

Algebraic Neural Network Theory



Kathlén Kohn

KTH
Digital Futures

digital futures

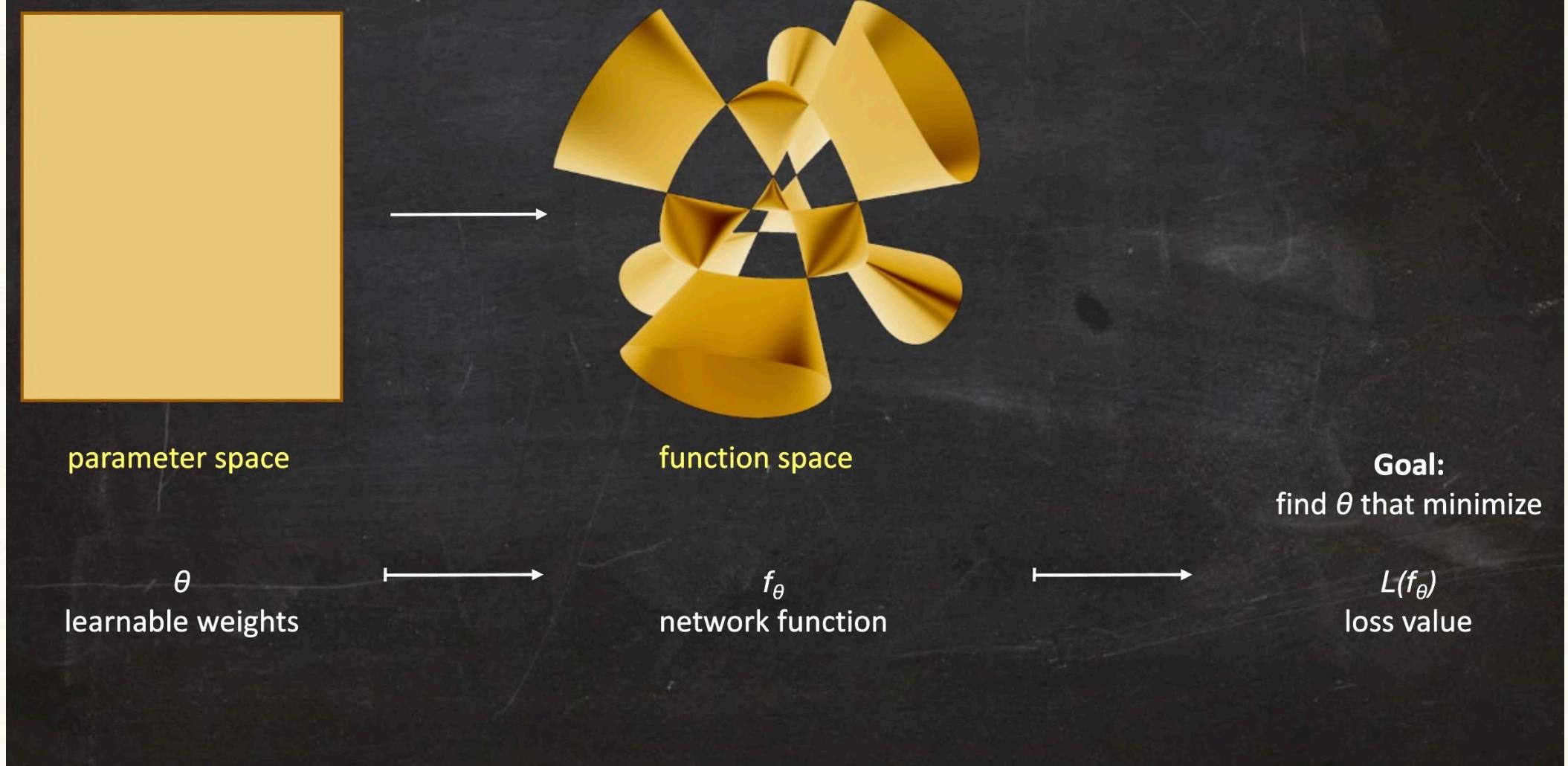
WASP | WALLENBERG AI
AUTONOMOUS SYSTEMS
AND SOFTWARE PROGRAM

**SF
SG** SWEDISH
FOUNDATIONS'
STARTING GRANT

 **Ragnar Söderbergs
STIFTELSE**

 Göran Gustafssons Stiftelser

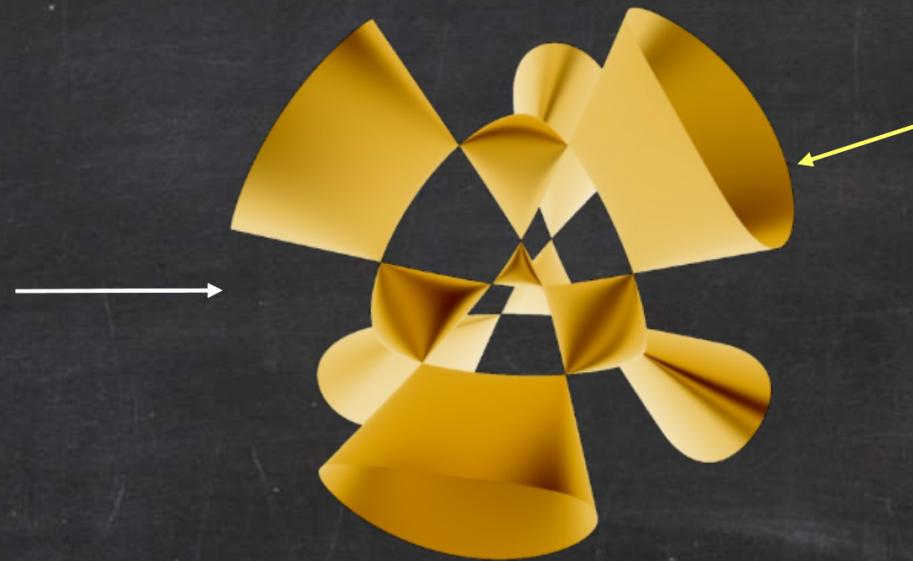
deep learning in a nutshell



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parameter space



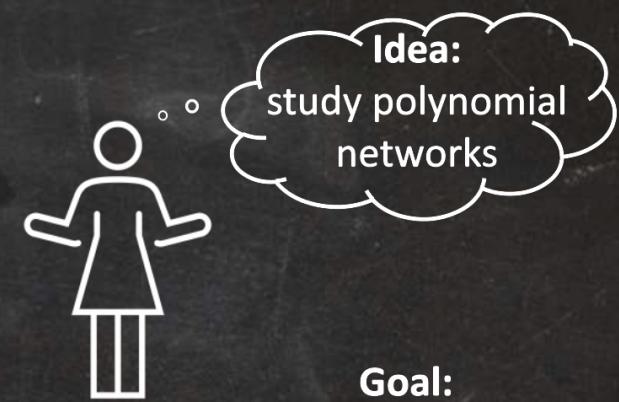
function space

θ
learnable weights



f_θ
network function

neuromaniifold (Amari et. al 2001)
extremely hard to understand!



Goal:
find θ that minimize

$L(f_\theta)$
loss value

Example: MLPs

multilayer perceptrons

$$\alpha_L \circ \sigma \circ \dots \circ \sigma \circ \alpha_2 \circ \sigma \circ \alpha_1$$

α_i = learnable affine linear functions

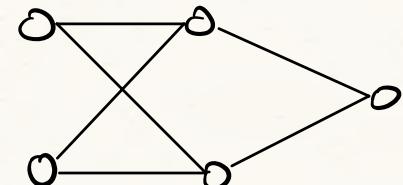
σ = nonlinear activation function, applied entrywise

we assume: σ is a univariate polynomial

Ex: $\sigma(x) = x^2$

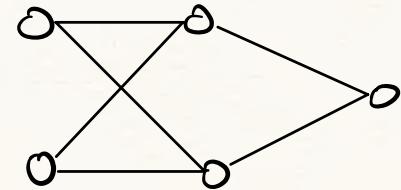
$$[e \ f] \sigma \left(\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \right)$$

Which functions does this MLP parametrize?



Ex: $\sigma(x) = x^2$

$$[e \ f] \sigma \left(\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \right)$$



Which functions does this MLP parametrize?

$$e^{(ax+by)^2} + f(cx+dy)^2$$

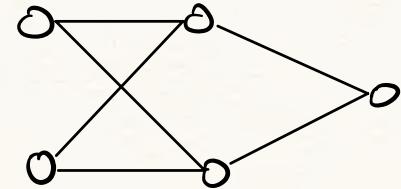
$$= \underbrace{(a^2e + c^2f)}_A x^2 + \underbrace{2(abe + cdf)}_B xy + \underbrace{(b^2e + d^2f)}_C y^2$$

Can you obtain all of $\mathbb{R}[x,y]_2$?

↖ homogeneous quadratic polynomials in x,y
 i.e., are all values for A, B, C possible?

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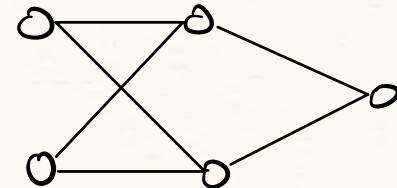
↖ homogeneous quadratic polynomials in x,y
 i.e., are all values for A, B, C possible?

YES

What about $\sigma(x) = x^3$?

Ex: $\sigma(x) = x^3$

$$\begin{bmatrix} e & f \end{bmatrix} \sigma \left(\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \right)$$



Which functions does this MLP parametrize?

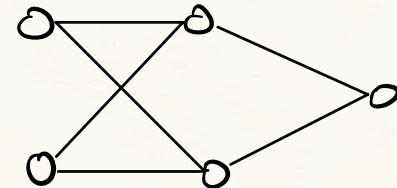
$$\begin{aligned} & e(ax+by)^3 + f(cx+dy)^3 \\ &= \underbrace{(a^3e + c^3f)}_A x^3 + \underbrace{3(a^2be + c^2df)}_B x^2y + \underbrace{3(ab^2e + cd^2f)}_C xy^2 + \underbrace{(b^3e + d^3f)}_D y^3 \end{aligned}$$

Can you obtain all of $\mathbb{R}[x,y]_3$?

i.e., are all values for A,B,C,D possible?
↗ homogeneous cubic polynomials in x,y

Ex: $\sigma(x) = x^3$

$$[e \ f] \sigma \begin{pmatrix} [a \ b] & [x] \\ [c \ d] & [y] \end{pmatrix}$$



Which functions does this MLP parametrize?

