Neuromanifolds

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KTH VETENSKAP OCH KONST

WASP WALLENBERG AI, AUTONOMOUS SYSTEMS AND SOFTWARE PROGRAM

SFSG SWEDISH FOUNDATIONS' STARTING GRANT

Ragnar Söderbergs STIFTELSE

based on joint works with

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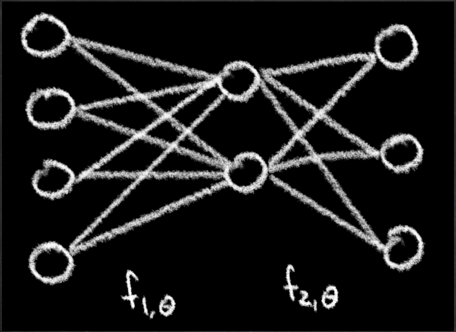
feedforward neural networks



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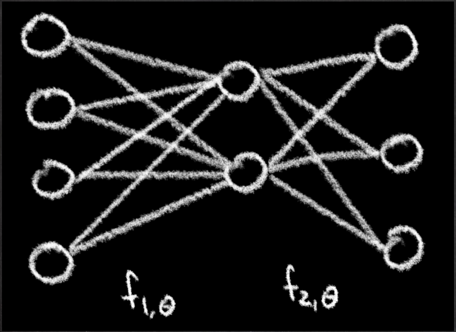

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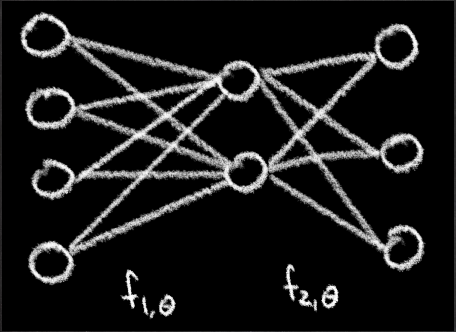

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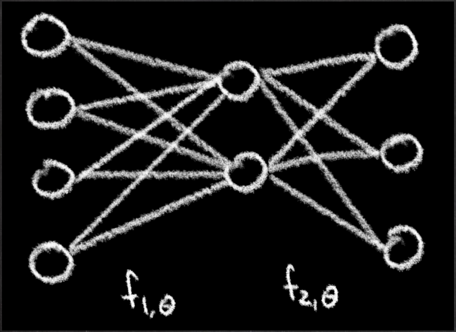

$\mathcal{M} = \mathrm{im}(\mu) =$ neuromanifold

it is a manifold with boundary and singularities

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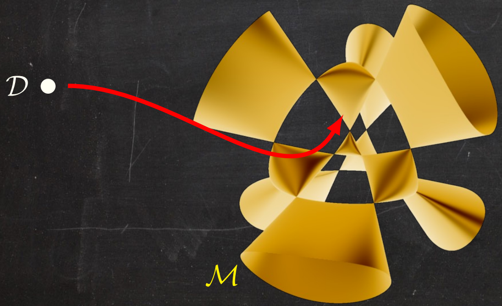
training a network

Given training data $\mathcal{D}$, the goal is to minimize the **loss**

$$\mathbb{R}^N \xrightarrow{\mu} \mathcal{M} \xrightarrow{\ell_{\mathcal{D}}} \mathbb{R}.$$



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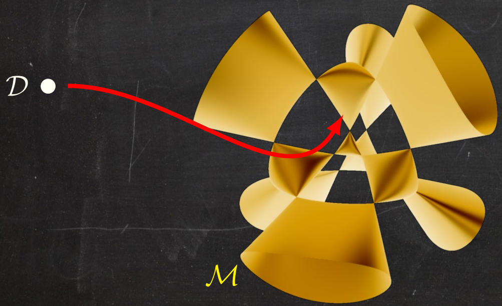

Geometric questions:

- How does the network architecture affect the geometry of the function space?
- How does the geometry of the function space impact the training of the network?

understanding networks via algebraic optimization

For piecewise algebraic activation, the neuromanifold is a semi-algebraic set (defined by polynomial equalities and inequalities).

