

The geometry of neural networks



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joint with

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Neural Networks

Neural Networks

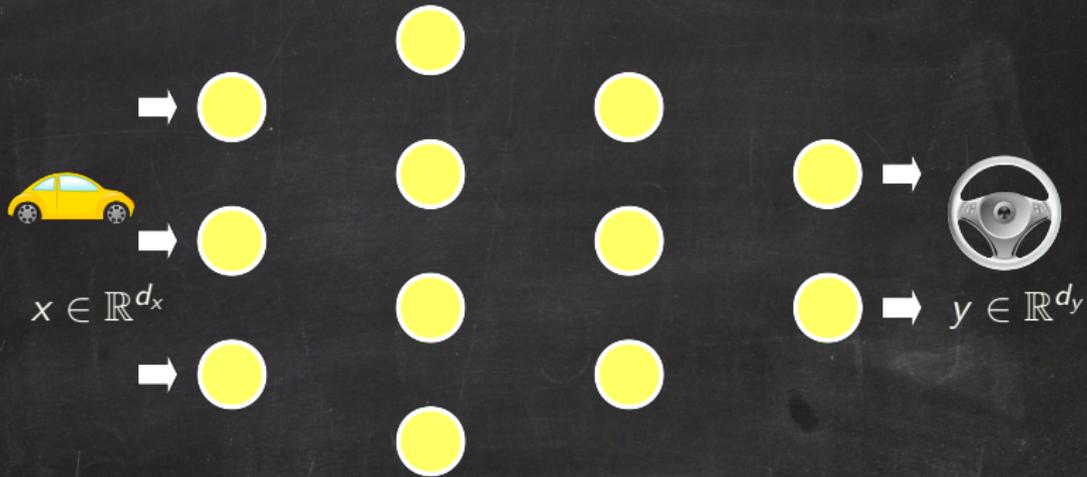


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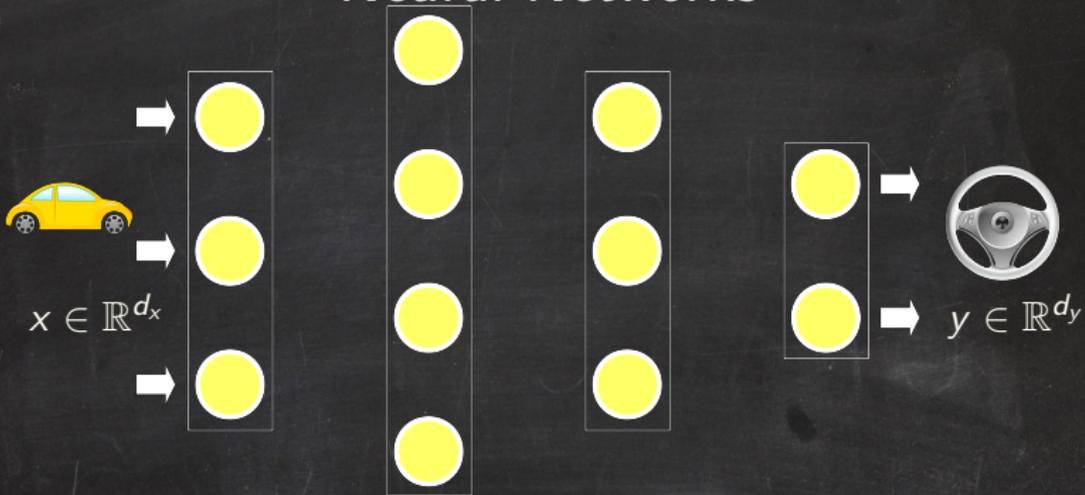


