MAD

NYU | COURANT INSTITUTE OF MATHEMATICAL SCIENCES

MATHEMATICS OF DEEP LEARNING

JOAN BRUNA , CIMS + CDS, NYU, SPRING'18

Lecture 13: Optimization Landscapes of deep networks. Open Problems

OBJECTIVES LECTURE 13

- Landscape of Optimization of Neural Networks

- Some Open Challenges

SPURIOUS VALLEYS

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- More generally, we are interested in certifying existence of descent paths.
- **Definition:** A *valley* is a connected component of the sublevel set Ω_u.

  Definition: A *spurious valley* is a connected component of the sublevel set Ω_u that does not contain a global minima.
- If a loss has no spurious valley, then one can continuously move from any point in parameter space to a global minima without increasing the loss:

  Given any initial parameter $\theta_0 \in \Theta$,
  $\exists$ continuous path $\theta : t \in [0,1] \mapsto \theta(t) \in \Theta$ st:
  $\theta(0) = \theta_0$, $\theta(1) \in \arg\min_{\theta} E(\theta)$, and
  $t \mapsto E(\theta(t))$ is non-increasing.

LINEAR VS NON-LINEAR DEEP MODELS

- Some authors have considered linear "deep" models as a first step towards understanding nonlinear deep models:

$$E(W_1, \ldots, W_K) = \mathbb{E}_{(X,Y)\sim P} \|W_K \ldots W_1 X - Y\|^2 \ .$$

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Theorem: [**Kawaguchi'16**] If $\Sigma = \mathbb{E}(XX^T)$ and $\mathbb{E}(XY^T)$ are full-rank and Σ has distinct eigenvalues, then $E(\Theta)$ has no poor local minima.

- studying critical points.
- later generalized in [Hardt & Ma'16, Lu & Kawaguchi'17]

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Proposition: [BF'16]

1. If $n_k > \min(n, m)$, $0 < k < K$, then $N_u = 1$ for all u.

2. (2-layer case, ridge regression)
   $E(W_1, W_2) = \mathbb{E}_{(X,Y)\sim P} \|W_2 W_1 X - Y\|^2 + \lambda(\|W_1\|^2 + \|W_2\|^2)$
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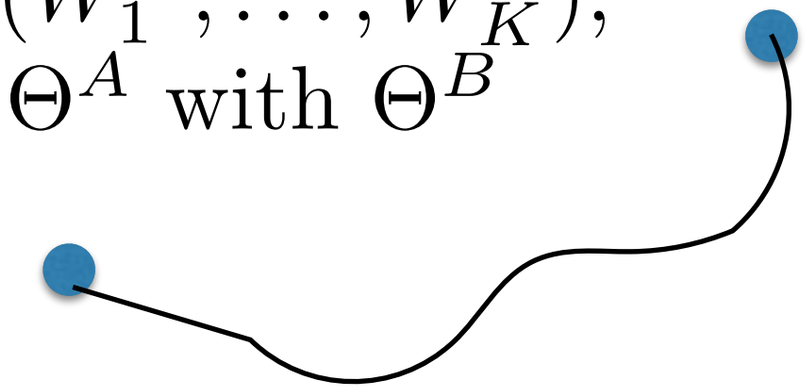
- We pay extra redundancy price to get simple topology.
- This simple topology is an "artifact" of the linearity of the network:

Proposition: [BF'16] For any architecture (choice of internal dimensions), there exists a distribution $P_{(X,Y)}$ such that $N_u > 1$ in the ReLU $\rho(z) = \max(0, z)$ case.

PROOF SKETCH

- Goal:

Given $\Theta^A = (W_1^A, \ldots, W_K^A)$ and $\Theta^B = (W_1^B, \ldots, W_K^B)$, we construct a path $\gamma(t)$ that connects Θ^A with Θ^B st $E(\gamma(t)) \leq \max(E(\Theta^A), E(\Theta^B))$.



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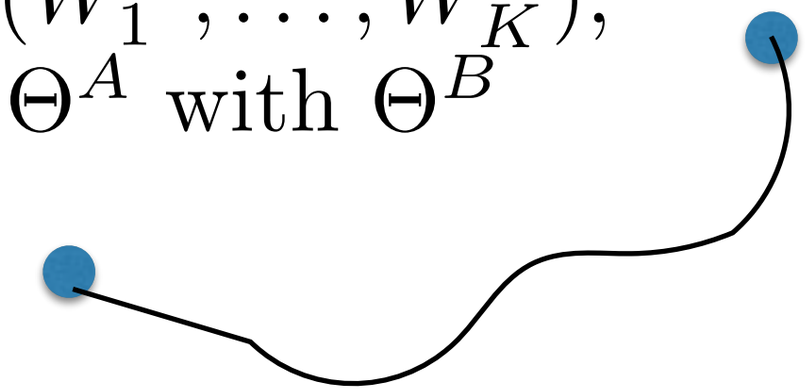

➤ Main idea:

1. Induction on K.
2. *Lift* the parameter space to $\widetilde{W} = W_1 W_2$: the problem is convex $\Rightarrow$ there exists a (linear) path $\widetilde{\gamma}(t)$ that connects Θ^A and Θ^B.
3. Write the path in terms of original coordinates by *factorizing* $\widetilde{\gamma}(t)$.

➤ Simple fact:
If $M_0, M_1 \in \mathbb{R}^{n \times n'}$ with $n' > n$,
then there exists a path $t : [0,1] \to \gamma(t)$
with $\gamma(0) = M_0$, $\gamma(1) = M_1$ and
$M_0, M_1 \in \text{span}(\gamma(t))$ for all $t \in (0,1)$.

MODEL SYMMETRIES

[with L. Venturi, A. Bandeira, '17]

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- We do the same analysis in the quotient space defined by the equivalence relationship .

Theorem: [BVV'18] The Multilinear regression $\mathbb{E}_{(X,Y)\sim P} \|W_K \dots W_1 X - Y\|^2$ has no spurious valleys.

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- Construct paths on the Grassmanian manifold of linear subspaces
- Generalizes best known results for multilinear case (no assumptions on covariance).

BETWEEN LINEAR AND RELU: POLYNOMIAL NETS

- Quadratic nonlinearities $\rho(z) = z^2$ are a simple extension of the linear case, by lifting or "kernelizing":

$$\rho(Wx) = \mathcal{A}_W X \ , \ X = xx^T \ , \ \mathcal{A}_W = (W_k W_k^T)_{k \leq M} \ .$$

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- No poor local minima with much better bounds in the scalar output two-layer case:

Theorem: [BBV'18] The two-layer quadratic network regression $\mathbb{E}_{(X,Y)\sim P}|U(WX)^2 - Y|^2$ has no spurious valleys if $M > 2N$.

ASYMPTOTIC CONNECTEDNESS OF RELU

- Good behavior is recovered with nonlinear ReLU networks, provided they are sufficiently overparametrized:

- Setup: two-layer ReLU network:

$$\Phi(X;\Theta) = W_2\rho(W_1X)\ ,\ \rho(z) = \max(0,z).W_1 \in \mathbb{R}^{m\times n}, W_2 \in \mathbb{R}^m$$

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Theorem [BF'16]: For any $\Theta^A, \Theta^B \in \mathbb{R}^{m\times n}, \mathbb{R}^m$, with $E(\Theta^{\{A,B\}}) \leq \lambda$, there exists path $\gamma(t)$ from Θ^A and Θ^B such that $\forall\ t\ , E(\gamma(t)) \leq \max(\lambda, \epsilon)$ and $\epsilon \sim m^{-\frac{1}{n}}$.

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- Overparametrisation "wipes-out" local minima (and group symmetries).

- The bound is cursed by dimensionality, ie exponential in n .

