

Geometry and AI

Daniel Platt
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Geometry is a discipline in pure maths. Geometry and AI have two connections: " \rightarrow ": geometry is used to invent machine learning algorithms, such as geometric kernel methods. " \leftarrow ": machine learning is used to answer questions in geometry, for example by using physics-informed neural networks as a PDE solver.

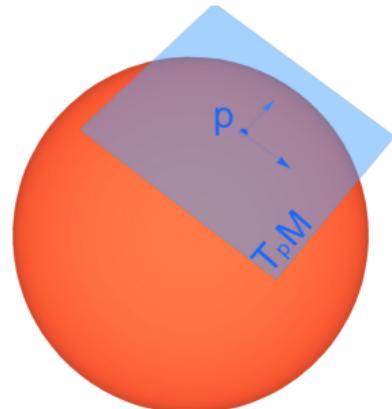
The structure of the tutorial is: (1) an introduction to Riemannian geometry, (2) positive definite kernels on metric spaces as example of the type " \rightarrow ", (3) a physics-informed neural network on the circle as an example of the type " \leftarrow ".



Tutorial materials, including these slides:
<https://github.com/danielplatt/geometry-ai-tutorial>

Riemannian geometry

- **Manifold:** space like



$$\{(x, y, z) \in \mathbb{R}^3 : x^2 + y^2 + z^2 - 1 = 0\}$$

- p point in M , **tangent space**:

$$T_p M = \{\text{directions you can go in from } p\}$$

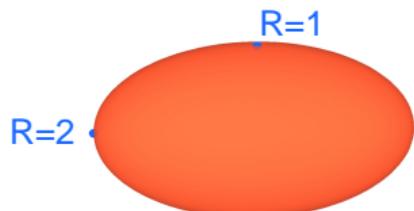
- **Riemannian metric**, "length of tangent vectors":

$$g : \{\text{tangent vectors}\} \rightarrow \mathbb{R}_+$$

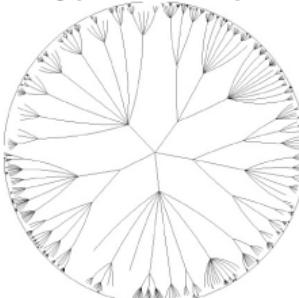
- \rightsquigarrow **curvature** $R : M \rightarrow \mathbb{R}$

Examples:

- Ellipsoid:



- Hyperbolic space:



- EEG data:

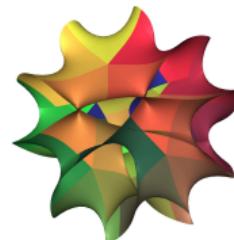
$$Q = \left\{ A \in \mathbb{R}^{m \times m} : \begin{array}{l} A \text{ symm.} \\ \text{and pos. def.} \end{array} \right\}$$

In neuroscience: ML on Q with different metrics

Riemannian geometry

- ▶ (Special case of) Yau's theorem: $f(z_1, \dots, z_4)$ is degree 5 polynomial \Rightarrow there exists a Riemannian metric "Calabi-Yau metric" with curvature $R \equiv 0$ on

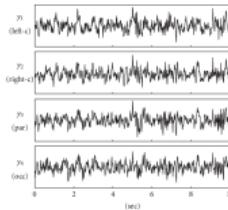
$$\{(z_1, \dots, z_4) \in \mathbb{C}^4 : f(z_1, \dots, z_4) = 0\}.$$



- ▶ Question: what does the metric look like?
Concretely: what's the length of a certain curve? Does the solution to the Poisson problem (defined later) have a zero?
- ▶ Best approach to approximately solve the equation $R \equiv 0$ are physics-informed neural networks; approximate solutions are used in two different ways
 1. Inspect approximate solution, formulate conjecture, prove theorem using traditional analysis
 2. Inspect solution, use computer for numerically verified proof
- ▶ Several problems in ML can be phrased in Riemannian geometry language

— Blackboard presentation for Riemannian metrics here —

Example 1: positive definite kernels



$$A \in \mathcal{P} := \{M \in \mathbb{R}^{n \times n} : M \text{ symmetric and pos. def.}\}$$

