So far, we have introduced…

- Mallat's invariant scattering transform networks
  - The deeper the network, the more invariant (translation, local deformation, scaling and rotation)
- Poggio et al. local (sparse), hierarchical, compositional functions
  - Avoid the curse of dimensionality
- Papyan et al. sparse cascaded convolutional dictionary learning
  - Uniqueness and stability guarantees of sparse recovery

Let's continue on …

- *Harmonic Analysis:* What are the optimal (transferrable) representations of functions as input signals (sounds, images, …)?

- *Approximation Theory:* When and why are deep networks better than shallow networks?

- ***Optimization:* What is the landscape of the empirical risk and how to minimize it efficiently?**

- ***Statistics:* How can deep learning generalize well without overfitting the noise?**

Generalization of Supervised Learning

Collect data: $\{(x_i, y_i) | \; i = 1, 2, \ldots, n\}$

Learn a model: $f: \mathcal{X} \rightarrow \mathcal{Y}, \; f \in \mathcal{H}$

Predict new data: $x \rightarrow f(x)$

All $(x, y) \sim \mathcal{D}$, where $\mathcal{D}$ is unknown

A common approach to learn:

ERM (Empirical Risk Minimization)

$$\min R_n(w) := \frac{1}{n} \sum_i l(w; x_i, y_i)$$

w: model parameters

$l(w; x, y)$: loss function w.r.t. data

Population Risk: $R(w) := \mathrm{E}[l(w; x, y)]$

Generalization Error

- We consider the standard ML setup:

$$\hat{E}(\Theta) = \mathbb{E}_{(X,Y)\sim\hat{P}}\ell(\Phi(X;\Theta),Y) + \mathcal{R}(\Theta)$$
$$E(\Theta) = \mathbb{E}_{(X,Y)\sim P}\ \ell(\Phi(X;\Theta),Y)\ .$$

$$\hat{P} = \frac{1}{n}\sum_{i\leq}\delta_{(xi,y_i)}$$

$\ell(z)$ convex

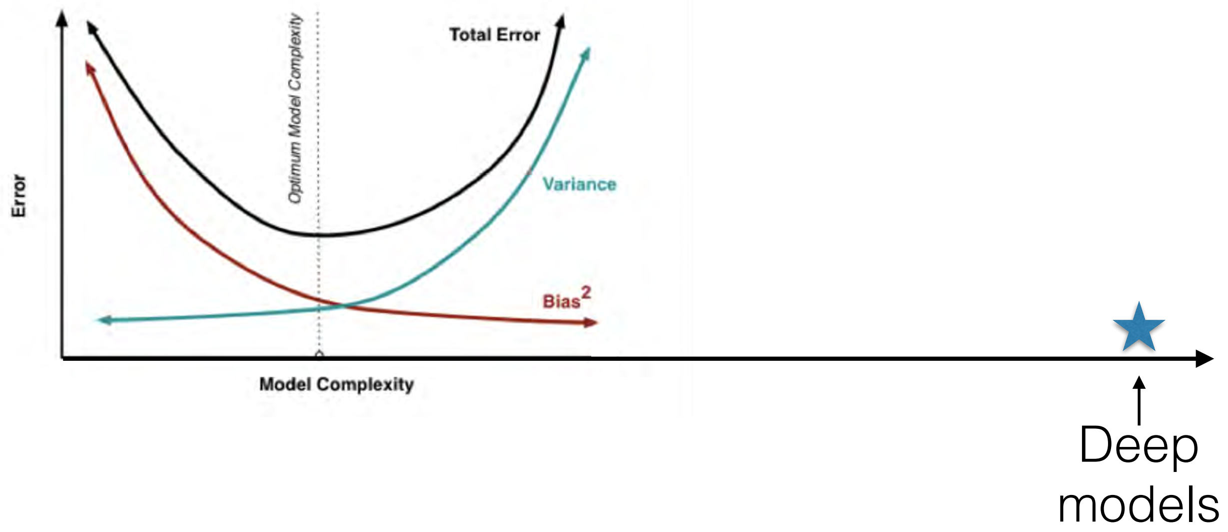
$\mathcal{R}(\Theta)$: regularization

- Population loss decomposition (*aka* "fundamental theorem of ML"):

$$E(\Theta^*) = \underbrace{\hat{E}(\Theta^*)}_{\text{training error}} + \underbrace{E(\Theta^*) - \hat{E}(\Theta^*)}_{\text{generalization gap}}\ .$$

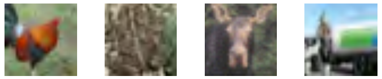
- Long history of techniques to provably control generalization error via appropriate regularization.
- Generalization error and optimization are entangled [Bottou & Bousquet]

Bias-Variance Tradeoff?



Models where p>20n are common

Why big models generalize well?