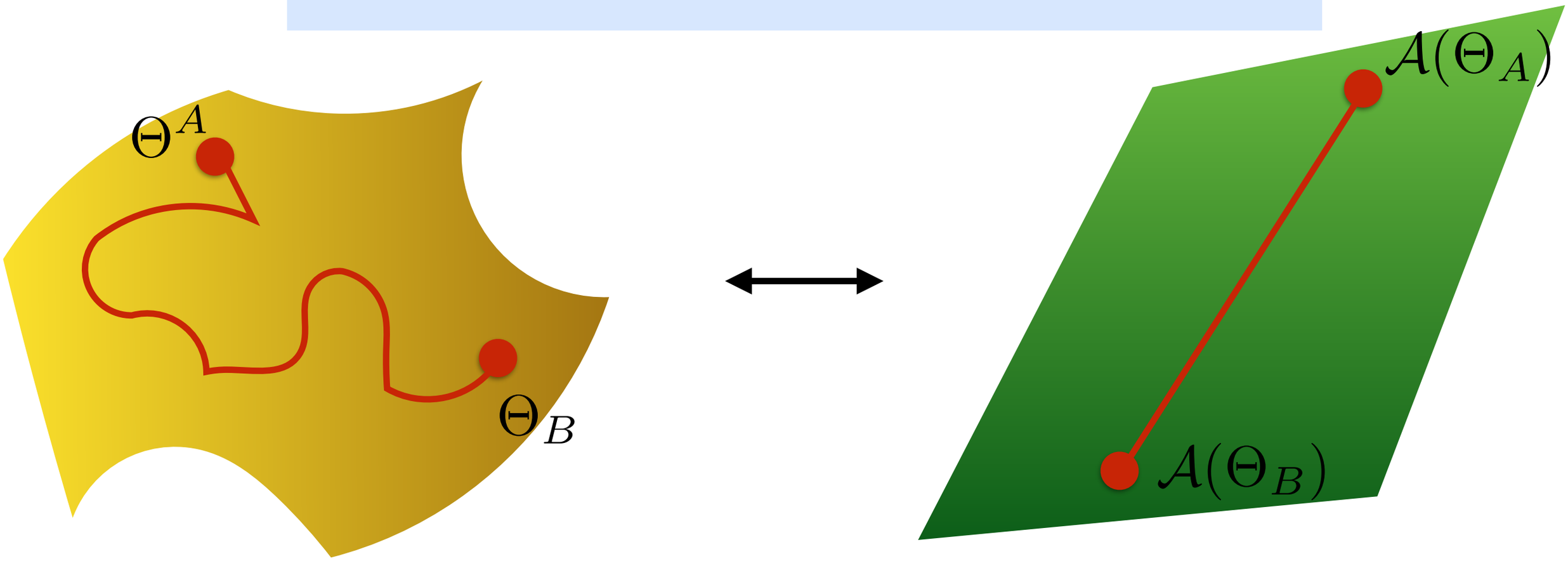
- Result is based on local linearization of the ReLU kernel (hence exponential price).

KERNELS ARE BACK?

$$\Phi(x;\Theta) = W_k \rho(W_{k-1} \dots \rho(W_1 X))) \ , \ \Theta = (W_1, \dots W_k) \ ,$$

- The underlying technique we described consists in "convexifying" the problem, by mapping *neural* parameters Θ to *canonical* parameters $\beta = \mathcal{A}(\Theta)$:

$$\Phi(X;\Theta) = \langle \Psi(X), \mathcal{A}(\Theta) \rangle \ .$$



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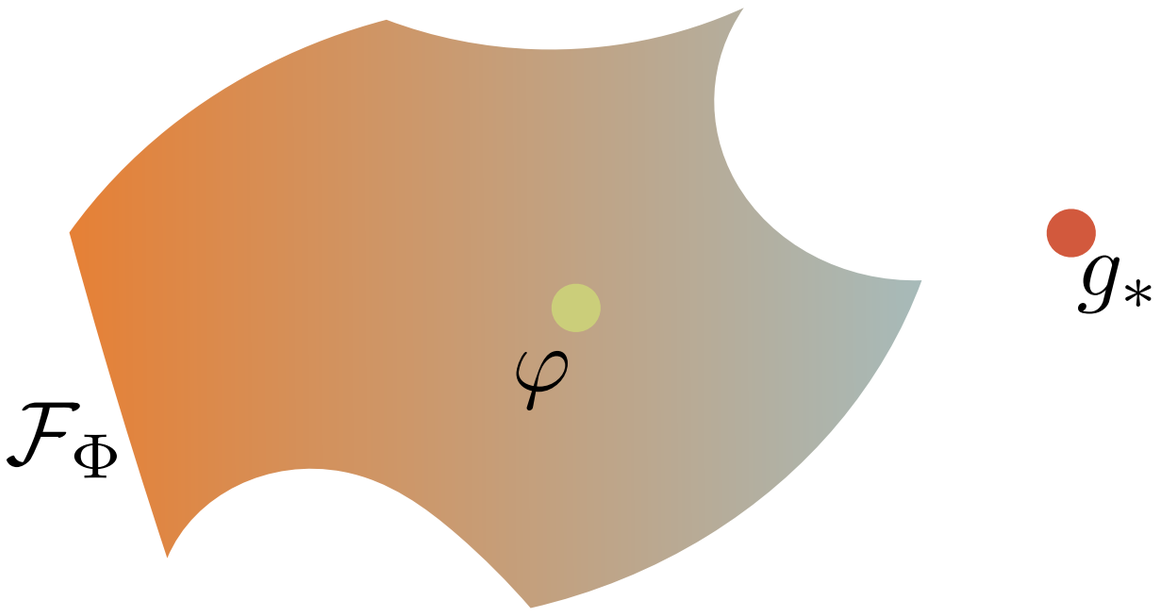
Theorem: [BVV'18] If $\dim\{\mathcal{A}(w),\, w \in \mathbb{R}^n\} = q < \infty$, then $L(U,W) = \mathbb{E}\|U\rho(WX) - Y\|^2$ has no spurious valley if $M \geq q$.

- This includes Empirical Risk Minimization (since RKHS is only queried on finite # of datapoints), and polynomial activations.
- See [Bietti&Mairal'17,Zhang et al'17, Bach'17] for related work.

PARAMETRIC VS MANIFOLD OPTIMIZATION

- This suggests thinking about the problem in the functional space generated by the model:

$$\mathcal{F}_\Phi = \{\varphi : \mathbb{R}^n \to \mathbb{R}^m \,; \varphi(x) = \Phi(x; \Theta) \text{ for some } \Theta\} \,.$$



$$\min_{\varphi \in \mathcal{F}_\Phi} \|\varphi - g_*\|_p$$

$$g_* : x \mapsto \mathbb{E}(Y|x)$$

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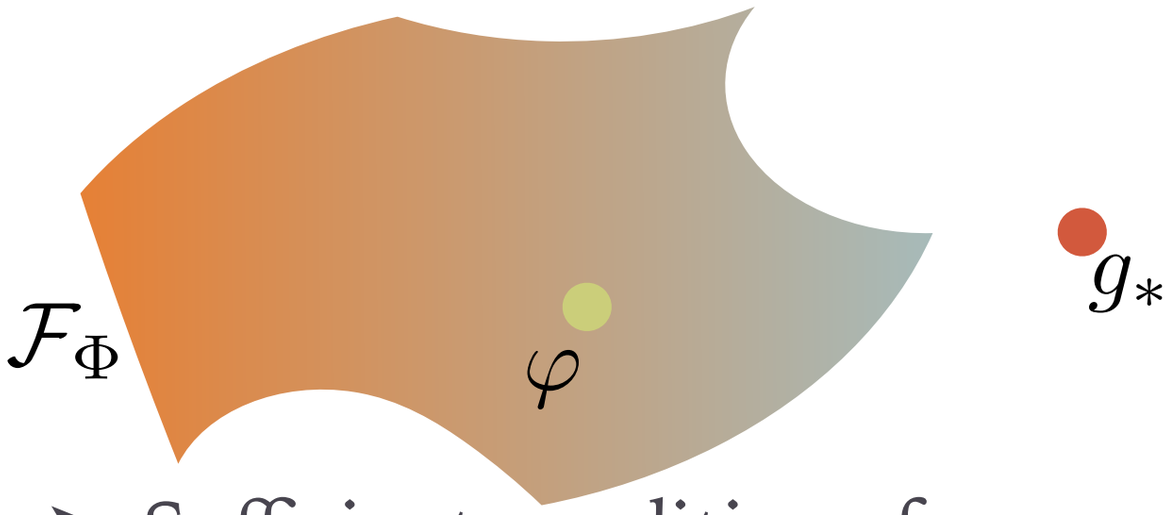

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- Sufficient conditions for success so far:
  - $\mathcal{F}_\Phi$ convex and Θ sufficiently large so that we can move freely within.
- Necessary condition: $\mathcal{F}_\Phi$ is *ball-connected:*
  $\mathcal{F}_\Phi \cap B_p(R, \epsilon)$ are connected for all p, R, ϵ.

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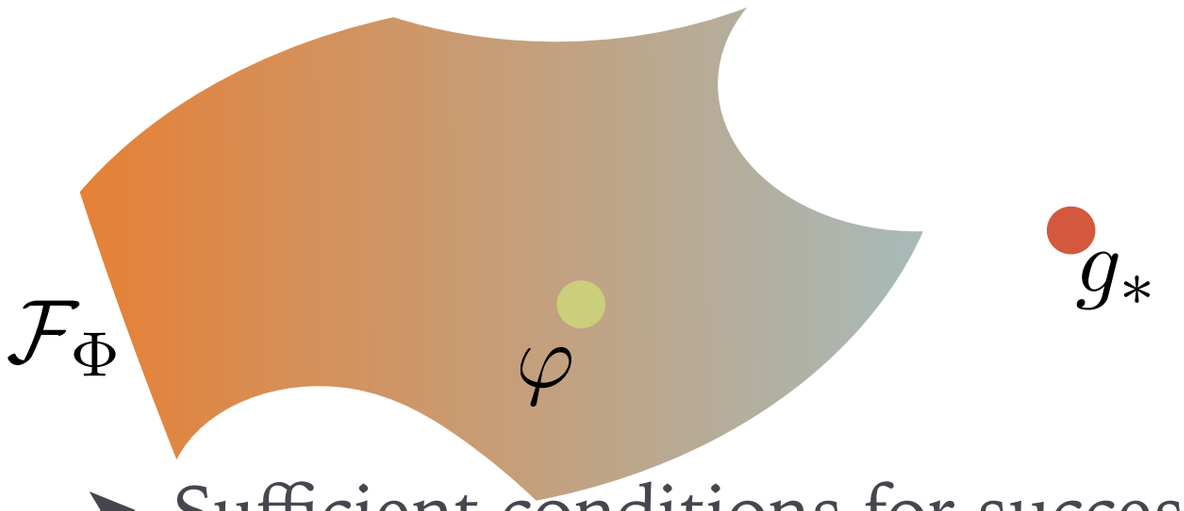

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- What happens when the model is not sufficiently overparametrised?

