Stat 212b: Topics in Deep Learning
Lecture 24

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Objective

- Tensor Decompositions and Deep Learning
  - Optimality certificates
  - Learning with high-order score function.
  - Hierarchical Tensor Decompositions
- Spin Glasses and Deep Learning
- Richard Zhang: "Colorful Image Colorization"
- Hoang Duong: "Learning Polynomial Factorization"

Tensor Methods in Deep Learning

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

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

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

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

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

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

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

- The dependencies on Θ are partly captured by the d-order tensor $\Theta^1 \bigotimes \Theta^2 \dots \bigotimes \Theta^d$.

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.

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

- 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:

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

  - 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 $\min_{U,V} \ell(Y, UV^T) + \lambda \sum_{i\le r} \|U_i\|_u \|V_i\|_v$ 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 $\phi(\Theta^1, \ldots, \Theta^d)$:

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

s: degree of homogeneity.

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

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- We construct models by adding *r* copies of homogenous maps:

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

- 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:

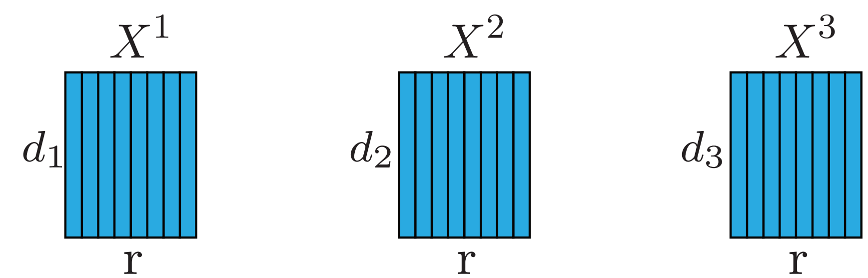
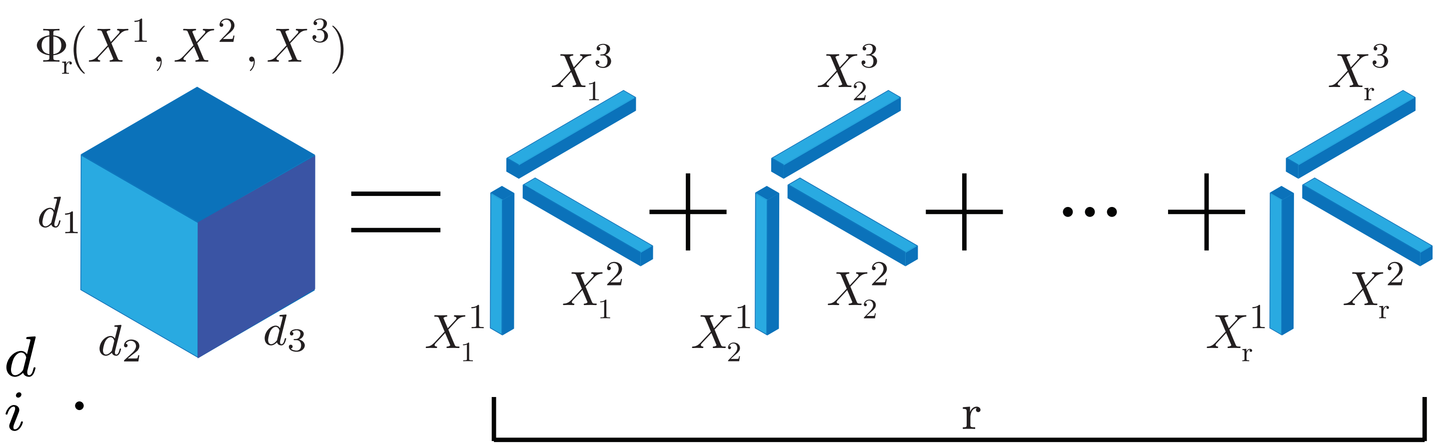