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Examples:

activation	loss
identity	
ReLU	
polynomial	

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Algebra Unveils Deep Learning - An Invitation to Neuroalgebraic Geometry.
ICML 2025: Spotlight & Position Paper

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Weierstrass Approximation Theorem:
Any activation function can be approximated by polynomial ones.
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Examples:

activation	loss	
identity	squared-error loss	$=$ Euclidean dist
ReLU	Wasserstein distance	$=$ polyhedral dist.
polynomial	cross-entropy	$\cong$ KL divergence

If the loss is also algebraic (or has at least algebraic derivatives), network training is an algebraic optimization problem.

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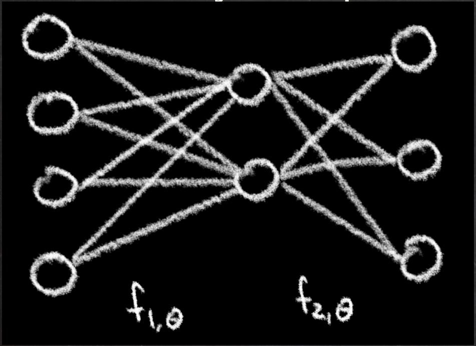
baby example: linear dense networks



In this example:

$$\mu : \mathbb{R}^{2\times 4} \times \mathbb{R}^{3\times 2} \longrightarrow \mathbb{R}^{3\times 4},$$
$$(W_1, W_2) \longmapsto W_2 W_1.$$

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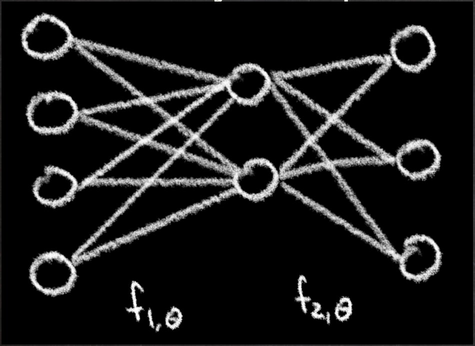

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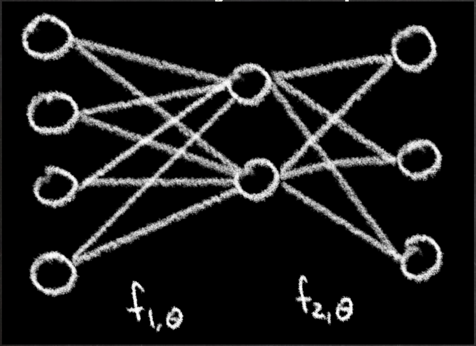

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In general:

$$\mu : \mathbb{R}^{k_1\times k_0} \times \mathbb{R}^{k_2\times k_1} \times \ldots \times \mathbb{R}^{k_L\times k_{L-1}} \longrightarrow \mathbb{R}^{k_L\times k_0},$$
$$(W_1, W_2, \ldots, W_L) \longmapsto W_L \cdots W_2 W_1.$$

$\mathcal{M} = \{W \in \mathbb{R}^{k_L\times k_0} \mid \mathrm{rank}(W) \leq \min(k_0, \ldots, k_L)\}$ is an algebraic variety and we know its singularities etc.

example: attention networks

A single-layer lightning self-attention network with weights $Q, K \in \mathbb{R}^{a\times d}$ and $V \in \mathbb{R}^{d'\times d}$ is

$$\begin{aligned} \mathbb{R}^{d\times t} &\longrightarrow \mathbb{R}^{d'\times t}, \\ X &\longmapsto VX\,X^\top K^\top QX. \end{aligned}$$

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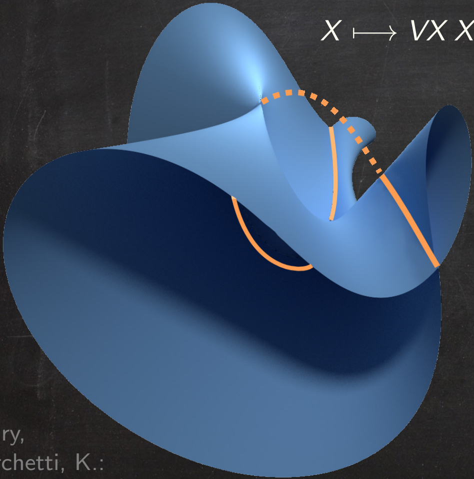

A slice of the 5-dimensional neuromanifold $\mathcal{M}$ for $a = d = t = 2, d' = 1$.

It is singular along the orange curve, and has boundary points where the curve leaves/enters $\mathcal{M}$.