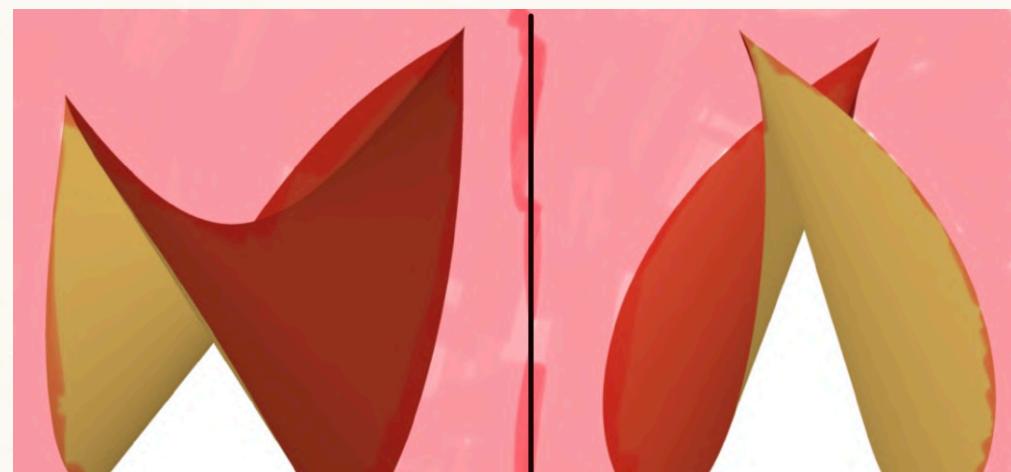
$$e(ax+by)^3 + f(cx+dy)^3$$

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Can you obtain all of $\mathbb{R}[x,y]_3$?

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No, e.g. $A = 1$
 $B = 0$
 $C = -1$
 $D = 0$



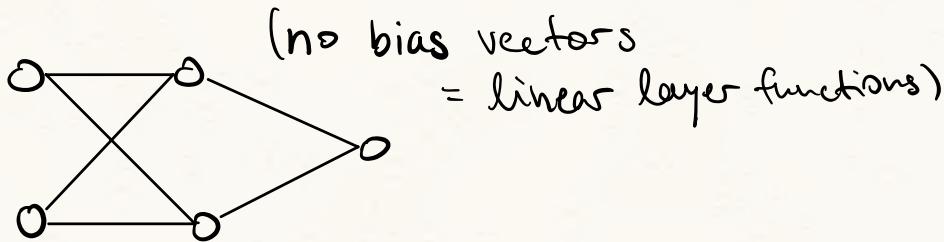
Neuromanifolds

A parametric machine learning model is a map $\mu: \Theta \times X \rightarrow Y$.

$\Theta \times X \xrightarrow{\text{parameters}} Y \xleftarrow{\text{inputs}} \text{outputs}$

Its **neuromanifold** is $M := \{\mu(\theta, \cdot): X \rightarrow Y \mid \theta \in \Theta\}$.

Example
MLPs:



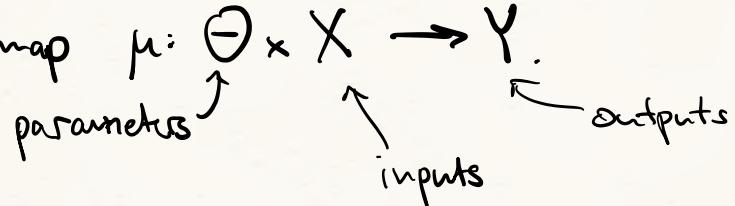
$$\sigma(x) = x^2 \Rightarrow M = \mathbb{R}[x_1, y]_2$$

$$\sigma(x) = x^3 \Rightarrow M \subsetneq \mathbb{R}[x_1, y]_3$$

$$\sigma(x) = x \Rightarrow ?$$

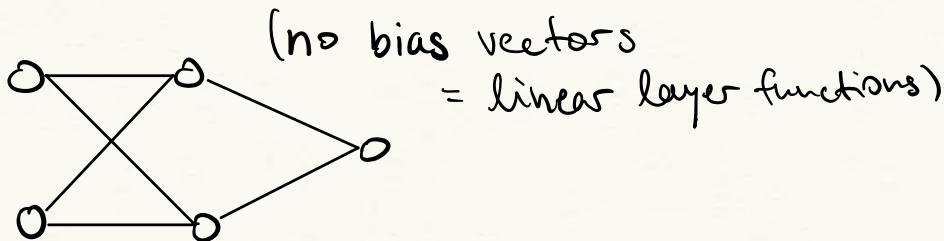
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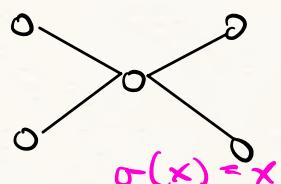
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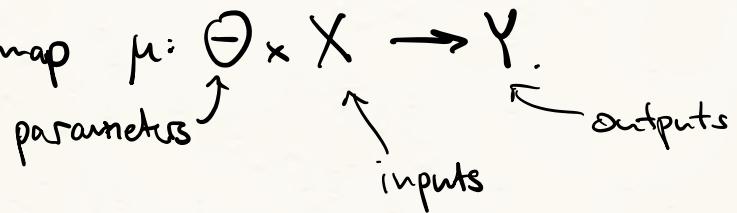
$$\sigma(x) = x \Rightarrow M = \mathbb{R}^{1 \times 2}$$



$$\begin{bmatrix} c \\ d \end{bmatrix} \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \Rightarrow M = ?$$

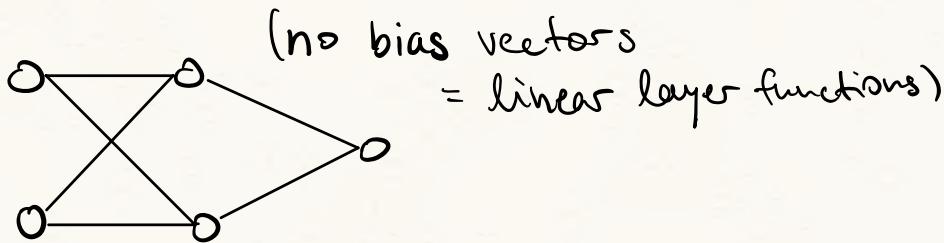
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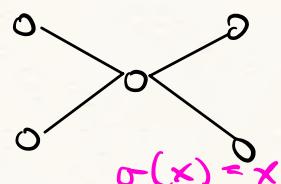
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$$\sigma(x) = x \Rightarrow M = \mathbb{R}^{1 \times 2}$$



$$\begin{bmatrix} c \\ d \end{bmatrix} \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \Rightarrow M = \{ W \in \mathbb{R}^{2 \times 2} \mid \text{rk}(W) \leq 1 \}$$

Linear MLPs: $\alpha_L \circ \dots \circ \alpha_2 \circ \alpha_1$, where

$\alpha_i: \mathbb{R}^{d_{i-1}} \rightarrow \mathbb{R}^{d_i}$ linear

$$\Rightarrow \mathcal{M} = \{W \in \mathbb{R}^{d_L \times d_0} \mid \text{rk}(W) \leq \min\{d_0, d_1, \dots, d_L\}\}$$

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Polynomial MLPs: $\alpha_L \circ \sigma \circ \dots \circ \sigma \circ \alpha_2 \circ \sigma \circ \alpha_1$, where
 $\alpha_i: \mathbb{R}^{d_{i-1}} \rightarrow \mathbb{R}^{d_i}$ affine linear
 $\sigma \in \mathbb{R}[x]_{\leq s}$
 $\Rightarrow \mathcal{M}$ lives in a finite-dimensional vector space, namely
 $(\mathbb{R}[x_1, \dots, x_{d_0}]_{\leq g^{L-1}})^{d_L}$

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Polynomial MLPs are the only ones with that property!

Universal Approximation Theorem

Leshno, Lin, Pinkus, Schocken: Multilayer feedforward networks with a non-polynomial activation function can approximate any function.
Neural Networks 6, 1993:

Theorem 1:

Let $\sigma \in M$. Set

$$\Sigma_n = \text{span} \{ \sigma(w \cdot x + \theta) : w \in R^n, \theta \in R \}.$$

Then Σ_n is dense in $C(R^n)$ if and only if σ is not an algebraic polynomial (a.e.).

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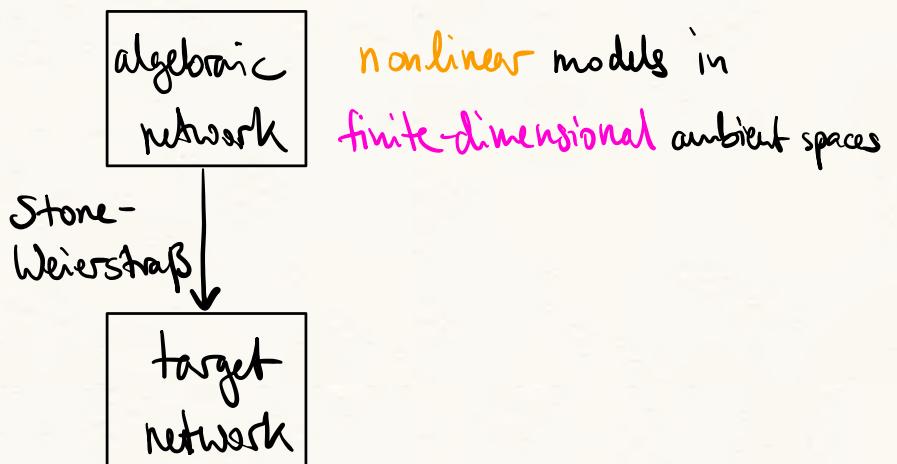
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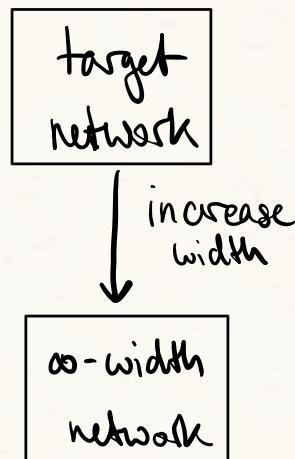
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polynomials are the choice
to approximate networks with
finite-dimensional models

AG approach



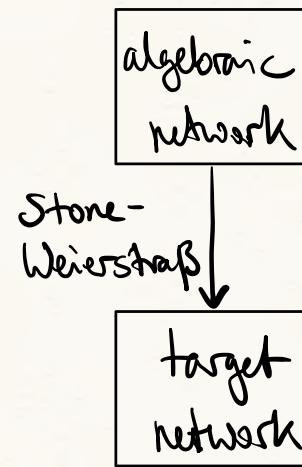
NTK approach



linearized models

at ∞ dimension

AG approach



nonlinear models in
finite-dimensional ambient spaces

Neural Tangent Kernel: Convergence and Generalization in Neural Networks

Arthur Jacot, Franck Gabriel, Clement Hongler

Advances in Neural Information Processing Systems 31 (NeurIPS 2018)

> 4000 citations

Network training = "distance" minimization

Let $M \subseteq V := \left(\mathbb{R}[x_1, \dots, x_{d_o}] \leq \mathcal{D} \right)^{d_L}$,
↑ neuromanifold

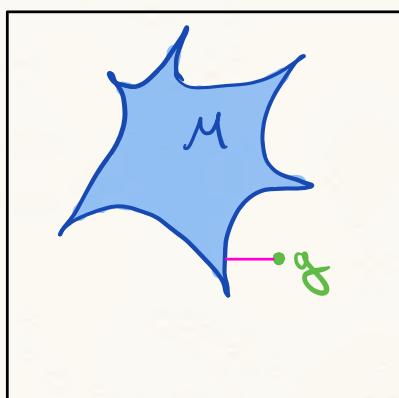
$S \subseteq \mathbb{R}^{d_o} \times \mathbb{R}^{d_L}$ finite dataset,

MSE loss: $\mathcal{L}(f) := \sum_{(a, b) \in S} \|f(a) - b\|^2$

↳ $\text{dist}(f, g) = 0$ possible for $f \neq g$

Proposition: There is a pseudometric $\text{dist}: V \times V \rightarrow \mathbb{R}_{\geq 0}$ and some $g \in V$ such that minimizing $\mathcal{L}(f)$ over $f \in M$ is equivalent to minimizing $\text{dist}(f, g)$ over $f \in M$.