CIFAR10

n=50,000
d=3,072
k=10

What happens when I turn off the regularizers?

Model	parameters	p/n	Train ***loss***	Test ***error***
CudaConvNet	145,578	2.9	0	23%
CudaConvNet (with regularization)	145,578	2.9	0.34	18%
MicroInception	1,649,402	33	0	14%
ResNet	2,401,440	48	0	13%

Ben Recht FoCM 2017

How to control generalization error?

- However, when $\Phi(X;\Theta)$ is a large, deep network, current best mechanism to control generalization gap has two key ingredients:
  - $\boxed{\text{– Stochastic Optimization}}$
    - ❖ "During training, it adds the sampling noise that corresponds to empirical-population mismatch" [Léon Bottou].
  - – Make the model *as large as possible*.
    - ❖ see e.g. "Understanding Deep Learning Requires Rethinking Generalization", [Ch. Zhang *et al*, ICLR'17].

Traditional Learning Theory

Common form of generalization bound (in expectation or high probability)

$$R(w) \leq R_n(w) + \sqrt{\frac{Capacity\ Measure}{n}}$$

Capacity Measurement	Complexity
VC-dimension	$VC \leq O(\|E\| \log \|E\|)$
***ε*-Covering number**	$\log_2 N_{l_1}(\mathcal{F}, \epsilon, m) \leq O\left(\frac{(AL_\phi)^{L(L+1)}}{\epsilon^{2L}}\right)$
Rademacher Average	$R_m(\mathcal{F}) \leq O(\mu^L)$

$|E|$: # of edges

L: # of layers

Big model should fail!

Training Algorithms for Deep Learning

Commonly Used Algorithms

Non-adaptive

- SGD
- SGD with momentum
- ……

Easy to implement

Adaptive

- Adam
- AdaGrad
- AdaDelta
- ……

Automatically tune parameters

Learn the curvature adaptively

Stochastic Gradient Descent

Objective loss function:

$$\min R_n(w) := \frac{1}{n}\sum_i l(w; x_i, y_i)$$

where $(x_i,\ y_i)$ is the data, w is the parameter vector.