FROM SIMPLE LANDSCAPES TO ENERGY BARRIER?

- Does a similar macroscopic picture arise in our setting?
- Given $\rho(z)$ homogeneous, assume
  - $\tilde{\rho}(\langle w, X\rangle) = \langle A_w, \psi(X)\rangle$, with $\dim(\psi(X)) = f(N)$.
- Define

$$\beta(M,N) = \inf_{S;\dim(S)=f^{-1}(M)} \inf_{\substack{U\in\mathbb{R}^{m\times M}\\ W\in\mathbb{R}^{M\times f^{-1}(M)}}} \sup_{\substack{\mathbb{E}\|Z\|\le N-f^{-1}(M),\\ P_S Z=0}} \mathbb{E}\|U\rho(WP_S X+Z)-Y\|^2$$

  - Best loss obtained by first projecting the data onto the best possible subspace of dimension $f^{-1}(M)$and adding bounded noise in the complement.
  - $\beta(M,N)$ decreases with M and $\beta(f(N),N) = \min_{U,W} E(U,W)$.

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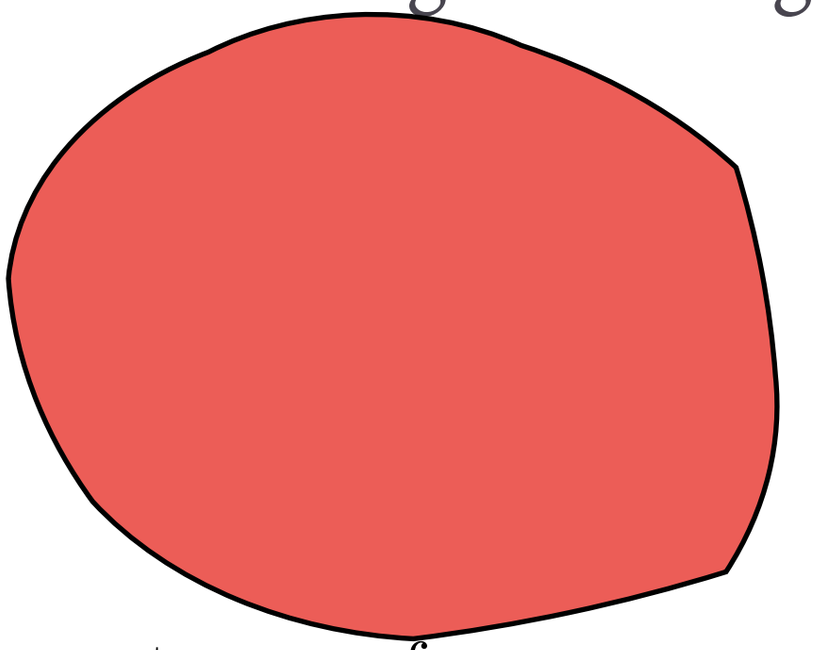
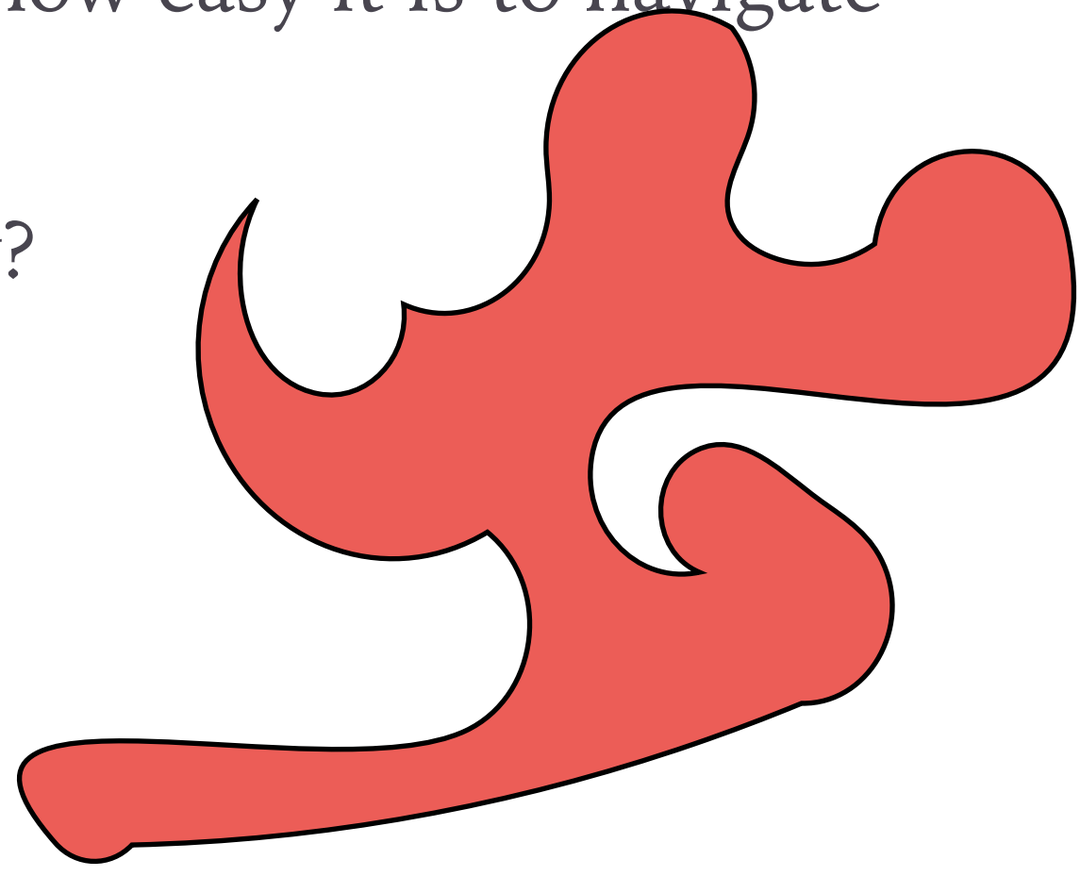
Conjecture [LBB'18]: The loss $L(U,W) = \mathbb{E}\|U\rho(WX)-Y\|^2$ has no poor local minima above the energy barrier $\beta(M,N)$.

FROM TOPOLOGY TO GEOMETRY

- The next question we are interested in is conditioning for descent.
- Even if level sets are connected, how easy it is to navigate through them?
- How "large" and regular are they?



easy to move from one energy level to lower one



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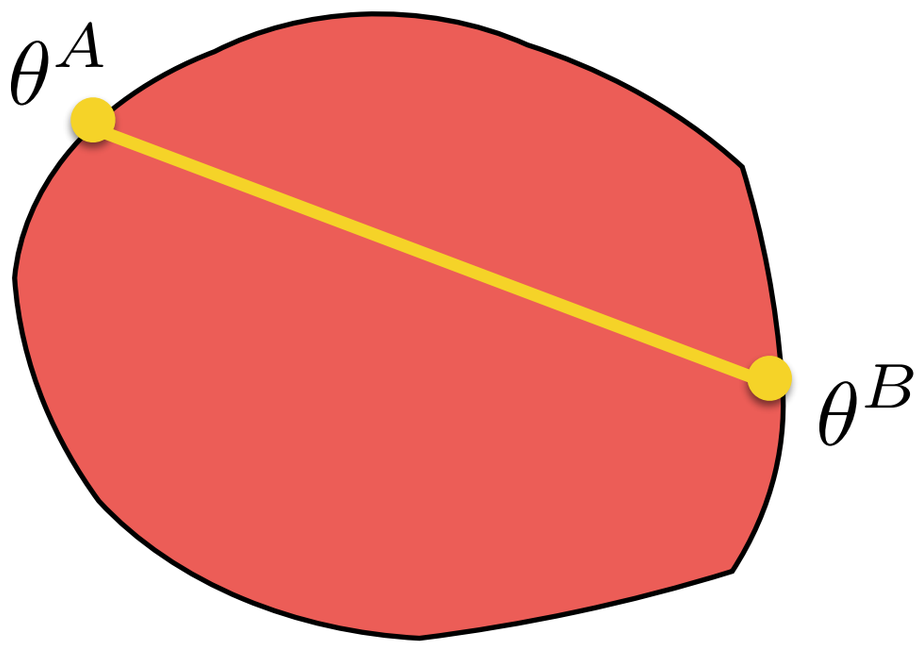
- We estimate level set geodesics and measure their length.