figure credit: R. Vidal



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

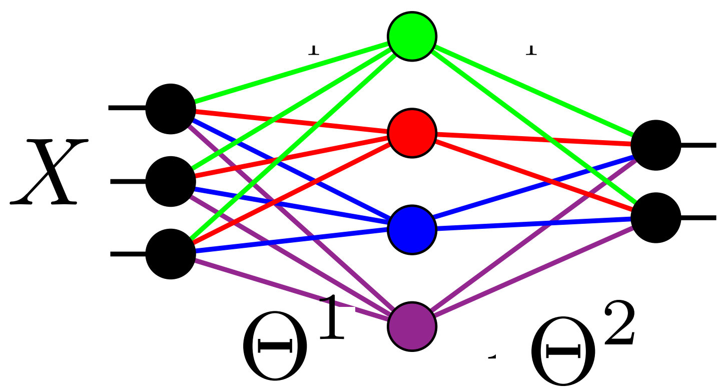
Candecomp/Parafac (CP) Tensor decomposition.

Adaptation to Deep Models

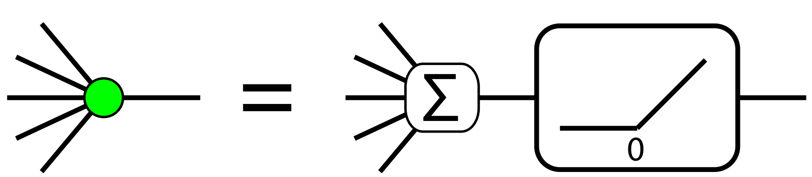
$$\Phi_r(\Theta^1, \ldots, \Theta^d) = \sum_{i=1}^{r} \phi(\Theta^1, \ldots, \Theta^d) \ .$$

ReLU Network:

ReLU Network with One Hidden Layer

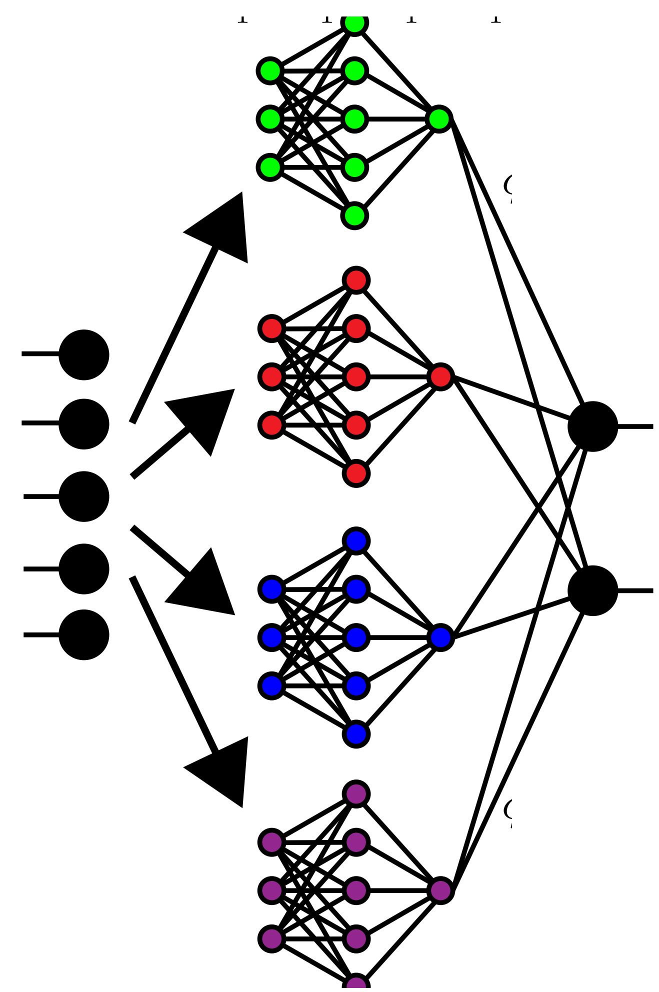


Rectified Linear Unit (ReLU)



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

Multilayer ReLU Parallel Network



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

Adaptation to Deep Models

- In the matrix case, the variational principle was

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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

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

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

$$\min_{\Theta} \ell(Y, \Theta) + \lambda \mathcal{R}(\Theta).$$

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

- 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]

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

- It results 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

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

[Cohen, Sharir, Shashua'15]

