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NYU | COURANT INSTITUTE OF MATHEMATICAL SCIENCES

MATHEMATICS OF DEEP LEARNING

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Lecture 10: Gradient Descent in non-convex Landscapes.

OBJECTIVES LECTURE 10

- Gradient Descent (stochastic and deterministic) Converges to local Minimisers.

- Role of Saddle points: exponential slowing-down. Efficiently escaping saddles with perturbations.

- Critical Point Analysis in Deep Learning: linear nets, spin glasses.

- Beyond Hessian analysis: sub-level set analysis

COMMENTS ON [RAGINSKY, RAKHLIN, TELGARSKY]

- **Theorem [Raginsky et al. '17, informal]:** The former decomposition terms are bounded as

$$\mathbb{E}g(\hat{\theta}) - \mathbb{E}g(\hat{\theta}_*) \simeq \epsilon \mathrm{Poly}\left(\beta^{-1}, d, \lambda_*^{-1}\right)$$

for $K \geq \mathrm{Poly}(\beta^{-1}, d, \lambda_*^{-1})\epsilon^{-4}$, and $\gamma \leq \dfrac{\epsilon^4}{\log(\epsilon^{-1})^4}$,

$$\mathbb{E}g(\hat{\theta}_*) - \mathbb{E}g_x(\hat{\theta}_*) \simeq \frac{(\beta^{-1} + d)^2}{\lambda_* n},$$

$$\mathbb{E}g_x(\hat{\theta}_*) - \inf_\theta g(\theta) \simeq \beta d \log(\beta^{-1} + 1).$$

- Only first term involves SGLD, other two only Gibbs sampler.
- λ_* is the spectral gap governing convergence of Markov chain.
  (it is independent of n)

COMMENTS ON [RAGINSKY, RAKHLIN, TELGARSKY]

- However, this spectral gap is exponential!
- We will see examples later where convergence to global optima is provably exponential.

NON-CONVEX OPTIMIZATION

- If optimization gradient-based algorithms converge to global minima in the convex case, what can we expect in non-convex optimization?

- Convergence to local minimisers?
- How many of those are global?
- How much can we be slowed down by saddle points?
- How much noise to add to gradient descent to escape those saddles?

NON-CONVEX OPTIMIZATION

- Vanilla Gradient descent scheme: $\theta_{k+1} = \theta_k - \gamma \nabla g(\theta_k)$
- Its equilibrium points satisfy $\nabla g(\theta_*) = 0$.

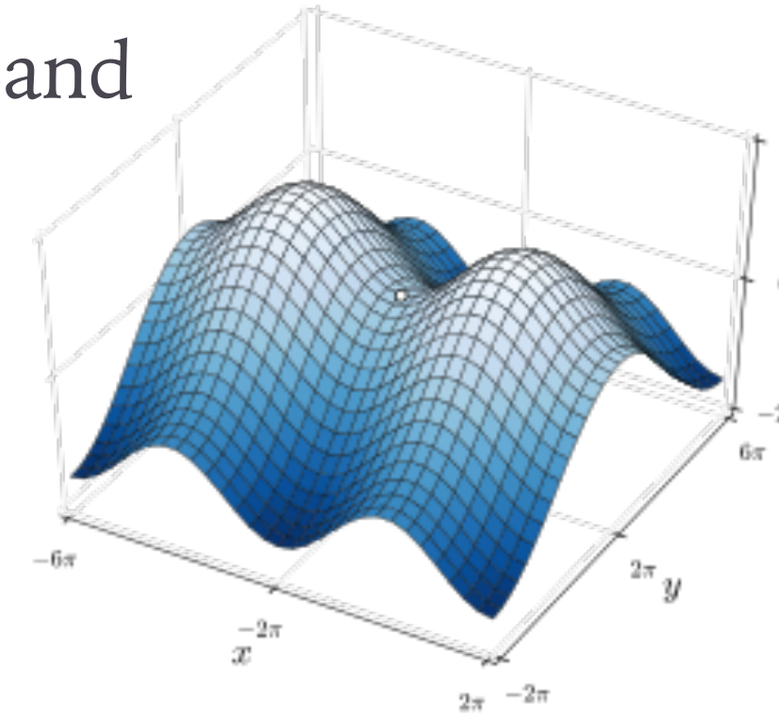
NON-CONVEX OPTIMIZATION

- Vanilla Gradient descent scheme: $\theta_{k+1} = \theta_k - \gamma \nabla g(\theta_k)$
- Its equilibrium points satisfy $\nabla g(\theta_*) = 0$.
- When g is convex, 1st order critical points are global minima.
- However, for general g, stationary points of gradient descent are not necessarily global minima.
- How can they be classified?

INDEX OF CRITICAL POINTS

- Suppose g is in $\mathcal{C}^2$ defined on $\mathbb{R}^d$.
- A *critical point* $\theta^* \in \mathbb{R}^d$ of g is such that $\nabla g(\theta^*) = 0$.
- θ^* is a *strict saddle point* if it is a critical point and its Hessian satisfies

$$\lambda_{\min}(\nabla^2 g(\theta_*)) < 0\,.$$



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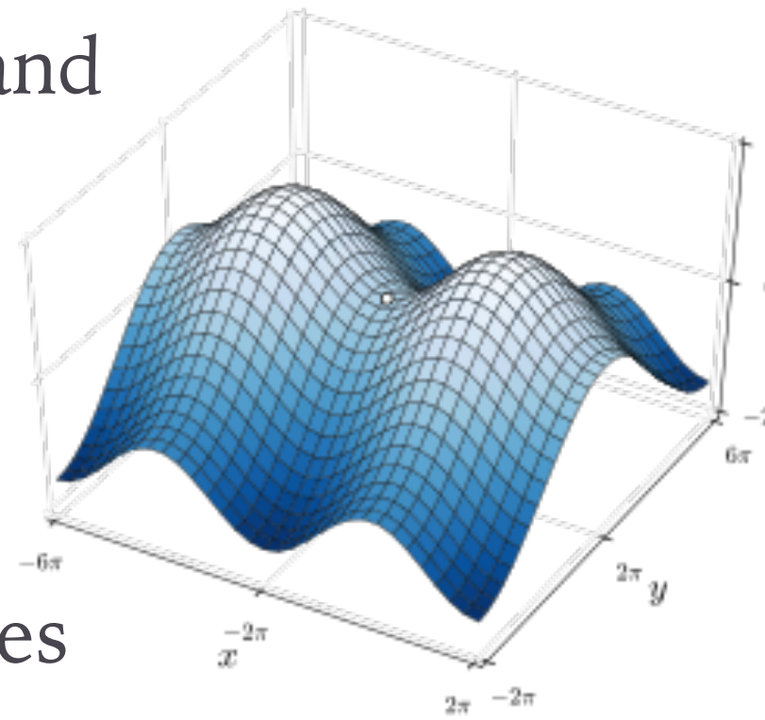

- A local minima (not necessarily strict) satisfies $\lambda_{\min}(\nabla^2 g(\theta_*)) \geq 0\,.$
- While every critical point is an equilibrium point of gradient descent, which are *stable* equilibria?

CHARACTERIZING STABLE EQUILIBRIA OF GRADIENT DESCENT

- Our intuition is that strict saddles are unstable equilibria, and thus it is unlikely that gradient descent reaches those points.
- We can find worst-case initializations of gradient descent that provably converge to saddle-points [Nesterov,'04].

CHARACTERIZING STABLE EQUILIBRIA OF GRADIENT DESCENT

- Our intuition is that strict saddles are unstable equilibria, and thus it is unlikely that gradient descent reaches those points.
- We can find worst-case initializations of gradient descent that provably converge to saddle-points [Nesterov,'04].
- On the other hand, we have just seen that adding noise to gradients can be used to escape saddle points.
- But, how likely is it that randomly initialized gradient descent gets stuck in a saddle point?
- We can study the region of attraction associated to each critical point.

STABLE MANIFOLD

- A discrete-time optimization algorithm is a mapping $\varphi : \mathbb{R}^d \to \mathbb{R}^d$
  - ex for gradient descent, $\varphi(\theta) = \theta - \gamma \nabla g(\theta)$.
  - iterate k is thus obtained as $\theta_k = \varphi^k(\theta_0)$.
- Denote by $\mathcal{X}^*$ the set of strict saddle points of g.
- **Definition** (Global Stable Set): The Global Stable Set of the strict saddles is

$$S_\varphi = \{\theta_0; \lim_{k \to \infty} \varphi^k(\theta_0) \in \mathcal{X}^*\} .$$

INTUITION: QUADRATIC CASE

- Consider the non-convex quadratic function

$$g(\theta) = \theta^\top H\theta\,, H = \mathrm{diag}(\lambda_1, \ldots, \lambda_d)\,, \lambda_1, \ldots \lambda_s > 0,\ \lambda_{s+1}, \ldots, \lambda_d < 0\,.$$

- A single critical point, $\theta^* = 0$, which is a strict saddle.
- Gradient descent initialised from θ_0 produces

$$\theta_{k+1} = \varphi(\theta_k) = \sum_{i=1}^{d} (1 - \gamma\lambda_i)^{k+1} \theta_{0,i} e_i\,.$$

- Suppose $\gamma < \dfrac{1}{\max_i |\lambda_i|}$. Then $\|\theta_k\| \to 0$ iff $\theta_0 \in \mathrm{span}\{e_1, \ldots, e_s\}$.
- It follows that if θ_0 is chosen at random, then we will avoid the strict saddle with probability 1.

INTUITION: GENERAL CASE

- In the case of gradient descent, in a neighborhood of a critical point θ_*, the local attractive set is well approximated by the span of eigenvectors corresponding to positive eigenvectors of the Hessian $\nabla^2 g(\theta_*)$.
- This local attractive set has zero measure within a small neighborhood, thus with probability 1 an initialization sufficiently close to θ_* will leave this neighborhood.
- From local stability to global stability?

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- From local stability to global stability?
- Not trivial: locally escaping a given saddle point does not guarantee we won't fall into another one later.

STABLE MANIFOLD THEOREM

- Given a diffeomorphism φ, we define an unstable fixed point set as

$$\mathcal{A}^*_\varphi = \{\theta;\, \varphi(\theta) = \theta;\, \max_i |\lambda_i(D\varphi(\theta))| > 1\}.$$

- **Theorem [Stable Manifold]:** Let φ be a C^1 mapping from $\mathcal{X} \to \mathcal{X}$ and $\det(D\varphi(\theta)) \neq 0$ for all $\theta \in \mathcal{X}$. Then the set of initial points that converge to an unstable fixed point has measure zero:

$$\mu\left(\{\theta_0 : \lim_k \varphi^k(\theta_0) \in \mathcal{A}^*_\varphi\}\right) = 0\,.$$

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- **Corollary:** If $\mathcal{X}^* \subseteq \mathcal{A}^*_\varphi$, then $\mu(S_\varphi) = 0$.

GRADIENT DESCENT AVOIDS STRICT SADDLES

- Assume ∇g is Lipschitz, with $\|\nabla^2 g(\theta)\| \leq L$.
- Fact 1: every strict saddle point of g is an unstable fixed point of gradient descent: $\mathcal{X}^* \subseteq \mathcal{A}_\varphi^*$

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- Fact 2: Moreover, if step size satisfies $\gamma < L^{-1}$, then $\det(D\varphi(\theta)) \neq 0 \, \forall \theta$.

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- Assume ∇g is Lipschitz, with $\|\nabla^2 g(\theta)\| \leq L$.
- Fact 1: every strict saddle point of g is an unstable fixed point of gradient descent: $\mathcal{X}^* \subseteq \mathcal{A}_\varphi^*$
- Fact 2: Moreover, if step size satisfies $\gamma < L^{-1}$, then $\det(D\varphi(\theta)) \neq 0 \, \forall \theta$.
- Consequence: [Lee et al.'16] Under these assumptions, the stable set of strict saddle points has measure zero.
- This result also holds for proximal point, coordinate descent, mirror descent.

COMMENTS

- This result establishes that gradient descent escapes strict saddles. It does not directly imply that it converges to local minimizers!
- The required additional property is that $\lim_k \theta_k$ exists.
- Two sufficient conditions are discussed in [Lee et al.'16]:
  - Isolated critical points and compact sublevel sets
  - Satisfies the local Lojasiewicz inequality

$$\|\nabla g(\theta)\| \geq m|g(\theta) - g(\theta^*)|^a \, , a < 1$$

- What happens in the stochastic case?

FIRST-ORDER STATIONARY POINTS IN GRADIENT DESCENT

- An *ϵ-first-order stationary point* of g is such that $\|\nabla g(\theta^*)\| \leq \epsilon$.
- We know that plain gradient descent converges to first-order stationary points in the class of L-smooth functions:

Theorem [Nesterov'98]: For any $\epsilon > 0$, gradient descent with step size $\gamma = L^{-1}$ requires $\frac{L(g(\theta_0)-g^*)}{\epsilon^2}$ iterations to reach an ϵ-first order stationary point of g.

- This result is not cursed by dimensionality.
- Whereas first-order stationary points are sufficient in convex optimization, not anymore when g is non-convex.

ESCAPING FROM SADDLE POINTS

- We are interested in the problem of finding ϵ-*second order stationary points:* Assuming $\nabla^2 g$ is Lipschitz, such points satisfy

$$\|\nabla g(\theta^*)\| \leq \epsilon \text{ and } \lambda_{\min}(\nabla^2 g(\theta^*)) \geq -\sqrt{\epsilon\rho}\,.$$

$$\rho = \mathrm{Lip}(\nabla^2 g)$$

- If all saddle points are strict, then second-order stationary points are all local minima.

ESCAPING FROM SADDLE POINTS

- Owing to the instability of strict saddle points, stochastic gradient descent is also robust:

Theorem [Ge et al.'15]: If $g(\theta)$ satisfies the strict saddle, then Noisy Stochastic Gradient Descent converges to a local minimum in polynomial time.

- The theorem requires robust strict saddle (away from 0).
- They consider the noisy SGD setting:

$$\theta_{k+1} = \theta_k - \gamma(\nabla g(\theta_k) + \epsilon_k + Z)\,, Z \sim \mathcal{N}(0, I)\,.$$

  - Gaussian noise guarantees exploration in all directions.
- However, Time is dimension-dependent $(\Omega(d^4))$.

ESCAPING FROM SADDLE POINTS

- We have established that both gradient descent and stochastic gradient descent escape (strict) saddles.

- How fast do they escape?

- Does the noise improve or decrease the efficiency?

- Dependency on input dimensionality of the problem?