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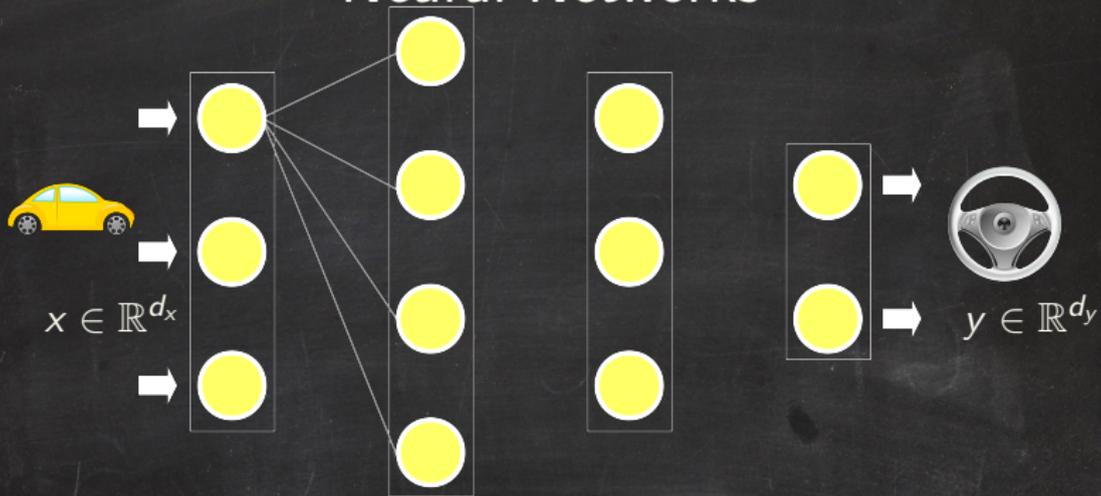
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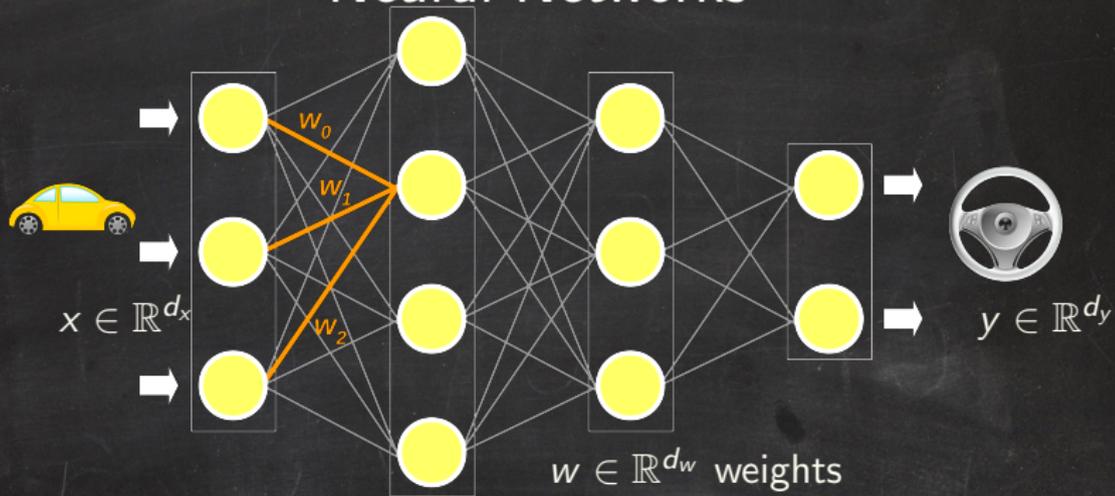
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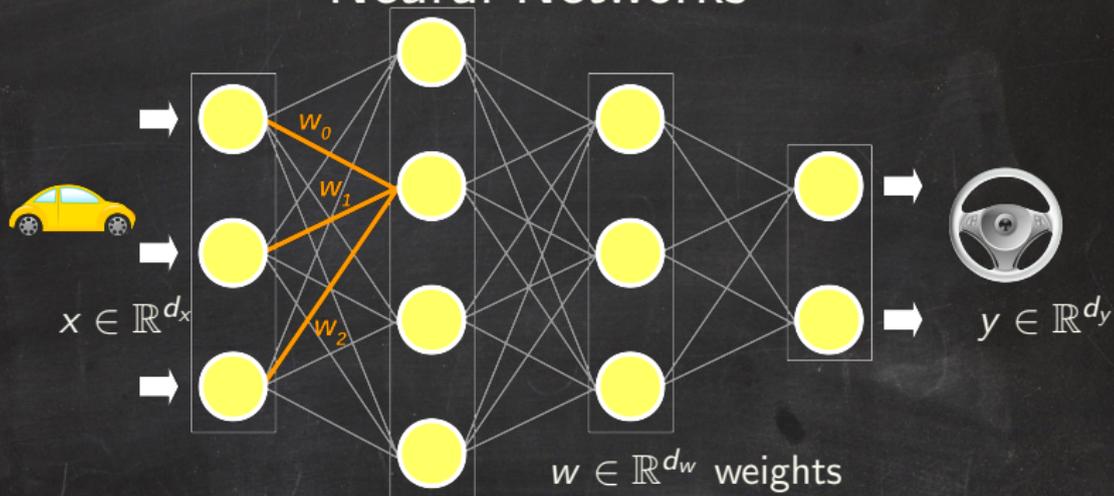
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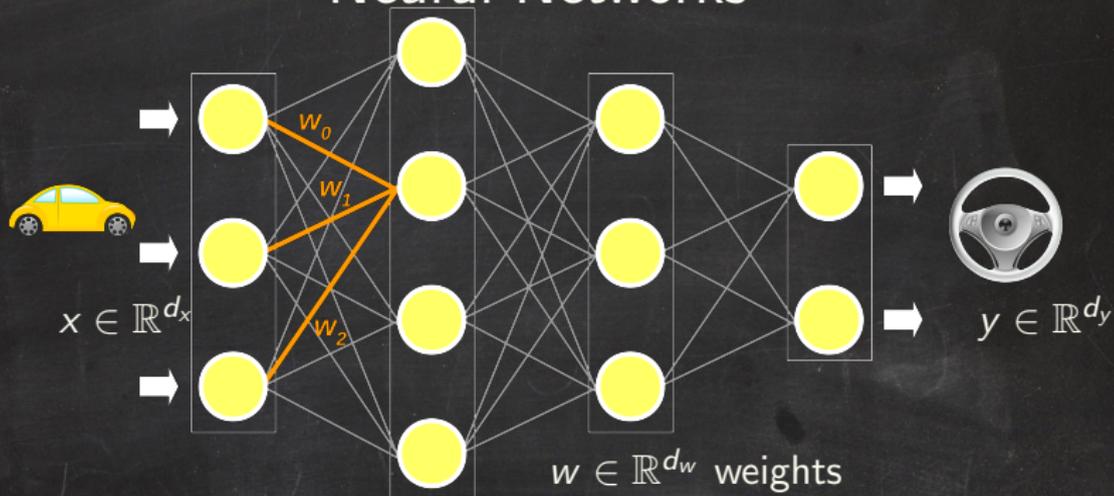