- Consider an input image x and its features extracted on dense, localized patches:

x

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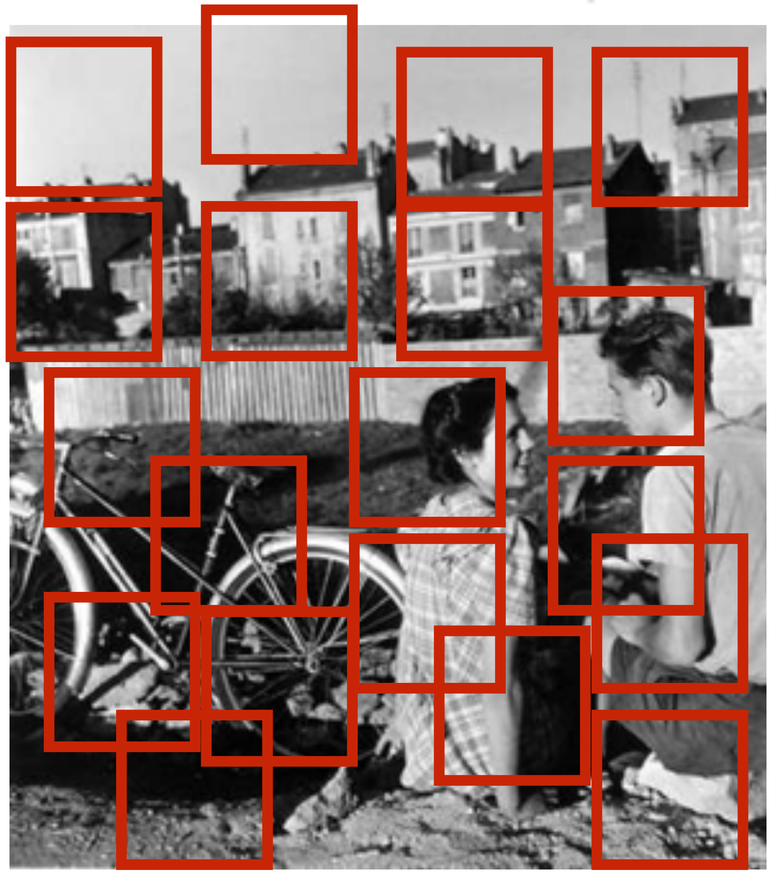

$\Phi(x^k)$

$$X = \{(\Phi(x^1), \ldots, \Phi(x^N)\} \ .$$

$$\Phi(x^k) \in \mathbb{R}^M \ .$$

- Aggregate features by combining high-order information:

$$p(y|x) = \sum_{d_1,\ldots d_N=1}^{M} A^y_{d_1,\ldots,d_N} \prod_{i=1}^{N} \Phi_{d_i}(x^i) \ ,$$

A^y: N-th order tensor of dimensions $M_k = M$.

[Cohen, Sharir, Shashua'15]

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- CP (Candecomp/Parafac) decomposition:

$$A = \sum_{k=1}^{K} \alpha_k a_1^k \otimes a_2^k \otimes \ldots a_N^k \ , \ a_i^k \in \mathbb{R}^M \ .$$

sum of K rank-1 N-th order tensors of size M.

Deep Nets and Hierarchical Tensor Decompositions

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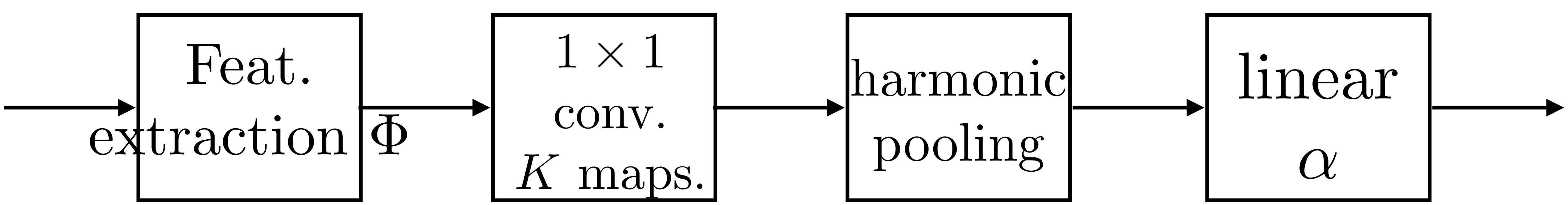
sum of K rank-1 N-th order tensors of size M.