ESCAPING FROM SADDLE POINTS WITH SGD

- [Jin et al.'17] study a similar version of SGD, where noise is added conditionally:
  - When the norm of the current gradient is smaller than a threshold, they add a small random perturbation, uniformly sampled from a d-dimensional ball.
- **Theorem [Jin et al.'17]:** Assume ∇g is L-Lipschitz and $\nabla^2 g$ is ρ-Lipschitz. Then with appropriate parameters, noisy Gradient Descent will output an ϵ-second order stationary point whp with

$$\tilde{O}\left(\frac{L(g(\theta_0)-g^*)}{\epsilon^2}\right) \text{ (up to polylog factors).}$$

ESCAPING FROM SADDLE POINTS WITH SGD

- The dimension appears in the rate as a $\log^4 d$ factor. It could be improved to a single log, but most probably not removed [open problem].
- When a current estimate θ_k is not an ϵ-second order stationary point, two things can happen:
  - $\|\nabla g(\theta_k)\|$ is large: not yet a 1st order stationary point.
  - $\nabla^2 g(\theta_k)$ has a large negative eigenvalue: noise added to updates enables descent in that case.
- Adding noise to the gradient is thus sufficient to escape saddles. Is noise also necessary to efficiently escape?

SMOOTH COUNTER-EXAMPLE

- Adversarially initializing Gradient Descent can stop any progress (for example, initialize exactly at a saddle point).
- As it turns out, even with uniform initialization, one can find smooth functions for which GD requires exponential time to escape:

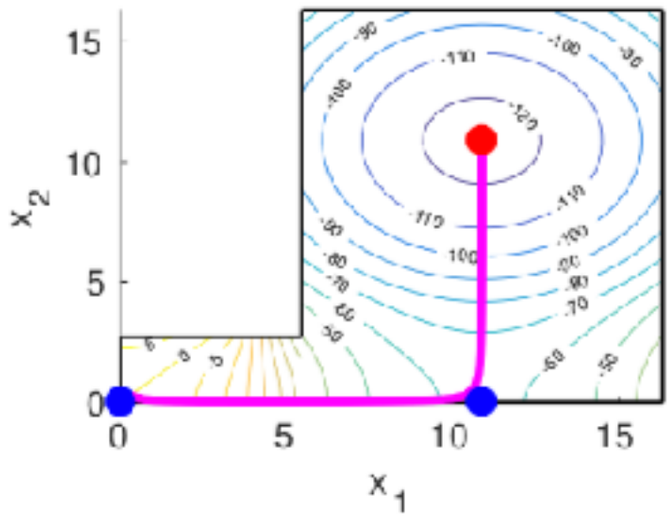
Theorem [Du et al.'17]: Suppose we initialize using uniform distribution on $[-1, 1]^d$. There exists a smooth function $g \in \mathbb{R}^d$ such that:

- with probability 1, GD will be $\Omega(1)$ distance away from any local minima for any $K \leq e^{\Omega(d)}$.
- for any $\epsilon > 0$, whp noisy GD finds a point θ such that $\|\theta - \theta^*\| \leq \epsilon$ for some local minimum θ^* in $\text{poly}(d, \epsilon^{-1})$ iterations.

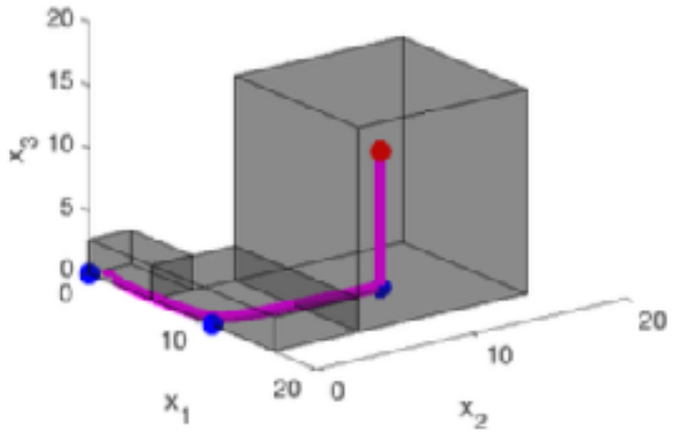
INTUITION

- The result can be generalized for initializations under any distribution that has most of its mass within a compact support (e.g. Gaussian).
- Key intuition: consider the function

$$g(\theta_1, \theta_2) = \begin{cases} -\gamma\theta_1^2 + L\theta_2^2 & \text{if } \theta_1 \in [0,1], \theta_2 \in [0,1] \\ L(\theta_1 - 2)^2 - \gamma\theta_2^2 & \text{if } \theta_1 \in [1,3], \theta_2 \in [0,1] \\ L(\theta_1 - 2)^2 + L(\theta_2 - 2)^2 - c & \text{if } \theta_1 \in [1,3], \theta_2 \in [1,3] \end{cases}$$

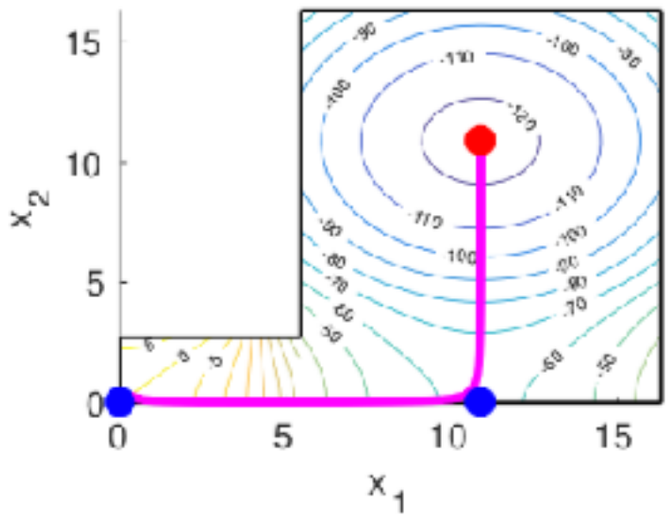


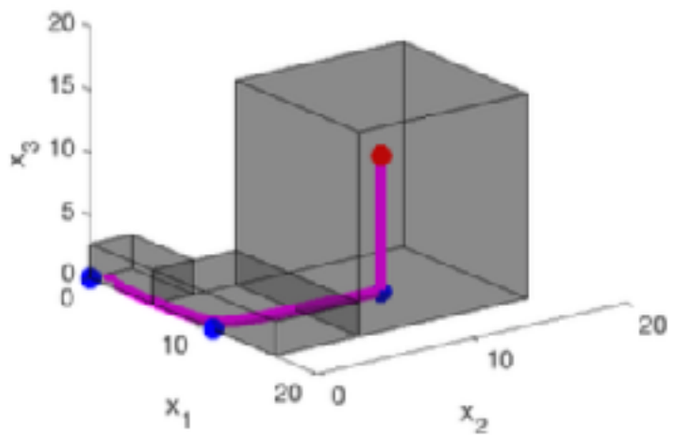
(a) Contour plot of the objective function and tube defined in 2D.



(b) Trajectory of gradient descent in the tube for $d = 3$.

INTUITION





$$R_1 = [0,1] \times [0,1].$$
$$R_2 = [1,3] \times [0,1].$$
$$R_3 = [1,3] \times [1,3].$$

- This function has minimum at (2,2) and saddle points at (0,0) and (2,0).
- Suppose initialization at R1; t_1:time to move from R1 to R2.
- Key observation: the time t_2 to transition R2->R3 is $t_2 \geq \kappa t_1$, with $\kappa > 1$.
- Therefore, escaping d saddle points requires $\Omega(\kappa^d)$ iterations.

BEYOND FIRST-ORDER METHODS

- There are other algorithms that efficiently escape saddle points, if allowed to use higher-order gradient information

- [Nesterov Polyak'06]: cubic regularization using Hessian.
- [Carmon et al,'16][Agarwal et al'16][Carmon & Duchi'16] showed convergence to second-order stationary points using only Hessian-vector product oracle.

LANDSCAPE OF CRITICAL POINTS

- Thus, studying the critical points of non-convex landscapes, and proving the strict-saddle property is a guarantee that gradient descent converges to global minima (eventually).
- Stochastic Gradient is theoretically motivated by escape time analysis (although not always with the correct noise).
- Successful analysis of strict saddles:
  - Tensor Decomposition [Lee et al.]
  - Matrix Completion [Ma et al.]
  - Deep Learning [Kawaguchi ‘16, Soltanolkotabi et al.’17]

TENSOR METHODS IN DEEP LEARNING

- Optimizing the training error with a generic deep network is a non-convex problem.

$$\min_{\Theta} \frac{1}{n} \sum_{i<n} \ell(y_i, \Phi(x_i; \Theta)) + \mathcal{R}(\Theta) \ .$$

- Consider a network of depth d with ReLU nonlinearities. Seen as a function of its parameters $\Theta, \Phi(x; \Theta)$ resembles a homogeneous piece-wise polynomial:

$$\Theta = \{\Theta^1, \ldots, \Theta^d\} \ .$$

$$\Phi(x; \Theta) = \sum_{p} \pi(x; \Theta) x_{p(1)} \prod_{j=1}^{d} \Theta^j_{p(j)} \ , \ \pi(x; \Theta) = \{0, 1\} \ .$$

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- Consider a network of depth d with ReLU nonlinearities. Seen as a function of its parameters Θ, $\Phi(x; \Theta)$ resembles a homogeneous "piece-wise" polynomial:

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$$\Theta = \{\Theta^1, \ldots, \Theta^d\} \ .$$

- The dependencies on Θ are partly captured by the d-order tensor

$$\Theta^1 \otimes \Theta^2 \ldots \otimes \Theta^d \ .$$

TENSOR METHODS

$$\min_{\Theta^1,\ldots,\Theta^d} F(Y, \Psi_X(\Theta^1,\ldots,\Theta^d)) + \mathcal{R}(\Theta^1,\ldots,\Theta^d) \ .$$

- Tensor factorizations are a broad class of non-convex optimization problems.

TENSOR METHODS

$$\min_{\Theta^1,\ldots,\Theta^d} F(Y, \Psi_X(\Theta^1,\ldots,\Theta^d)) + \mathcal{R}(\Theta^1,\ldots,\Theta^d) \ .$$

- Tensor factorizations are a broad class of non-convex optimization problems.

- A particularly famous instance is the matrix factorization problem:

$$\min_{U,V} \ \ell(Y, UV^T) + \mathcal{R}(U,V) \ , \ Y \in \mathbb{R}^{n\times m}, U \in \mathbb{R}^{n\times d}, V \in \mathbb{R}^{m\times d} \ .$$

  - Low-rank factorizations (e.g. PCA)
  - Sparse factorizations (Dictionary Learning, NMF)

MOTIVATION: MATRIX FACTORIZATION

- Example: low-rank factorization.

$$\min_{U,V} \ell(Y, UV^T) \ , \ \text{s.t. } \operatorname{rank}(UV^T) \leq r \ .$$

  - When $\ell(Y, X) = \|Y - X\|_{op}$, $\ell(Y, X) = \|Y - X\|_F$OK

- We can *lift* the problem and relax the constraint:

$$\min_X \ell(Y, X) + \lambda \|X\|_* \ , \quad \|X\|_* = \text{Nuclear norm of } X.$$

- Factorized and relaxed formulations are connected via a variational principle:

$$\|X\|_* = \min_{UV^T = X} \frac{1}{2}(\|U\|_F^2 + \|V\|_F^2) \ .$$

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- Q: General case?

TENSOR NORMS [BACH, HAEFFELE&VIDAL]

- A first generalization is the tensor norm

$$\|X\|_{u,v} = \inf_r \min_{UV^T=X} \frac{1}{2}\left(\sum_i \|U_i\|_u^2 + \|V_i\|_v^2\right) .$$

Theorem [H-V]: A local minimizer of the factorized problem $\min_{U,V} \ell(Y, UV^T) + \lambda \sum_{i<r} \|U_i\|_u \|V_i\|_v$ such that for some i $U_i = V_i = 0$ is a global minimizer of the convex problem $\min_X \ell(Y, X) + \lambda \|X\|_{u,v}$ as well as the factorized problem.

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- This produces an *optimality certificate:* we use a surrogate convex problem to obtain a guarantee that a non-convex problem is solved optimally.

FROM TENSOR FACTORIZATIONS TO DEEP NETS

- We start by generalizing a multilinear mapping (tensor) to homogeneous maps $\phi(\Theta^1, \ldots, \Theta^d)$:

s: degree of homogeneity.

$$\forall\ \Theta, \forall\ \alpha \geq 0\ ,\ \phi(\alpha\Theta^1, \ldots, \alpha\Theta^d) = \alpha^s \phi(\Theta^1, \ldots, \Theta^d)\ .$$

Ex: ReLU $\rho(x) = \max(0, x)$ is homogeneous of degree 1.

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$$\Phi_r(\Theta^1, \ldots, \Theta^d) = \sum_{i \leq r} \phi(\Theta_i^1, \ldots, \Theta_i^d)\ .$$

- We consider

$$\min_{\Theta^1, \ldots, \Theta^d} \ell(Y, \Phi_r(\Theta^1, \ldots, \Theta^d)) + \lambda \mathcal{R}(\Theta^1, \ldots, \Theta^d)\ ,$$

Key assumption: $\mathcal{R}$ is positively homogeneous of the same degree as Φ.

FROM TENSOR FACTORIZATIONS TO DEEP NETS

$$\Phi_r(\Theta^1, \ldots, \Theta^d) = \sum_{i=1}^{r} \phi(\Theta^1, \ldots, \Theta^d) \ .$$

Examples

Matrices: $\Phi(U, V) = UV^T = \sum_{i=1}^{r} U_i V_i^T \ \ (\phi(U_i, V_i) = U_i V_i^T) \ .$

Higher-order Tensors:

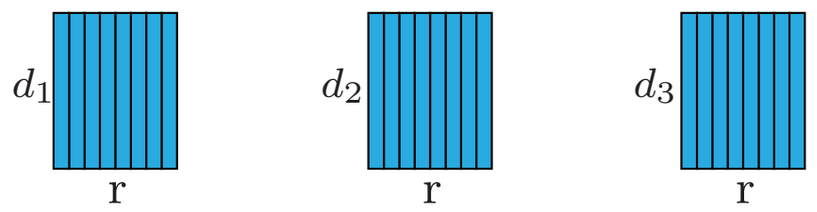
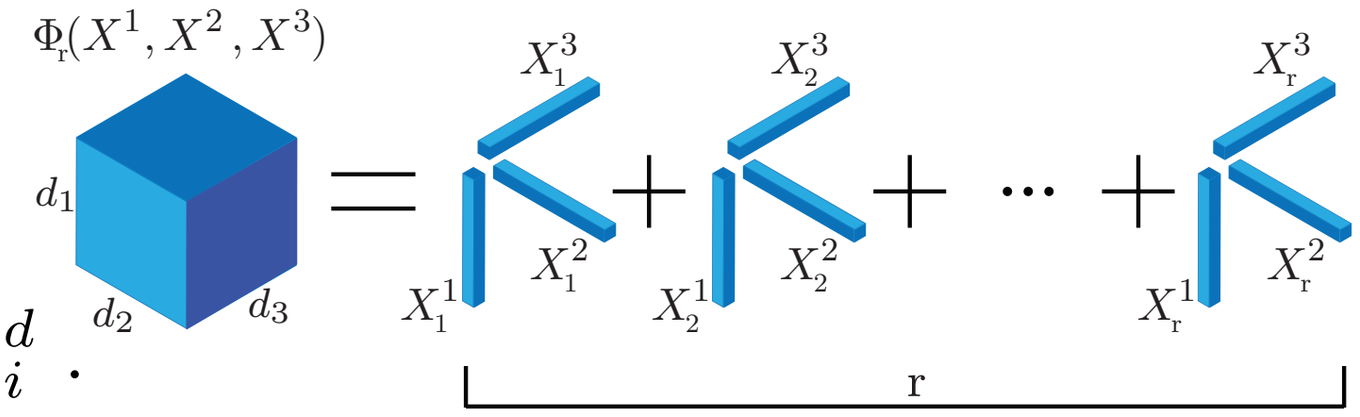


figure credit: R. Vidal



$$\phi(\Theta_i^1, \ldots, \Theta_i^d) = \Theta_i^1 \otimes \cdots \otimes \Theta_i^d \ .$$

Candecomp/Parafac (CP) Tensor decomposition.

