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:

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

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

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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.

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

  - 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:

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

- 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.

- 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.

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

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

- 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

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

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:

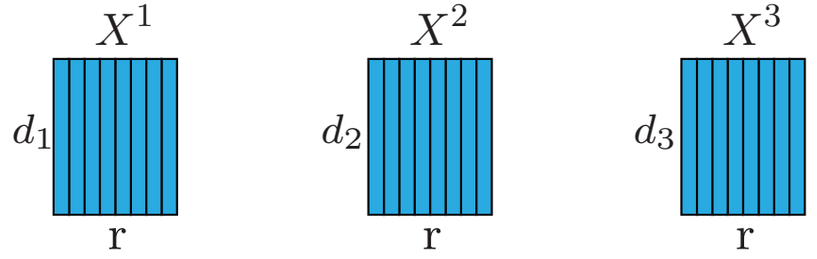
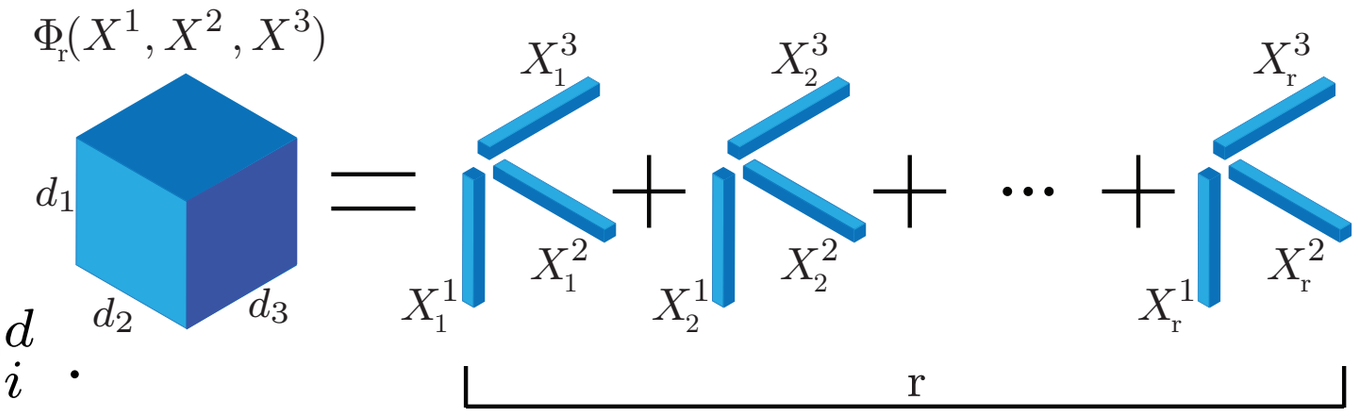


figure credit: R. Vidal

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



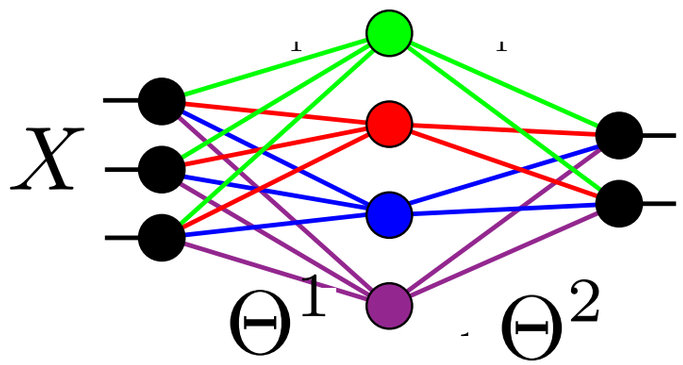
Candecomp/Parafac (CP) Tensor decomposition.