Henry, Marchetti, K.: Geometry of Lightning Self-Attention: Identifiability and Dimension. **ICLR 2025**

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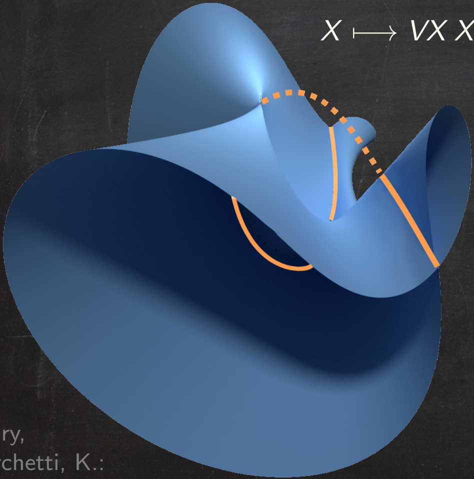

A slice of the 5-dimensional neuromanifold $\mathcal{M}$ for $a = d = t = 2, d' = 1$.

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It is not a variety, but a semialgebraic set.

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a dictionary

machine learning	algebraic geometry
sample complexity & expressivity	dimension, degree, covering number
subnetworks & implicit bias	singularities
identifiability & hidden symmetries	fibers of the parametrization
optimization & gradient descent	critical point theory, discriminants, dynamical invariants

dimension, degree, covering number

The dimension of the neuromanifold $\mathcal{M}$ measures how many functions can be exactly expressed by the network.

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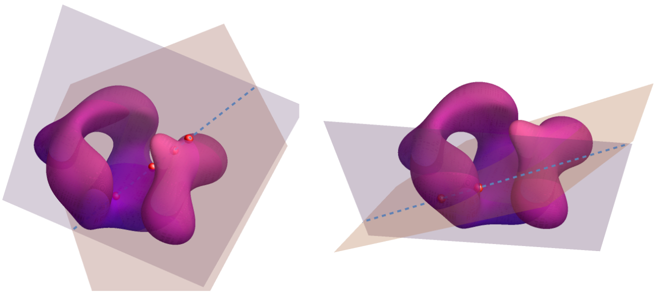
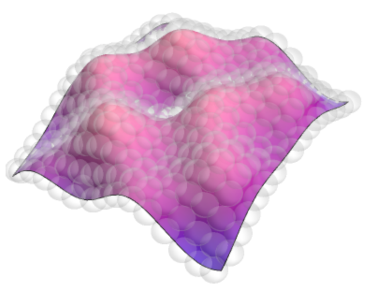
The degree of an algebraic variety is the number of intersections (over $\mathbb{C}$) with a generic linear space (of the correct dimension).

It measures how curvy/twisted the variety is.



dimension, degree, covering number



covering number $\mathcal{N}_\varepsilon(\mathcal{M})$ = minimum number of metric balls of radius ε required to cover $\mathcal{M}$

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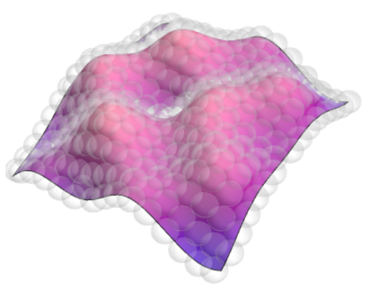

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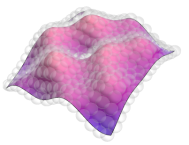
$$\log \mathcal{N}_\varepsilon(\mathcal{M}) = \mathcal{O}\left(\dim(\mathcal{M}) \cdot \log \frac{\mathrm{degree}(\mathcal{M})}{\varepsilon} + C \right)$$

(cf. Weyl's Tube Formula)

dimension, degree, covering number



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relation to sample complexity:
the number of data samples required to infer the function that best approximates the distribution of data (with high probability, and within a given generalization loss margin ε) scales logarithmically in $\mathcal{N}_\varepsilon(\mathcal{M})$.

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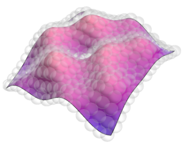

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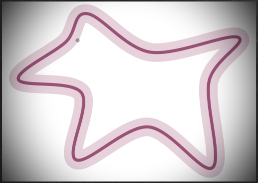
relation to approximative expressivity:



the volume of the ε-tube around $\mathcal{M}$ measures how many functions can be approximated within an error of ε.

it is $\leq \mathcal{N}_\varepsilon(\mathcal{M}) \cdot \mathrm{vol}(\text{ball of radius } 2\varepsilon)$

dimension, degree, covering number

Takeaway

Dimension and degree are the most fundamental invariants of an algebraic neuromanifold.