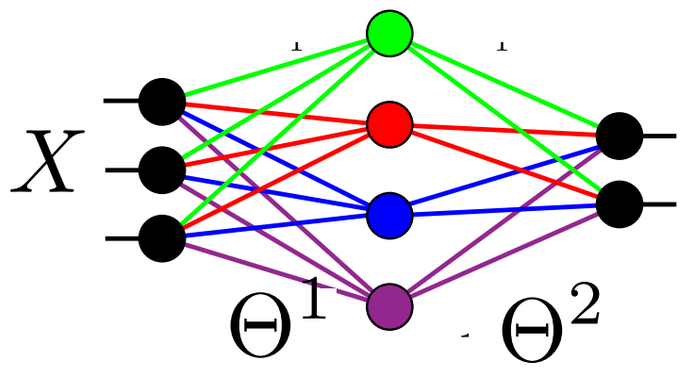
ADAPTATION TO DEEP MODELS

$$\Phi_r(\Theta^1, \ldots, \Theta^d) = \sum_{i=1}^{r} \phi(\Theta^1, \ldots, \Theta^d) \ .$$

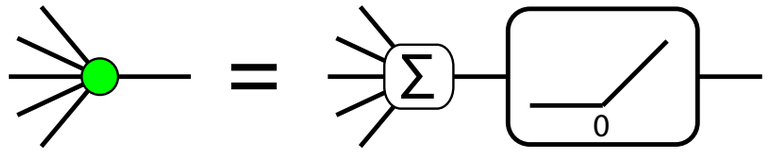
➤

ReLU Network:

ReLU Network with One Hidden Layer



Rectified Linear Unit (ReLU)



$\phi(\Theta^1, \Theta^2)$

Multilayer ReLU
Parallel Network

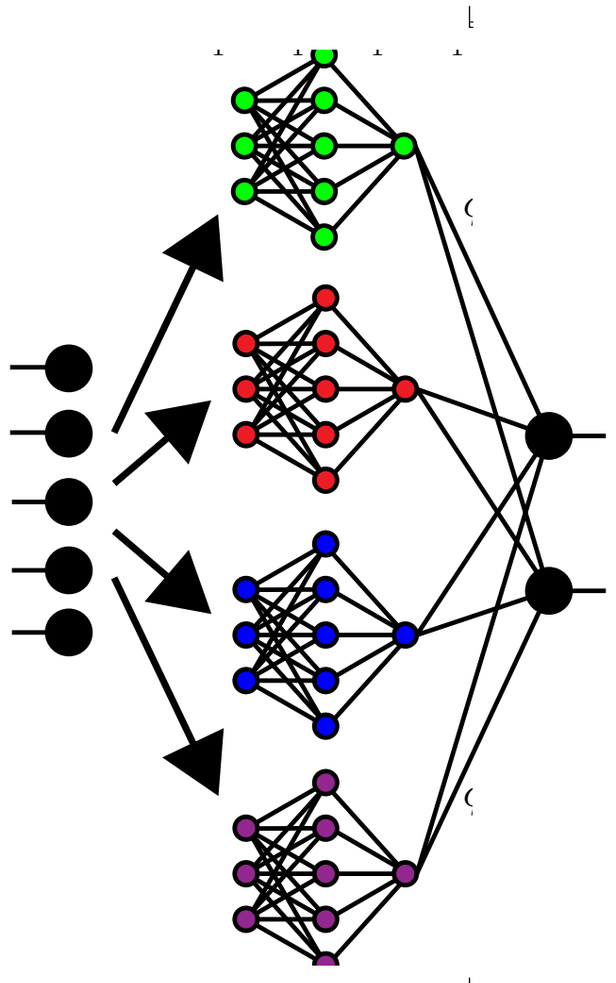


figure credit: R. Vidal

$$\Phi(\Theta^1, \ldots, \Theta^d) = \sum_i \phi(\Theta_i^1, \ldots, \Theta_i^d) \ .$$

ADAPTATION TO DEEP MODELS

- In the matrix case, the variational principle was

$$\|X\|_{u,v} = \min_{UV^T=X} \sum_{i\leq r} \|U_i\|_u \|V_i\|_v \ .$$

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$$\|X\|_{u,v} = \min_{UV^T=X} \sum_{i\leq r} \|U_i\|_u \|V_i\|_v \ .$$

- This is generalized to

$$\mathcal{R}(\Theta) = \min_{\Theta^1,\ldots,\Theta^d} \sum_{i\leq r} g(\Theta_i^1,\ldots,\Theta_i^d) \ , \ s.t. \ \Phi_r(\Theta^1,\ldots,\Theta^d) = \Theta \ .$$

Proposition [H-V]: $\mathcal{R}$ is convex.
Also, if g is positively homogeneous of degree s, so is $\mathcal{R}$.

ADAPTATION TO DEEP MODELS

Theorem [H-V]: A local minimizer of the factorized problem

$$\min_{\Theta^k} \ell(Y, \sum_{i \leq r} \phi_r(\Theta_i^k)) + \lambda \sum_{i \leq r} g(\Theta_i^k)$$

such that for some i and all k $\Theta_i^k = 0$ is a global minimizer for both factorized problem and the convex formulation

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- Global optimality certificate for a broad class of non-convex optimization problems, including some form of deep learning architectures.
- Q: How to use this certificate in practice?

ADAPTATION TO DEEP MODELS

- Pros
  - Global optimality certificate, easy to check
  - Inclues nonlinear models as long as they are homogeneous.
  - Provides a possible meta-algorithm: increase the lifting value r progressively is local optimum does not very condition.

- Cons
  - How much do we need to increase r in practice?
  - How stringent is the homogenous regularization condition?

TENSOR DECOMPOSITIONS AND NEURAL NETS

- Suppose a label generating model of the form

$$\mathbb{E}(y|x) = f_0(x) = \langle a_2, \sigma(A_1 x + b_1) \rangle + b_2 \ ,$$

$\sigma(\cdot)$: point-wise nonlinearity
$A_1 \in \mathbb{R}^{d \times k}$.

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- Q: Given training samples $\{(x_i, y_i)\,;\, y_i = f_0(x_i)\}_{i \leq n}$, can we estimate the parameters a_2, A_1, b_1, b_2 with provable risk?
- Q: Using a computationally efficient algorithm?

BREAKING THE PERILS OF (...) [Janzamin, Sedghi, Anandkumar]

- If one assumes knowledge of the input distribution $p(x)$, then one can exploit the relationship between score functions and conditional expectations:

Def: The m-th order score function $S_m(x)$ is the m-th order tensor

$$S_m(x) = (-1)^m \frac{\nabla^m p(x)}{p(x)} \ .$$

Proposition: If $f(x) = \mathbb{E}(y|x)$, then

$$\mathbb{E}(y \cdot S_3(x)) = \mathbb{E}(\nabla^3 f(x)) \ .$$

BREAKING THE PERILS OF (. . .) [Janzamin, Sedghi, Anandkumar]

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- It follows that when $\mathbb{E}(y|x) = f_0(x)$, we have

$$\mathbb{E}(y \cdot S_3(x)) = \sum_{j \leq k} \lambda_j (A_1)_j \otimes (A_1)_j \otimes (A_1)_j \ \in \mathbb{R}^{d \times d \times d}, \ \lambda_j \in \mathbb{R} \ .$$

BREAKING THE PERILS OF (...) [Janzamin, Sedghi, Anandkumar]

➤ Learning generalization bound in the "realizable" setting:

Theorem: The tensor algorithm *NN-Lift* learns the target function $\mathbb{E}(y|x) = f_0(x)$ up to error ϵ when the number of samples is of the order of

$$n \geq O\left(\frac{kd^3}{\epsilon^2}\frac{\lambda_{max}(A_1)^2}{\lambda_{min}(A_1)^6}\right) .$$

(k: size of hidden layer)
(d: input dimension)

➤ Comments:

- ➤ Polynomial sample complexity.
- ➤ Algorithm has polynomial complexity as well.
- ➤ Extension to non-realizable setting (see paper for details).

BREAKING THE PERILS OF (. . .) [Janzamin, Sedghi, Anandkumar]

- Pros
  - Statistical Guarantees that also incorporate computational feasibility.
  - Learning is essentially reduced to finding low-rank tensor factorizations.

- Cons
  - very strong hypothesis: knowledge of p(x).
  - only a particular Neural network architecture (one hidden layer so far).
  - restrictive class of nonlinearities? : the proof requires

$$\mathbb{E}(\sigma'''(z)) \ , \ \mathbb{E}(\sigma''(z))$$

DEEP NETWORKS AND SPIN GLASSES

- Suppose we have a linear deep network:

$$\Phi(x; \Theta_1, \ldots, \Theta_K) = \Theta_K \Theta_{K-1} \ldots \Theta_1 x \ .$$

- And suppose we train using least squares regression:

$$E(\Theta) = \frac{1}{n} \sum_{i \leq n} \|y_i - \Phi(x_i; \Theta)\|^2 \ .$$

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$$(\Theta_1 x)^j = \sum_l \Theta_1^{j,l} x^l \ ,$$

- In coordinates,

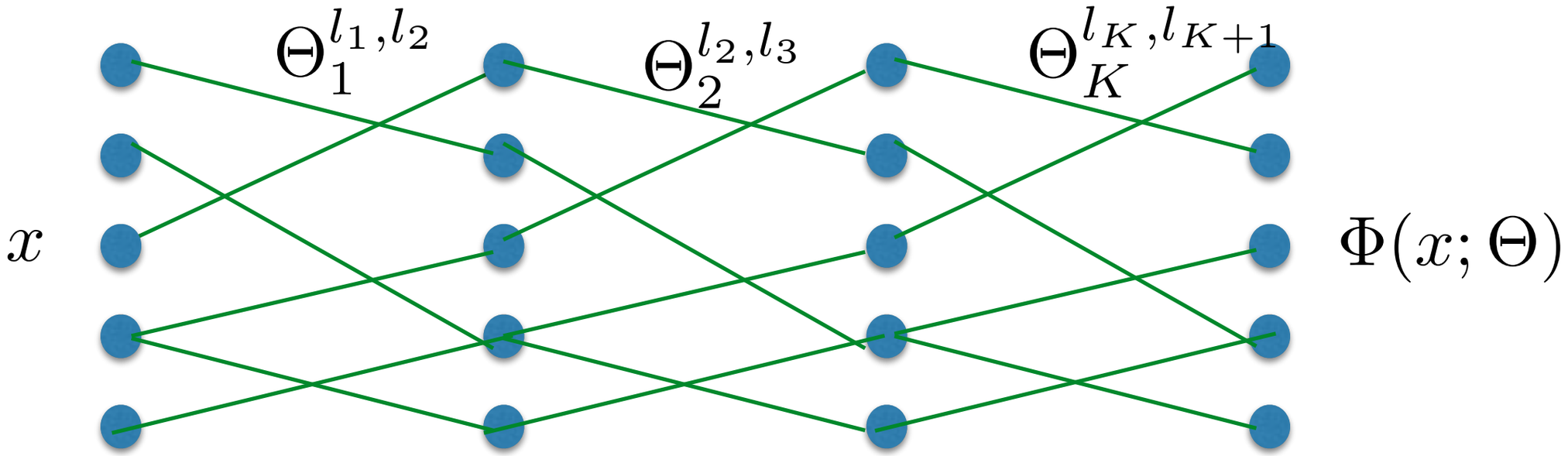
$$(\Theta_2 \Theta_1 x)^j = \sum_{l_1, l_2} \Theta_2^{j,l_2} \Theta_1^{l_2,l_1} x^{l_1} \ ,$$

$$(\Theta_K \ldots \Theta_2 \Theta_1 x)^j = \sum_{l_1, \ldots l_K} x^{l_1} \Theta_K^{j,l_K} \prod_{k=2}^{K-1} \Theta_k^{l_k, l_{k-1}} \ .$$

[Choromaska, Henaff, Mathieu, LeCun, Ben Arous,'14]

DEEP NETWORKS AND SPIN GLASSES

- Equivalently, we can define *paths*



$$p = (l_0, l_1, \ldots, l_{K+1})$$

$$\mathcal{P} = \{p = (l_0, \ldots, l_{K+1}); 1 \leq l_k \leq M_k\}$$

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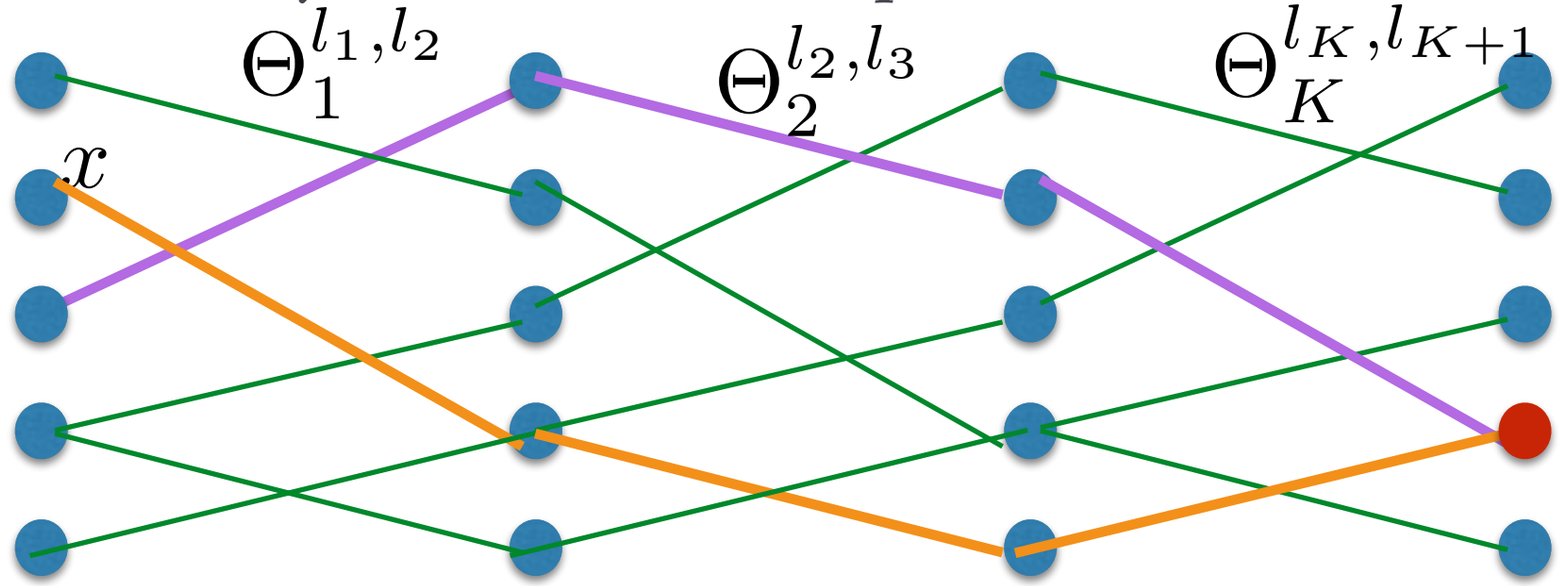