Neural Networks



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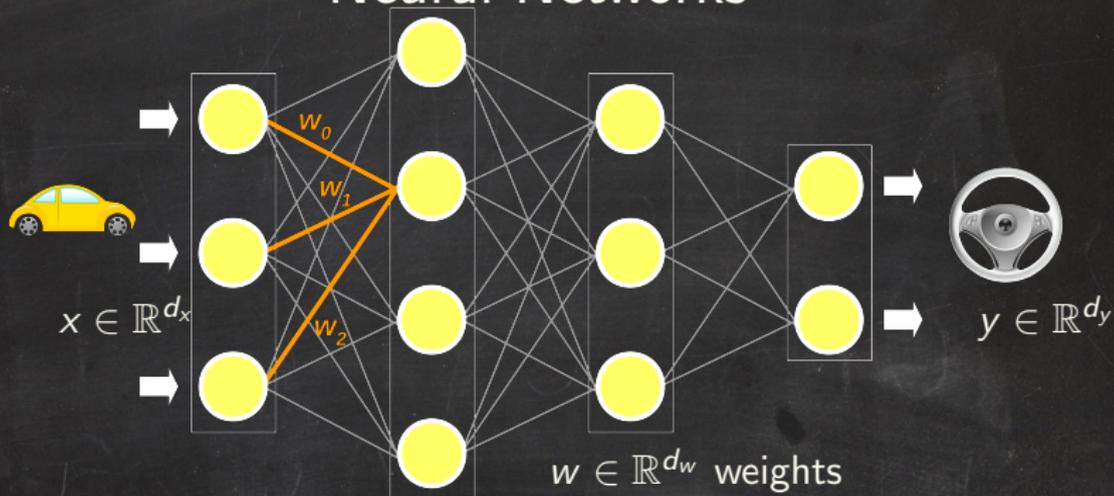


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Definition $\mathcal{M}_\Phi := \left\{ \Phi(w, \cdot) : \mathbb{R}^{d_x} \rightarrow \mathbb{R}^{d_y} \mid w \in \mathbb{R}^{d_w} \right\}$

is called the **neuromanifold** of Φ .