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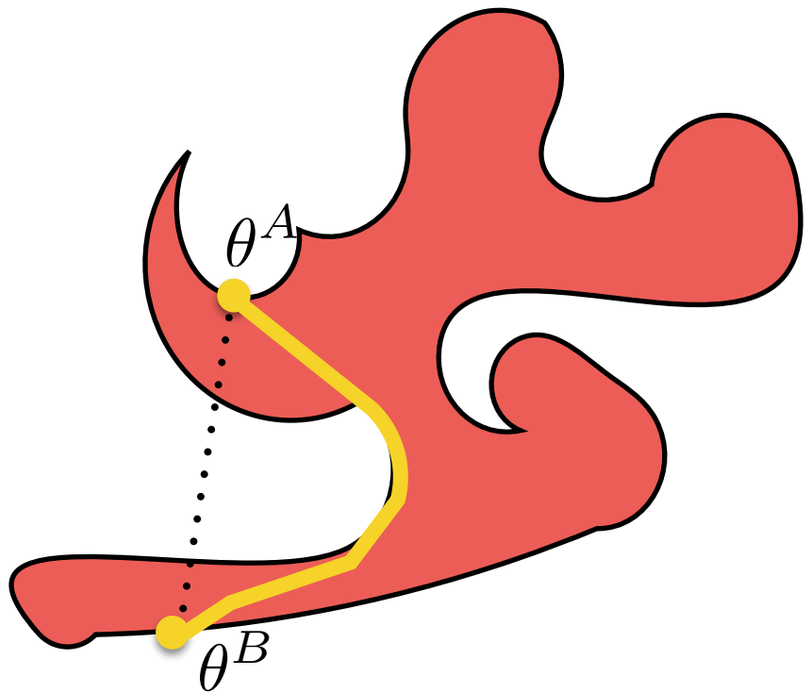

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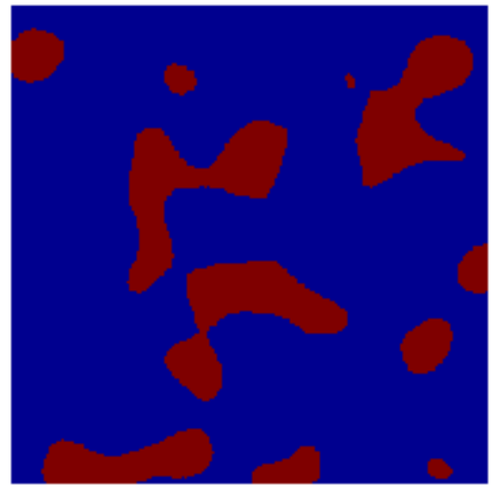
FINDING CONNECTED COMPONENTS



- Suppose $\theta_1,\ \theta_2$ are such that $E(\theta_1) = E(\theta_2) = u_0$
  - They are in the same connected component of Ω_{u_0} iff

    there is a path $\gamma(t),\ \gamma(0) = \theta_1, \gamma(1) = \theta_2$ such that
    $\forall\ t \in (0,1)\ ,\ E(\gamma(t)) \leq u_0\ .$

- Moreover, we penalize the length of the path:

$$\forall\ t \in (0,1)\ ,\ E(\gamma(t)) \leq u_0 \quad \text{and} \quad \int \|\dot{\gamma}(t)\| dt \leq M\ .$$

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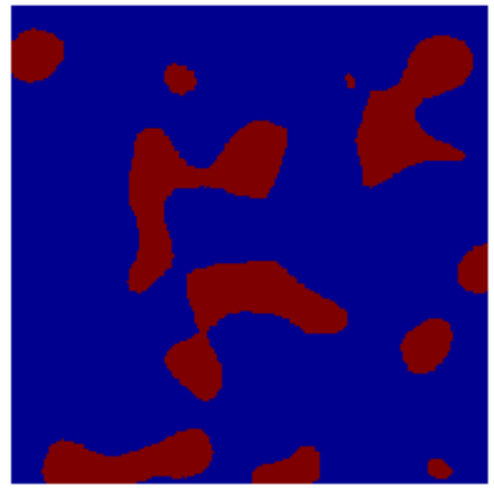

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θ_1

θ_2

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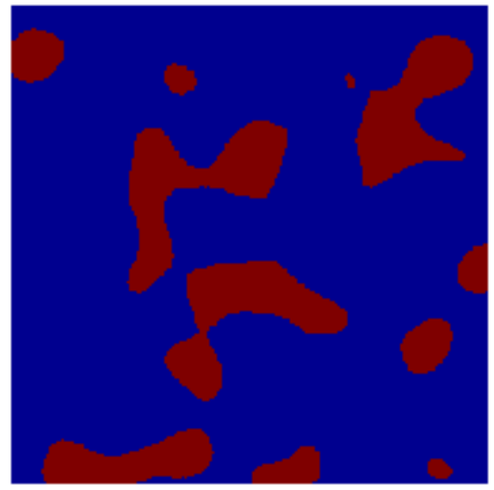

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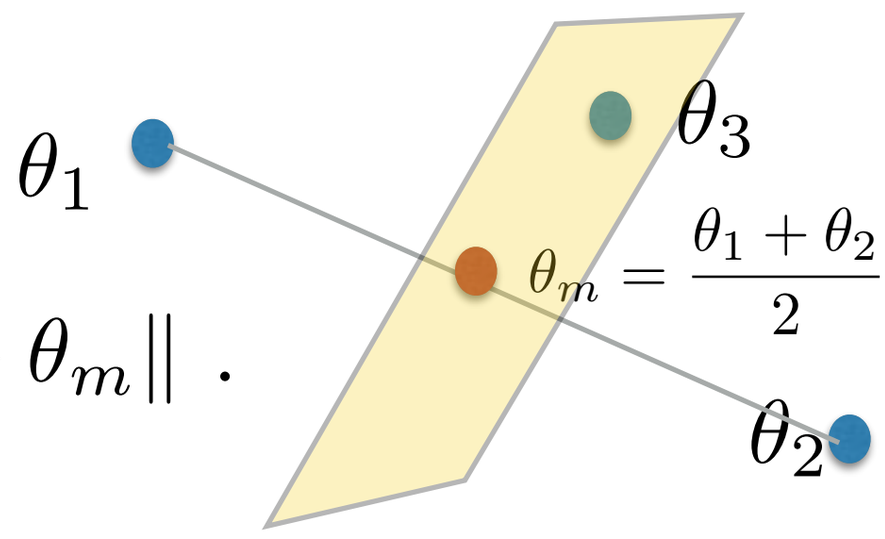
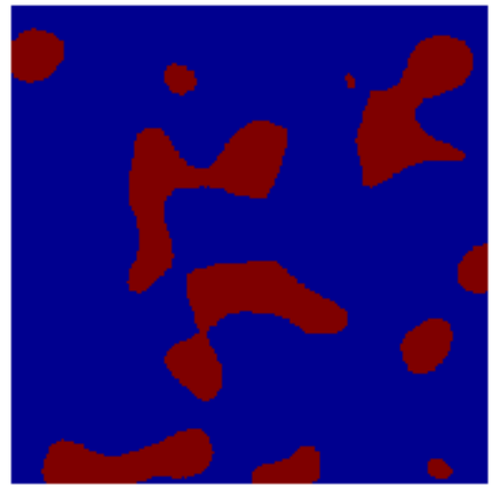
- Dynamic programming approach:

$$\theta_3 = \arg \min_{\theta \in \mathcal{H};\, E(\theta) \leq u_0} \|\theta - \theta_m\|\ .$$



FINDING CONNECTED COMPONENTS



- Suppose θ_1, θ_2 are such that $E(\theta_1) = E(\theta_2) = u_0$
  - They are in the same connected component of Ω_{u_0} iff

there is a path $\gamma(t),\ \gamma(0) = \theta_1, \gamma(1) = \theta_2$ such that
$\forall\ t \in (0,1)\ ,\ E(\gamma(t)) \leq u_0\ .$

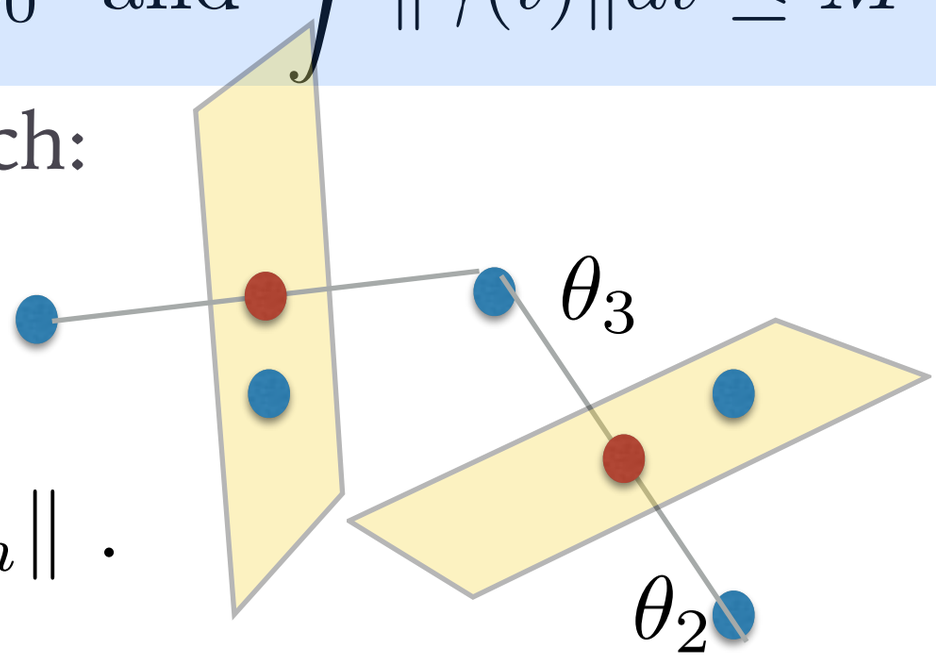
- Moreover, we penalize the length of the path:

$$\forall\ t \in (0,1)\ ,\ E(\gamma(t)) \leq u_0 \quad \text{and} \quad \int \|\dot{\gamma}(t)\| dt \leq M\ .$$