$\Phi(x;\Theta)$

$$p = (l_0, l_1, \ldots, l_{K+1})$$

$$\mathcal{P} = \{p = (l_0, \ldots, l_{K+1}); 1 \leq l_k \leq M_k\}$$

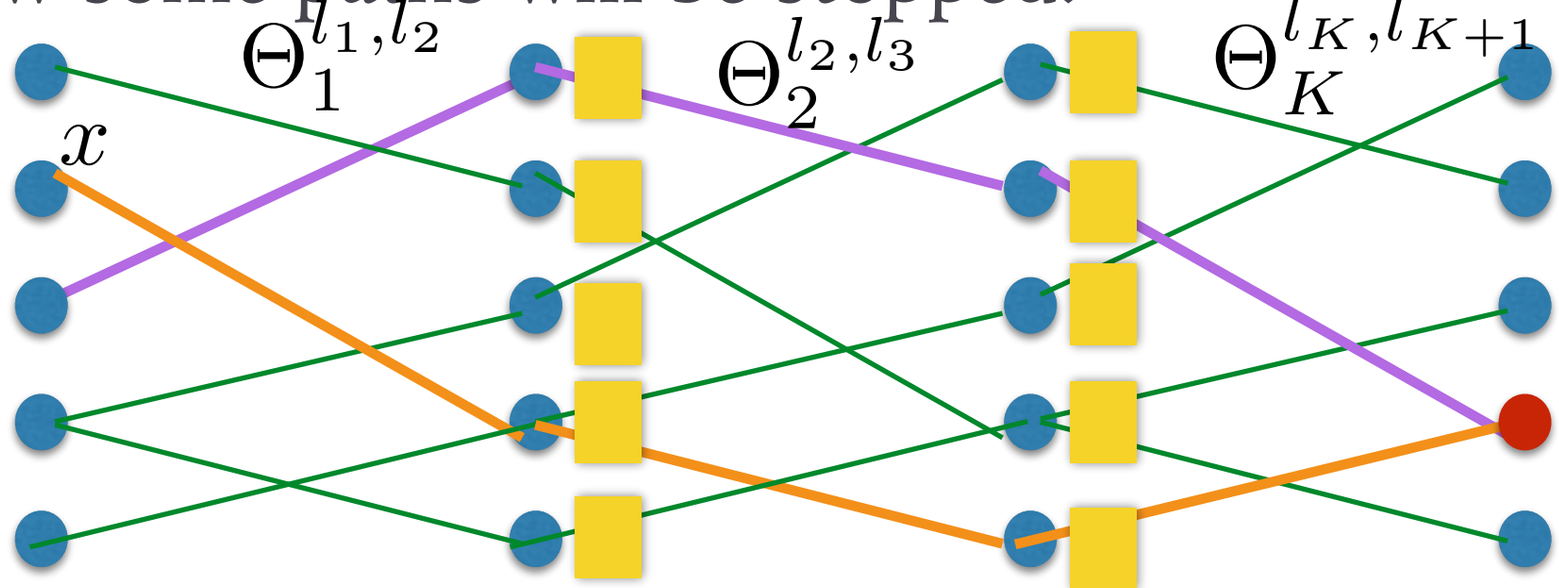
- Homogeneous polynomial on Θ.
- Q: What about a ReLU network instead?

$$\Phi(x;\Theta)^j = \sum_{p \in \mathcal{P}; p(K+1)=j} x^{p(1)} \prod_{k \leq K} \Theta_k^{p(k),p(k+1)} .$$

[Choromaska, Henaff, Mathieu, LeCun, Ben Arous,'14]

DEEP NETWORKS AND SPIN GLASSES

- Now some paths will be stopped:



-

$$\Phi(x;\Theta)^j = \sum_{p\in\mathcal{P};p(K+1)=j} \pi(p,x,\Theta)\cdot x^{p(1)} \prod_{k\leq K} \Theta_k^{p(k),p(k+1)} \ , \ \pi(p,x,\Theta) = \{0,1\}$$

$$p = (l_0,\ldots,l_K) \ , \ \tilde{p} = (l_0,\ldots,l_{K-1})$$

- Biases produce low-order terms (we ignore them for now)

$$\pi(p,x,\Theta) = \pi(\tilde{p},x,\Theta)\cdot\left(\sum_{p'\in\tilde{\mathcal{P}};p'(K)=p(K)} \pi(p',x,\Theta)\prod_{k<K}\Theta_k^{p'(k),p'(k+1)} > 0\right) .$$

[Choromaska, Henaff, Mathieu, LeCun, Ben Arous,'14]

DEEP NETWORKS AND SPIN GLASSES

- Loss becomes

$$E(\Theta) = \frac{1}{n}\sum_{i\leq n} \|y_i - \Phi(x_i;\Theta)\|^2$$

$$= \frac{1}{n}\sum_{i\leq n}\sum_{j=1}^{M_K}\left(y_i^j - \sum_{p\in\mathcal{P};p(K+1)=j} \pi(p,x_i,\Theta)\cdot x_i^{p(1)}\prod_{k\leq K}\Theta_k^{p(k),p(k+1)}\right)^2$$

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$$\stackrel{n\to\infty}{\to} C + \sum_{p\in\mathcal{P}} q(X,Y,\Theta,p)\prod_{k\leq K}\Theta_k^{p(k),p(k+1)}$$

$$+ \sum_{p,p'\in\mathcal{P}} Q(X,\Theta,p,p')\prod_{k\leq K}\Theta_k^{p(k),p(k+1)}\Theta_k^{p'(k),p'(k+1)} \ , \text{ with}$$

$$q(X,Y,\Theta,p) = \mathbb{E}_{X,Y}\left(\pi(p,X,\Theta)Y^{p(K)}X^{p(1)}\right) \ ,$$

$$Q(X,\Theta,p,p') = \mathbb{E}_X\left(\pi(p,X,\Theta)\pi(p',X,\Theta)X^{p(1)}X^{p'(1)}\right) \ .$$

[Choromaska, Henaff, Mathieu, LeCun, Ben Arous,'14]

DEEP NETWORKS AND SPIN GLASSES

- The loss "looks" like a polynomial in Θ provided we **break the dependency** of $\pi(p, x, \Theta)$ with respect to Θ .
  - It means that thresholding is independent of Θ.
- For large enough n (assuming iid samples), it results that

$$q(X, Y, p) \sim \mathcal{N}(\mu_p, \sigma_p^2) \ ,$$

$$Q(X, p, p') \sim \mathcal{N}(\mu_{p,p'}, \sigma_{p,p'}^2) \ ,$$

[Choromaska, Henaff, Mathieu, LeCun, Ben Arous,'14]

DEEP NETWORKS AND SPIN GLASSES

- Furthermore, if one also assumes *redundancy* (weights shared across layers), *uniformity* (same weights are not used too often along surviving paths) and *normalized weights,* authors arrive at

$$E(\Theta) \simeq \mathcal{L}_{\Lambda,K}(\Theta) = \frac{1}{\Lambda^{(K-1)/2}} \sum_{l_1,\ldots,l_K=1}^{\Lambda} Z_{l_1,\ldots,l_K}\Theta_{l_1}\ldots\Theta_{l_K} \ ,$$

with $\|\Theta\|^2 = \Lambda$.

$\mathcal{L}_H(\Theta)$: Hamiltonian of the H-spin spherical spin glass model.

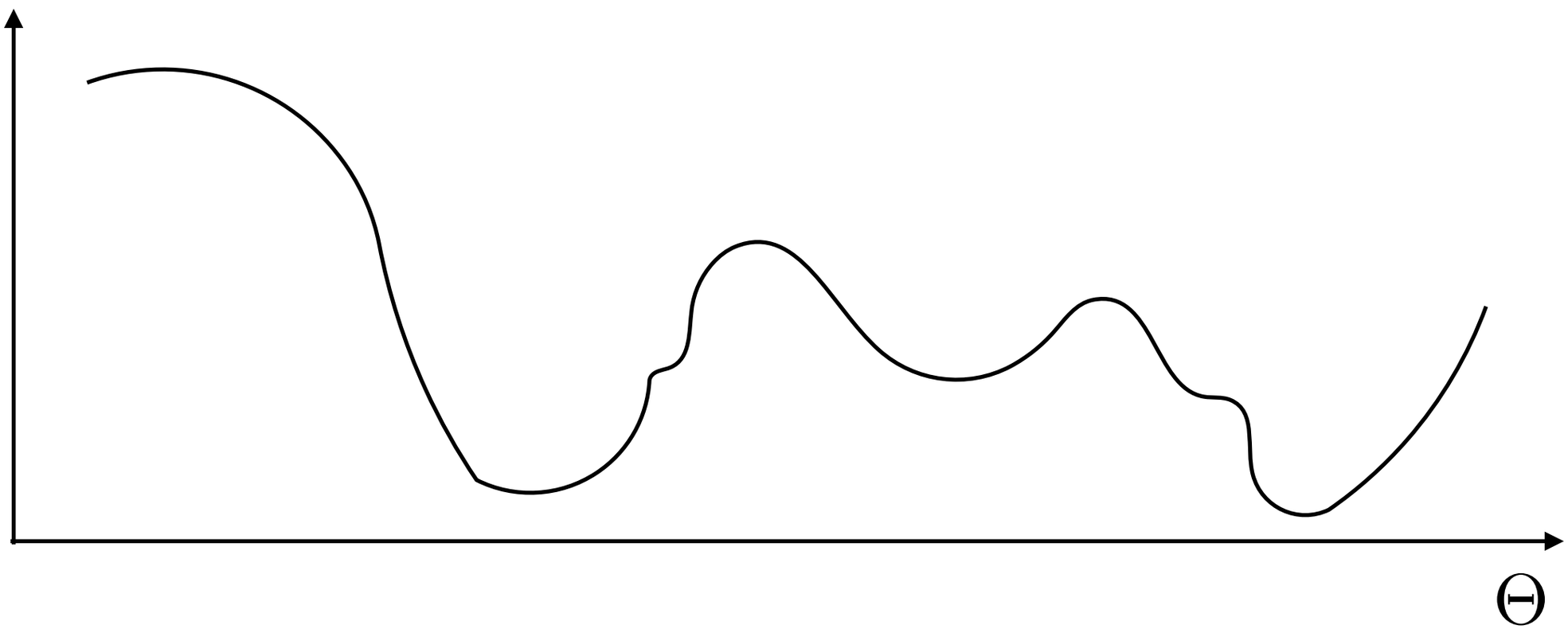
$Z_p \sim \mathcal{N}(0,\sigma^2)$.

[Choromaska, Henaff, Mathieu, LeCun, Ben Arous,'14]

DEEP NETWORKS AND SPIN GLASSES

- [Auffinger et al '10] [Auffinger, Ben Arous'13], obtained a complete description of the behavior of critical points of spherical spin glasses.

- In particular, critical points (ratio of negative to positive eigenvalues of the Hessian) occur at different energy bands:



LANDSCAPE OF SPHERICAL SPIN GLASSES

- The energy landscape of several prototypical models in statistical physics exhibit a so-called *energy barrier,* e.g. spherical spin glasses:

$$H_{N,p}(\sigma) = N^{-(p-1)/2} \sum_{i_1,\dots i_p=1}^{N} J_{i_1,\dots,i_p}\sigma_{i_1}\cdots\sigma_{i_p} \ , \ \sigma \in S^{N-1}(\sqrt{N}) \ , J_i \sim \mathcal{N}(0,1).$$

$$\lim_{N\to\infty} \frac{1}{N} \log \mathbb{E}\,\mathrm{Crt}_{N,k}(u) = \Theta_{k,p}(u).$$

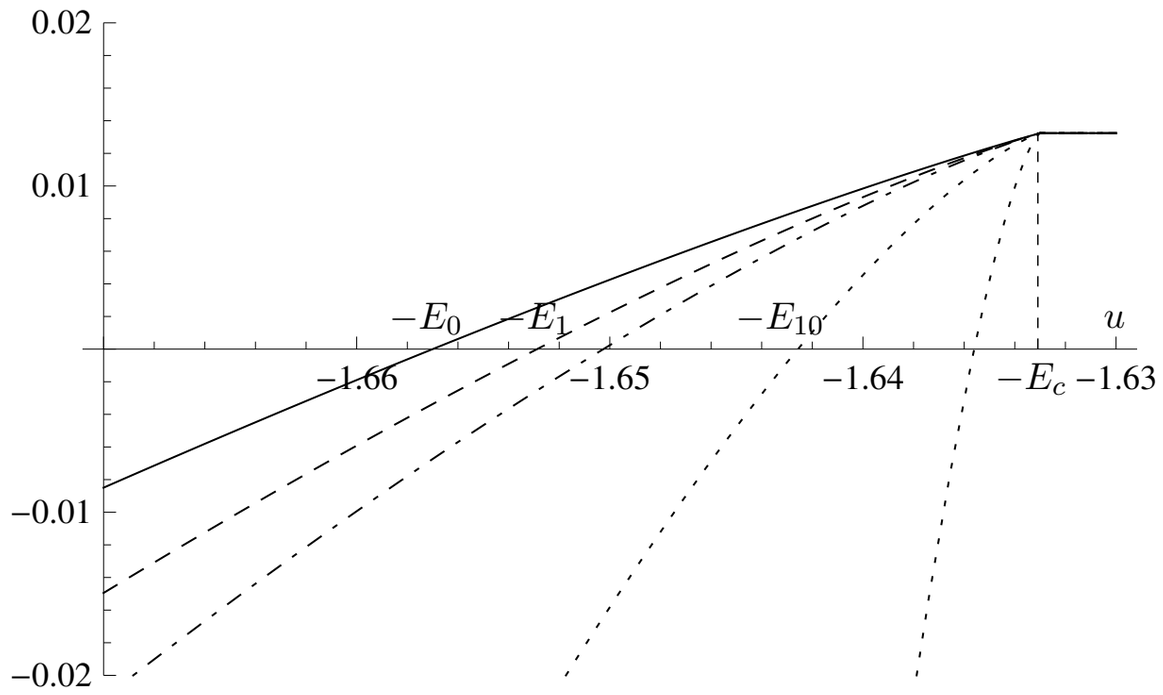


FIGURE 1. The functions $\Theta_{k,p}$ for $p = 3$ and $k = 0$ (solid), $k = 1$ (dashed), $k = 2$ (dash-dotted), $k = 10$, $k = 100$ (both dotted). All these functions agree for $u \geq -E_\infty$.