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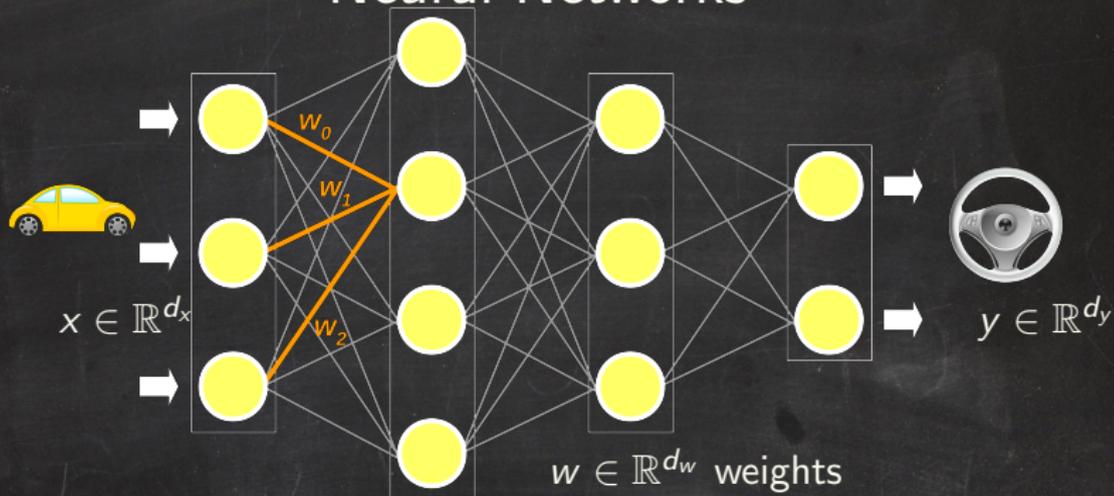
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Observation

1. Φ piecewise smooth $\Rightarrow \mathcal{M}_\Phi$ manifold with singularities
2. $\dim \mathcal{M}_\Phi \leq d_w$

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Example The neuromanifold of the linear network Φ is

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Loss Landscapes

A **loss function** on a neural network $\Phi : \mathbb{R}^{d_w} \times \mathbb{R}^{d_x} \rightarrow \mathbb{R}^{d_y}$ is of the form

$$\begin{array}{ccc} L : \mathbb{R}^{d_w} & \xrightarrow{\mu} & \mathcal{M}_\Phi & \xrightarrow{\ell|_{\mathcal{M}_\Phi}} & \mathbb{R}, \\ w & \longmapsto & \Phi(w, \cdot) & & \end{array}$$

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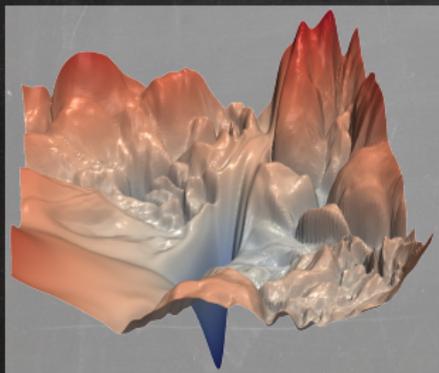
where ℓ is a functional defined on a subset of $C(\mathbb{R}^{d_x}, \mathbb{R}^{d_y})$ containing \mathcal{M}_Φ .