- Dynamic programming approach:

$$\theta_m = \frac{\theta_1 + \theta_2}{2}$$

$$\theta_3 = \arg \min_{\theta \in \mathcal{H};\, E(\theta) \leq u_0} \|\theta - \theta_m\|\ .$$



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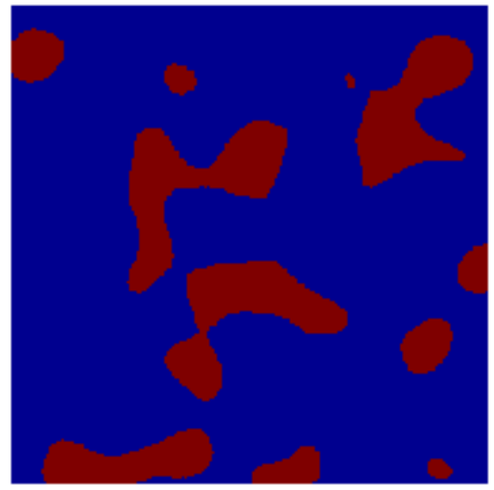

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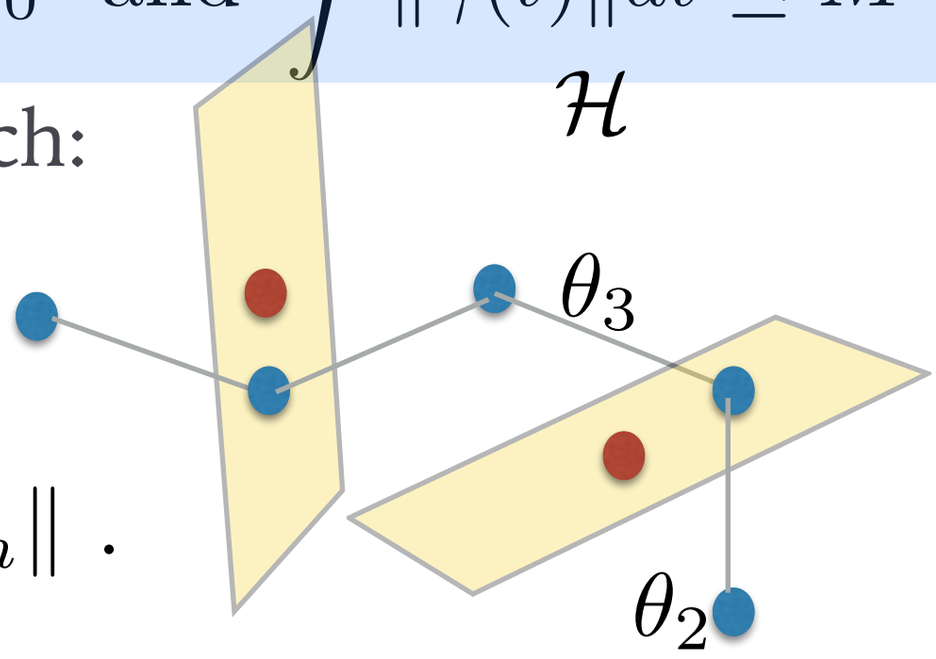
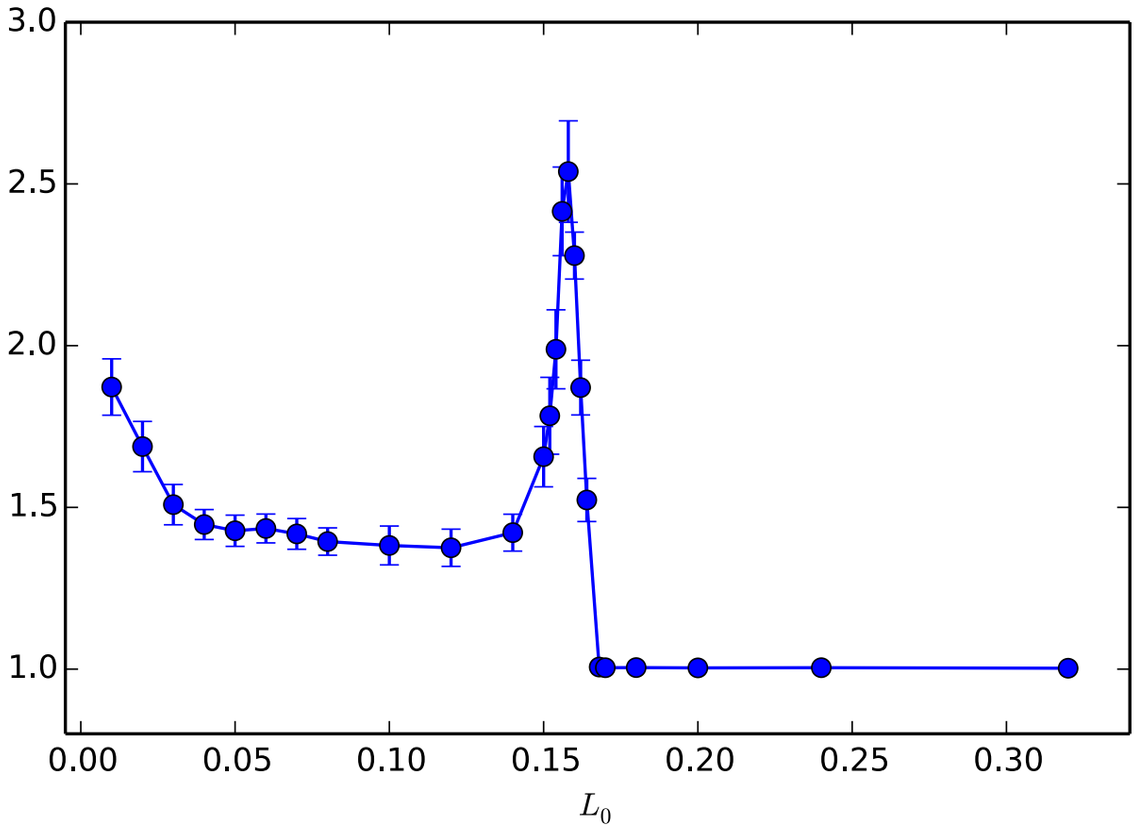
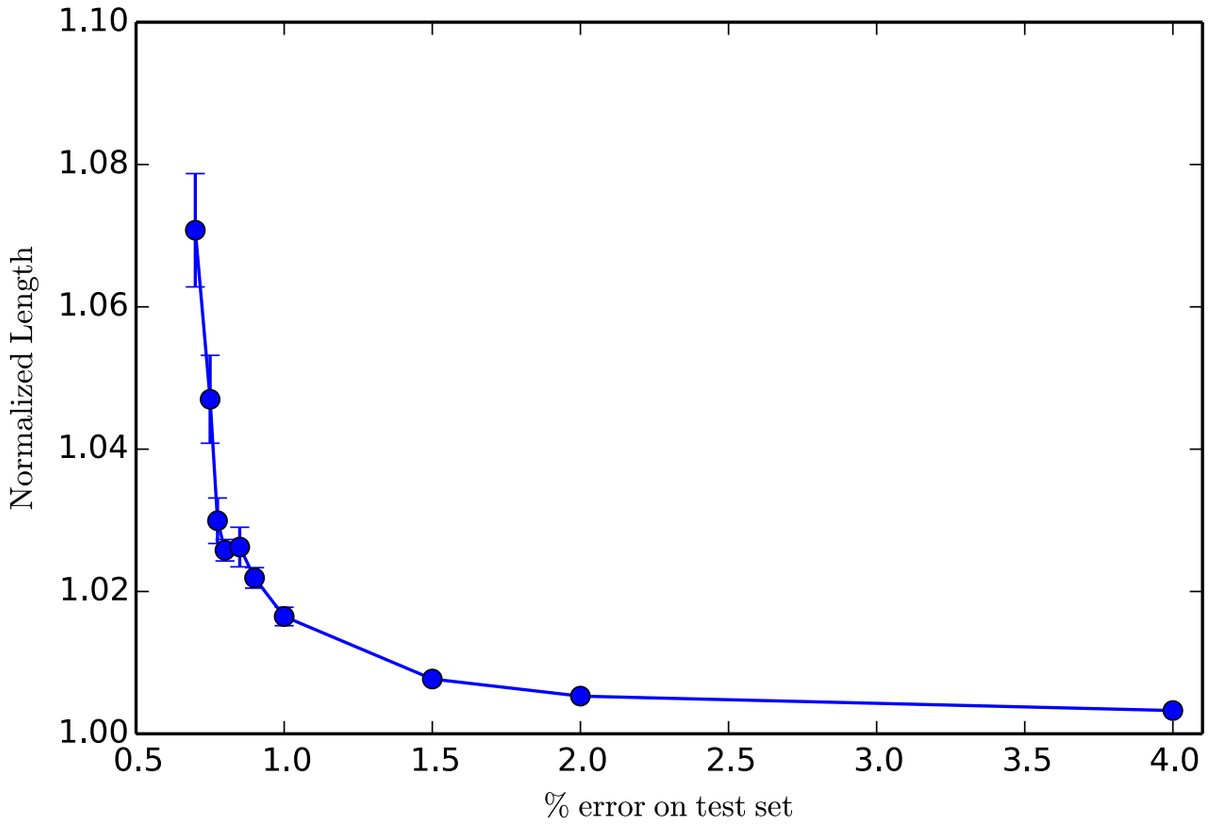