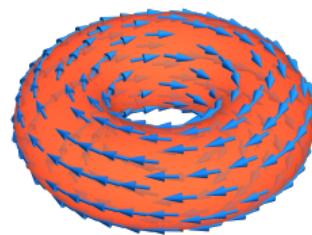
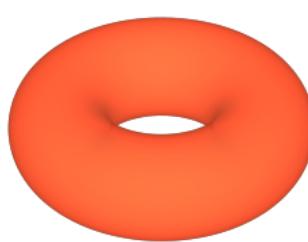
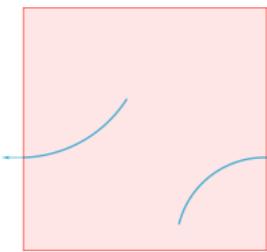
- ▶ Goal: classify patient $x_1, \dots, x_k \in \mathcal{P}$ EEG readings (e.g. diseased/non-diseased)
- ▶ Riemannian metric g on \mathcal{P} and $\lambda > 0 \Rightarrow$ Gaussian kernel $k : \mathcal{P} \times \mathcal{P} \rightarrow \mathbb{R} \Rightarrow \phi : \mathcal{P} \rightarrow \mathcal{H}$ and use linear classifier for $\phi(x_1), \dots, \phi(x_k)$ on Hilbert space \mathcal{H}
- ▶ Different g give different ϕ (Log-Euclidean, Affine-invariant, ...)
- ▶ Gaussian kernel: $k(x, y) = \exp(-d(x, y)^2/(2\lambda))$
- ▶ Positive definite : \Leftrightarrow

$(k_{ij}) = (k(x_i, x_j))$ is positive semidefinite for all $x_i \in \mathcal{P}$.

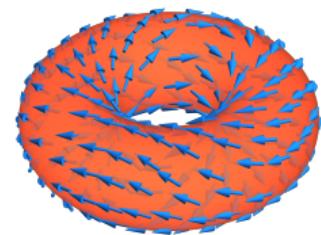
- ▶ Heuristic: classification works well if kernel is pos. def.
- ▶ Theorem: If k is pos. def. for all $\lambda > 0$, then the space has curvature $R = 0$.
Theorem: If ex. isometric $S^1 \hookrightarrow \mathcal{P}$, then k not pos. def. for any $\lambda > 0$.
- ▶ Open question: ex. space on which k pos. def. for some λ ?

Example 2: the Poisson problem

- ▶ 3-torus $([0, 1] \times [0, 1] \times [0, 1]) / \sim$, where \sim identifies opposing faces



(standard metric)



(funny metric)

- ▶ Vector field: $X : T^3 \rightarrow \{\text{tangent vectors}\}$
- ▶ Laplace operator $\Delta : \{\text{vector fields}\} \rightarrow \{\text{vector fields}\}$
- ▶ Question: does there exist a "Calabi-Yau" metric on T^3 such that **every** vector field X satisfying $\Delta X = 0$ has a zero?
- ▶ Easier question: does there exist **any** metric on T^3 such that every (or some) vector field X satisfying $\Delta X = 0$ has a zero?
- ▶ Approach: **numerically verified proof**:
 1. Use physics-informed neural network (PINN) to solve $\Delta X = 0 \rightarrow$ approximate solution X_{PINN} with zero
 2. Prove an error bound for residual $|\Delta X_{\text{PINN}}|$ of the PINN solution (\leftarrow exercise)
 3. Conclude that the **nearby genuine solution X** also must have a zero (\leftarrow pure maths)

Thank you for the attention!

Image credit: Calabi-Yau variety by Andrew J. Hanson - Ticket#2014010910010981, CC BY-SA 3.0, <https://commons.wikimedia.org/w/index.php?curid=30579072>

EEG recording cap: A cap holds electrodes in place while recording an EEG. 29 October 2012, 17:44:31. https://www.flickr.com/photos/tim_uk/8135755109/. Chris Hope. CC BY 2.0.

Time series data: Luca Faes, Silvia Erla, Giandomenico Nollo: Measuring Connectivity in Linear Multivariate Processes: Definitions, Interpretation, and Practical Analysis