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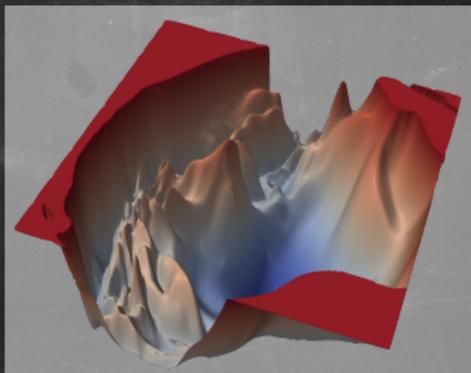
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Visualizations
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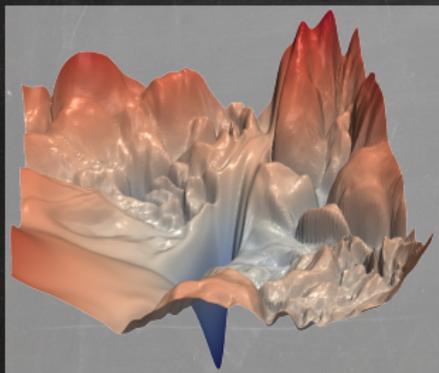
Source: Li, Hao, et al. "Visualizing the loss landscape of neural nets."
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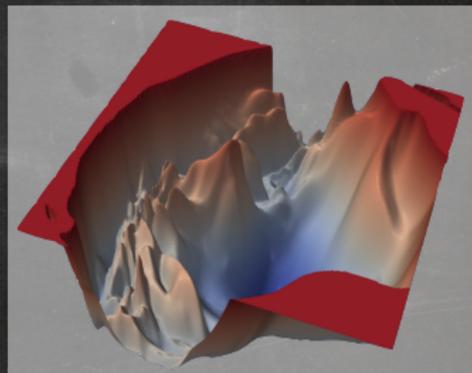
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Observation If $\varphi \in \text{Crit}(\ell|_{\mathcal{M}_\Phi})$, then $\mu^{-1}(\varphi) \subset \text{Crit}(L)$.

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$$(W_h, \dots, W_1) \longmapsto W_h \cdots W_1$$

Recall: $\mathcal{M}_\Phi = \{M \in \mathbb{R}^{d_h \times d_0} \mid \text{rk}(M) \leq r\}$, where $r := \min \{d_0, d_1, \dots, d_h\}$.

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Theorem Let $M \in \mathcal{M}_\Phi$.

1. If $\text{rk}(M) = r$, then $\mu^{-1}(M)$ has 2^b path-connected components

where $b := \#\{i \mid 0 < i < h, d_i = r\}$.

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L has non-global minima $\Leftrightarrow \ell|_{\mathcal{M}_\Phi}$ has non-global minima.

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(**even in the non-filling case!**)

The Quadratic Loss

Fixed data matrices $X \in \mathbb{R}^{d_0 \times s}$ and $Y \in \mathbb{R}^{d_h \times s}$ define a **quadratic loss**

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Minimizing $\ell_{X,Y}$ on the determinantal variety $\mathcal{M}_\Phi = \{M \mid \text{rk}(M) \leq r\}$ is equivalent to minimizing the Euclidean distance of YX^T to \mathcal{M}_Φ .

Euclidean Distance to Varieties

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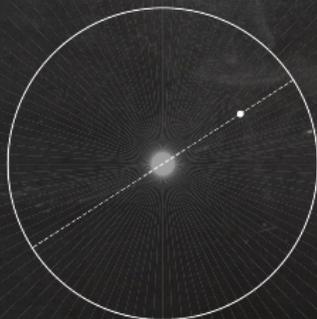
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$$\delta(\text{circle}) = 2$$