They control metric quantities such as covering numbers,
which in turn measure approximate expressivity and sample complexity.

singularities

Singularities of a variety are points where the variety does not look locally like a smooth manifold.

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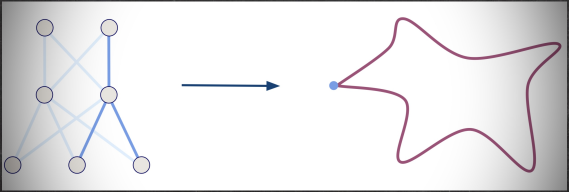
Conjecture: The singularities of neuromanifolds correspond to subnetworks. (known for convolutional & fully-connected networks with polynomial activation)



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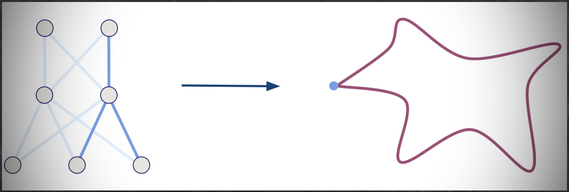

Potential explanation for *lottery ticket hypothesis*: the tendency of deep networks to discard weights during learning.

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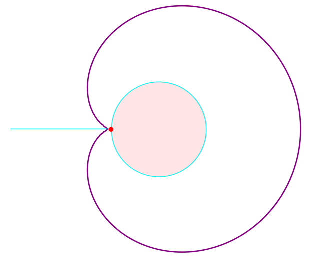
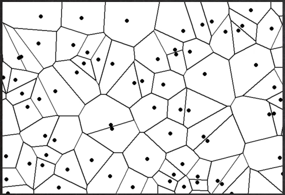


voronoi cells

Given a set $\mathcal{M} \subseteq \mathbb{R}^n$, the Voronoi cell of $x \in \mathcal{M}$ consists of all $u \in \mathbb{R}^n$ such that x is "closest" among all points in $\mathcal{M}$.



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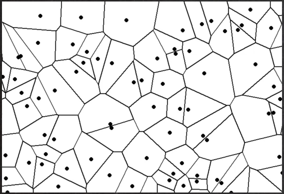

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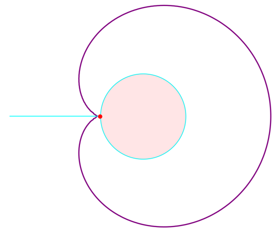

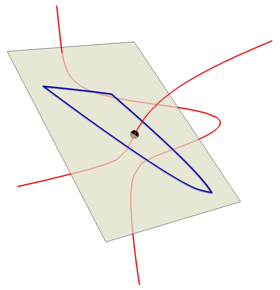

or a manifold, variety, semi-algebraic set, etc.

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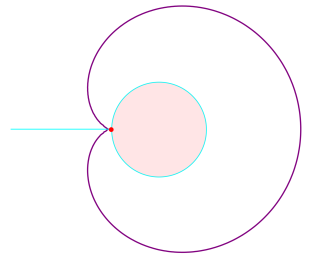

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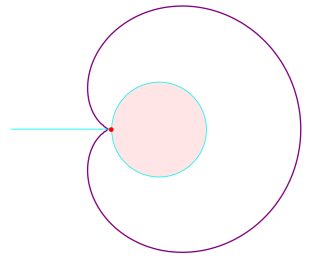

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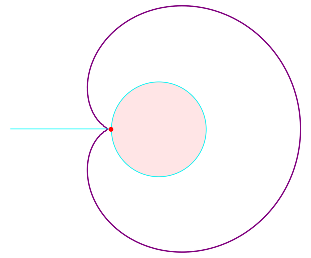

- $\mathcal{M} \subseteq \mathbb{R}^2$ is the purple curve
- loss $=$ Euclidean distance
- at all smooth points $x \in \mathcal{M}$, the Voronoi cell is a line segment
- the Voronoi cell at the singularity is 2-dimensional, i.e., that point is the closest with positive probability

singularities

Takeaway

Singularities of the neuromanifold can introduce implicit biases in the learning process.