[Auffinger, Ben Arous Cerny,'11]

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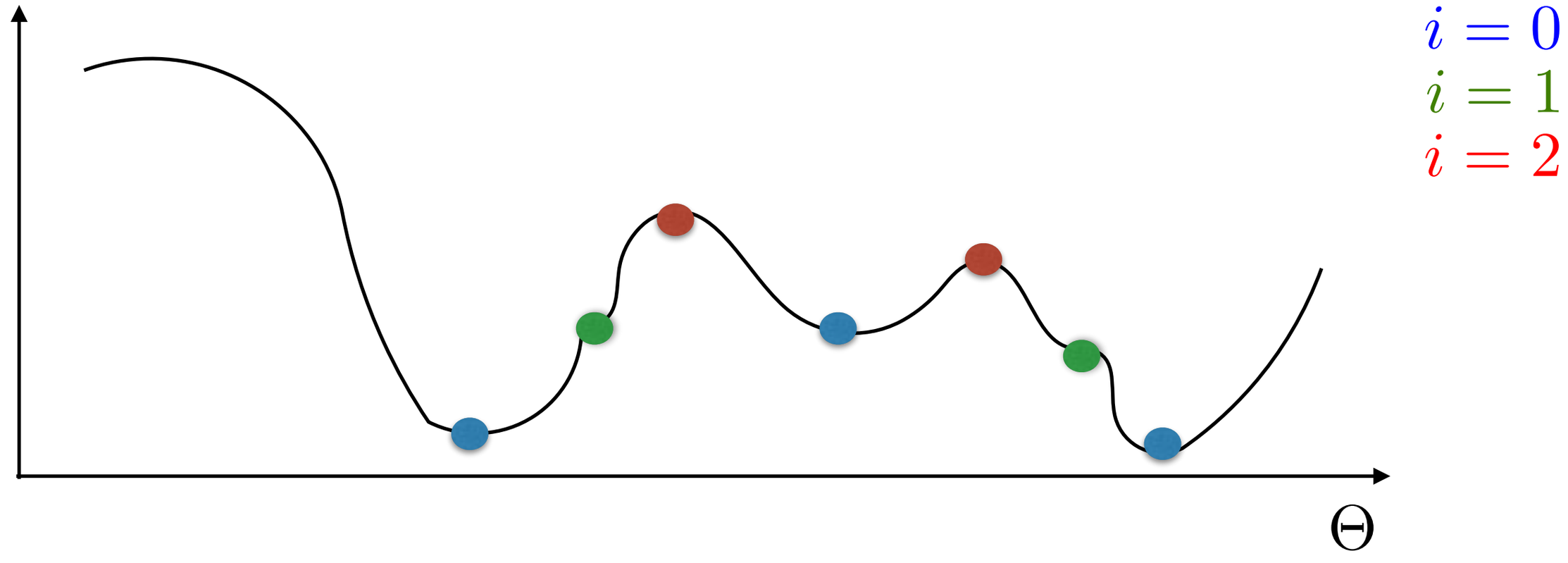
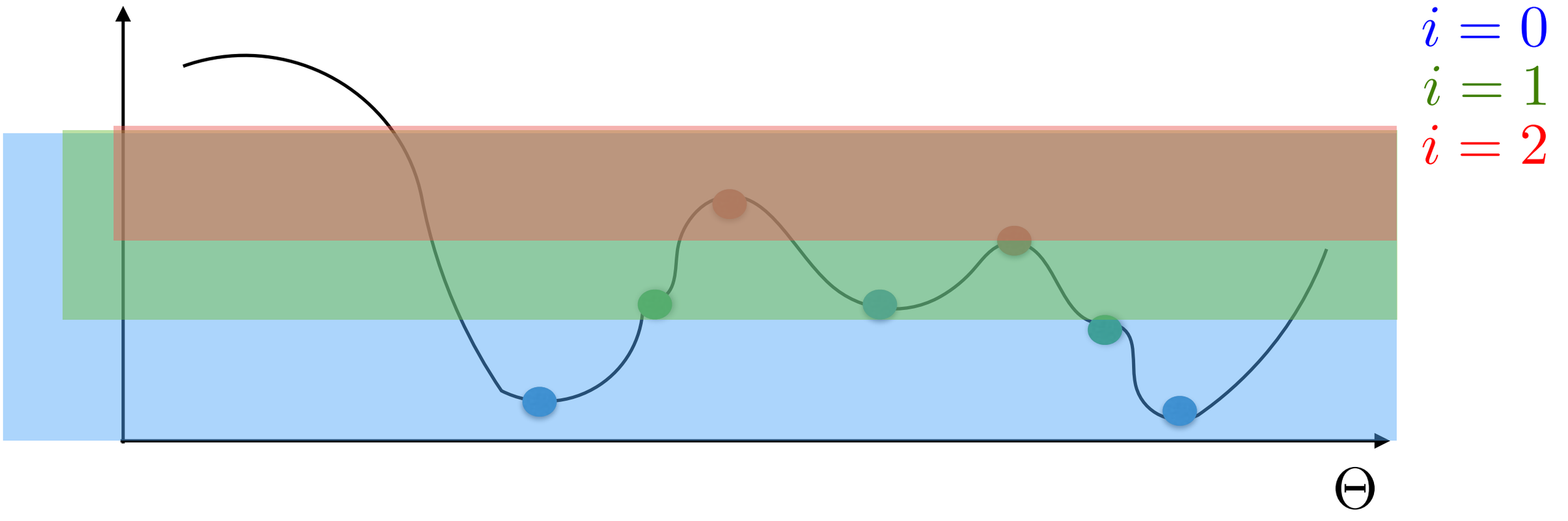


DEEP NETWORKS AND SPIN GLASSES

- As $\Lambda \to \infty$, the distributions concentrate along different bands: each index concentrates in different bands.

- As $\Lambda \to \infty$, the number of local minima dominate the rest of the indices.



DEEP NETWORKS AND SPIN GLASSES

- See also:
  - *"The effect of Gradient Noise on the Energy Landscape of Deep Networks"*, Chaudhari & Soatto. They study exterior magnitude field and its associated smoothing annealing schemes to reduce number of critical points.
  - *"Explorations on high dimensional landscapes"*, Sagun, Guney, Ben Arous, LeCun. Study the existence of a narrow band containing the bulk of the critical points of deep energy landscapes in the high-dimensional setting.

PRIOR RELATED WORK

- Models from Statistical physics have been considered as possible approximations [Dauphin et al.'14, Choromanska et al.'15, Segun et al.'15]
- Tensor factorization models capture some of the non convexity essence [Anandukar et al'15, Cohen et al. '15, Haeffele et al.'15]

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- [Tian'17] studies learning dynamics in a gaussian generative setting.
- [Chaudhari et al'17]: Studies local smoothing of energy landscape using the local entropy method from statistical physics.
- [Pennington & Bahri'17]: Hessian Analysis using Random Matrix Th.
- [Soltanolkotabi, Javanmard & Lee'17]: layer-wise quadratic NNs.

NON-CONVEXITY ≠ NOT OPTIMIZABLE

- We can perturb any convex function in such a way it is no longer convex, but such that gradient descent still converges.
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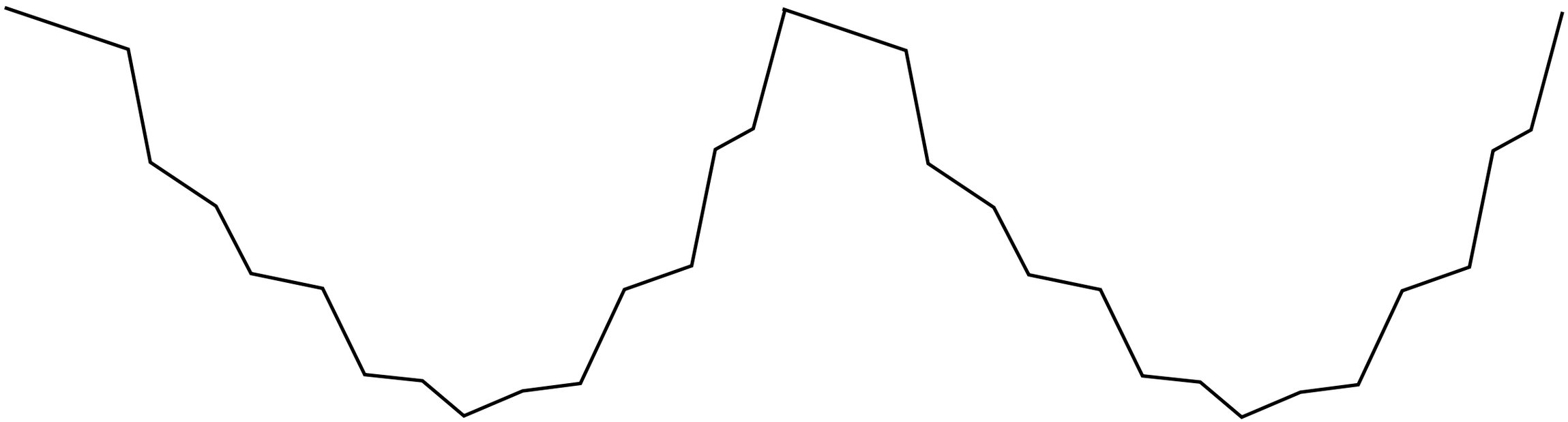
- E.g. quasi-convex functions.
- In particular, deep models have internal symmetries.

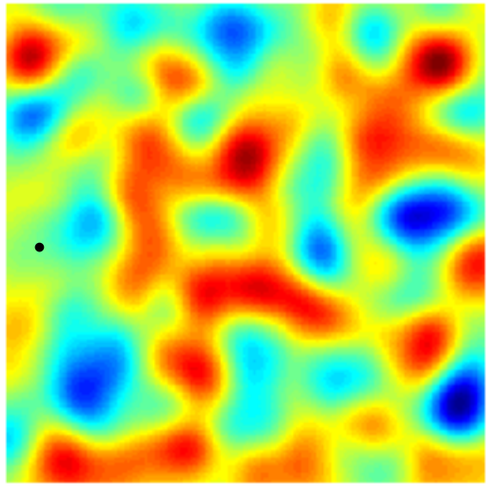
$$F(\theta) = F(g.\theta) \ , \ g \in G \text{ compact.}$$



ANALYSIS OF NON-CONVEX LOSS SURFACES

- Given loss $E(\theta)$, $\theta \in \mathbb{R}^d$, we consider its representation in terms of level sets:

$$E(\theta) = \int_0^\infty \mathbf{1}(\theta \in \Omega_u) du \ , \ \Omega_u = \{y \in \mathbb{R}^d \ ; \ E(y) \leq u\} \ .$$



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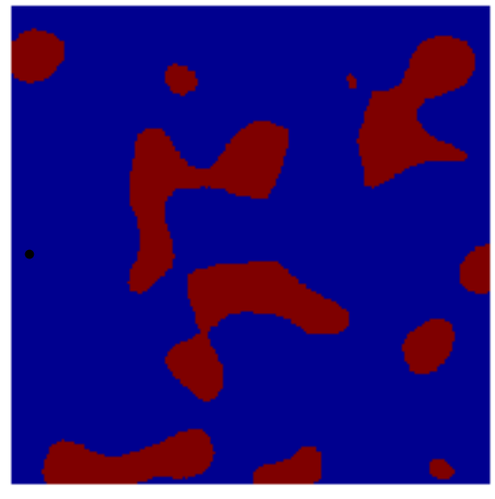

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- In particular, we ask how connected they are, i.e. how many connected components N_u at each energy level u ?

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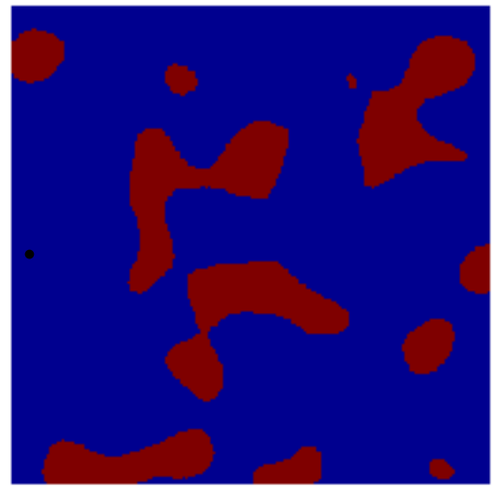

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- Related to presence of poor local minima:

Proposition: If $N_u = 1$ for all u then E has no poor local minima.

(i.e. no local minima y^* s.t. $E(y^*) > \min_y E(y)$)

SPURIOUS VALLEYS

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- **Definition:** A *valley* is a connected component of the sublevel set Ω_u.

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- **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:

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

$$X \in \mathbb{R}^n \ , \ Y \in \mathbb{R}^m \ , \ W_k \in \mathbb{R}^{n_k \times n_{k-1}} \ .$$

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$$X \in \mathbb{R}^n \ , \ Y \in \mathbb{R}^m \ , \ W_k \in \mathbb{R}^{n_k \times n_{k-1}} \ .$$

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]

LINEAR VS NON-LINEAR DEEP MODELS

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

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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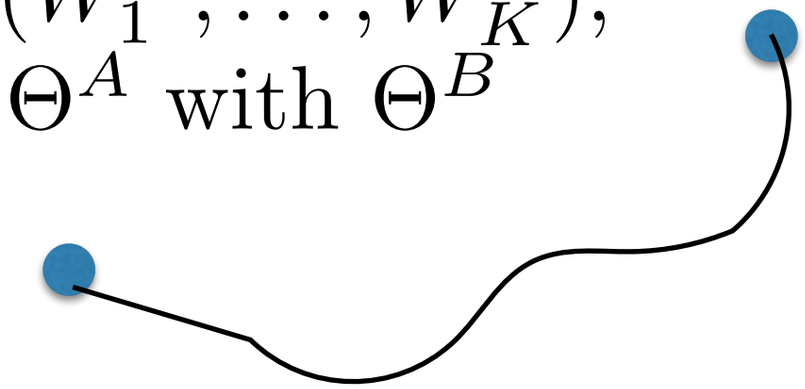
- We pay extra redundancy price to get simple topology.
- This simple topology is an "artifact" of the linearity of the network:

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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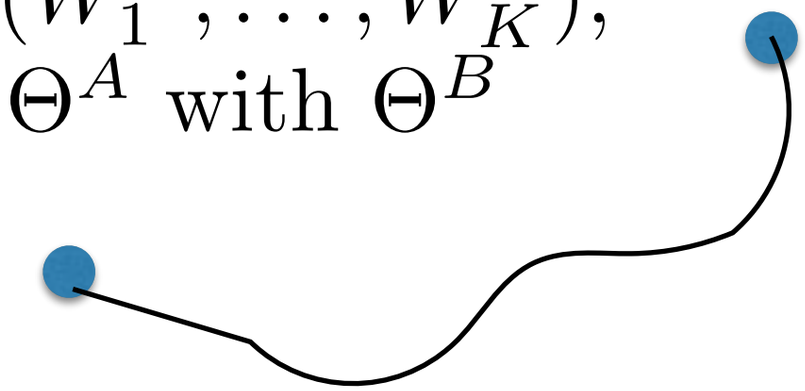

➤ Main idea:

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 $t \in (0,1)$.