V



Why?

Network training = "distance" minimization

Let $M \subseteq V := \left(\mathbb{R}[x_1, \dots, x_{d_o}] \leq D \right)^{d_L}$,
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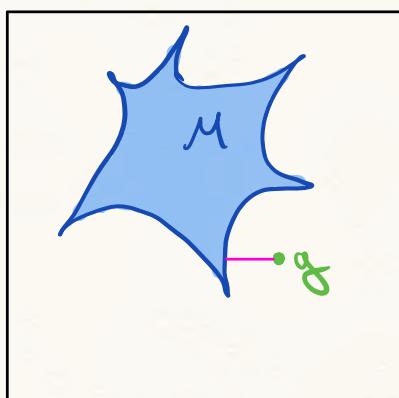
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V



Assume: $d_L = 1$

Let $v_D: (x_1, \dots, x_{d_o}) \mapsto (\text{all monomials in } x_1, \dots, x_{d_o} \text{ of degree } \leq D)$,
 c_f be coefficient vector of $f \in V$ such that $f(x) = v_D(x) \cdot c_f$,

Veronese
embedding ↗

Network training = "distance" minimization

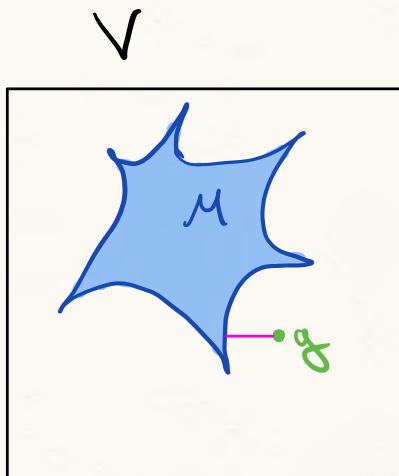
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 A & B matrices whose rows are $v_D(a) \& b$, resp., over all $(a, b) \in S$

Veronese
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$$\Rightarrow \mathcal{L}(f) = \|A c_f - B\|^2$$

Network training = "distance" minimization

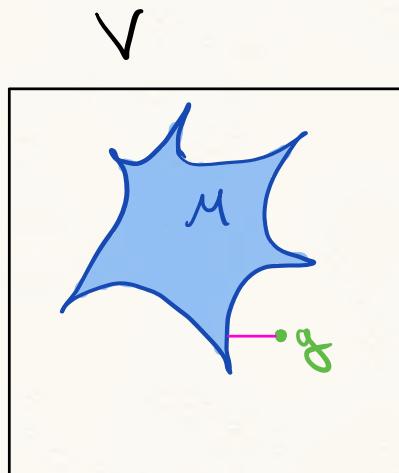
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 A & B matrices whose rows are $v_D(a) \& b$, resp., over all $(a, b) \in S$

Veronese
embedding ↗

$$\Rightarrow \mathcal{L}(f) = \|A c_f - B\|^2 = \|c_f - A^+ B\|^2 \xrightarrow{\text{pseudoinverse}} + \text{const.}$$

$$\sim \|c\|_Q := c^T Q c$$

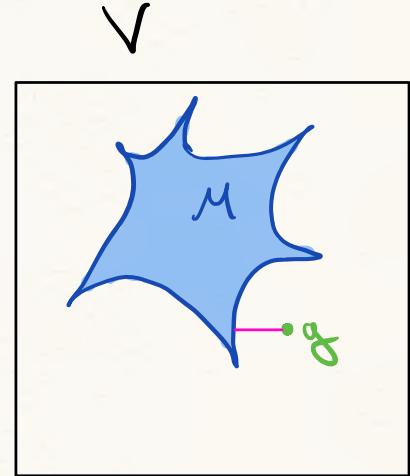
$$\underset{f \in M}{\operatorname{argmin}} \quad L(f) = \underset{f \in M}{\operatorname{argmin}} \quad \| C_f - A^T B \|_{A^T A}^2$$

Observations ($d_L=1$):

① $A^T A$ depends only on input data,
 $A^T B$ on both input & output

② $A^T A \in \mathbb{R}^{\dim V \times \dim V}$ is rank-deficient whenever $|S| < \dim V \Rightarrow$ pseudometric
 \downarrow
(LLMs: $|S| < \dim M$)

③



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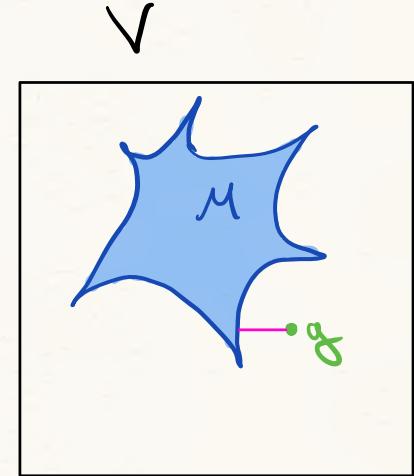
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③ even when $|S| \geq \dim V$, $A^T A$ is not an arbitrary symmetric PD matrix,
while $A^T B$ yields all vectors $\in \mathbb{R}^{\dim V}$

Why?

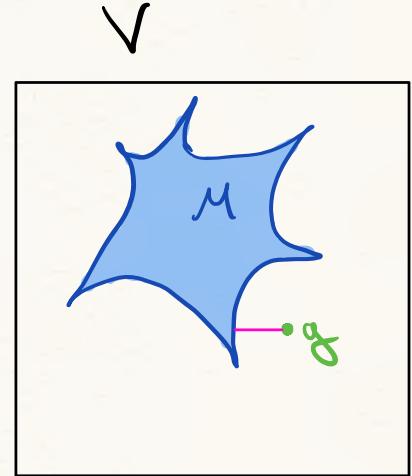
Which matrices can be obtained?

(try for $d_L=1$: $v(x) = (1, x, x^2, \dots, x^D)$)



$$\underset{f \in M}{\operatorname{argmin}} \quad L(f) = \underset{f \in M}{\operatorname{argmin}} \quad \| C_f - A^T B \|^2_{A^T A}$$

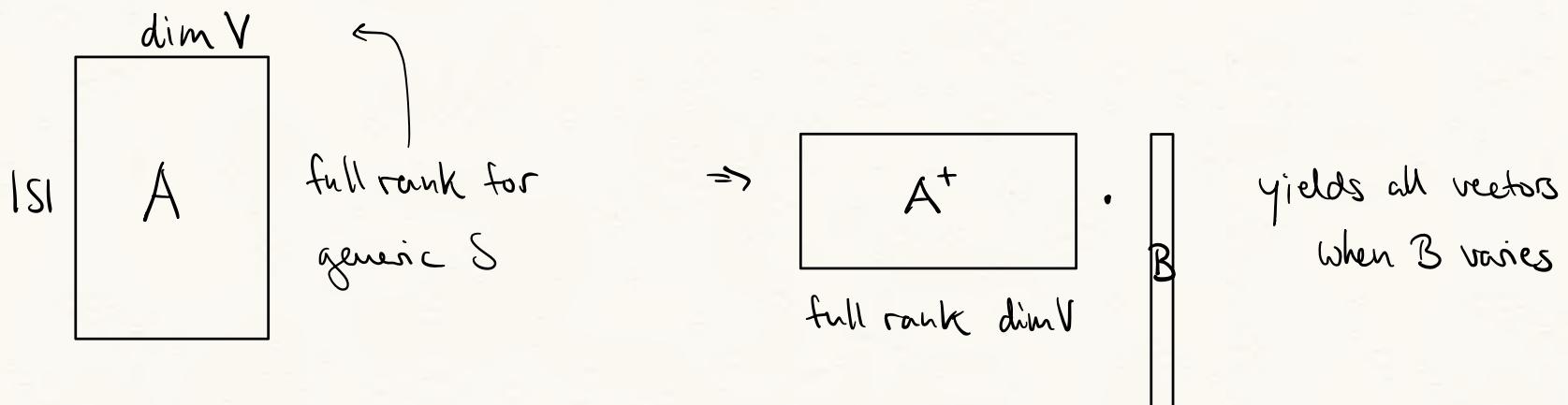
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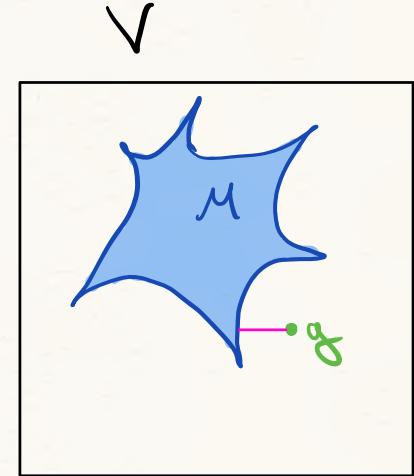
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$$A^T A = \begin{array}{c|c|c|c} & & & \\ \downarrow i & & & \\ \boxed{\begin{array}{c|c|c} v(a_1) & \cdots & v(a_{|S|}) \\ \hline & & \end{array}} & \boxed{\begin{array}{c} v(a_1) \\ \vdots \\ v(a_{|S|}) \end{array}} & & \end{array}$$

has (i, j) entry $\sum_{(a, b) \in S} v_i(a) v_j(b)$
 monomial of degree $\leq 2D$
 that can be factored in several ways

Ex.: $d_0 = 1$

$$\Rightarrow v(x) = (1, x, x^2, \dots, x^D)$$

$$\Rightarrow A = \begin{bmatrix} 1 & a_1 & a_1^2 & \dots & a_1^D \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & a_{151} & a_{151}^2 & \dots & a_{151}^D \end{bmatrix} \text{ Vandermonde matrix}$$

$$\Rightarrow A^T A = \begin{bmatrix} |S| & \sum a_k & \sum a_k^2 & \dots & \sum a_k^D \\ \sum a_k & \sum a_k^2 & \sum a_k^3 & \dots & \sum a_k^{D+1} \\ \sum a_k^2 & \sum a_k^3 & \sum a_k^4 & \dots & \sum a_k^{D+2} \\ \vdots & \vdots & \vdots & & \vdots \\ \sum a_k^D & \sum a_k^{D+1} & \sum a_k^{D+2} & \dots & \sum a_k^{2D} \end{bmatrix} \text{ Hankel matrix}$$