They often correspond to subnetworks, favoring the selection of simpler models.

singularities

of polynomial networks that are fully-connected (MLP) or convolutional (CNN) correspond to subnetworks

MLP singularities cause implicit bias, CNN singularities don't

Shahverdi, Marchetti, K.: Learning on a Razor's Edge – the Singularity Bias of Polynomial Neural Networks. **preprint 2025**

fibers of the parametrization

Recall: The neuromanifold is the image of parametrization map

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Identifiability / hidden symmetries:
Which network parameters give rise to the same function?

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fiber-dimension theorem:
The dimension of the image of an algebraic map equals the co-dimension of its generic fiber. (nonlinear version of rank-nullity theorem)

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More generally: All geometric features of the neuromanifold are caused by μ.

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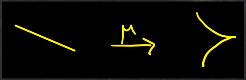
For instance, singularities on $\mathcal{M}$ can arise in 2 ways:

- from critical points of μ



- from special (i.e., non-generic) fibers of μ

example: polynomial convolutional networks

Theorem: Let activation σ be a generic polynomial of large degree with $\sigma(0) = 0$.

Shahverdi, Marchetti, K.:
On the Geometry and Optimization of Polynomial CNNs. **AISTATS 2025**
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Away from the zero function $0 \in \mathcal{M}$, the network parametrization map is

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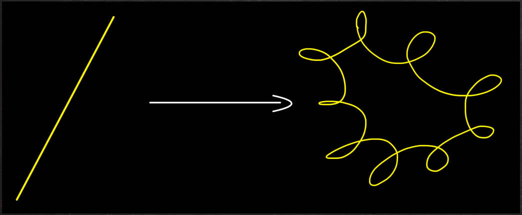

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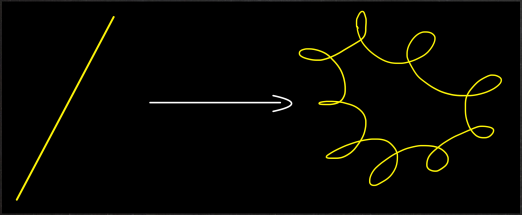

The singularities correspond to subnetworks.

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comparison: polynomial MLPs

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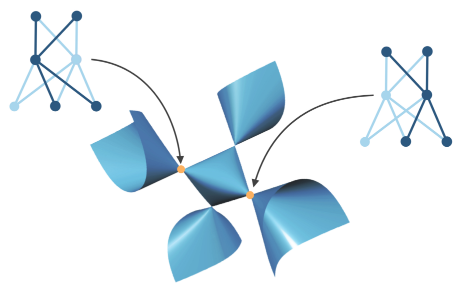
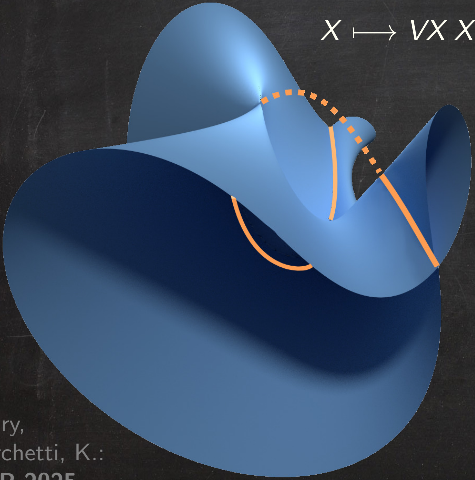
Infinite fibers exist.
They cause rank drop of the Jacobian and singularities with implicit bias.



comparison: lightning self-attention

A single-layer lightning self-attention network with weights $Q, K \in \mathbb{R}^{a \times d}$ and $V \in \mathbb{R}^{d' \times d}$ is

$$\begin{aligned} \mathbb{R}^{d \times t} &\longrightarrow \mathbb{R}^{d' \times t}, \\ X &\longmapsto V X X^\top K^\top Q X. \end{aligned}$$



The neuromanifold is semialgebraic but not a variety (polynomial inequalities needed!)

It has both nodal and cuspidal singularities.