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

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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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- 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 $\beta = \mathcal{A}(\Theta)$:

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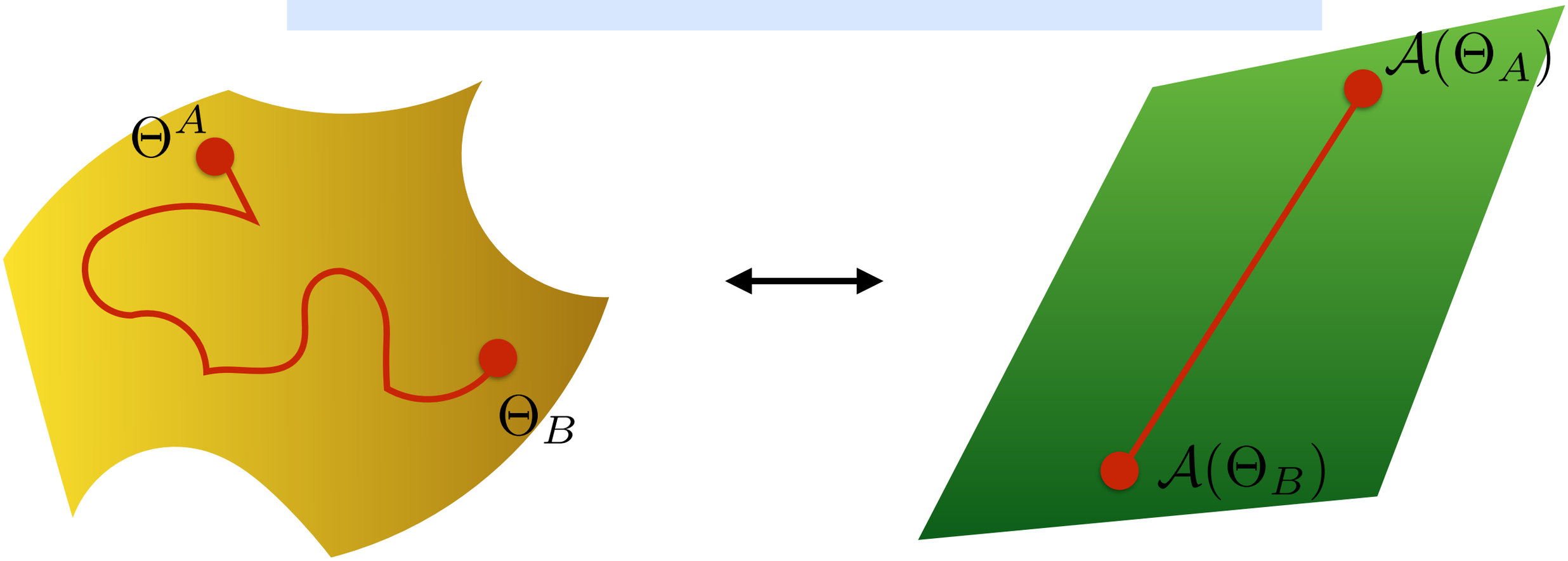

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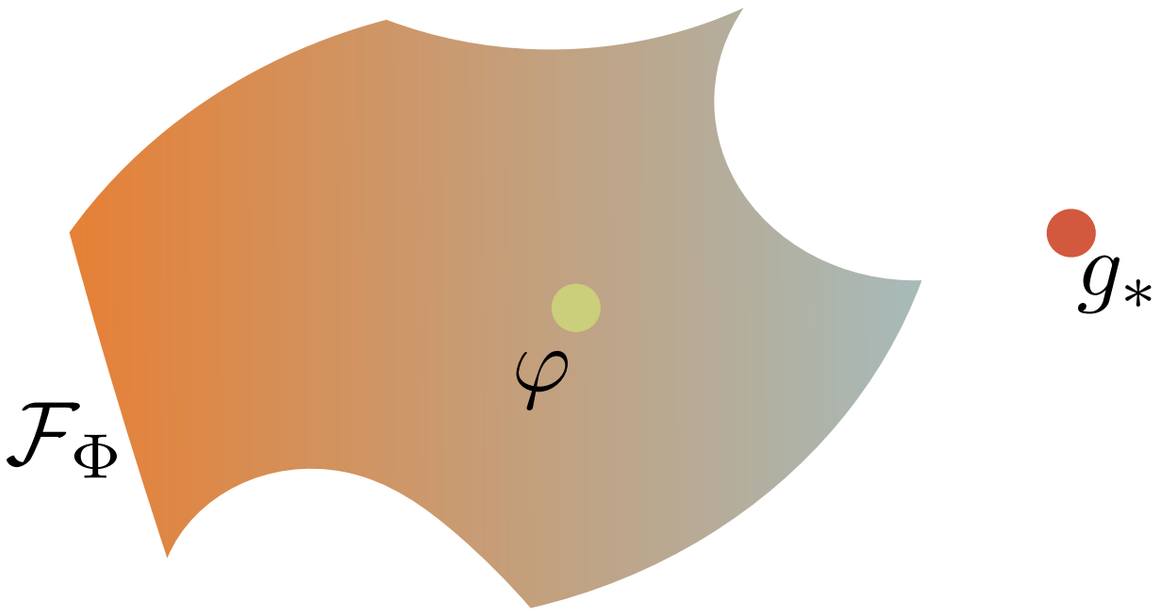
Theorem: [BVV'18] If $\dim\{\mathcal{A}(w),\, w \in \mathbb{R}^n\} = q < \infty$, then $L(U,W) = \mathbb{E}\|U\rho(WX) - Y\|^2$ has no spurious valley if $M \geq q$.

- 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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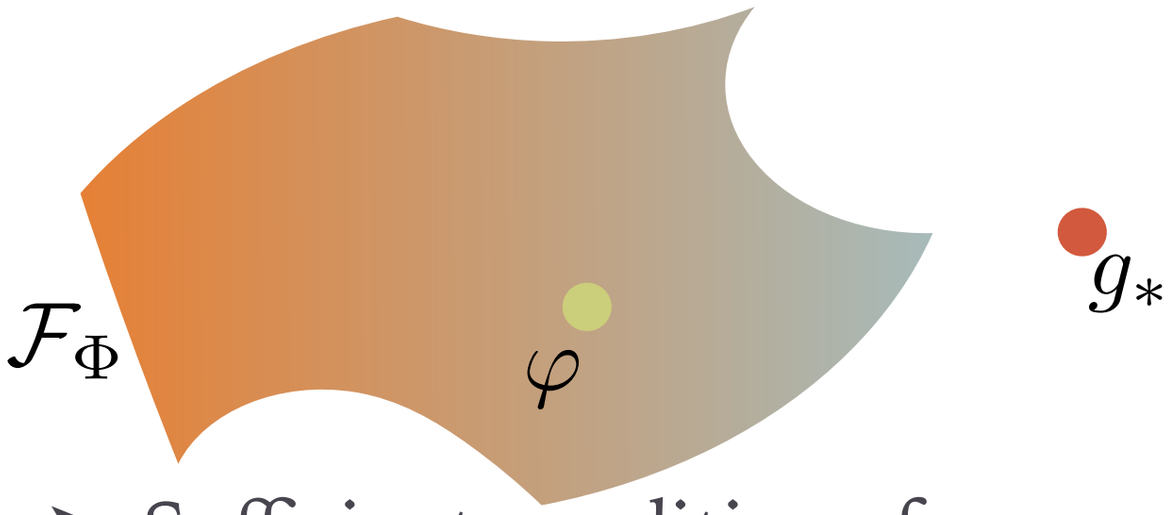

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  - $\mathcal{F}_\Phi$ convex and Θ sufficiently large so that we can move freely within.
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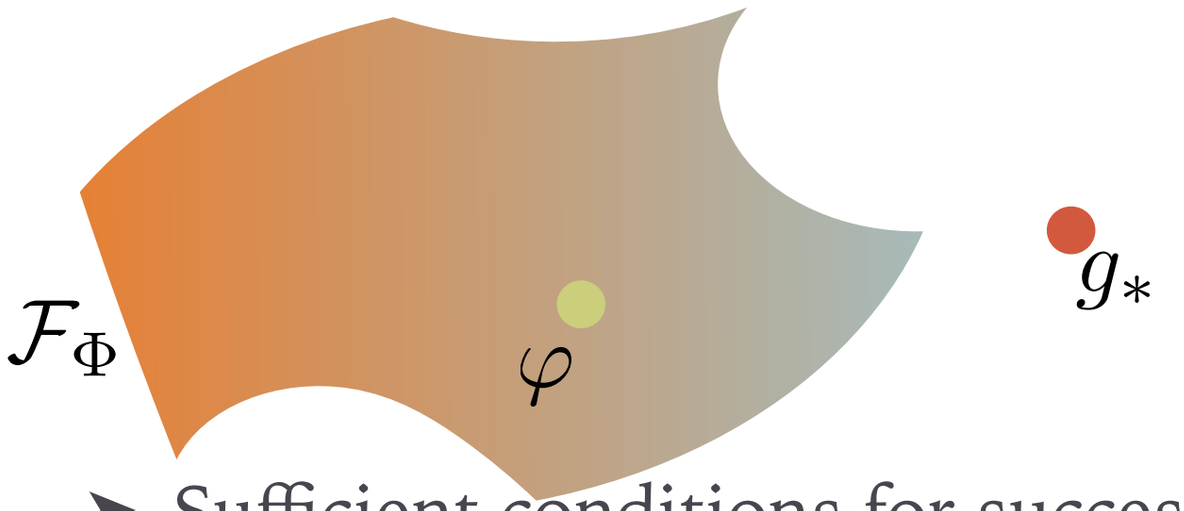

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- What happens when the model is not sufficiently overparametrised?

FROM SIMPLE LANDSCAPES TO ENERGY BARRIER

- The energy landscape of several prototypical models in statistical physics exhibit a so-called *energy barrier,* e.g. spherical spin glasses:

$$H_{N,p}(\sigma) = N^{-(p-1)/2} \sum_{i_1,\dots i_p=1}^{N} J_{i_1,\dots,i_p}\sigma_{i_1}\cdots\sigma_{i_p} \ , \ \sigma \in S^{N-1}(\sqrt{N}) \ , J_i \sim \mathcal{N}(0,1).$$

$$\lim_{N\to\infty} \frac{1}{N} \log \mathbb{E}\,\mathrm{Crt}_{N,k}(u) = \Theta_{k,p}(u).$$

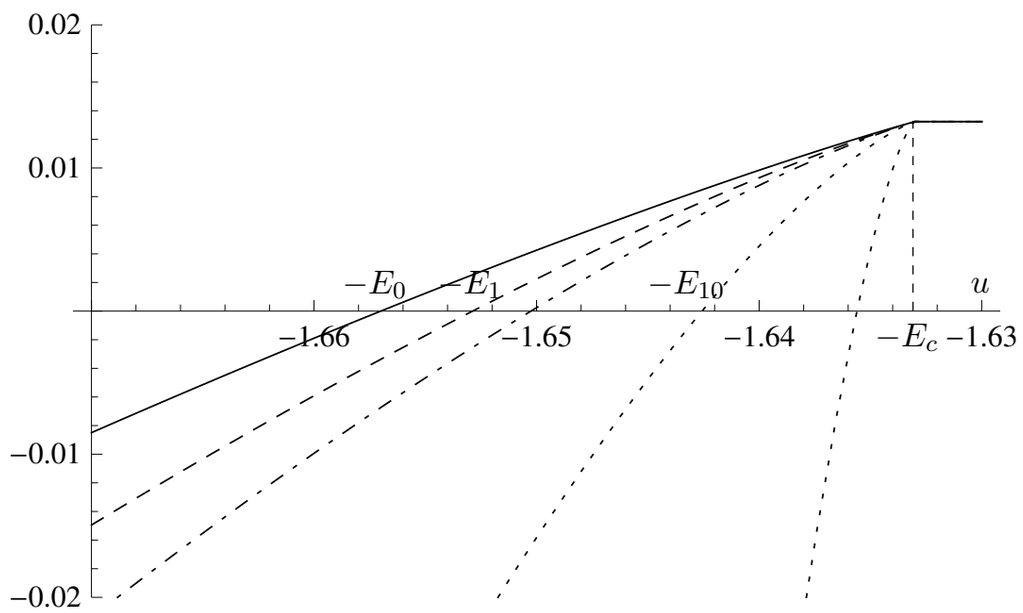

FIGURE 1. The functions $\Theta_{k,p}$ for $p = 3$ and $k = 0$ (solid), $k = 1$ (dashed), $k = 2$ (dash-dotted), $k = 10$, $k = 100$ (both dotted). All these functions agree for $u \geq -E_\infty$.