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$$\Rightarrow v(x) = (1, x, x^2, \dots, x^D)$$

$$\Rightarrow A = \begin{bmatrix} 1 & a_1 & a_1^2 & \dots & a_1^D \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & a_{151} & a_{151}^2 & \dots & a_{151}^D \end{bmatrix} \text{ Vandermonde matrix}$$

$$\Rightarrow A^T A = \begin{bmatrix} \sum a_k & \sum a_k^2 & \sum a_k^3 & \dots & \sum a_k^D \\ \sum a_k^2 & \sum a_k^4 & \sum a_k^6 & \dots & \sum a_k^{D+1} \\ \sum a_k^3 & \sum a_k^6 & \sum a_k^9 & \dots & \sum a_k^{D+2} \\ \vdots & \vdots & \vdots & & \vdots \\ \sum a_k^D & \sum a_k^{D+1} & \sum a_k^{D+2} & \dots & \sum a_k^{2D} \end{bmatrix} \text{ Hankel matrix}$$

Ex.: $d_0 = 2, D = 2$

$$\Rightarrow v(x, y) = (1, x, y, x^2, xy, y^2)$$

$$\Rightarrow A^T A = \sum_{\substack{(a,b) \in S \\ a = (x,y)}} \begin{bmatrix} 1 & x & y & x^2 & xy & y^2 \\ 1 & x & y & x^2 & xy & y^2 \\ x & x^2 & xy & x^3 & x^2y & xy^2 \\ y & xy & y^2 & x^3y & x^2y^2 & y^3 \\ x^2 & x^3 & x^2y & x^4 & x^3y & x^2y^2 \\ xy & x^2y & xy^2 & x^3y & x^2y^2 & xy^3 \\ y^2 & xy^2 & y^3 & x^2y^2 & x^3y^3 & y^4 \end{bmatrix} \begin{bmatrix} 1 \\ x \\ y \\ x^2 \\ xy \\ y^2 \end{bmatrix}$$

Network training = "distance" minimization

Let $M \subseteq V := \left(\mathbb{R}[x_1, \dots, x_{d_o}] \leq \mathbb{D} \right)^{d_L}$,
 ↪ neuromaniifold

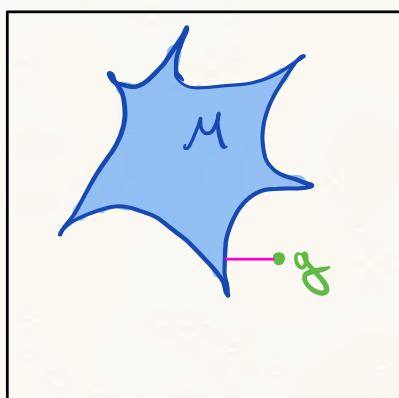
$S \subseteq \mathbb{R}^{d_o} \times \mathbb{R}^{d_L}$ finite dataset,

MSE loss: $\mathcal{L}(f) := \sum_{(a, b) \in S} \|f(a) - b\|^2$

↳ $\text{dist}(f, g) = 0$ possible for $f \neq g$

Proposition: There is a pseudometric $\text{dist}: V \times V \rightarrow \mathbb{R}_{\geq 0}$ and some $g \in V$ such that minimizing $\mathcal{L}(f)$ over $f \in M$ is equivalent to minimizing $\text{dist}(f, g)$ over $f \in M$.

V



$d_L > 1$

$$f = (f_1, \dots, f_{d_L}), \quad C_f := \begin{bmatrix} | & | \\ c_{f_1} & \cdots & c_{f_{d_L}} \\ | & | \end{bmatrix}$$

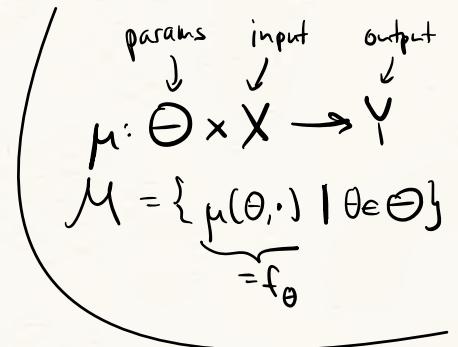
$$\Rightarrow f(x) = v_g(x) \cdot C_f$$

$$\|C\|_Q^2 := \text{tr}(C^T Q C)$$

$$\Rightarrow \mathcal{L}(f) = \|A C_f - B\|_{\text{Frob}}^2 = \|C_f - A^T B\|_{A^T A}^2 + \text{const.}$$

Loss Landscape

$$= \{(\theta, \mathcal{L}(f_\theta)) \mid \theta \in \Theta\}$$



Loss Landscape

$$= \{(\theta, \mathcal{L}(f_\theta)) \mid \theta \in \Theta\}$$

params \downarrow input \downarrow output \downarrow
 $\mu: \Theta \times X \rightarrow \mathbb{Y}$
 $M = \underbrace{\{\mu(\theta, \cdot) \mid \theta \in \Theta\}}_{=f_\theta}$

can be studied in a decoupled way:

$$\Theta \xrightarrow{\quad} M \xrightarrow{\mathcal{L}} \mathbb{R}$$

$$\theta \xrightarrow{\quad} f_\theta$$

$\left. \begin{matrix} \\ \\ \end{matrix} \right\}$
 Loss landscape in function space:

$$= \{(f, \mathcal{L}(f)) \mid f \in M\} \subseteq V \times \mathbb{R}$$

Loss Landscape

$$= \{(\theta, \mathcal{L}(f_\theta)) \mid \theta \in \Theta\}$$

params input output

$$\mu: \Theta \times X \rightarrow \mathbb{Y}$$

$$\mathcal{M} = \underbrace{\{\mu(\theta, \cdot) \mid \theta \in \Theta\}}_{= f_\theta}$$

can be studied in a decoupled way:

$$\begin{array}{ccc} \Theta & \xrightarrow{\quad} & \mathcal{M} \\ \theta & \xrightarrow{\quad} & f_\theta \end{array}$$

}

loss landscape in function space:

$$= \{(f, \mathcal{L}(f)) \mid f \in \mathcal{M}\} \subseteq \mathbb{V} \times \mathbb{R}$$

Geometry of \mathcal{M} affects loss landscape!

How?

Which geometric properties does \mathcal{M} have?

***Position: Algebra Unveils Deep Learning
An Invitation to Neuroalgebraic Geometry***

Giovanni Luca Marchetti ^{* 1} Vahid Shahverdi ^{* 1} Stefano Mereta ^{* 1} Matthew Trager ^{* 2} Kathlén Kohn ^{* 1}

Machine Learning Algebraic Geometry

sample complexity and expressivity

dimension, degree, and covering number

subnetworks and implicit bias

singularities

identifiability and invariance

fibers of the parameterization

optimization and gradient descent

critical point theory, discriminants, and dynamical invariants

Identifiability

$$\begin{array}{ccc} \Theta & \xrightarrow{\mu} & \mathcal{M} \\ \theta & \longmapsto & f_\theta \end{array}$$

Given (generic) $f \in \mathcal{M}$,
what is $\hat{\mu}^{-1}(f)$?

Identifiability

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Given (generic) $f \in \mathcal{M}$,
what is $\hat{\mu}^{-1}(f)$?

For monomial MLP with $\sigma(x) = x^r, r >> 0$:

$$\begin{aligned} \mu: \mathbb{R}^{d_L \times d_{L-1}} \times \cdots \times \mathbb{R}^{d_1 \times d_0} &\longrightarrow \mathcal{M} \\ ((w_L, \dots, w_1)) &\longmapsto w_L \circ \sigma \circ \cdots \circ \sigma \circ w_2 \circ \sigma \circ w_1 \end{aligned}$$

What is the generic fiber?

Identifiability

$$\begin{array}{ccc} \Theta & \xrightarrow{\mu} & \mathcal{M} \\ \theta & \longmapsto & f_\theta \end{array}$$

Given (generic) $f \in \mathcal{M}$,
what is $\hat{\mu}(f)$?

For monomial MLP with $\sigma(x) = x^r, r > 0$:

$$\begin{array}{ccc} \mu: \mathbb{R}^{d_L \times d_{L-1}} \times \cdots \times \mathbb{R}^{d_1 \times d_0} & \longrightarrow & \mathcal{M} \\ ((w_L, \dots, w_1)) & \longmapsto & w_L \circ \sigma \circ \cdots \circ \sigma \circ w_2 \circ \sigma \circ w_1 \end{array}$$

Observation: $D_i \in GL(d_i)$ diagonal

$P_i \in GL(d_i)$ permutation matrix

$$\begin{aligned} \Rightarrow \mu(w_L D_{L-1}^{-r} P_{L-1}^T, \dots, P_2 D_2 w_2 D_1^{-r} P_1^T, P_1 D_1 w_1) \\ = \mu(w_L, \dots, w_2, w_1) \end{aligned}$$

On the Expressive Power of
Deep Polynomial Neural Networks 2019

Joe Kileel*
Princeton University

Matthew Trager*
New York University

Joan Bruna
New York University

Identifiability

$$\begin{array}{ccc} \Theta & \xrightarrow{\mu} & \mathcal{M} \\ \theta & \longmapsto & f_\theta \end{array}$$

Given (generic) $f \in \mathcal{M}$,
what is $\tilde{\mu}(f)$?

For monomial MLP with $\sigma(x) = x^r, r \gg 0$:

Activation degree thresholds and expressiveness of
polynomial neural networks 2024

Bella Finkel*, Jose Israel Rodriguez†, Chenxi Wu, Thomas Yahl

Proven that those para-
meter symmetries are
the generic fiber
(implicitly described all fibers!)

follow-ups (2025):

THE ALEXANDER-HIRSCHOWITZ THEOREM FOR NEUROVARIETIES

ALEX MASSARENTI AND MASSIMILIANO MELLA

Identifiability of Deep Polynomial Neural Networks

Konstantin Usevich*, Ricardo Borsoi, Clara Dérand, Marianne Clausel†
Université de Lorraine, CNRS, CRAN

Identifiability

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Activation degree thresholds and expressiveness of
polynomial neural networks 2024

Bella Finkel*, Jose Israel Rodriguez†, Chenxi Wu, Thomas Yahl

Proposition 16. Let \mathbb{K} be a subfield of \mathbb{C} . Given integers d, k , there exists an integer $\tilde{r} = \tilde{r}(k)$ with the following property. If $r > \tilde{r}(k)$ and $p_1, \dots, p_k \in \mathbb{K}[x_1, \dots, x_d]$ are pairwise non-proportional, then p_1^r, \dots, p_k^r are linearly independent (over \mathbb{K}). Moreover, $\tilde{r}(k) = 6(k-1)^2 - 6(k-1) + 1$ has the desired property.

Identifiability

$$\begin{array}{ccc} \Theta & \xrightarrow{\mu} & \mathcal{M} \\ \theta & \longmapsto & f_\theta \end{array}$$

Given (generic) $f \in \mathcal{M}$,
what is $\tilde{\mu}^{-1}(f)$?

For polynomial MLP with $\sigma(x) \in \mathbb{R}[x]$ generic, $\sigma \gg 0$:

Conjecture: Generic fiber $\tilde{\mu}^{-1}(f)$ consists only of permutations.

