: simple example + symmetries.
- Riemannian **metric**  $\iff$  Relevant **kernel**.

#### 2. The metric $g_{\boldsymbol{x}}$ is simple – path shortening:

- Discretize the path energy  $\ell^2(\gamma) \simeq \frac{1}{N} \sum_{i=1}^{N} N^2 \|\gamma(i/N) \gamma((i-1)/N)\|_{\gamma(i/N)}^2$ .
- "Mean curvature flow": gradient descent with respect to the snapshot positions.

## 3. The cometric $K_a = (g_a)^{-1}$ is simple – geodesic shooting:

- Implement the exponential  $(q_0,p_0)\mapsto \exp_{q_0}(p_0)$  by integrating the Hamilton ODE.
- Solve the inverse problem  $p_0 \mapsto \exp_A(p_0) \cong B$  with an optimizer or a network.

#### Riemannian metrics provide:

- Expressive vocabulary: trees, balls, shapes and probability distributions.
- Complete **toolbox**: local metric  $\longrightarrow$  geodesics, exponentials and barycenters.
- Appealing **message**:

simple paths on a curved space > complex paths on a flat space.

This framework is the cornerstone of several applied fields, and provides an **inspiring** outlook in many other settings.

#### $\implies$ Lab session with GeomStats. $\Leftarrow$

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