- The resulting model is a shallow network:

$$p_A(y|x) = \sum_{k=1}^{K} \alpha_k^y \prod_{i=1}^{N} \left(\sum_{m=1}^{M} a_i^k(m) \Phi_m(x^i) \right) \ .$$



Deep Nets and Hierarchical Tensor Decompositions

[Cohen, Sharir, Shashua'15]

- Q: How to parametrize/factorize the tensors A^y ?
- Hierarchical-Tucker (HT) decompositions:

$$\phi^{1,j,\gamma} = \sum_{\alpha=1}^{r_0} a_\alpha^{1,j,\gamma} \phi^{0,2j-1,\alpha} \otimes \phi^{0,2j,\alpha} \ , \ \text{order } 2$$

$$\ldots$$

$$\phi^{l,j,\gamma} = \sum_{\alpha=1}^{r_{l-1}} a_\alpha^{l,j,\gamma} \phi^{l-1,2j-1,\alpha} \otimes \phi^{l-1,2j,\alpha} \ , \ \text{order } 2^l$$

$$\ldots$$

$$A^y = \sum_{\alpha=1}^{r_{L-1}} a_\alpha^{L,j,\gamma} \phi^{L-1,2j-1,\alpha} \otimes \phi^{L-1,2j,\alpha} \ , \ \text{order } 2^L = N \ .$$

– Corresponds to a deep representation with $L = \log N$ layers.

Deep Nets and Hierarchical Tensor Decompositions

[Cohen, Sharir, Shashua'15]

- In both decompositions, given enough terms, any tensor can be approximated arbitrarily well.

- *Depth efficiency* question: for tensors that require a polynomial size in the HT decomposition, how many parameters in the CP representation do we need?
- and vice-versa?

[Cohen, Sharir, Shashua'15]

Theorem: Let A be a tensor of order N and dimension M in each slice, generated by the HT formula using ranks $r_l = r = O(M)$. Then A will have CP-rank at least $r^{N/2}$ almost everywhere.

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Then A will have CP-rank at least $r^{N/2}$ almost everywhere.

- The HT space with rank r blocks has $O(r^2 N)$ parameters.
- Besides a negligible set, all functions that can be realized by a polynomially sized HT model require exponential size in order to be approximated by a CP model.
- The converse is not true: a CP model of size $O(NMK)$ can be represented in HT with $O(NK\max(K, M)) \simeq O(NK^2)$

Deep Nets and Hierarchical Tensor Decompositions

[Cohen, Sharir, Shashua'15]

- Pros
  - Framework that explains that depth efficiency is universal: *all* hierarchical decompositions require exponentially more effort to parametrize using non-hierarchical factorizations.
  - Role of Convolution: weight sharing in a CP decomposition reduces to symmetric tensors. Not the case in the HT decomposition.

- Cons
  - Nonlinearities are multiplicative in this model: numerically and statistically unstable. Logarithms do not fully resolve unstability.
  - Approximation error results. Interplay with estimation and optimization error?

Deep Networks and Spin Glasses

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

- Suppose we have a linear deep network:

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

- 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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- In coordinates, $(\Theta_1 x)^j = \sum_l \Theta_1^{j,l} x^l~,$