Conjecture: Let $d \in \mathbb{Z}_{>0}$.

There is $\tilde{r} \in \mathbb{Z}_+$ such that all $r > \tilde{r}$ satisfy:

There is $U \subset \mathbb{R}[x] \subset$ Zariski open such that:

For all $\sigma \in U$ and all $p_1, \dots, p_k \in \mathbb{R}[x_1, \dots, x_d]$ non-constant & pairwise distinct:

$\sigma(p_1), \dots, \sigma(p_k)$ are linearly independent.

Geometry of Newmannifolds

$\mu: \Theta \times X \rightarrow Y$ polynomial (in both $\theta \in \Theta$ & $x \in X$)

$$\begin{array}{ccc} \Theta & \longrightarrow & M \\ \theta & \longmapsto & \mu(\theta, \cdot) \end{array}$$

What kind of object is M ?

A **semialgebraic** set!

↑
describable by
polynomial equations
& inequalities

Geometry of Newmannifolds

$\mu: \Theta \times X \rightarrow Y$ polynomial (in both $\theta \in \Theta$ & $x \in X$)

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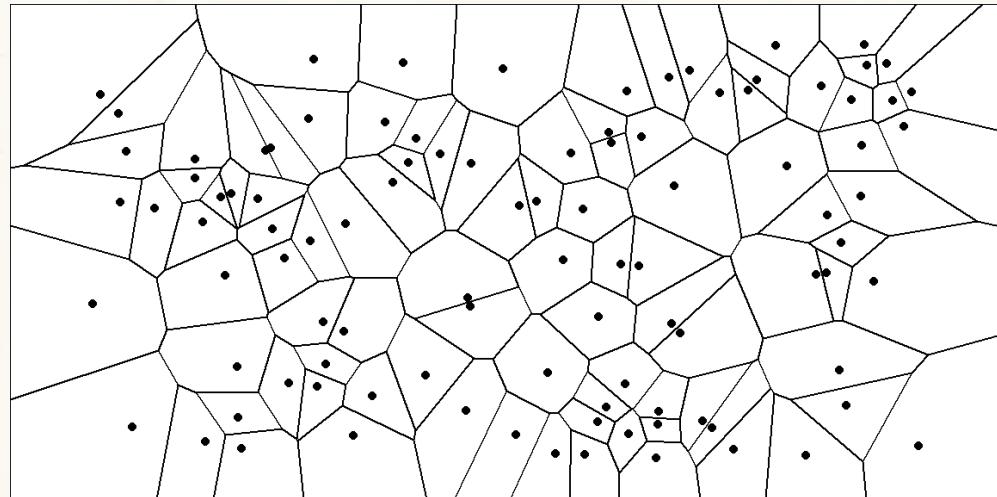
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Euclidean distance
minimization can be
implicitly biased to
singularities & boundaries of M

Voronoi cells



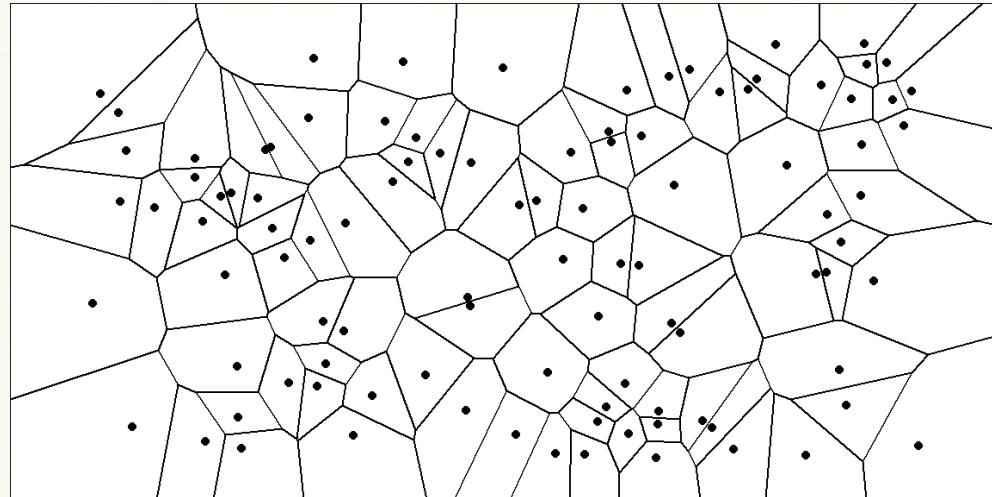
For $S \subseteq \mathbb{R}^n$, the **Voronoi cell** at $p \in S$ is
$$\text{Vor}_S(p) := \{u \in \mathbb{R}^n \mid \forall q \in S, q \neq p: \|p-u\|_2 < \|q-u\|_2\}$$

$$M \in \mathbb{R}^2$$
$$x^2 + y^2 = 1, y \geq 0$$

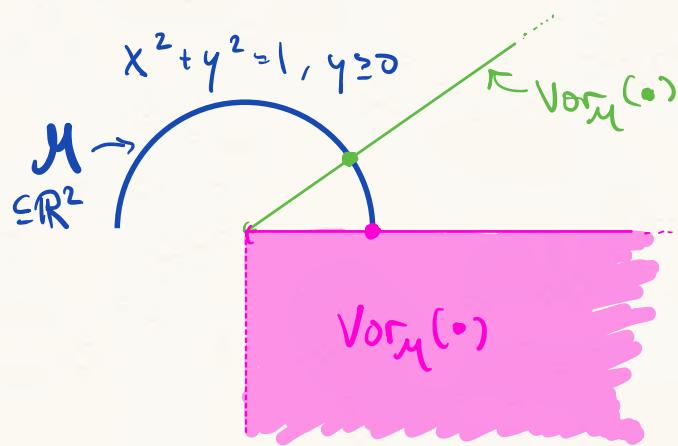
What is the Voronoi cell at •?

What is the Voronoi cell at •?

Voronoi cells



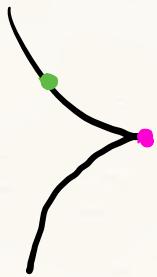
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The **2 relative boundary points** are the only points on M with full-dimensional Voronoi cells!
 ↗ **implicit bias** towards ∂M

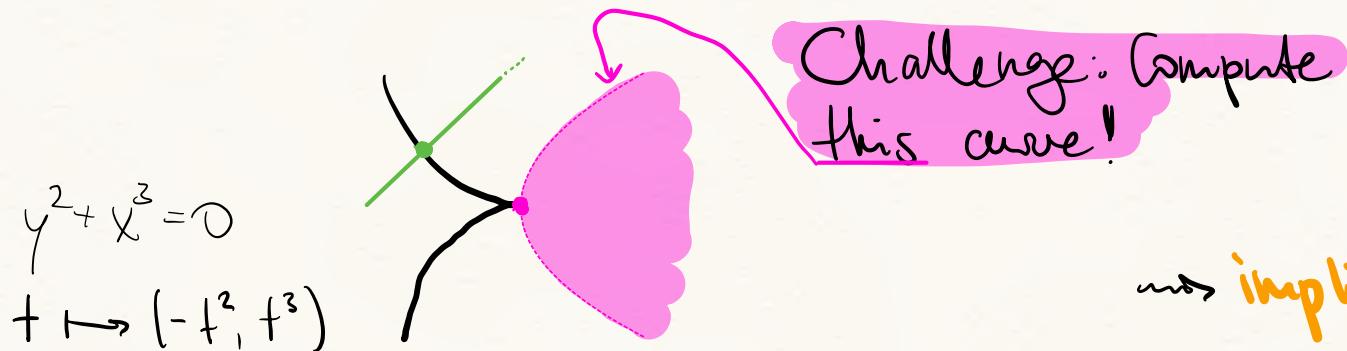
points in ∂M are global minima with positive probability on data u

singularities



What are the Voronoi cells at \bullet and \circ ?

singularities

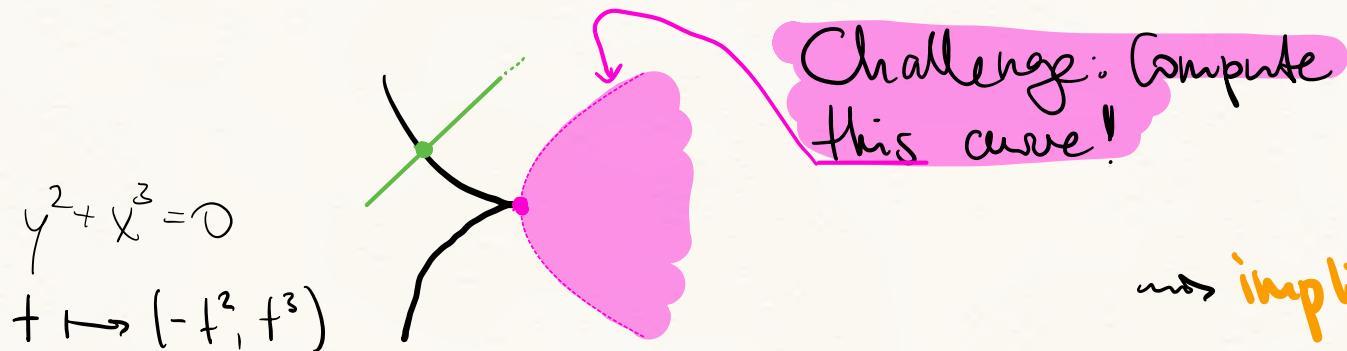


Challenge: Compute
this curve!

→ implicit bias towards $\text{Sing}(M)$

What are the Voronoi cells at \bullet and \bullet ?

singularities



→ **implicit bias** towards $\text{Sing}(M)$

What are the Voronoi cells at and ?

Tradeoff



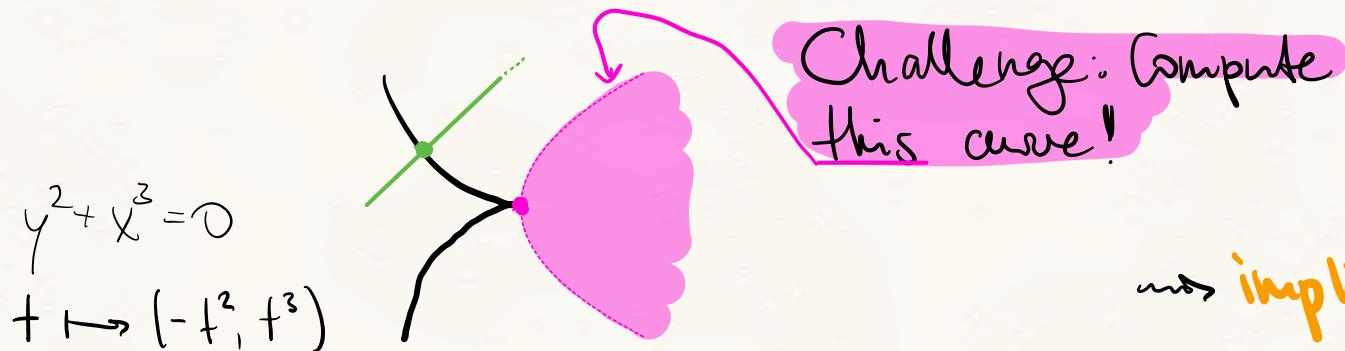
learning close to singularity
→ slow & numerical instability

[Amari et al]



singular solution generalizes better:
① stable global minimum when perturbing data
② **Conjecture:** singularities of neural manifolds
are sparse subnetworks
[We've proven this for MLPs & CNNs]

singularities



→ **implicit bias** towards $\text{Sing}(M)$

What are the Voronoi cells at and ?