Gradient Descent: $w_{t+1} = w_t - \frac{\eta}{n}\sum \nabla l(w_t; x_i, y_i)$

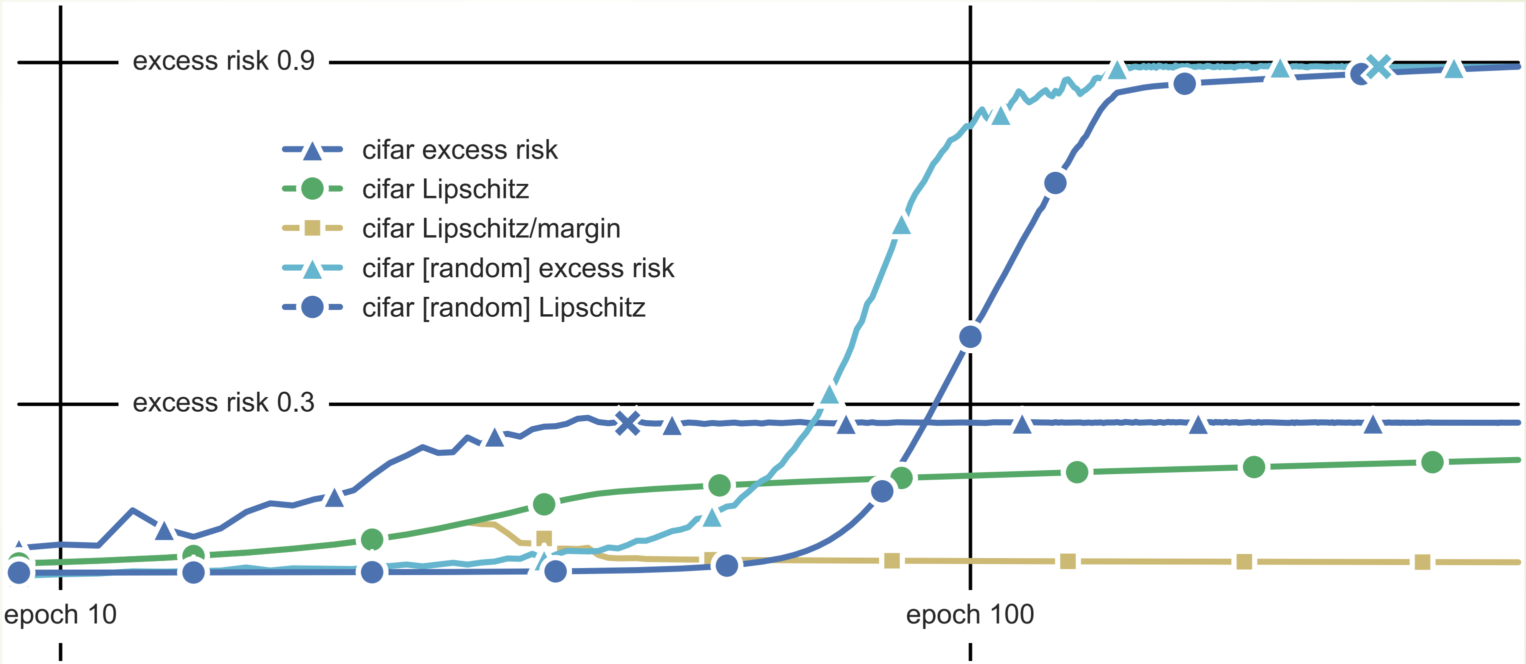
O(n) time complexity

SGD: $w_{t+1} = w_t - \eta \nabla l(w_t; x_{i_t}, y_{i_t})$, where i_t is uniform in {1, …, n}

O(1) time complexity

Extensions: mini-batch SGD

SGD with early stopping regularizes



Bartlett et al. 2017. Generalization error of AlexNet in Cifar10

Margin and Network Lipschitz based Generalization error bound (Bartlett et al. 2017)

Theorem 1.1. *Let nonlinearities* $(\sigma_1, \ldots, \sigma_L)$ *and reference matrices* $(M_1, \ldots, M_L)$ *be given as above (i.e.,* σ_i *is* ρ_i*-Lipschitz and* $\sigma_i(0) = 0$*). Then for* $(x, y), (x_1, y_1), \ldots, (x_n, y_n)$ *drawn iid from any probability distribution over* $\mathbb{R}^d \times \{1, \ldots, k\}$*, with probability at least* $1 - \delta$ *over* $((x_i, y_i))_{i=1}^n$*, every margin* $\gamma > 0$ *and network* $F_\mathcal{A} : \mathbb{R}^d \to \mathbb{R}^k$ *with weight matrices* $\mathcal{A} = (A_1, \ldots, A_L)$ *satisfy*

$$\Pr\left[\arg\max_j F_\mathcal{A}(x)_j \neq y\right] \leq \widehat{\mathcal{R}}_\gamma(F_\mathcal{A}) + \widetilde{\mathcal{O}}\left(\frac{\|X\|_2 R_\mathcal{A}}{\gamma n}\ln(W) + \sqrt{\frac{\ln(1/\delta)}{n}}\right),$$

where $\widehat{\mathcal{R}}_\gamma(f) \leq n^{-1}\sum_i \mathbb{1}\left[f(x_i)_{y_i} \leq \gamma + \max_{j \neq y_i} f(x_i)_j\right]$ *and* $\|X\|_2 = \sqrt{\sum_i \|x_i\|_2^2}$.

The *spectral complexity* $R_{F_\mathcal{A}} = R_\mathcal{A}$ of a network $F_\mathcal{A}$ with weights $\mathcal{A}$ is the defined as

$$R_\mathcal{A} := \left(\prod_{i=1}^L \rho_i \|A_i\|_\sigma\right)\left(\sum_{i=1}^L \frac{\|A_i^\top - M_i^\top\|_{2,1}^{2/3}}{\|A_i\|_\sigma^{2/3}}\right)^{3/2}.$$

Stochastic Gradient/Discrete Langevin Dynamics (SGLD)

SGLD is a variant of SGD:

$$w_{t+1} = w_t - \eta \nabla l\left(w_t; x_{i_t}, y_{i_t}\right) + \sqrt{\frac{2\eta}{\beta}} z_t, \text{ where } z_t \sim \mathcal{N}(0, I_d)$$

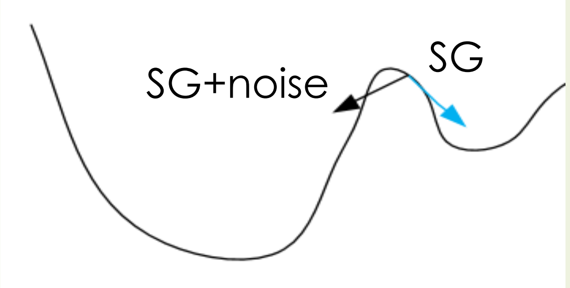
Injection of Gaussian noise makes SGLD completely different with SGD

For small enough step size η_t, Gaussian noise will dominate the stochastic gradient.