Adaptation to Deep Models

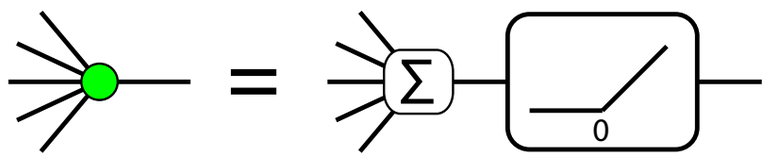
- ReLU Network:

figure credit: R. Vidal

ReLU Network with One Hidden Layer

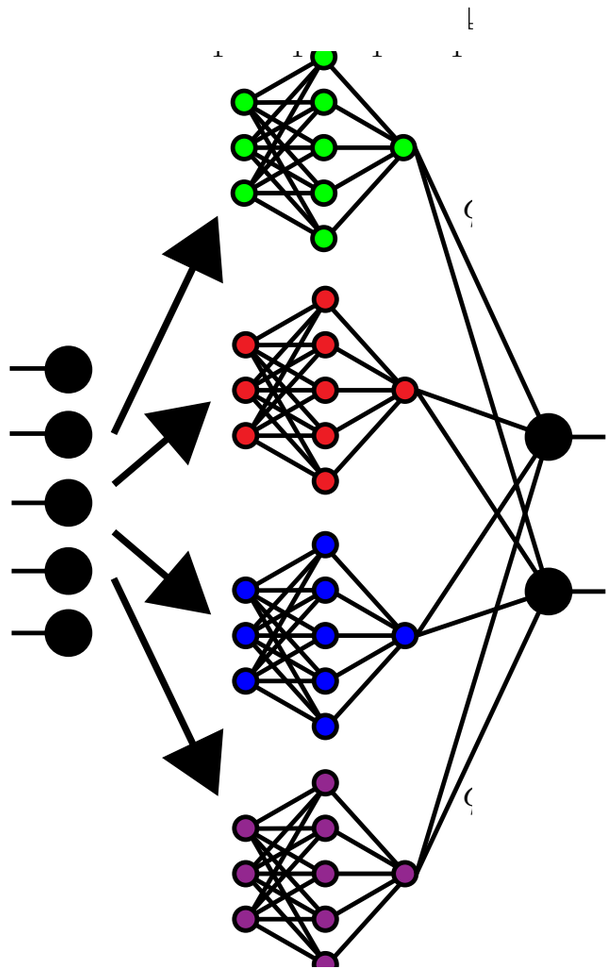


Rectified Linear Unit (ReLU)



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

Multilayer ReLU Parallel Network



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

Adaptation to Deep Models

- In the matrix case, the variational principle was

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

- 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

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

- 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
$A_1 \in \mathbb{R}^{d \times k}$.

- 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 needs

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

Deep Nets and Hierarchical Tensor Decompositions

[Cohen, Sharir, Shashua'15]

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

x

Deep Nets and Hierarchical Tensor Decompositions

[Cohen, Sharir, Shashua'15]

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

x  $\Phi(x^k)$

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

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

- 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 $M_k = M$.

Deep Nets and Hierarchical Tensor Decompositions

[Cohen, Sharir, Shashua'15]

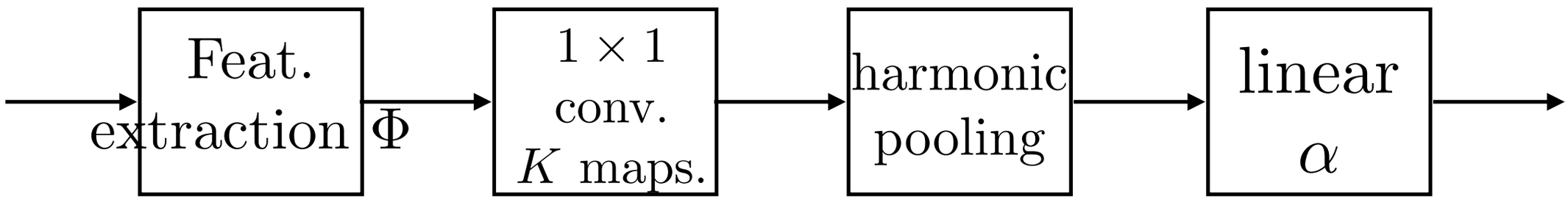
- Q: How to parametrize/factorize the tensors A^y ?
- CP (Candecomp/Parafac) decomposition:

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

$$\text{sum of } K \text{ rank-1 } N\text{-th order tensors of size } M.$$

- 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:

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

$$\dots$$

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

$$\dots$$

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

– 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 viceversa?

Deep Nets and Hierarchical Tensor Decompositions

[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.