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[Amari et al]



singular solution generalizes better:
① stable global minimum when perturbing data
② **Conjecture:** singularities of neural manifolds
are sparse subnetworks

[We've proven this for MLPs & CNNs]

In general: depends on **type** of singularity



MLP

$\sigma(x) =$ generic
polynomial
of large
degree



CNN

These singularities have that tradeoff, while these don't!

In both cases, they are sparse subnetworks ^

What about smooth interior points?

$M \subseteq \mathbb{R}^n$ algebraic variety (i.e. described by polynomial equations)

Q symmetric PD $n \times n$ matrix

Fact: For almost all $u \in \mathbb{R}^n$, the number of complex critical points of

$$\min_{x \in M \setminus \text{Sing}(M)} \|x - u\|_Q^2$$

is the same, called the Euclidean Distance Degree: $\text{EDD}_Q(u)$.

What is $\text{EDD}_{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}(0)$?

What about smooth interior points?

$M \subseteq \mathbb{R}^n$ algebraic variety (i.e. described by polynomial equations)

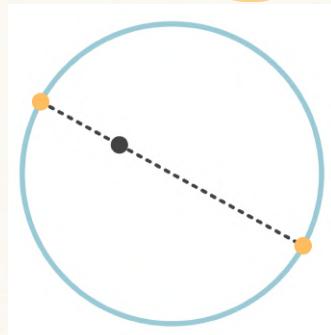
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What is $\text{EDD}_{\begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}}(\bigcirc)$?

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$M \subseteq \mathbb{R}^n$ algebraic variety (i.e. described by polynomial equations)

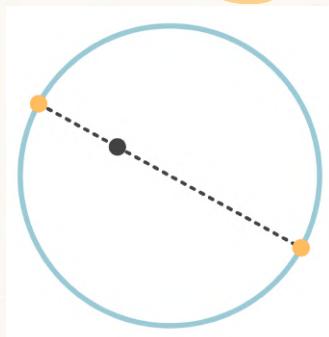
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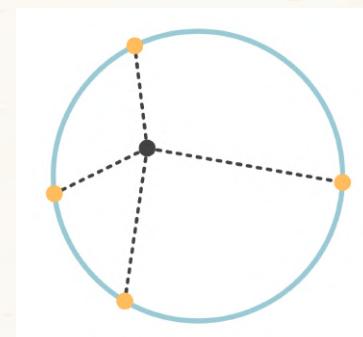
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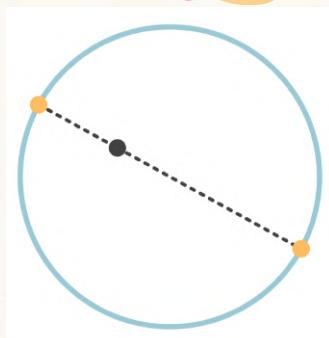
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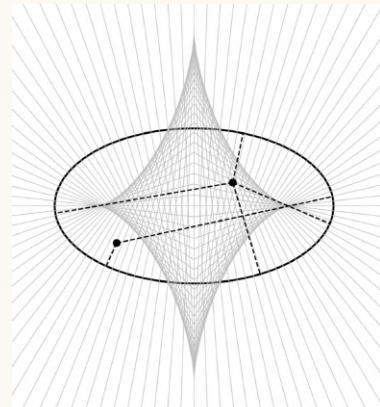
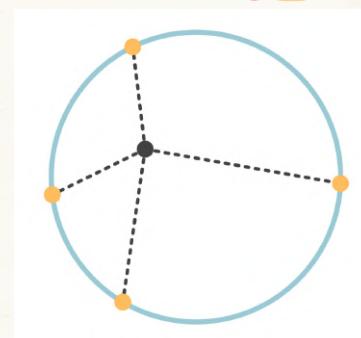
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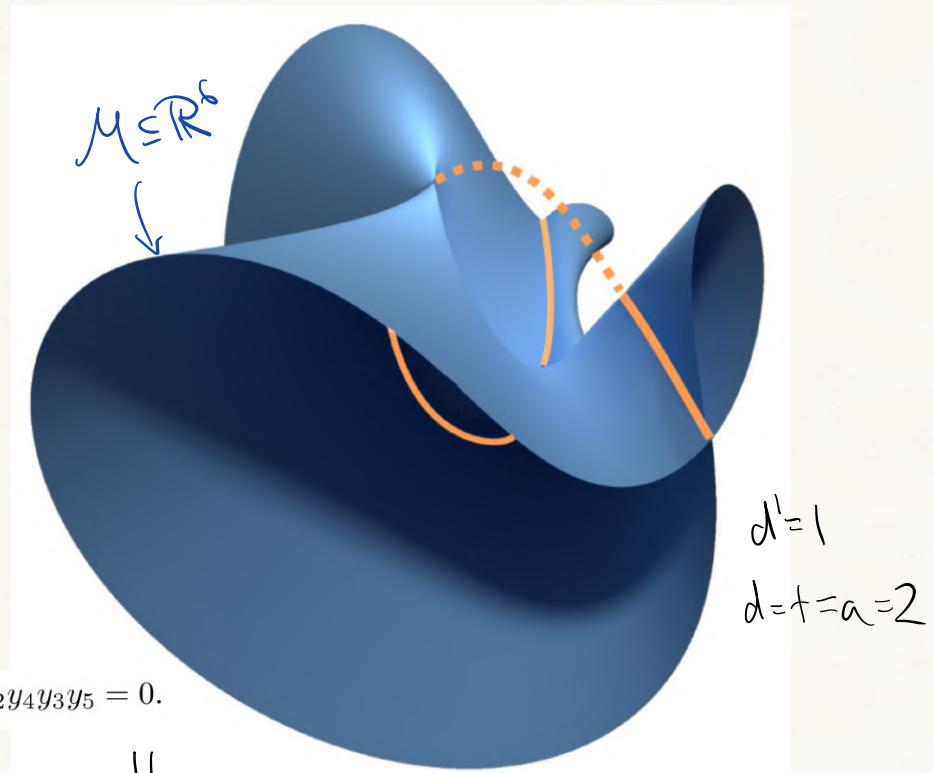


Lightning Self-Attention (single head, single layer)

$$\begin{array}{ccc}
 \mathbb{R}^{d \times t} & \xrightarrow{\quad} & \mathbb{R}^{d \times t} \\
 X & \mapsto & \mathbb{V} X X^T K^T Q X
 \end{array}$$

learnable parameters
 $\mathbb{V} \in \mathbb{R}^{d \times d}$, $K, Q \in \mathbb{R}^{a \times d}$

$$y_1^2 y_6^2 + y_4^2 y_3^2 + y_1 y_3 y_5^2 + y_2^2 y_4 y_6 - 2 y_1 y_4 y_3 y_6 - y_2 y_1 y_6 y_5 - y_2 y_4 y_3 y_5 = 0.$$



For almost all PD matrices Q ,
 $\text{EDD}_Q(M) = 14$.

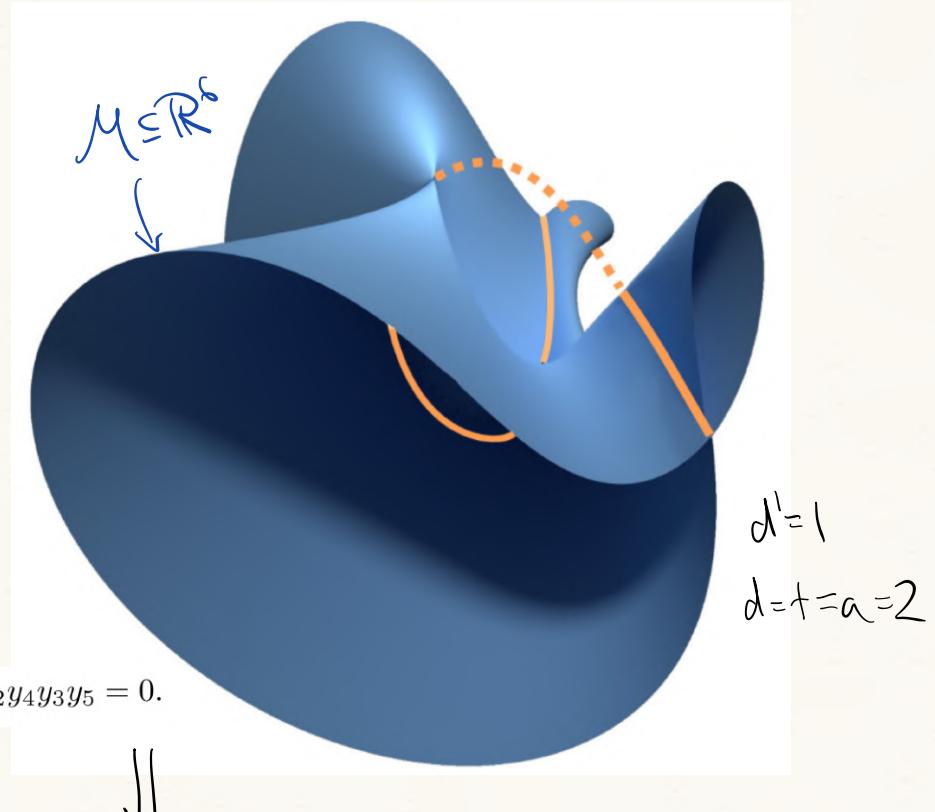
What happens if Q becomes degenerate?