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

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

Deep Networks and Spin Glasses

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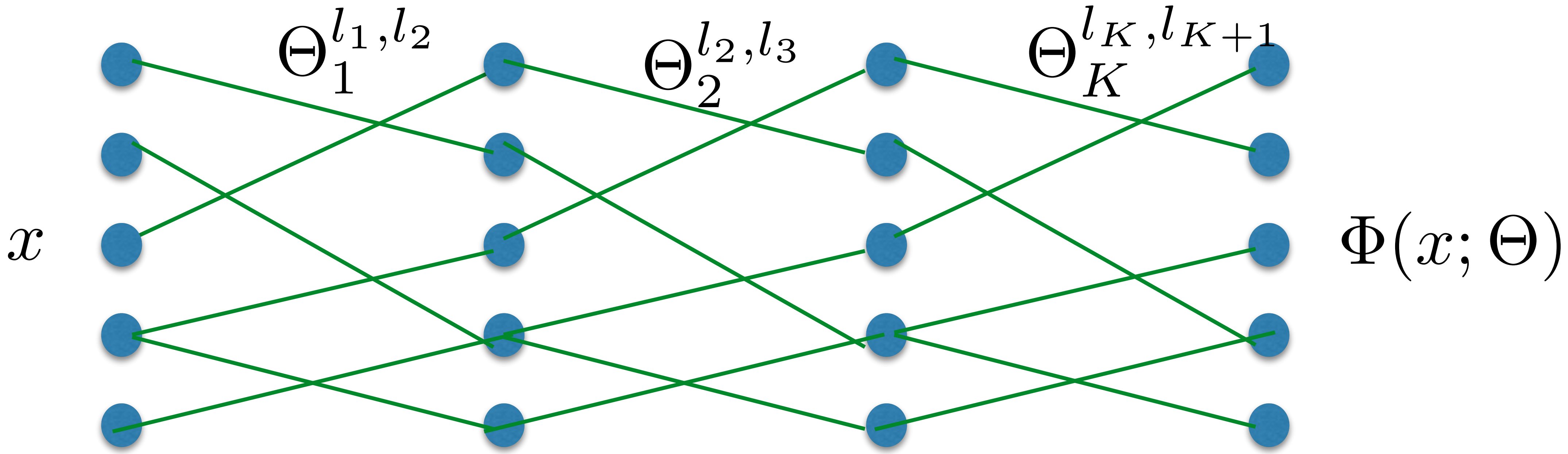

- Equivalently, we can define *paths* $p = (l_0, l_1, \dots, l_{K+1})$

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

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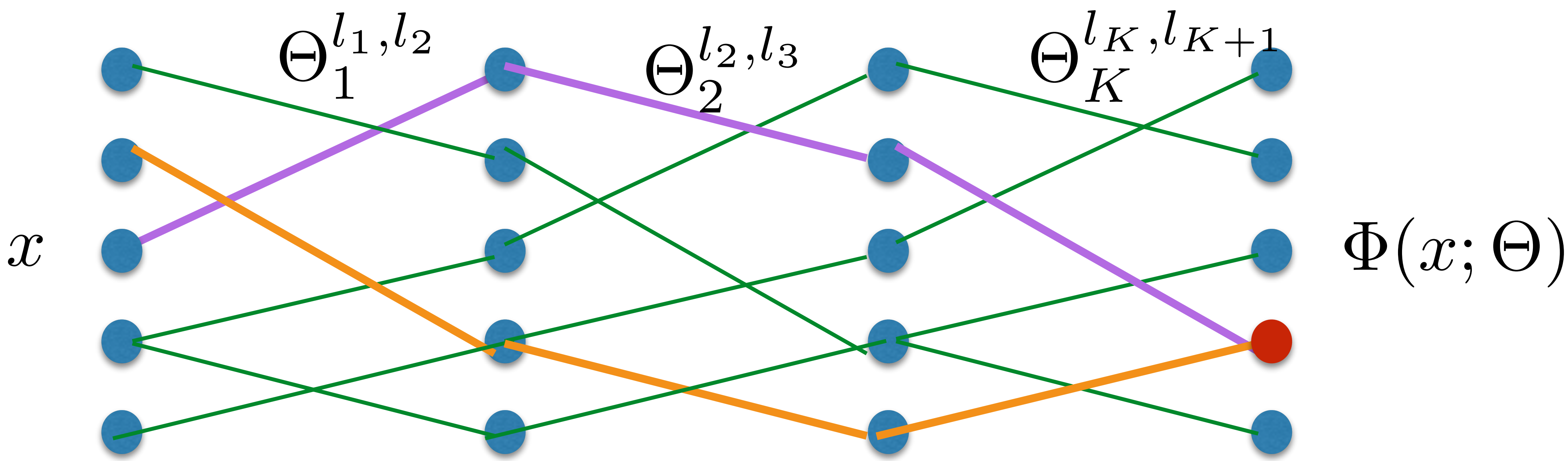