- $\mathrm{The\ HT\ space\ with\ rank}\ r\ \mathrm{blocks\ has}\ O(r^2 N)\ \mathrm{parameters.}$
- 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:

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

- And suppose we train using least squares regression:

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

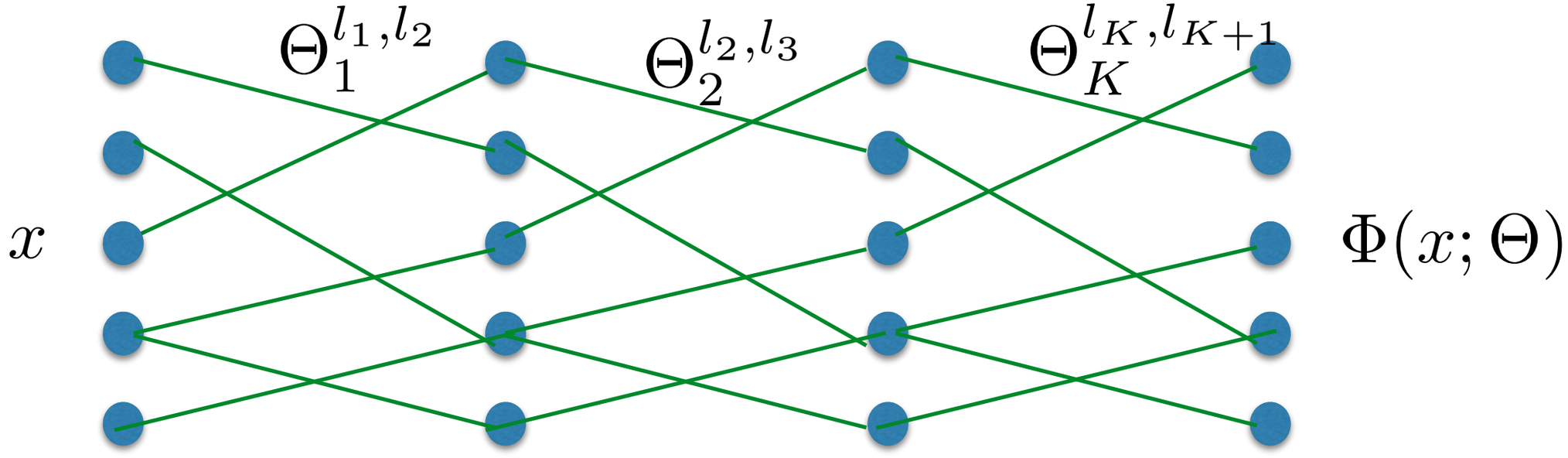
- In coordinates, $(\Theta_1 x)^j = \sum_l \Theta_1^{j,l} x^l \ ,$