(i.e., Q is symmetric positive semidefinite)

Lightning Self-Attention (single head, single layer)

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 X & \mapsto & \mathbb{V} X X^T K^T Q X \\
 & & \uparrow \quad \quad \quad \uparrow \\
 & & \text{learnable parameters} \\
 & & \mathbb{V} \in \mathbb{R}^{d \times d}, K, Q \in \mathbb{R}^{a \times d}
 \end{array}$$

$$y_1^2 y_6^2 + y_4^2 y_3^2 + y_1 y_3 y_5^2 + y_2^2 y_4 y_6 - 2 y_1 y_4 y_3 y_6 - y_2 y_1 y_6 y_5 - y_2 y_4 y_3 y_5 = 0.$$



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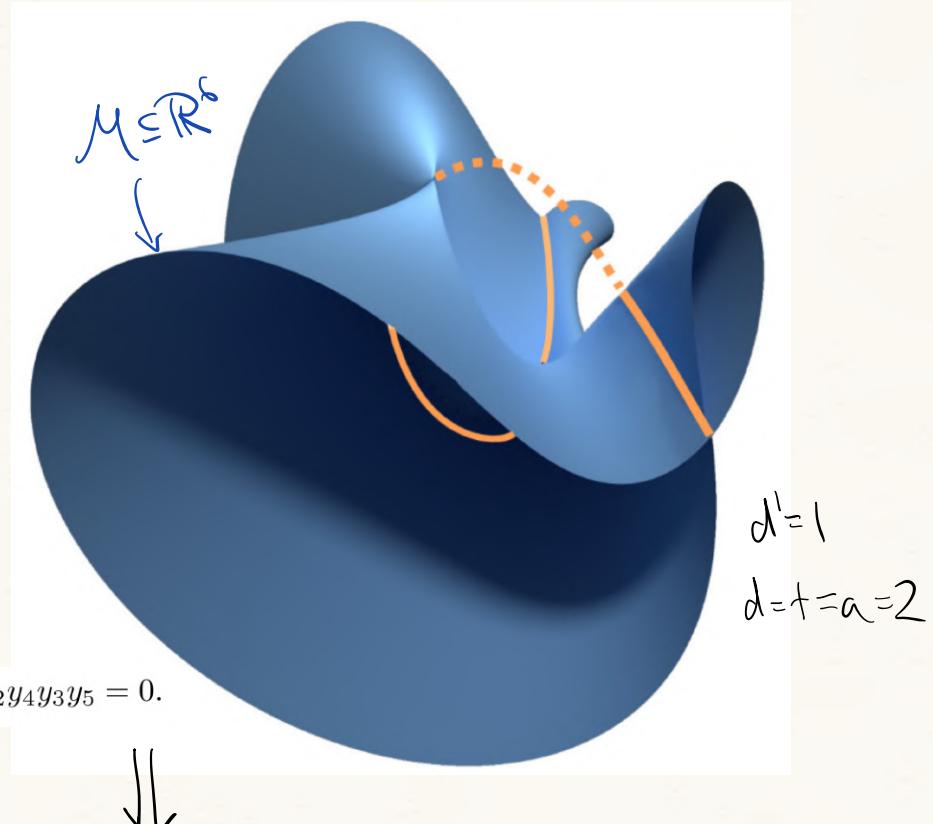
k	complex critical point set
0	14 points
1	14 points
2	4 points + a curve
3	a surface
4	a 3-dimensional subvariety
5	a 4-dimensional subvariety

$K := \dim \ker Q$

Lightning Self-Attention (single head, single layer)

$$\begin{array}{ccc}
 \mathbb{R}^{d \times t} & \xrightarrow{\quad} & \mathbb{R}^{d \times t} \\
 X & \mapsto & V X X^T K^T Q X \\
 & & \uparrow \quad \quad \quad \uparrow \\
 & & \text{learnable parameters} \\
 & & V \in \mathbb{R}^{d \times d}, K, Q \in \mathbb{R}^{a \times d}
 \end{array}$$

$$y_1^2 y_6^2 + y_4^2 y_3^2 + y_1 y_3 y_5^2 + y_2^2 y_4 y_6 - 2 y_1 y_4 y_3 y_6 - y_2 y_1 y_6 y_5 - y_2 y_4 y_3 y_5 = 0.$$



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$K := \dim \ker Q$

$M \cap (\ker(Q) + u)$
 \hookrightarrow zero loss solutions!

In general

$M \subseteq \mathbb{R}^n$ algebraic variety, $d := \dim M$.

Q symmetric positive semi-definite $n \times n$ matrix
 $K := \ker Q$

$\pi: \mathbb{R}^n \rightarrow K^\perp$

turns Q into nondegenerate quadric

In general

$M \subseteq \mathbb{R}^n$ algebraic variety, $d := \dim M$.

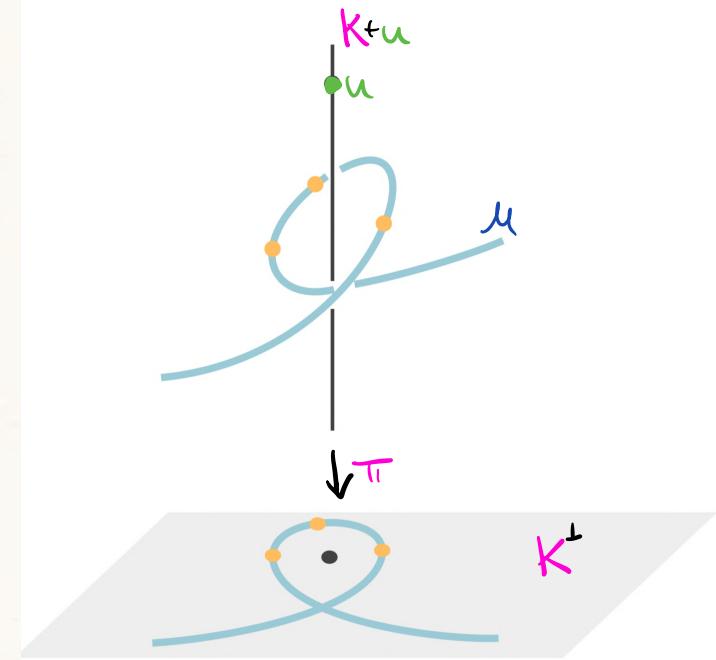
Q symmetric positive semi-definite $n \times n$ matrix $K := \ker Q$	$\pi: \mathbb{R}^n \rightarrow K^\perp$ turns Q into nondegenerate quadric
---	---

Case 1: let $k < n-d$.

For almost all Q with $k = \dim K$ and almost all $u \in \mathbb{R}^n$,

$$\begin{array}{c}
\text{EDD}_Q(M) \\
\parallel \\
\text{EDD}_{\pi(Q)}(\pi(M))
\end{array}
\left\{
\begin{array}{l}
\text{critical points of } \min_{x \in M \setminus \text{Sing}(M)} \|x-u\|_Q^2 \\
\text{critical points of } \min_{x \in \pi(M) \setminus \text{Sing}(\pi(M))} \|x-\pi(u)\|_{\pi(Q)}^2
\end{array}
\right.$$

\uparrow
1:1
 \downarrow



In general

$M \subseteq \mathbb{R}^n$ algebraic variety, $d := \dim M$.

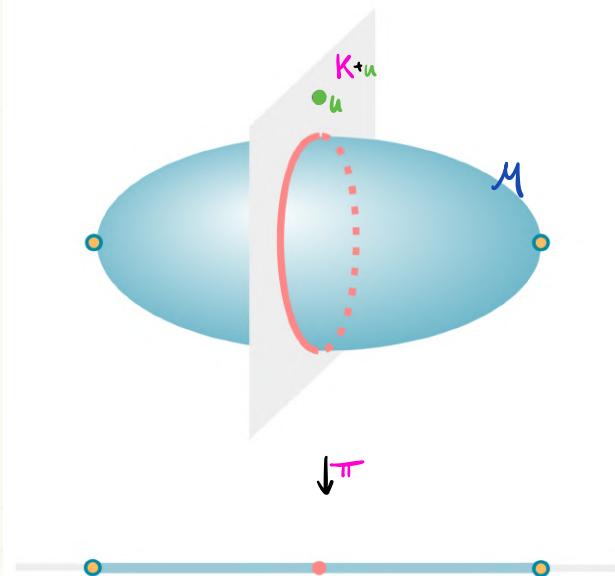
Q symmetric positive semi-definite $n \times n$ matrix
 $K := \ker Q$

$\pi: \mathbb{R}^n \rightarrow K^\perp$
turns Q into nondegenerate quadric

Case 2: let $k \geq n-d$.

For almost all Q with $k = \dim K$ and almost all $u \in \mathbb{R}^n$, we have
2 types of critical points of $\min_{x \in M \setminus \text{Sing}(u)} \|x-u\|_Q^2$:

(A) $(K+u) \cap M$: zero loss solutions



In general

$M \subseteq \mathbb{R}^n$ algebraic variety, $d := \dim M$.

Q symmetric positive semi-definite $n \times n$ matrix
 $K := \ker Q$

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turns Q into nondegenerate quadric

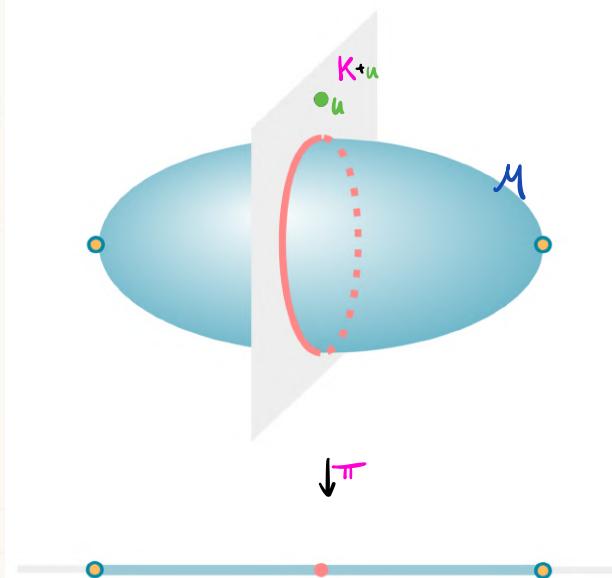
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For almost all Q with $k = \dim K$ and almost all $u \in \mathbb{R}^n$, we have

2 types of critical points of $\min_{x \in M \setminus \text{Sing}(u)} \|x-u\|_Q^2$:

A $(K+u) \cap M$: zero less solutions

B finitely many on the ramification locus $\text{Ram}(\pi|_X)$
 $:= \{\text{critical points of } \pi|_X\}$



In general

$M \subseteq \mathbb{R}^n$ algebraic variety, $d := \dim M$.

Q symmetric positive semi-definite $n \times n$ matrix
 $K := \ker Q$ $\pi: \mathbb{R}^n \rightarrow \mathbb{K}^1$
turns Q into nondegenerate quadratic

Case 2: let $k \geq n - d$.