[Auffinger, Ben Arous Cerny,'11]

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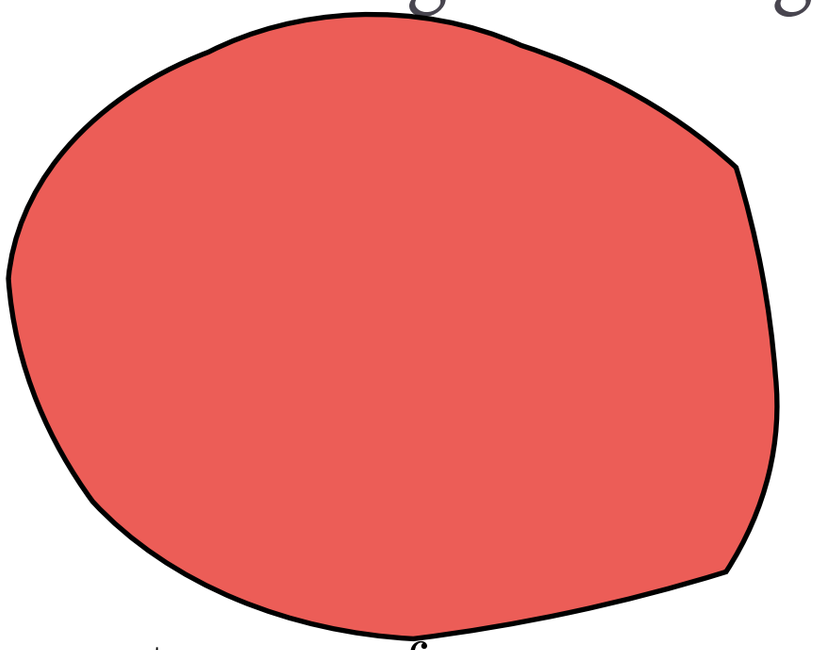
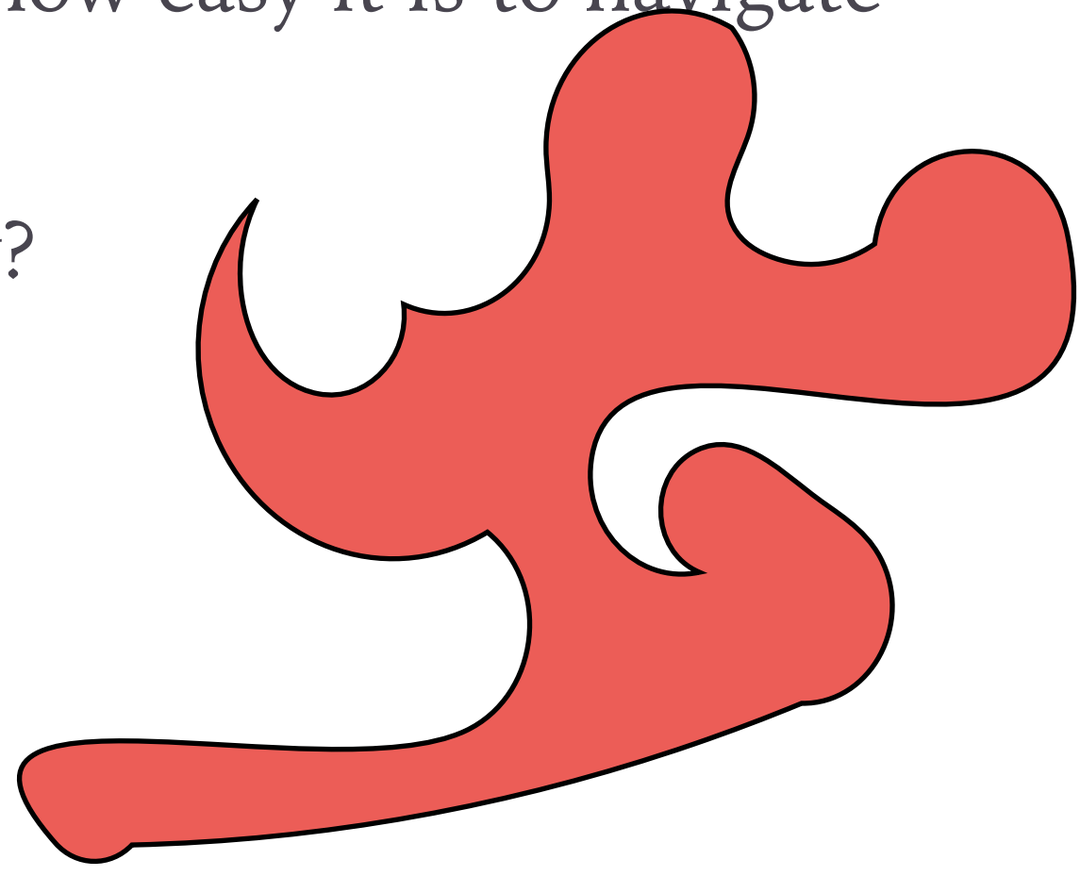
Conjecture [LBB'18]: The loss $L(U,W) = \mathbb{E}\|U\rho(WX)-Y\|^2$ has no poor local minima above the energy barrier $\beta(M,N)$.

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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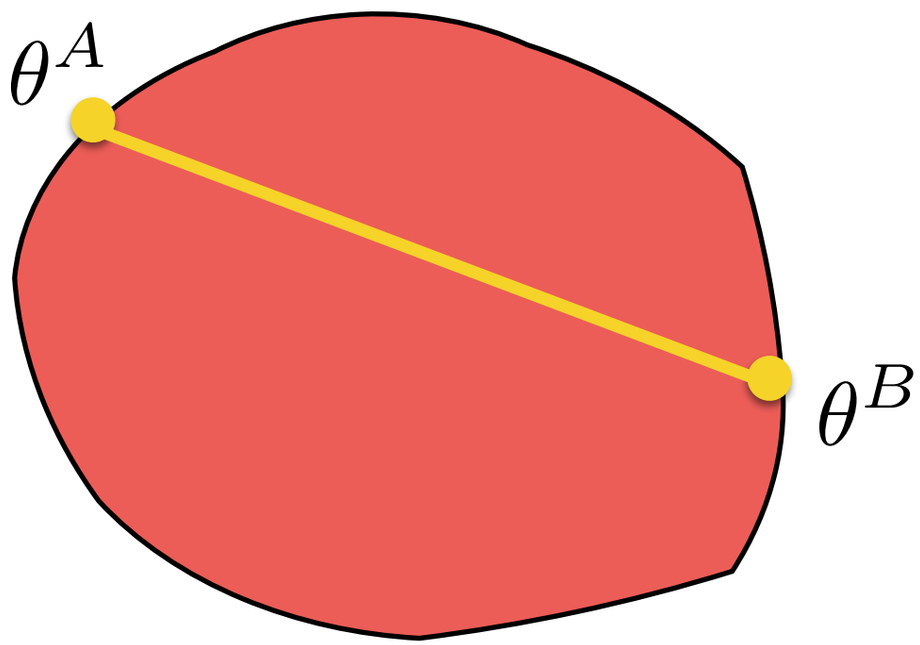
- Even if level sets are connected, how easy it is to navigate through them?
- We estimate level set geodesics and measure their length.



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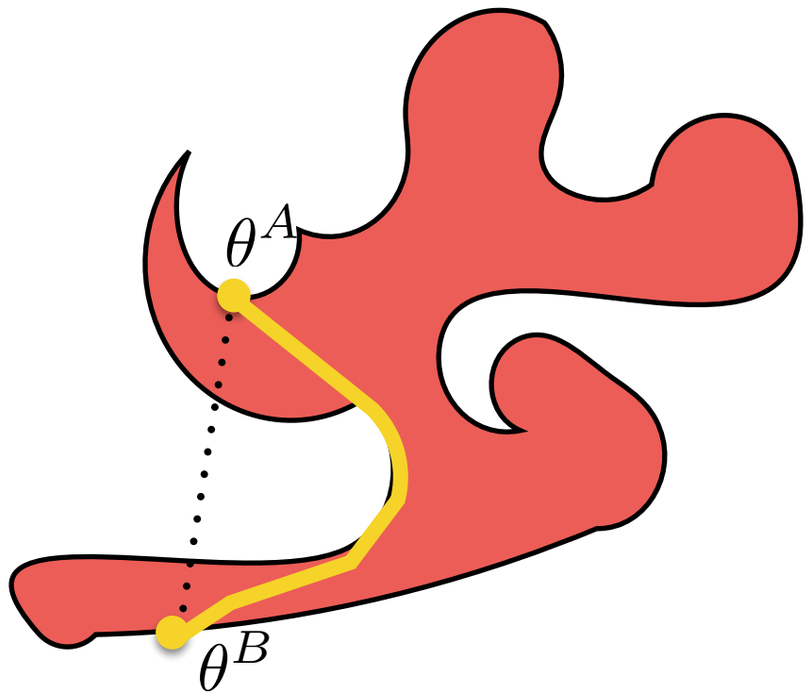

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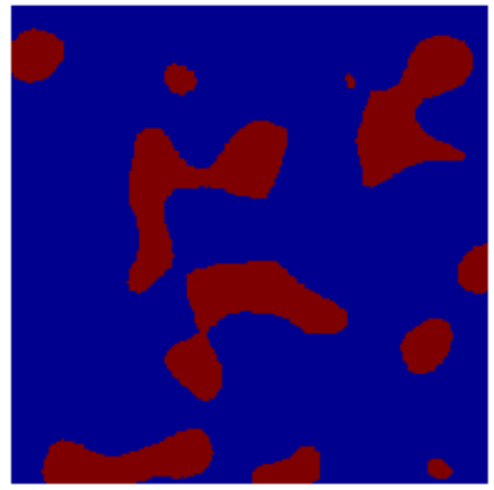
FINDING CONNECTED COMPONENTS



- Suppose $\theta_1,\ \theta_2$ are such that $E(\theta_1) = E(\theta_2) = u_0$
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- Moreover, we penalize the length of the path:

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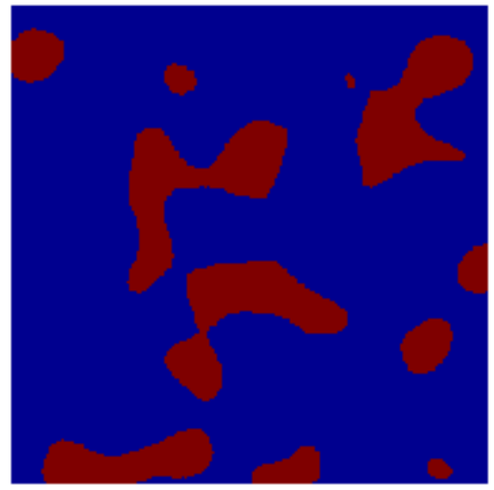

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- Dynamic programming approach:

θ_1

θ_2

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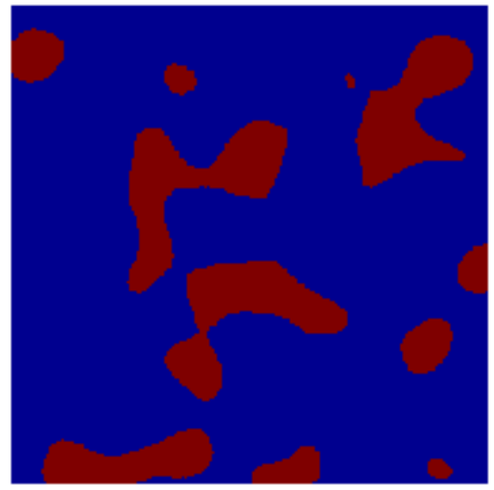

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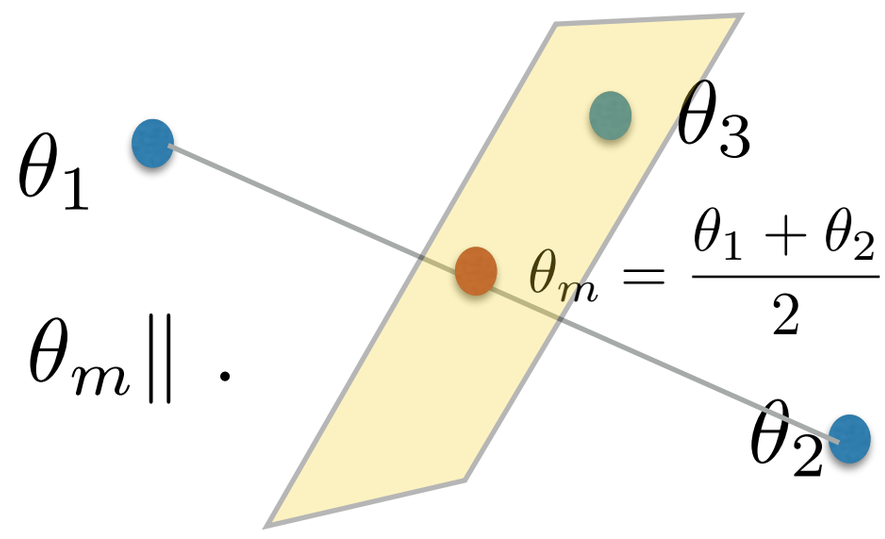

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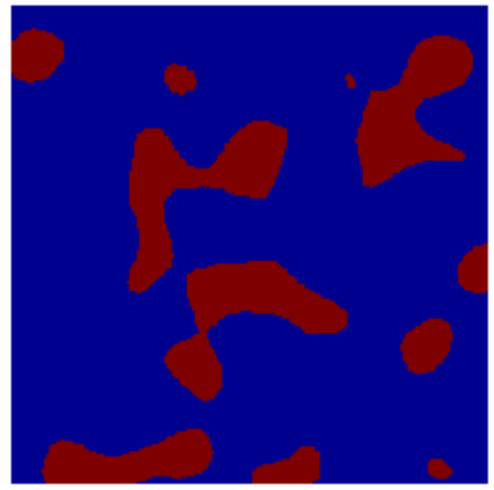

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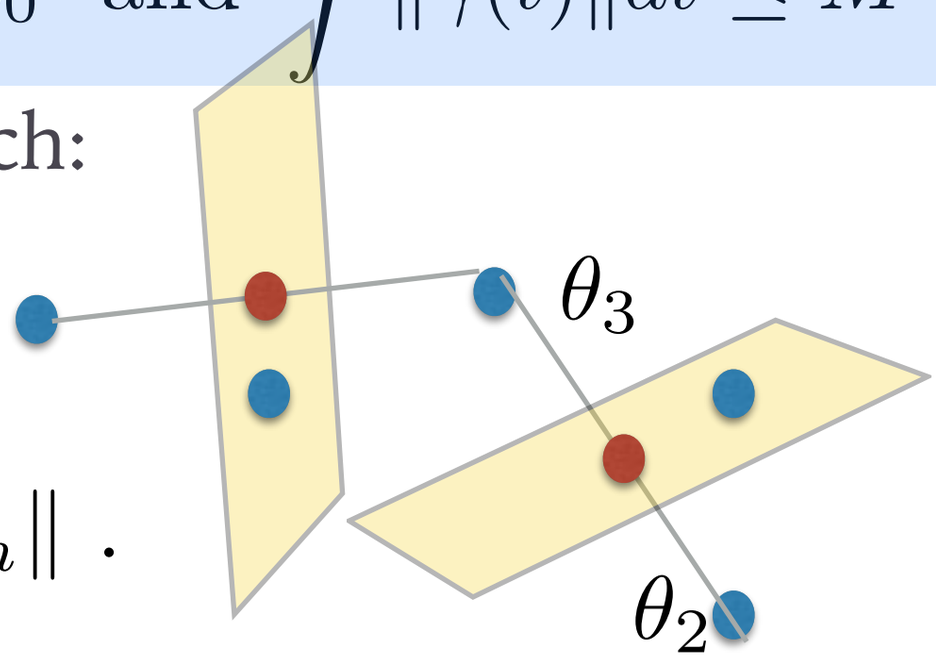
$$\forall\ t \in (0,1)\ ,\ E(\gamma(t)) \leq u_0 \quad \text{and} \quad \int \|\dot{\gamma}(t)\| dt \leq M\ .$$

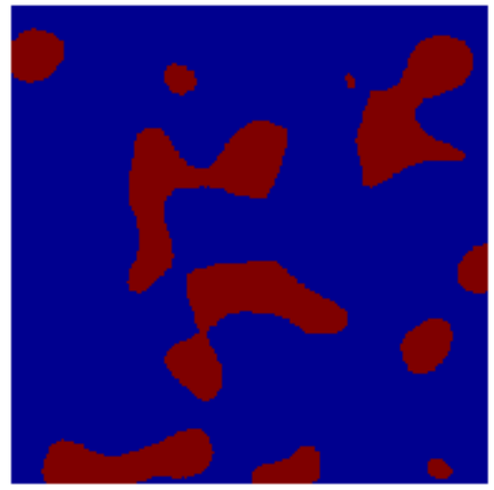
- Dynamic programming approach:

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

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



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
$\forall\ t \in (0,1)\ ,\ E(\gamma(t)) \leq u_0\ .$