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

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

Deep Networks and Spin Glasses

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

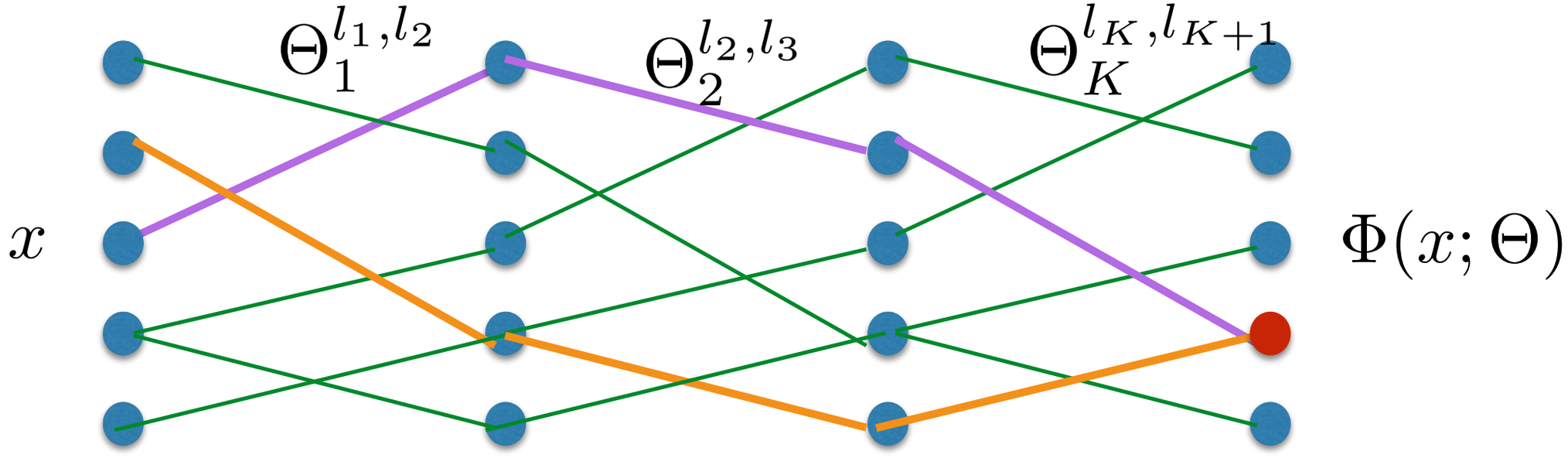


- Equivalently, we can define *paths* $p = (l_0, l_1, \ldots, l_{K+1})$

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

Deep Networks and Spin Glasses

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



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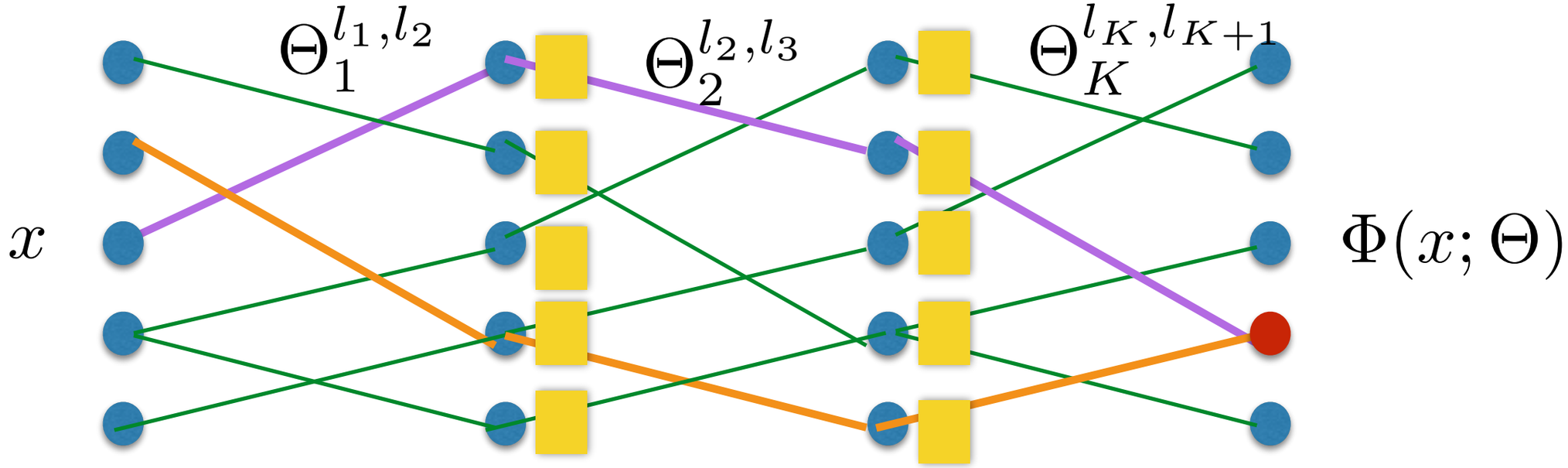
$$\mathcal{P} = \{p = (l_0, \ldots, l_{K+1}); 1 \leq l_k \leq M_k\}$$

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

- 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: $\blacksquare : \rho(z) = \max(0, z)$.

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

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

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

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

Deep Networks and Spin Glasses

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

- Loss becomes

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

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

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

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

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

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

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 (and 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