For almost all Q with $k = \dim K$ and almost all $u \in \mathbb{R}^n$, we have

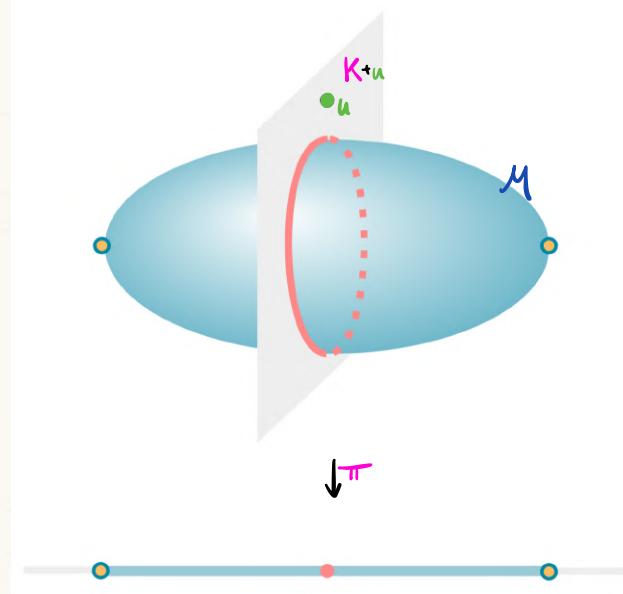
2 types of critical points of $\min_{x \in \text{M}(\text{Sing}(u))} \|x - u\|^2_Q$

(A) $(K+u) \cap M$: zero less solutions

③ finitely many on the ramification locus $\text{Ram}(\mathbb{T}|_X)$
 $\quad := \{\text{critical points of } \mathbb{T}|_X\}$

1 : 1

$\text{EDD}_{\pi(Q)}(\text{Br}) \leftarrow$ critical points of $\min_{x \in \text{Br}(\pi|_X)} \|x - \pi(u)\|_{\pi(Q)}^2$ ← Branch locus $\pi(\text{Ram})$



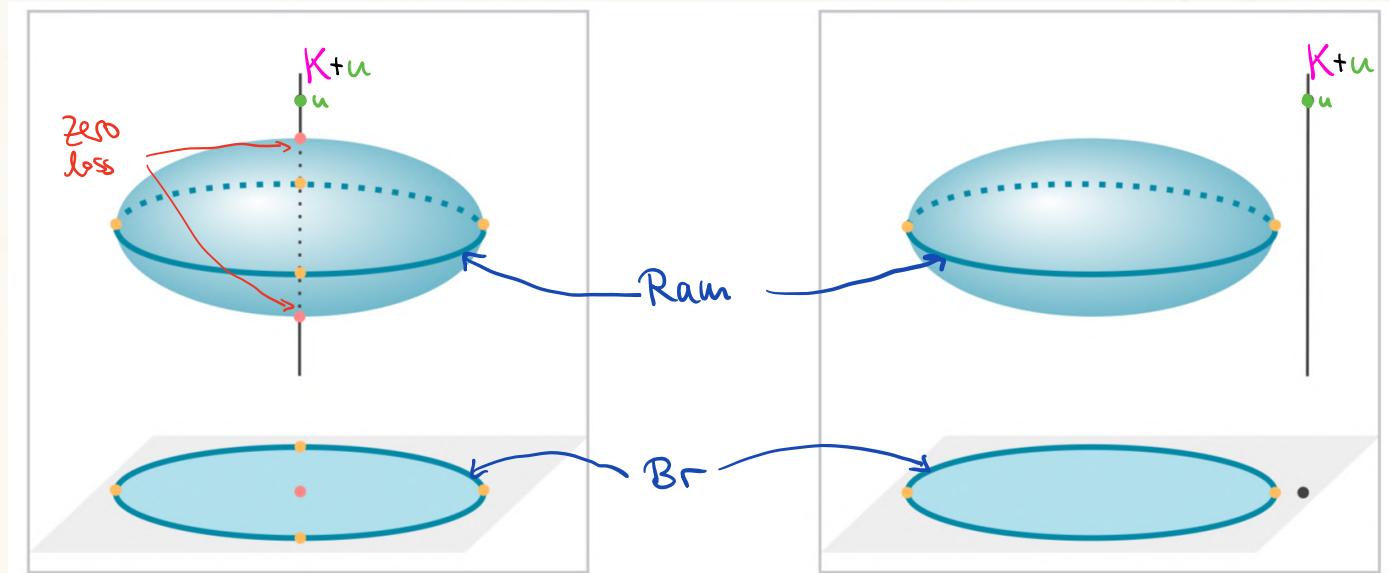
In general

$M \subseteq \mathbb{R}^n$ algebraic variety, $d := \dim M$.

Q symmetric positive semi-definite $n \times n$ matrix
 $K := \ker Q$

$\pi: \mathbb{R}^n \rightarrow K^\perp$
turns Q into nondegenerate quadric

Case 2: let $k \geq n-d$.



Induced bias towards Ran !

depends only on K (not on Q) \uparrow & not on u

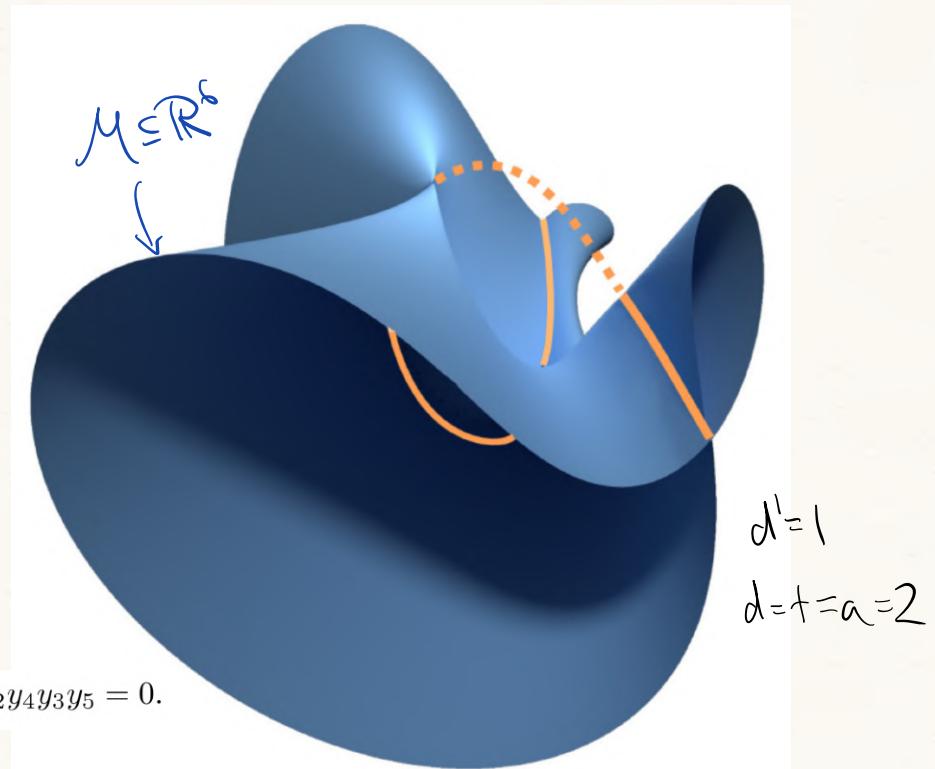
Lightning Self-Attention (single head, single layer)

$$\begin{array}{ccc}
 \mathbb{R}^{d \times t} & \xrightarrow{\quad} & \mathbb{R}^{d \times t} \\
 X & \mapsto & \nabla X X^T K^T Q X \\
 & & \uparrow \quad \quad \quad \uparrow \\
 & & \text{learnable parameters} \\
 & & V \in \mathbb{R}^{d \times d}, K, Q \in \mathbb{R}^{a \times d}
 \end{array}$$

$$y_1^2 y_6^2 + y_4^2 y_3^2 + y_1 y_3 y_5^2 + y_2^2 y_4 y_6 - 2 y_1 y_4 y_3 y_6 - y_2 y_1 y_6 y_5 - y_2 y_4 y_3 y_5 = 0.$$

Q = from MSE loss with general dataset S

$ S $	$k = \dim K$	complex critical point set
≥ 3	0	14 points
2	2	a curve and two lines
1	4	a 3-dimensional subvariety



$Q = \underline{\text{general}} \text{ symmetric positive } \underline{\text{semidefinite}}$

k	complex critical point set
0	14 points
1	14 points
2	4 points + a curve
3	a surface
4	a 3-dimensional subvariety
5	a 4-dimensional subvariety

$K := \dim \ker Q$

$M \cap (\ker(Q) + u)$
 \hookrightarrow zero loss solutions!

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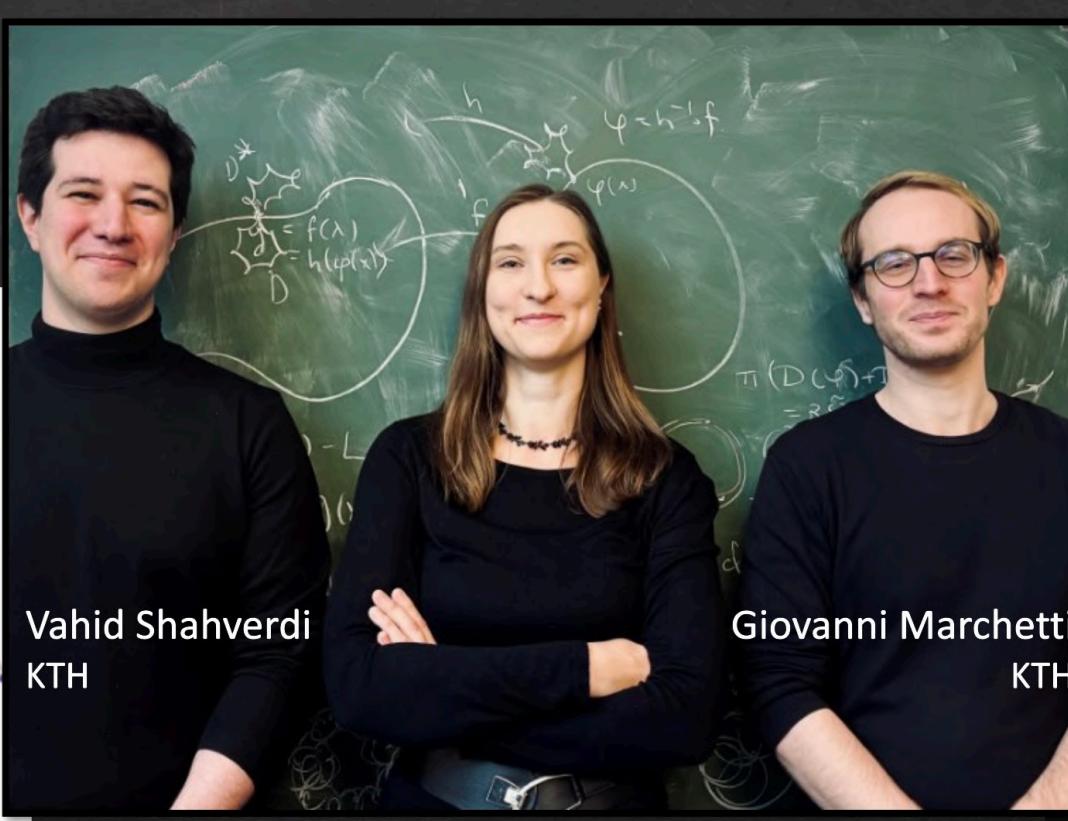
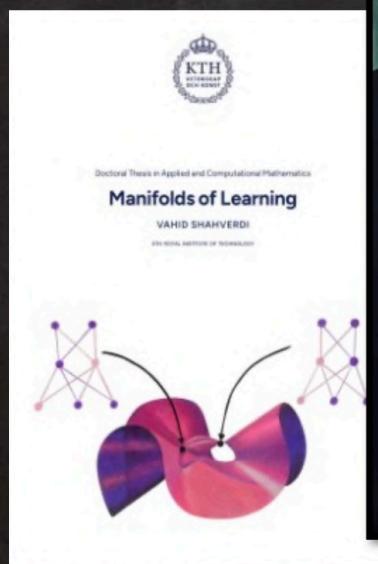
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