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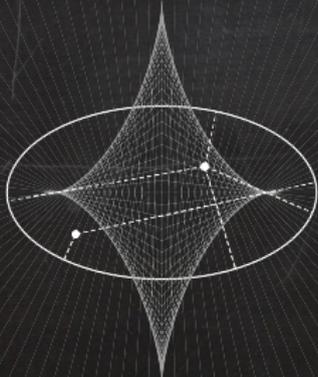
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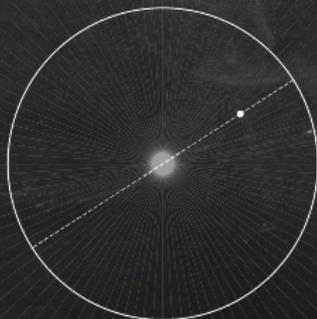
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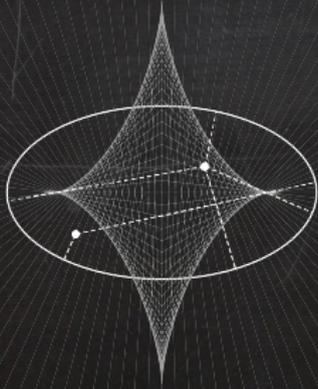
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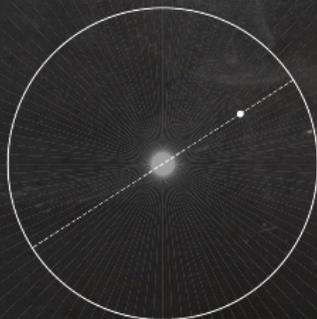
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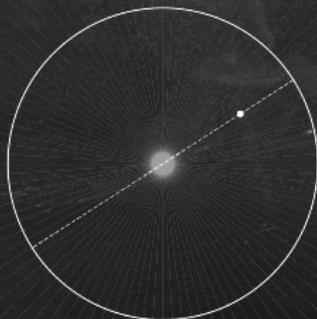
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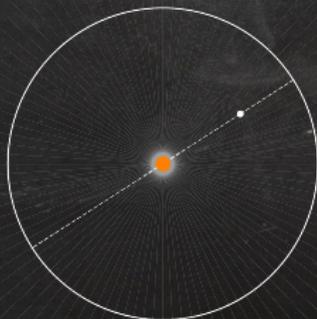
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Corollary [Baldi & Hornik '89, Kawaguchi '16]

If ℓ is a **quadratic loss**, then all local minima for the loss $L = \ell \circ \mu$ on a **linear network** are global. **(even in the non-filling case!)**

Linear Networks Can Have Bad Local Minima

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There is a constant $\delta^{\text{gen}} \in \mathbb{Z}_{>0}$ such that for almost all linear coordinate changes $f : \mathbb{R}^N \rightarrow \mathbb{R}^N$ the ED degree of $f(\mathcal{Z})$ is δ^{gen} .

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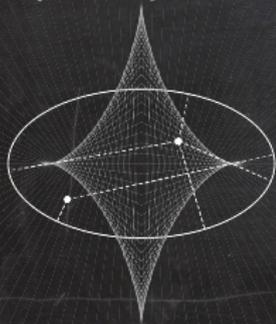
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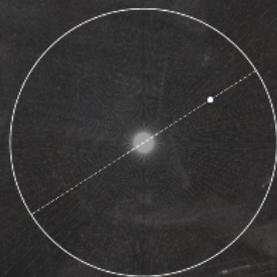
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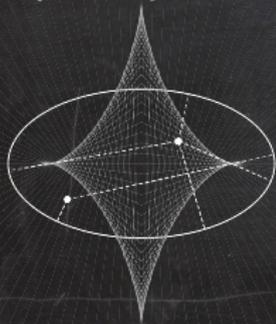
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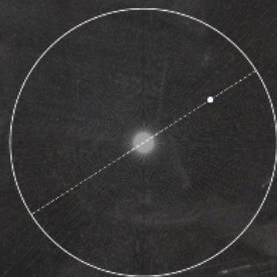
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Equivalently: δ^{gen} is the ED degree of \mathcal{Z}

under the perturbed Euclidean distance $\|f(\cdot)\|_2$.