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

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

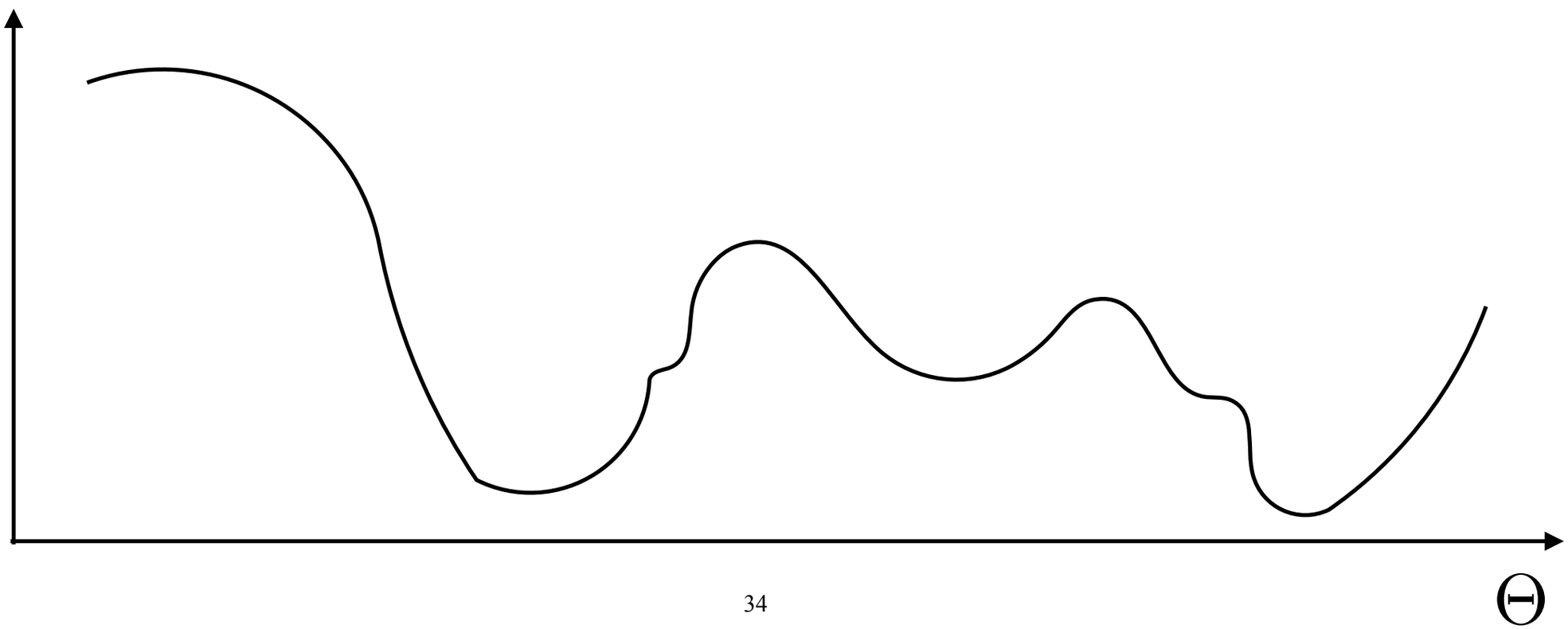
$\mathcal{L}_H(\Theta)$: Hamiltonian of the H-spin spherical spin glass model.

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:



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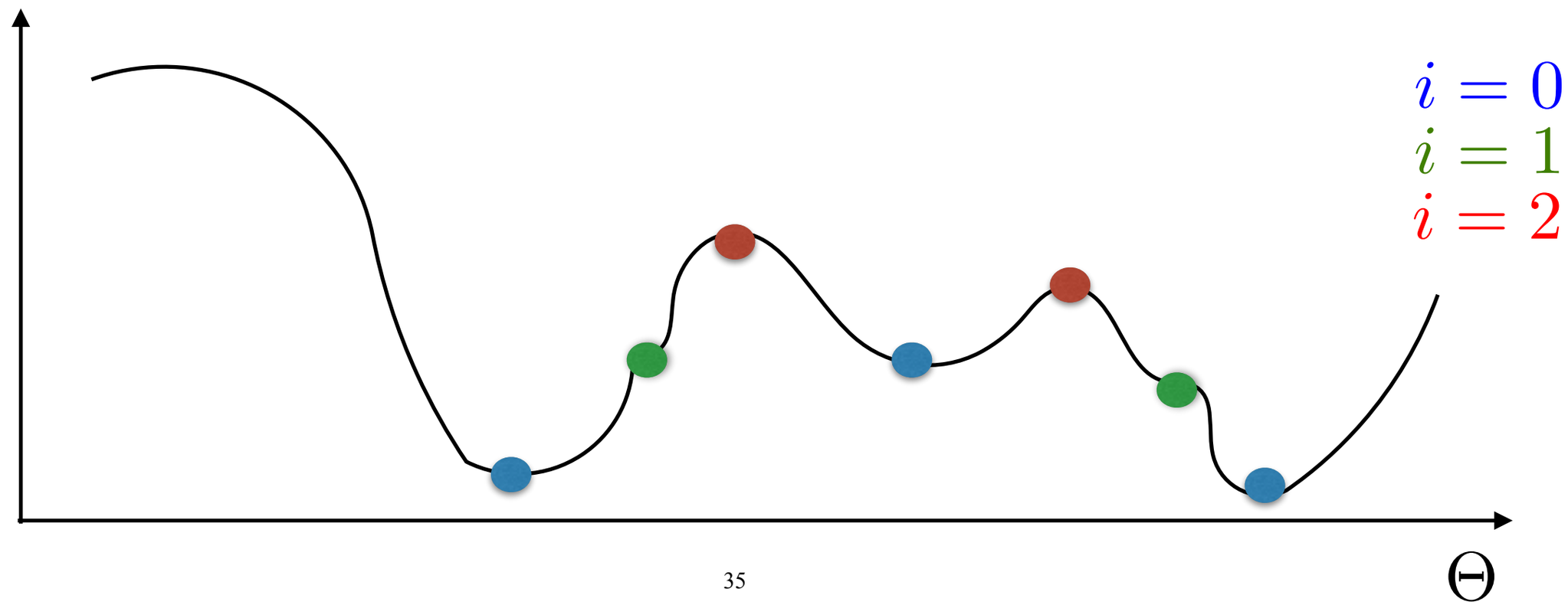
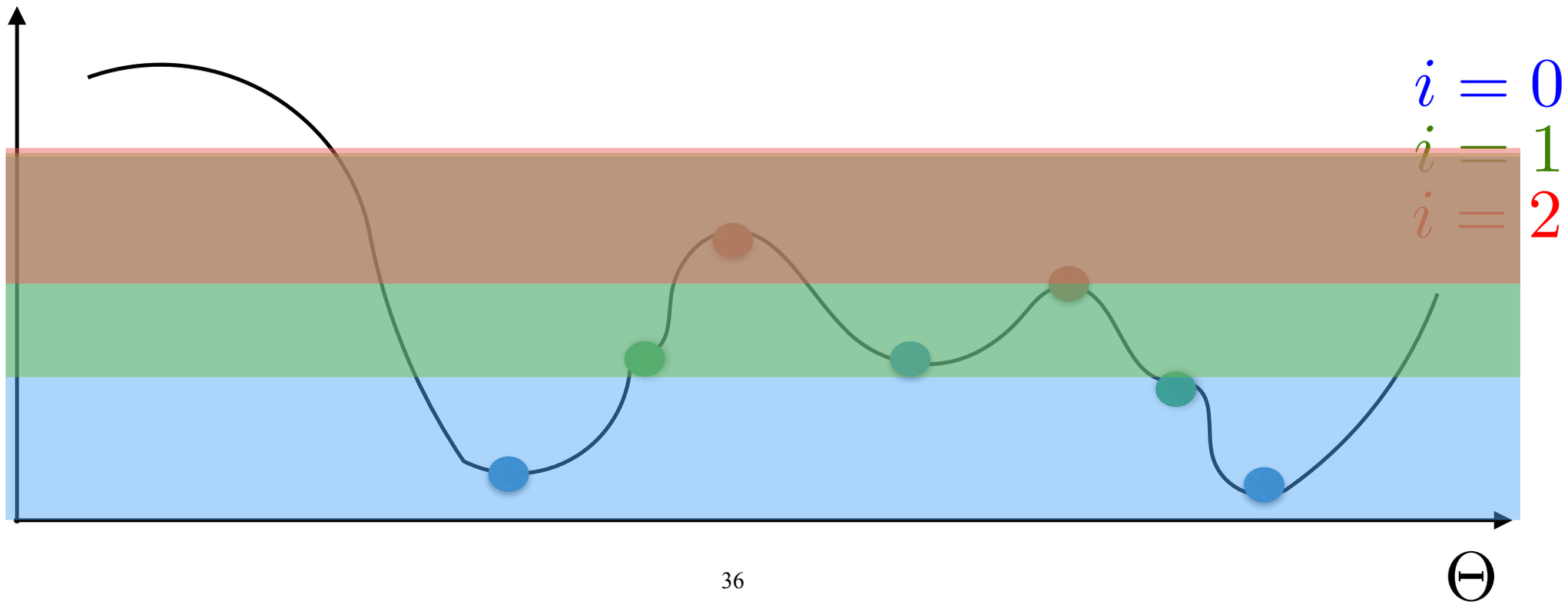


Deep Networks and Spin Glasses

[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

[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.