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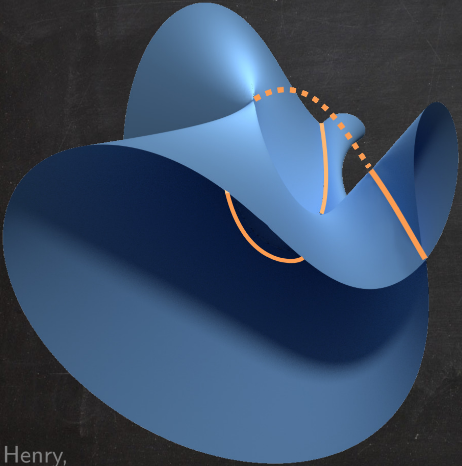
comparison: lightning self-attention

$$VXX^\top K^\top QX$$



cusps 

$\Leftrightarrow$ boundary points

$\Leftrightarrow$ Jacobian rank drops

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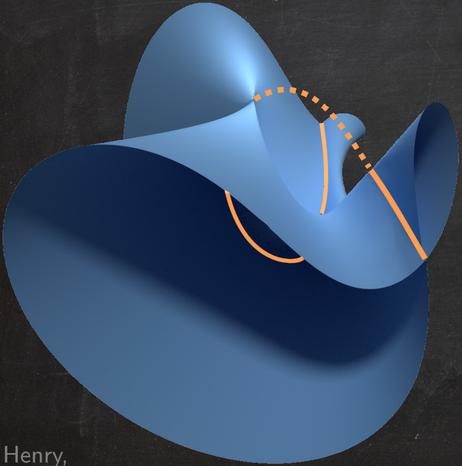

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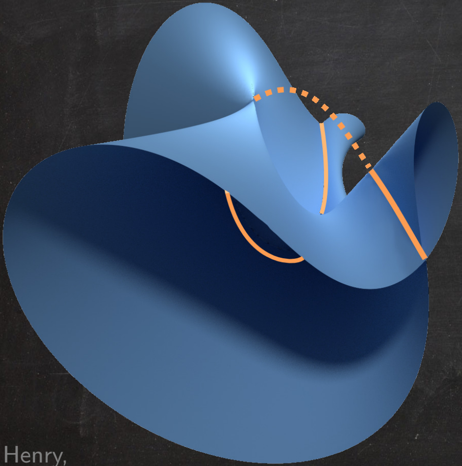

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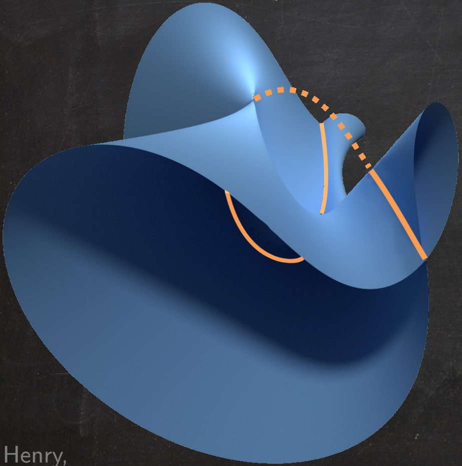

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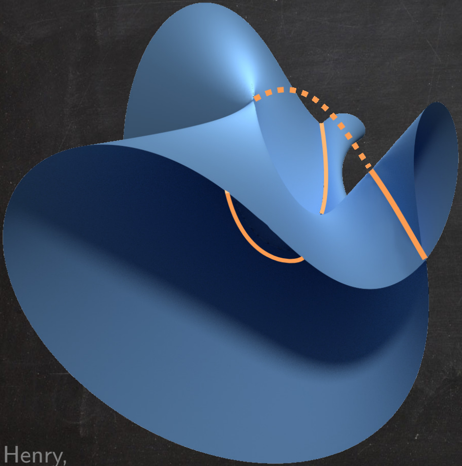

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- $\mathrm{GL}(d)$-symmetries of V and $K^\top Q$ of neighboring layers

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fibers of the parametrization

Takeaway

Fibers of the parameterization control the dimension and symmetries of the neuromanifold.