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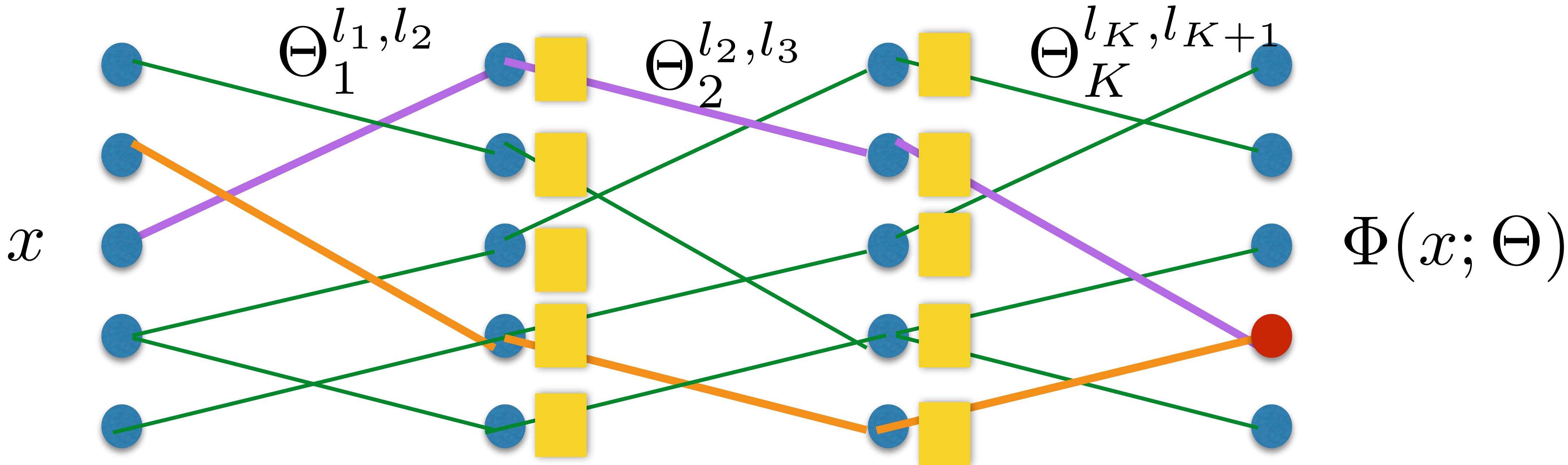
$$\Phi(x;\Theta)^j = \sum_{p \in \mathcal{P}; p(K+1)=j} x^{p(1)} \prod_{k \leq K} \Theta_k^{p(k),p(k+1)} .$$

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

Deep Networks and Spin Glasses

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



- Now some paths will be stopped: ■ : $\rho(z) = \max(0, z)$.