NUMERICAL EXPERIMENTS

- Compute length of geodesic in Ω_u obtained by the algorithm and normalize it by the Euclidean distance. Measure of curviness of level sets.



cubic polynomial



CNN/MNIST

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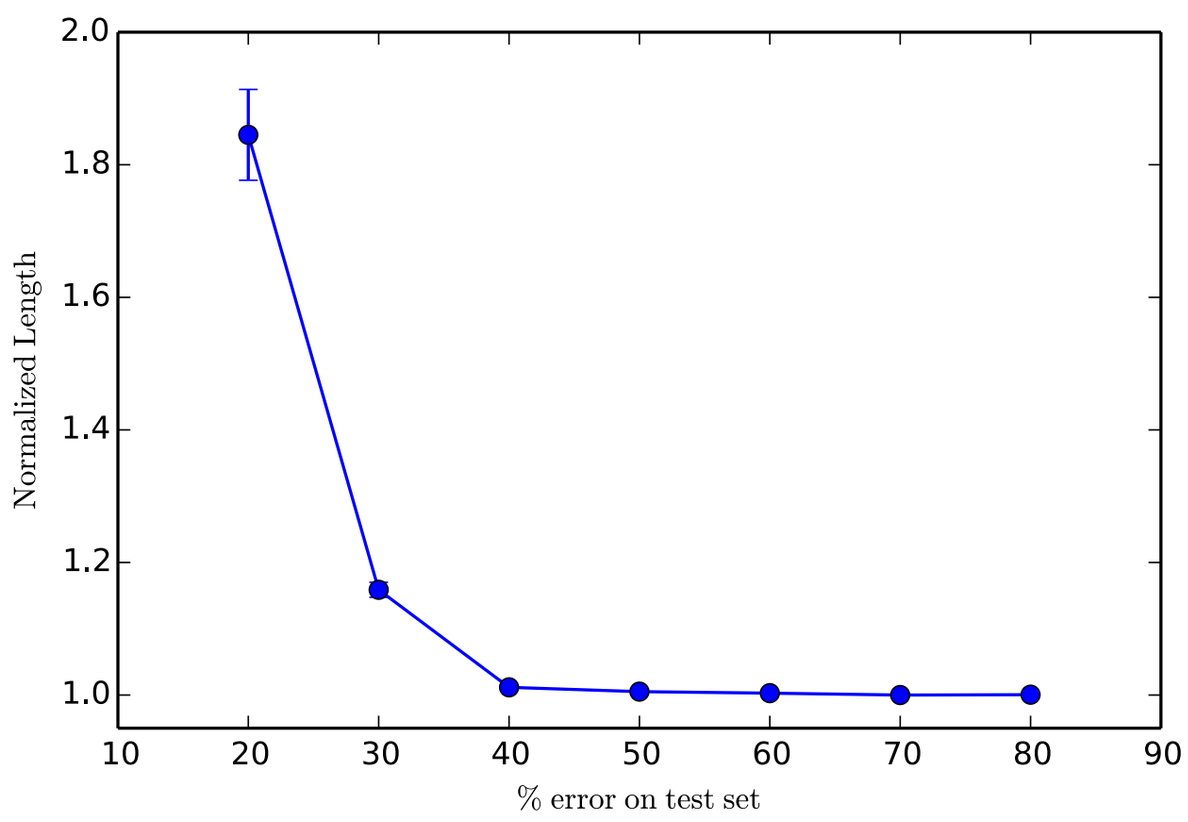
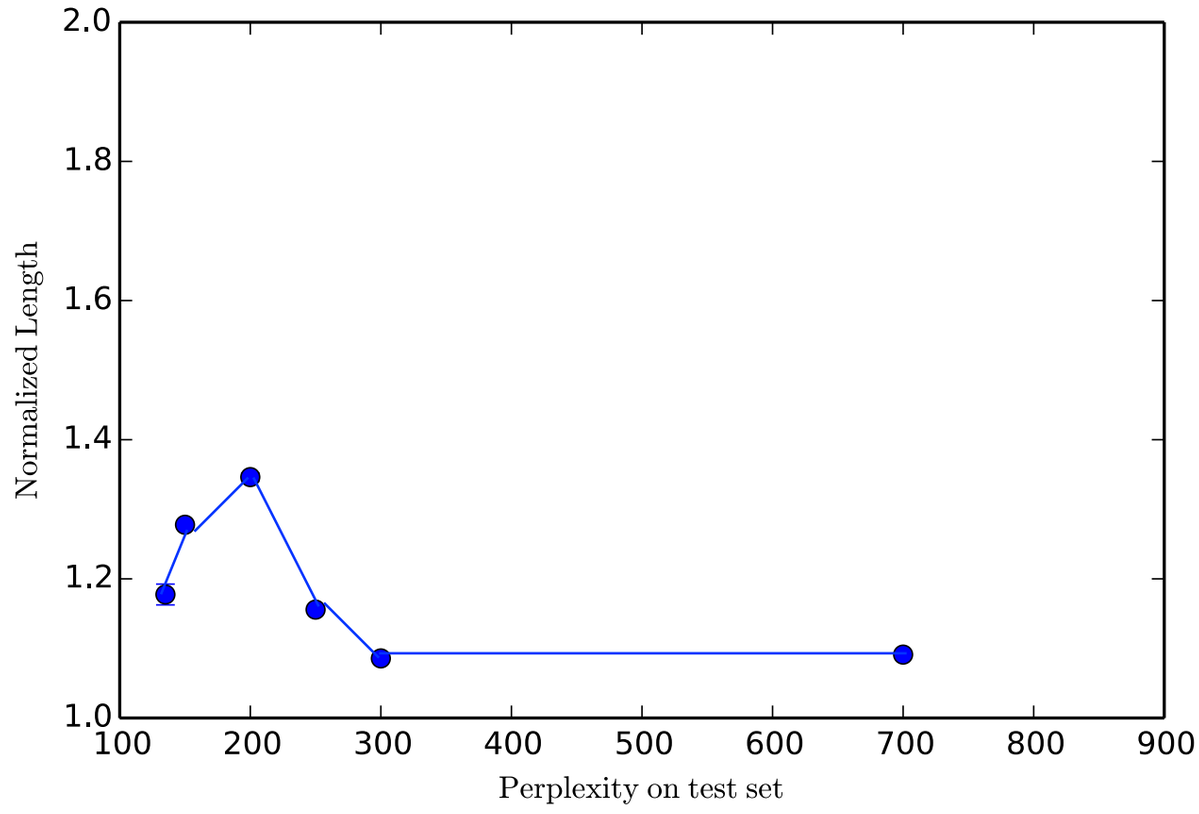


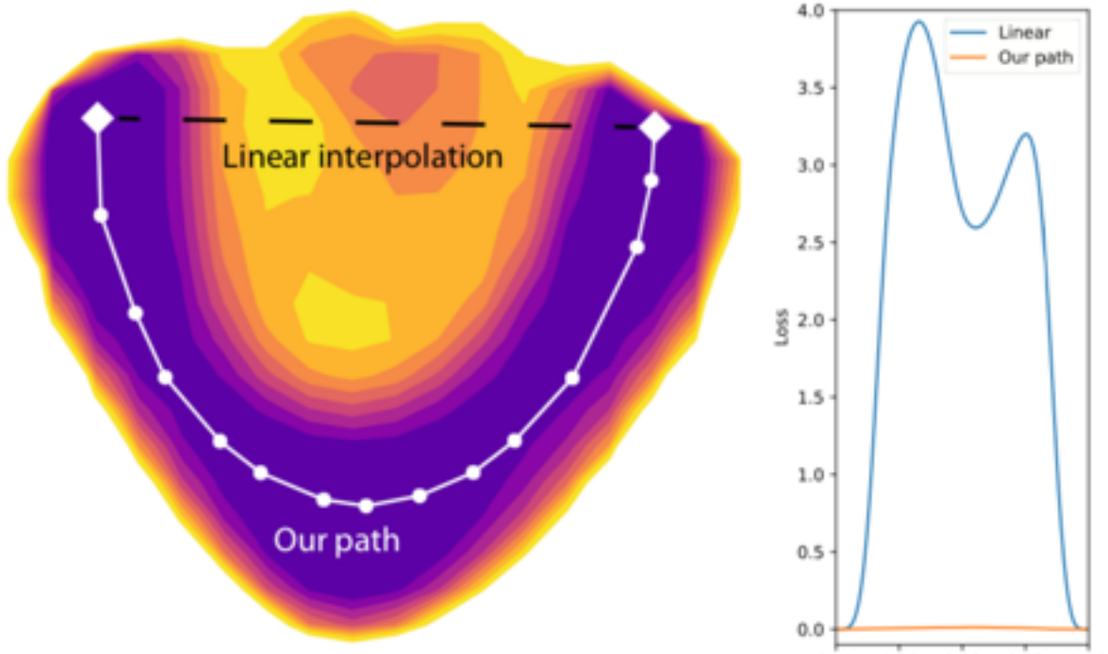
CNN/CIFAR-10



LSTM/Penn

FOLLOW-UPS

- Extensions to larger models and using a more sophisticated path interpolation method in [Draxler et al.'18]



- Using *Nudged Elastic Band* method.