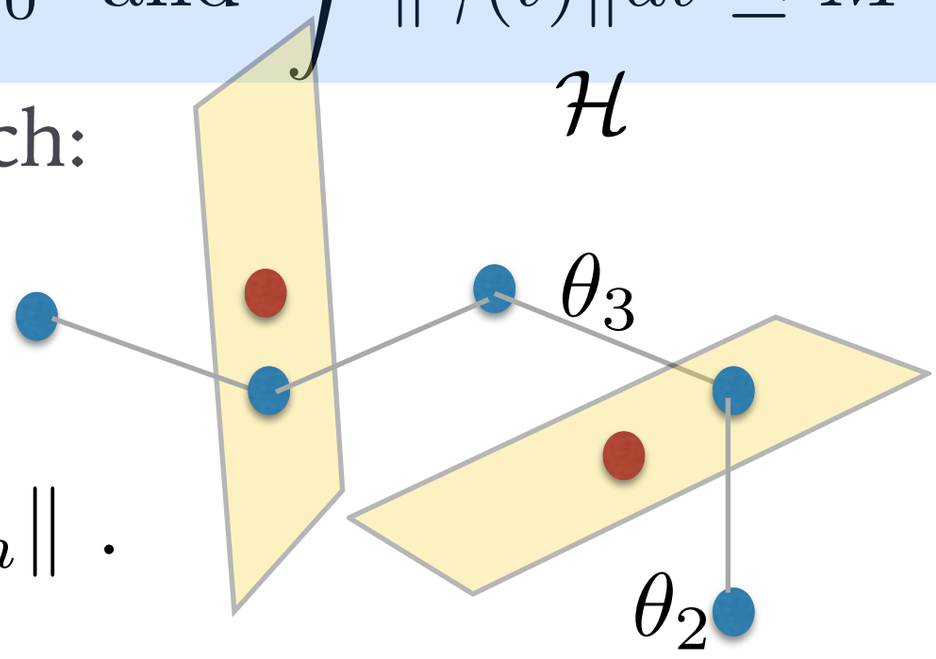
- Moreover, we penalize the length of the path:

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

- Dynamic programming approach:

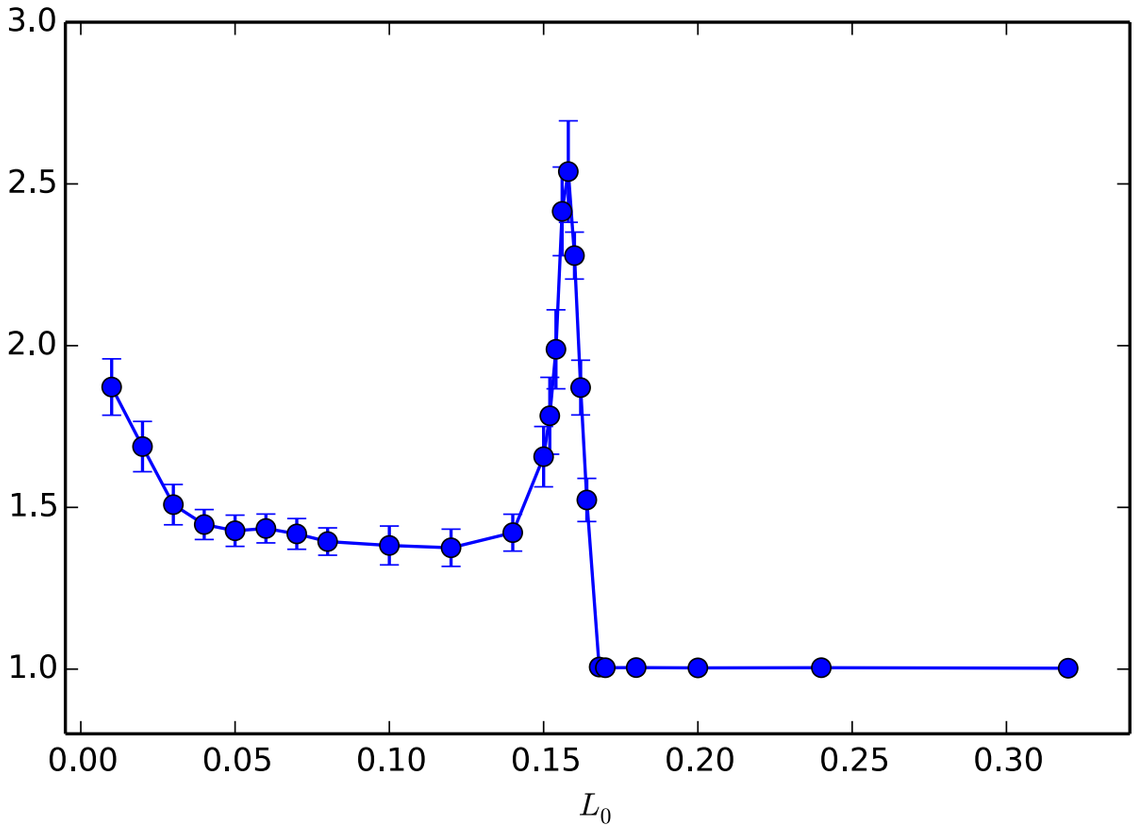
$$\theta_m = \frac{\theta_1 + \theta_2}{2}$$

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

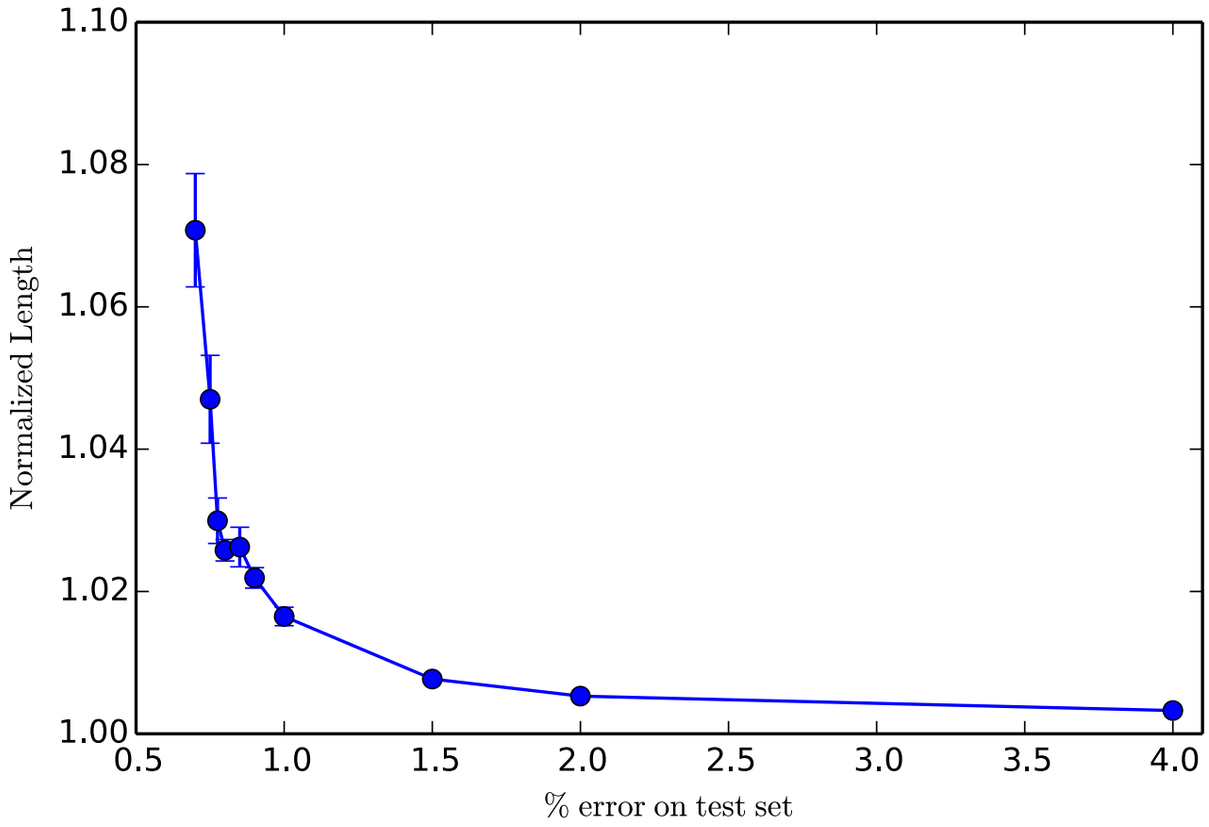


NUMERICAL EXPERIMENTS

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



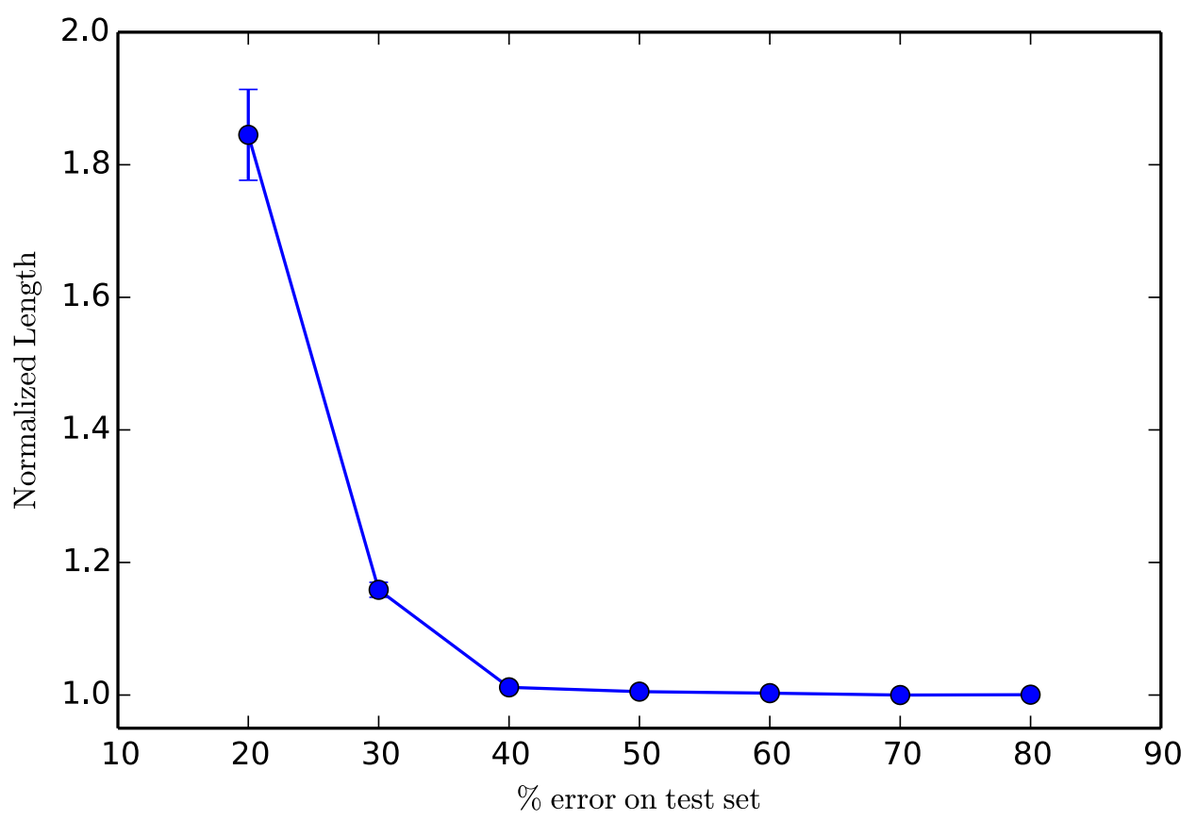
cubic polynomial



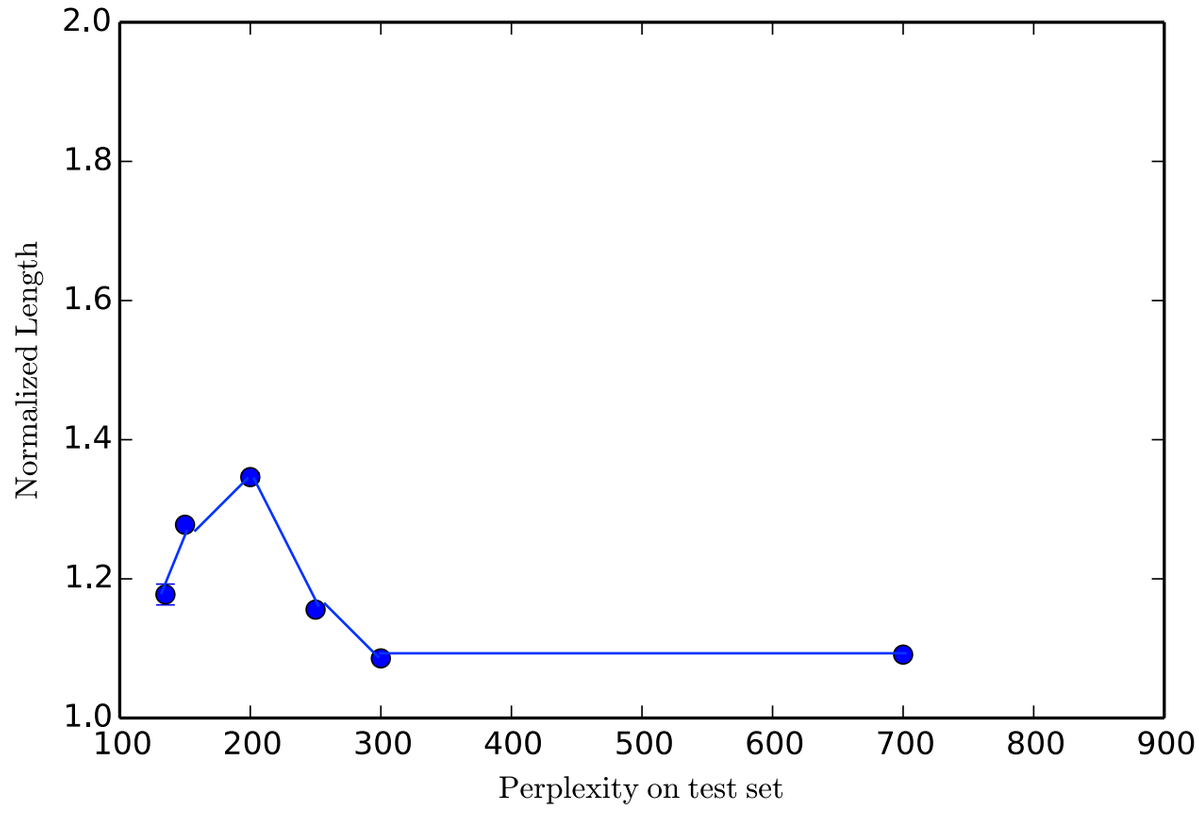
CNN/MNIST

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.



CNN/CIFAR-10



LSTM/Penn

ANALYSIS AND PERSPECTIVES

- #of components does not increase: no detected poor local minima so far when using typical datasets and typical architectures (at energy levels explored by SGD).
- Level sets become more irregular as energy decreases.
- Presence of “energy barrier”? extend to truncated Taylor?
- Kernels are back? CNN RKHS
- Open: “sweet spot” between overparametrisation and overfitting?
- Open: Robustness to noise in specification of activation function. Connection with Stochastic Gradient descent?