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

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

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

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

Deep Networks and Spin Glasses

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

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

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

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

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

Deep Networks and Spin Glasses

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

- 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

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

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

Deep Networks and Spin Glasses

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

- 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

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

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

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

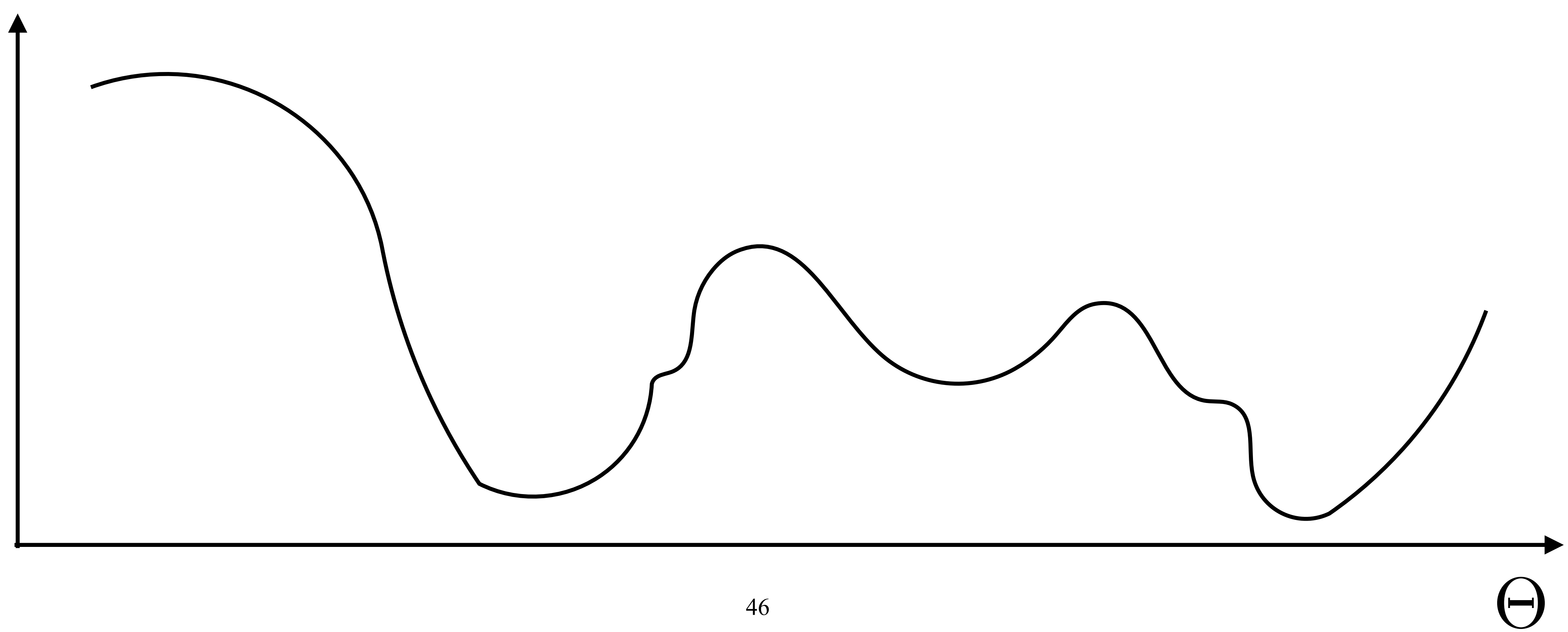
$\mathcal{L}_H(\Theta)$: Hamiltonian of the H-spin spherical spin glass model.

Deep Networks and Spin Glasses

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

- [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:



Deep Networks and Spin Glasses

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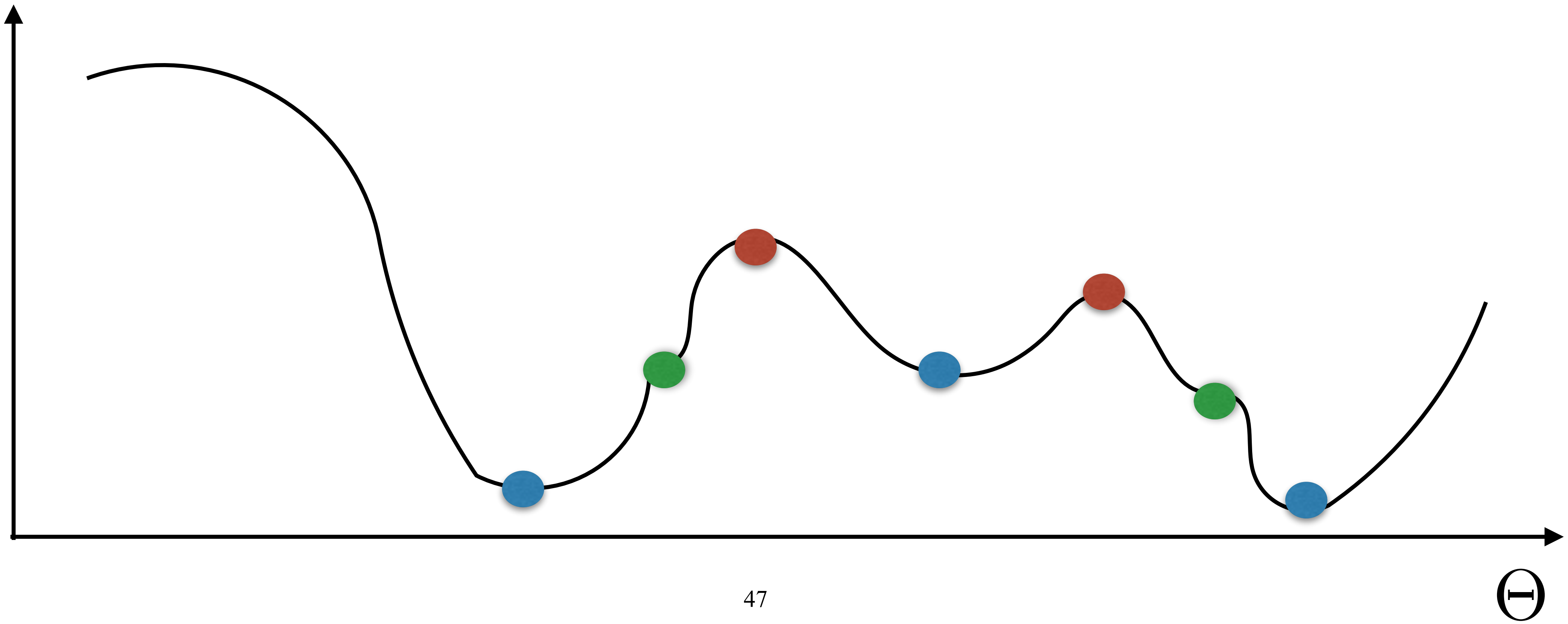
- [Auffinger et al '10] [Auffinger, Ben Arous'13], obtained a complete description of the behavior of critical points of spherical spin glasses.