Together with the parameterization's critical points, they explain the singularities of the neuromanifold.

critical point theory & discriminants

Goal: minimize the loss

$$\mathcal{L}_{\mathcal{D}} : \mathbb{R}^N \xrightarrow{\mu} \mathcal{M} \xrightarrow{\ell_{\mathcal{D}}} \mathbb{R}.$$

critical point theory & discriminants

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Critical points of $\mathcal{L}_{\mathcal{D}}$ arise in various ways:

1. they can be caused by the parametrization μ
   (i.e., $\theta \in \mathrm{Crit}(\mu)$) such that $\theta \in \mathrm{Crit}(\mathcal{L}_{\mathcal{D}})$ but $\mu(\theta) \notin \mathrm{Crit}(\ell_{\mathcal{D}})$)

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Morse theory

critical point theory & discriminants

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critical point theory & discriminants

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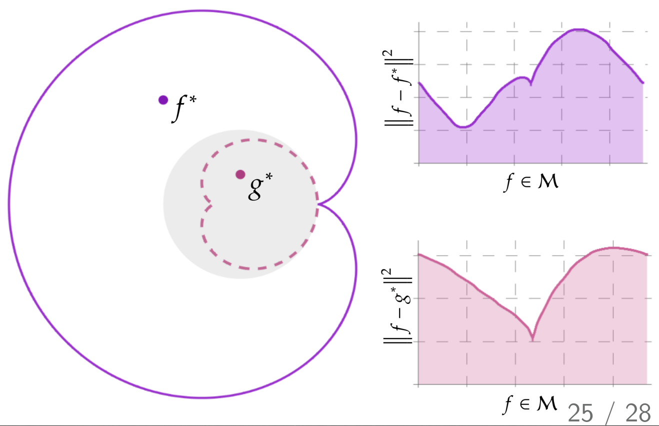
over $\mathbb{C}$: always 4 critical points

over $\mathbb{R}$: 4 or 2 critical points

discriminant = dashed



critical point theory, discriminants, dynamical invariants

Takeaway

The critical points of the loss arise from the geometry of the neuromanifold and its parametrization.

Their number and type can change suddenly as data crosses discriminants.

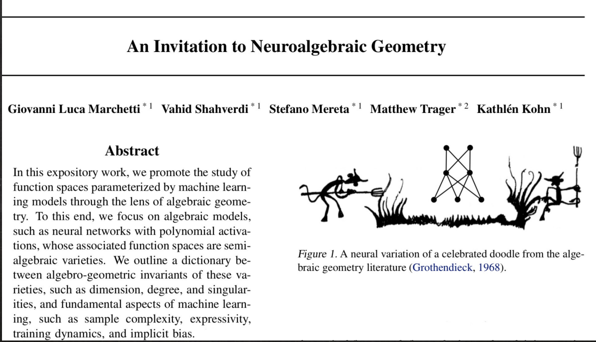
Moreover, algebraic invariants of gradient flow govern the training dynamics...

many future questions

- Describe **all** singularities of MLPs & attention neuromanifolds explicitly, and compute their Voronoi cells. ($\rightsquigarrow$ implicit bias?)
- Compare the type of critical points and more generally the loss landscape of
  - attention networks
  - polynomial convolutional networks
  - polynomial MLPs
- How do skip connections and inhomogeneous activations regularize μ (i.e., less spurious critical points) and smoothen out singularities?
- What happens to the neuromanifold when imposing group equivariance?
- What about ReLU networks, or more generally piecewise rational activation?
- Beyond algebraic geometry: tame geometry of o-minimal structures

thanks for your attention!

machine learning	algebraic geometry
sample complexity & expressivity	dimension, degree, covering number
subnetworks & implicit bias	singularities
identifiability & hidden symmetries	fibers of the parametrization
optimization & gradient descent	critical point theory, discriminants, dynamical invariants



An Invitation to Neuroalgebraic Geometry

Giovanni Luca Marchetti [*1] Vahid Shahverdi [*1] Stefano Mereta [*1] Matthew Trager [*2] Kathlén Kohn [*1]

Abstract

In this expository work, we promote the study of function spaces parameterized by machine learning models through the lens of algebraic geometry. To this end, we focus on algebraic models, such as neural networks with polynomial activations, whose associated function spaces are semi-algebraic varieties. We outline a dictionary between algebro-geometric invariants of these varieties, such as dimension, degree, and singularities, and fundamental aspects of machine learning, such as sample complexity, expressivity, training dynamics, and implicit bias.

Figure 1. A neural variation of a celebrated doodle from the algebraic geometry literature (Grothendieck, 1968).

Neuroalgebraic Geometry

algebraic NNs

↓ polynomial approximation

target NN

studies nonlinear models
in finite-dimensional ambient space

aims to draw conclusions
in the limit

NTK approach

target NN

↓ increase width

∞-width NN

studies linearized models
in ∞-dimensional ambient space

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