BEYOND FINITE INTRINSIC DIMENSION

- For generic activation function and data distribution, should one expect presence of spurious valleys/minima?
  - Yes [more later]
- What characterization should one pursue in that case?

BEYOND FINITE INTRINSIC DIMENSION

- For generic activation function and data distribution, should one expect presence of spurious valleys/minima?
  - Yes [more later]
- What characterization should one pursue in that case?
- *Towards energy barrier characterizations*: certify that spurious minima lie below a certain energy level.

PRESENCE OF POOR LOCAL MINIMA [YUN ET AL.18]

- Consider a one-hidden layer nonlinear network trained with mean-squared error:

$$L(U, W) = \widehat{\mathbb{E}}\|U\rho(WX) - Y\|^2, \text{ with}$$

$$\rho(x) = \begin{cases} s_+ x & , x \geq 0 \\ s_- x & , x < 0 \end{cases}$$

- Assume $Y \neq RX + b$ for any $R \in \mathbb{R}^{d_y \times d_x}$, $b \in \mathbb{R}^{d_y}$.

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- Assume $Y \neq RX + b$ for any $R \in \mathbb{R}^{d_y \times d_x}$, $b \in \mathbb{R}^{d_y}$.
- **Theorem [YSJ'18]:** If samples are distinct and $m > 1$, then there are poor local minima of L whose empirical risk is the same as the linear fitting.

PRESENCE OF POOR LOCAL MINIMA

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PRESENCE OF POOR LOCAL MINIMA

- Linear fitting is a very weak property: any interesting dataset won't be linearly solvable.
- The proof relies heavily in the piece-wise linear structure of the activation function.
- What is the situation for generic activations?
- We advance towards results somewhat between positive and negative: the landscape is "nice" above a certain energy level.

RESNETS VS LINEAR MODELS

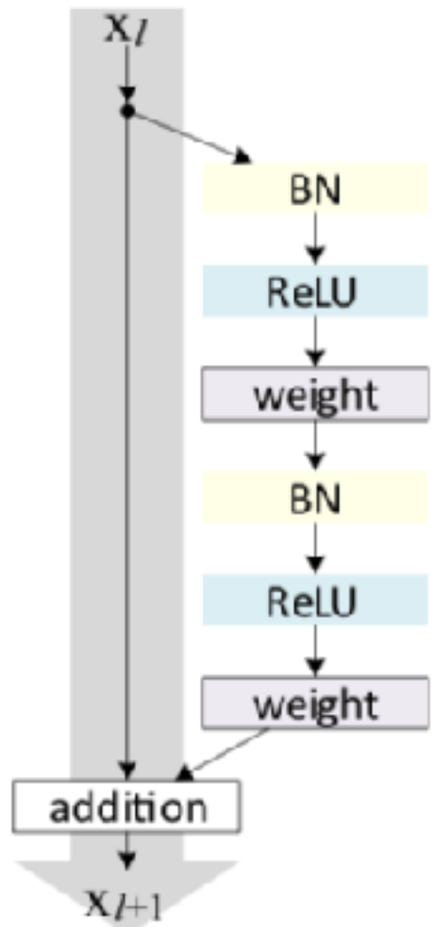
- [Shamir '18] studies the landscape of optimization of generic *Residual Networks* with linear preactivations:

$$f_{k+1}(x) = f_k(x) + h(f_k(x); \theta_k)$$

- The resulting network and loss becomes

$$\Phi_\Theta(x) = w^\top (x + V F_\theta(x)) \,, \; \Theta = \{w, V, \theta\} \,.$$

$$L(w, V, \theta) = \mathbb{E}[\ell(\Phi_\Theta(x), y)] \,.$$



[He et al.'16]

RESNETS VS LINEAR MODELS

- Linear models correspond to a specific slice of the parameter space:

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$$L(w, 0, \theta) = \mathbb{E}[\ell(w^\top x, y)] \,.$$

- **Theorem [Shamir'18]:** Suppose L is twice-differentiable and suppose M is a subset of the parameter domain such that $\max_M(\|w\|, \|V\|) \leq b$. Then any $(w, V, \theta) \in M$ which is an ϵ-second order stationary point satisfies

$$L(w, V, \theta) \leq \min_{\|w'\| \leq r} L(w', 0, \theta) + (\epsilon + \epsilon^{1/4})\text{poly}(b, r, \mu) \,.$$

(μ: Lipschitz constants of L and its derivatives)

- Consequence for spurious local minima?

RESNETS VS LINEAR MODELS

- Taking $\epsilon = 0$, we obtain

Corollary [Shamir'18]: Suppose L is twice-differentiable and continuous Hessians at any compact subset of its domain. Then every local minimum (w, V, θ) of L satisfies

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- Does this directly imply that SGD will provably converge efficiently to a model outperforming linear regression?
- No, because the bound depends on the norm of the stationary point (parameter b).
- Also, this energy barrier is typically very high.

CONCLUSIONS ON OPTIMIZATION LANDSCAPE

- Lots of recent results covering both positive, negative and *mixed* cases.
- Positive results:
  - Many results are distribution-independent, but not architecture independent. Universality should contain a bit of both.
- Negative results:
  - Most construct *planted* solutions: $Y = \Phi(X, \theta_0)$ for some θ_0. Towards more realistic negative examples?
- Mixed cases: energy barriers are a reasonable mathematical picture of realistic landscapes with the right universality properties.

SOME OPEN CHALLENGES

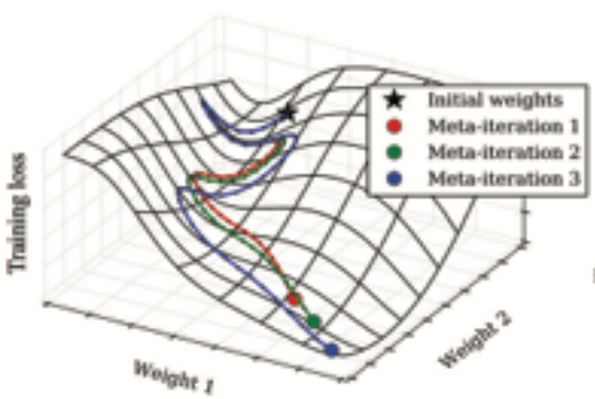
CONVOLUTIONS AND GENERALIZATION IN SUPERVISED LEARNING

- We saw last week that size of the model does not directly impact its generalization error…
- … provided it has the appropriate architecture.
- In the case of natural images, CNNs capture the correct inductive bias.

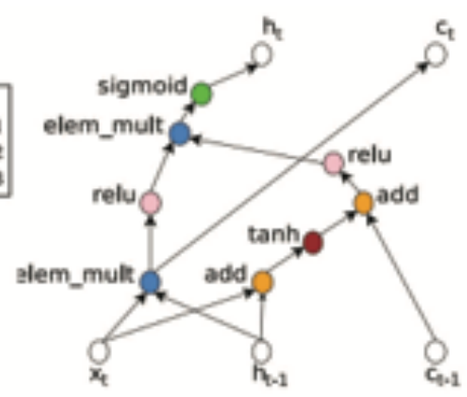
- Open: **construct statistical models for natural images that explain this mathematically.**
- Need to combine tools from signal processing (e.g. wavelets) with statistical learning.
- Geometric measures of generalization.