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



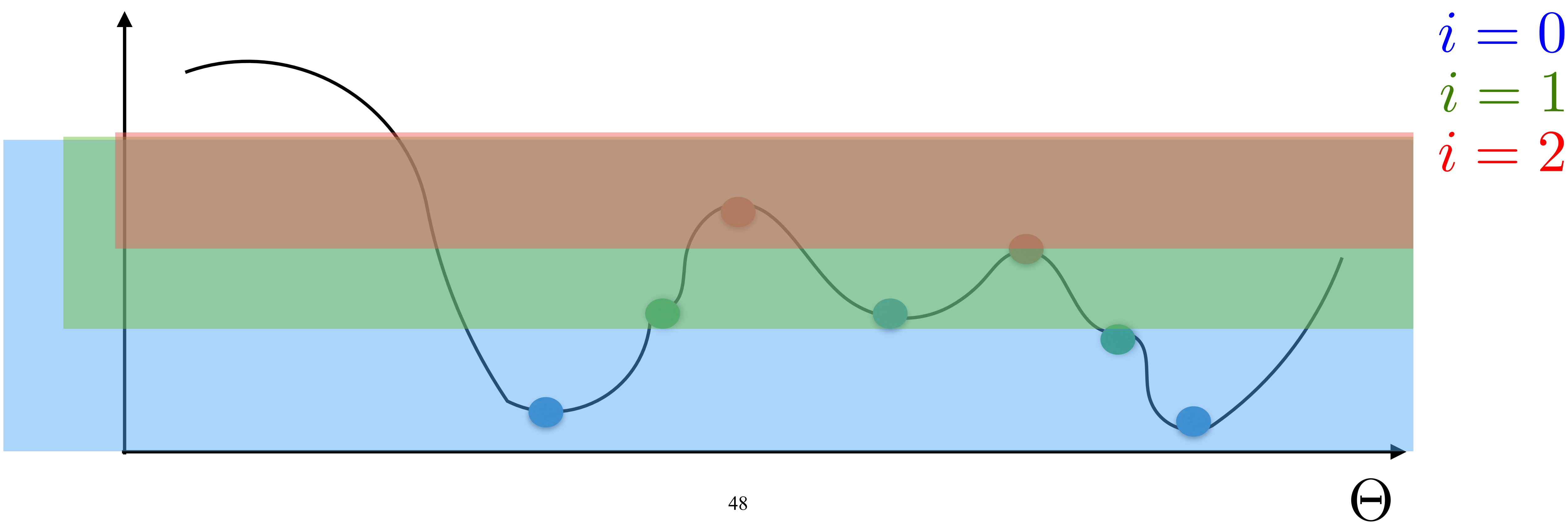
$i = 0$
$i = 1$
$i = 2$

Deep Networks and Spin Glasses

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

- 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.

Deep Networks and Spin Glasses

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

- Pros
  - Macroscopic picture that explains *some* of the behavior of stochastic gradient descent on deep neural networks.
  - Analysis tools from Random Matrix theory that explain non-local behavior and might complement invariance/symmetry arguments.
- Cons
  - The simplifications on the model are very strong.
  - Does not inform about the role of convolutions in the energy landscape
  - Does not really inform about the role of depth in the optimization.