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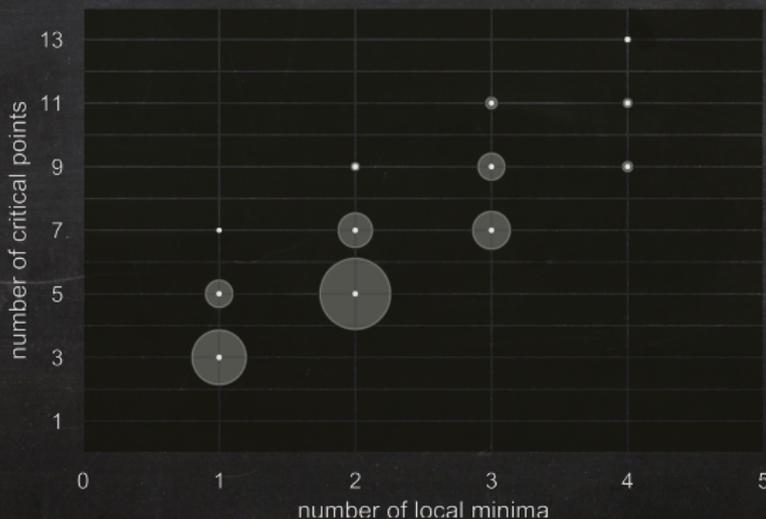
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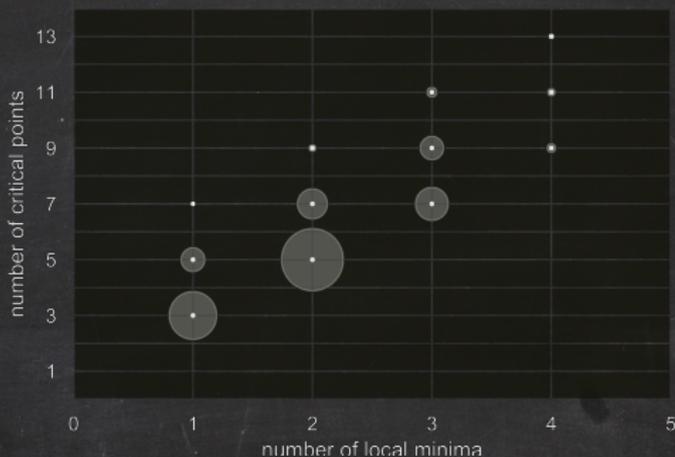
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3. Also: different number of local minima in different open regions of $\mathbb{R}^{3 \times 3}$, not all of them global !

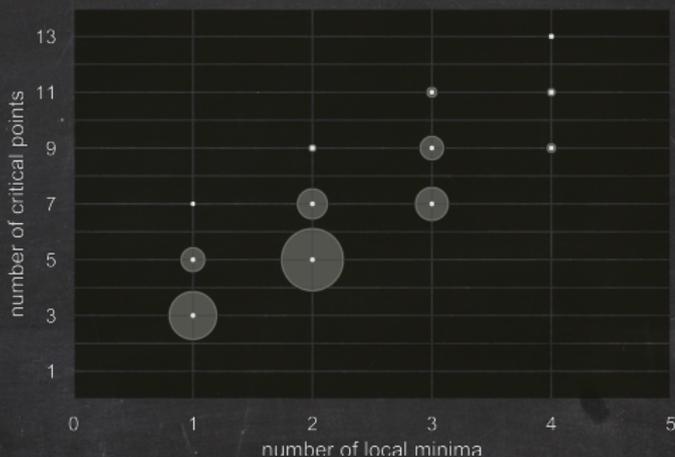


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		# real critical points						
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# local minima	1	0	476	120	1	0	0	0
	2	0	0	805	190	10	0	0
	3	0	0	0	228	116	21	0
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All determinantal varieties behave like this ! XI - XIV

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$$\delta(\mathcal{M}_1) = \min\{m, n\}$$

Take Away

- ◆ determinantal varieties are examples of neuromanifolds
- ◆ for linear networks with smooth convex losses:

	quadratic loss	other loss
filling	no bad min.	no bad min.
non-filling	no bad min.	bad min.

convex optimization
on vector space

special embedding of
determinantal varieties

- ◆ future extensions to
 - ◇ convolutional networks
(ongoing work with T. Merkh, G. Montúfar, M. Trager)
 - ◇ networks with polynomial activation functions or
 - ◇ ReLU networks (using semi-algebraic sets)

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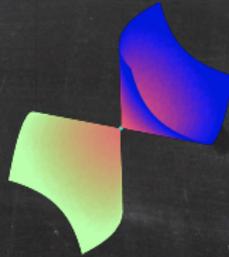
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- ◆ In the non-filling case, the neuromanifold is a semi-algebraic set whose boundary is contained in the discriminant hypersurface of polynomials.
- ◆ **Example:** If there are 2 filters of even width, the complement of the neuromanifold is a union of two convex cones.