NON-STATIONARY AND FEW-SHOT LEARNING

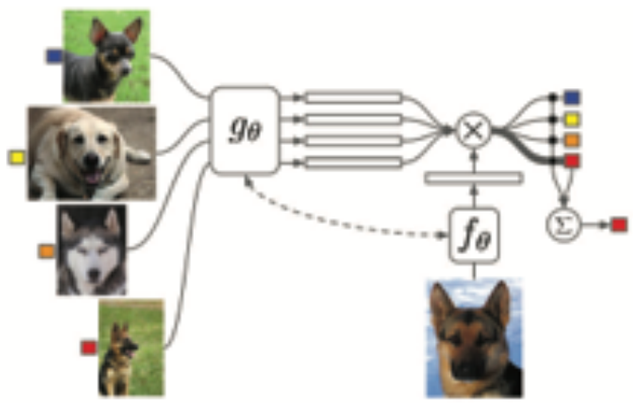
- Many practical scenarios fall outside the traditional iid setup of a large training set $X_i \sim P$.
  - Few-shot learning [Lake et al.'15]
  - Meta-learning [Schmidhuber,'90s, ...]
  - "Learning to Learn"



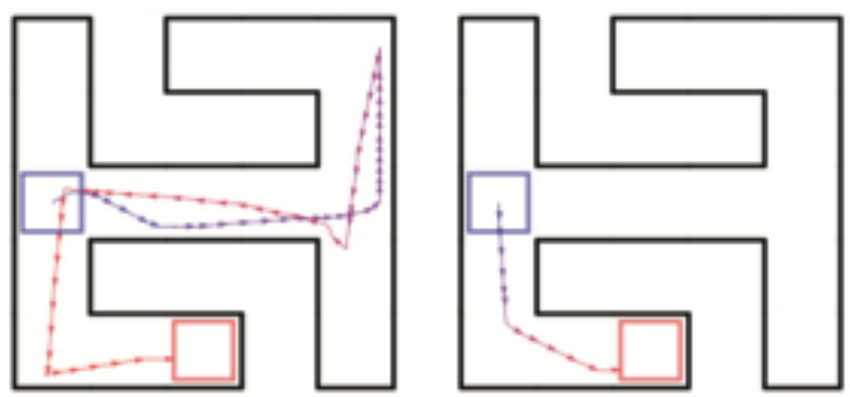
hyperparameter optimization
Maclaurin et al. '15



learned recurrent cell
Zoph & Le '17



few-shot image classifier
Vinyals et al. '16


learning to quickly navigate new mazes
Duan et al. '16

- *C. Finn, Bair blog*

NON-STATIONARY AND FEW-SHOT LEARNING

- Most of these instances can be reduced to a supervised learning task by lifting the input to be the set

$$S_i = (\{x_1, y_1, \ldots x_K, y_K, x_t\}, y_t)$$

  - and then assuming one has an iid collection of such sets.

- How to formalize this setup and quantify the resulting bias-variance tradeoffs?
- Which properties of high-dimensional landscapes and stability translate into this setting?

DEEP LEARNING APPLICATIONS

- In numerical methods
  - Develop Data-driven Integrators that replace fixed integrators (e.g. Projective Dynamics, RK).
  - Fast Multipole Methods.
  - **Need certificate guarantees.**
- In statistical/computational complexity
  - Tool for high-dimensional algorithmic search?
  - **Need ability to interpret.**

DEEP LEARNING IN PHYSICAL SCIENCES

- In Quantum mechanics, current surge of interest for exploiting deep learning models to approximate wave functions Ψ.
- In an N-body system, this wave function describes the quantum state of the system and is defined in a (complex) Hilbert space of dimension N.
- Observables correspond to the spectrum o adjoint operators of this Hilbert space.
- Challenge: construct tractable *ansatz* with approximation properties

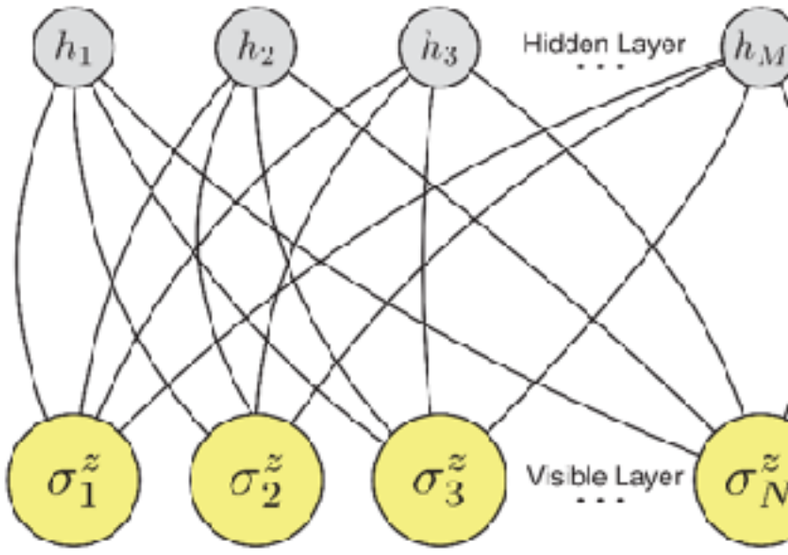
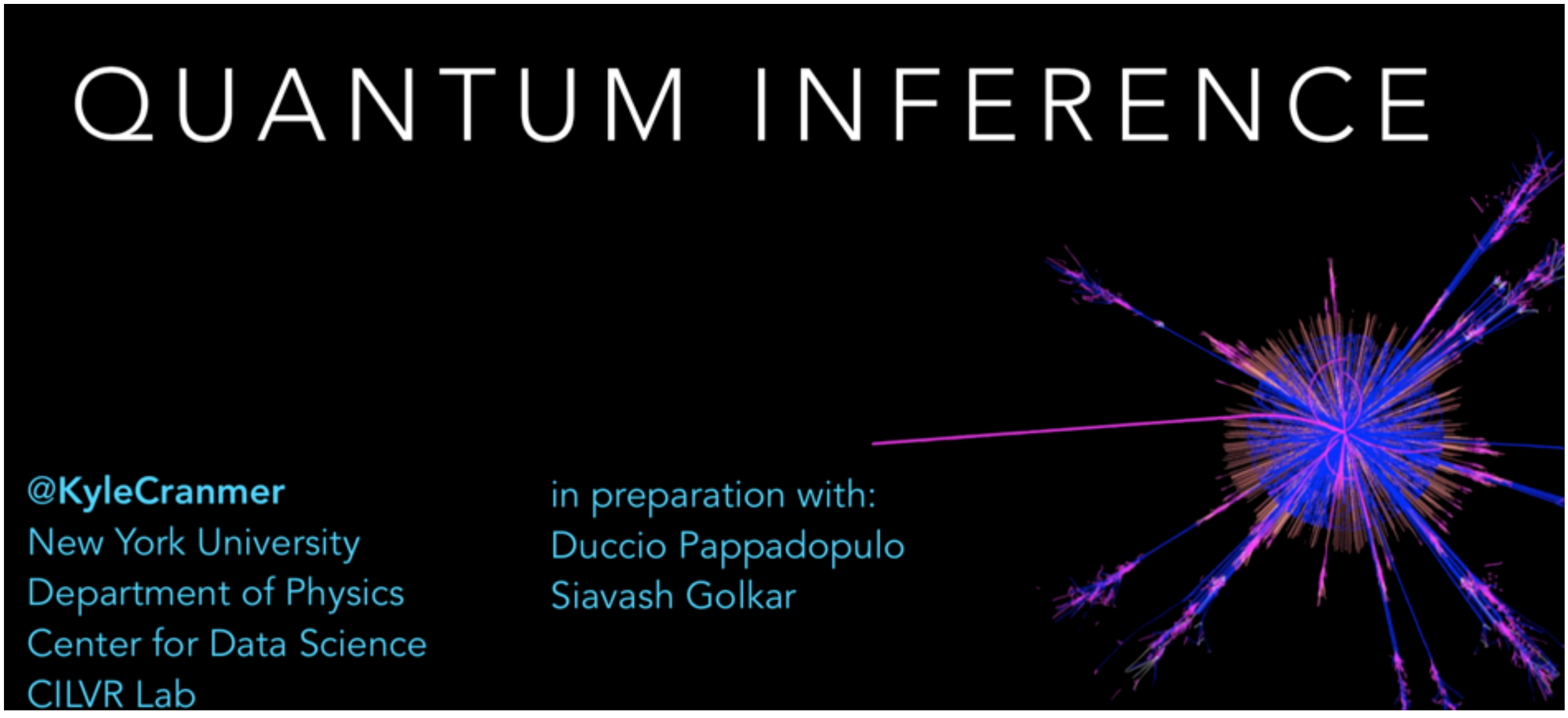


Fig. 1. Artificial neural network encoding a many-body quantum state of N spins. A Boltzmann machine architecture that features a set of N visible artificial neurons (yellow d set of M hidden neurons (gray dots) is shown. For each value of the many body spin co $\mathcal{S} = (\sigma_1^z, \sigma_2^z, \ldots, \sigma_N^z)$, the artificial neural network computes the value of the wave function

Carleo et al, Science'17

DEEP LEARNING IN PHYSICAL SCIENCES

- In particular, how to perform quantum variational inference?



MULTI-AGENT SYSTEMS

- Beyond potential systems: not even a landscape of optimization, but a more general dynamical system:

$$\dot{\theta}_k = \nabla_{\theta_k} f_k(\theta_1, \ldots, \theta_N) \ , \ (k \leq N) \, .$$

The Mechanics of n-Player Differentiable Games

David Balduzzi [1] Sébastien Racaniere [1] James Martens [1] Jakob Foerster [2] Karl Tuyls [1] Thore Graepel [1]

- Framework that goes beyond matrix games (e.g. prisoners dilemma)?
- High-dimensional dynamics, no Nash equilibria in general.

THANKS FOR LISTENING!