Distinctions of SGLD

Intuitively, injected isotropic Gaussian noise helps escape saddle points or local minimum

SGLD is the discretization of following SDE



$$\boxed{dW(t)} = -\nabla F\big(W(t)\big)dt + \sqrt{\frac{2}{\beta}}dB(t)$$

where $F(\cdot)$ is the empirical loss function, $B(t)$ is the standard Brownian motion

Its distribution converges to Gibbs distribution $\propto \exp(-\beta F(w))$

Large β will concentrate on the global minimizer of $F(w)$

Liwei Wang et al. 2017

From the view of stability theory:

Under mild conditions of (surrogate) loss function, the generalization error of SGLD at N-th round satisfies

$$E[l(w_S, z)] - E_S[l(w_S, z)] \leq O\left(\frac{1}{n}\left(k_0 + L\sqrt{\beta \sum_{k=k_0+1}^{N} \eta_k}\right)\right)$$

where L is the Lipschitz constant, and $k_0 \coloneqq \min\ \{k: \eta_k \beta L^2 < 1\}$

If consider high probability form, there is an additional $\tilde{O}(\sqrt{1/n})$ term

Lipschitz Bound by Liwei Wang et al. 2017

From the view of PAC-Bayesian theory:

For regularized ERM with $R(w) = \lambda||w||^2/2$. Under mild conditions, with high probability, the generalization error of SGLD at N-th round satisfies

$$E[E[l(w_S, z)]] - E_S[E[l(w_S, z)]] \leq O\left(\sqrt{\frac{\beta}{n}\sum_{k=1}^{N}\eta_k e^{-\lambda(T_N - T_k)/2} E[||g_k||^2]}\right)$$

where $T_k = \sum_{j=1}^{k}\eta_k$, g_k is the stochastic gradient in each round.

Comparison Two Results

Both bounds suggest "train faster, generalize better", which explain the random label experiments in ICLR17

- In expectation, stability bound has a faster $O\left(\frac{1}{n}\right)$ rate.
- PAC-Bayes bound is data dependent, and doesn't rely on Lipschitz condition.
- Effect of step sizes in PAC-Bayes exponentially decay with time.

The Landscape of Risks

- However, when $\Phi(X;\Theta)$ is a large, deep network, current best mechanism to control generalization gap has two key ingredients:
  - Stochastic Optimization
    - ❖ "during training, it adds the sampling noise that corresponds to empirical-population mismatch" [Léon Bottou].
  - Make the model *as large as possible*.
    - ❖ see e.g. "Understanding Deep Learning Requires Rethinking Generalization", [Ch. Zhang *et al*, ICLR'17].

- We first address how overparametrization affects the energy landscapes $E(\Theta), \hat{E}(\Theta)$.

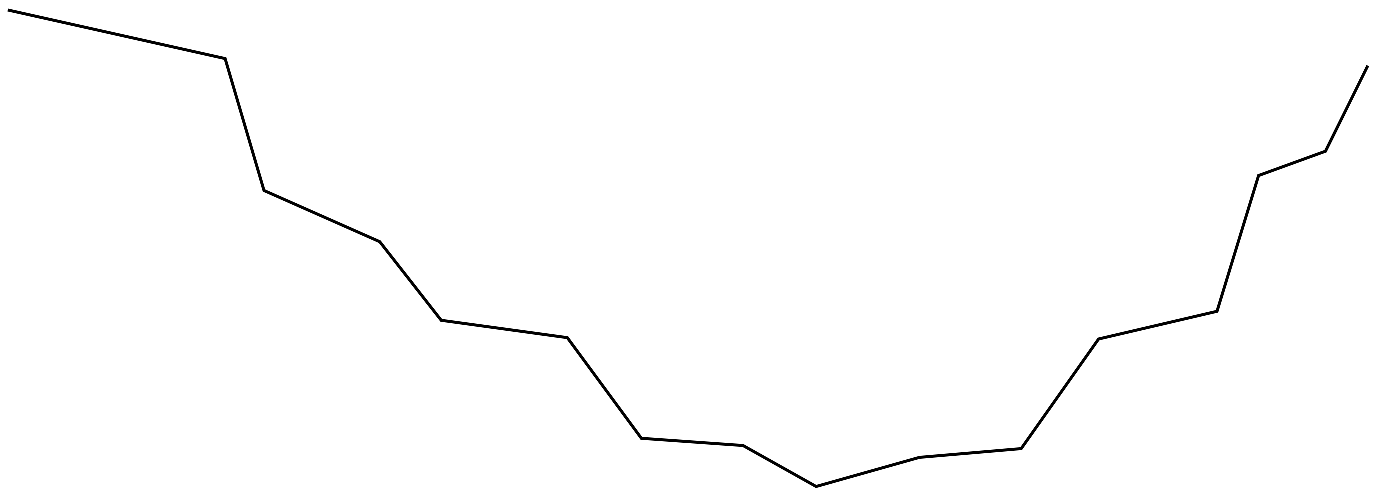
A `Deep' Dream:
All Critical Point/local optima = Global Optima?

- Choromanska-LeCun-Ben Arous'15: most of critical values are concentrated in a narrow bind of global optima, using random Morse theory on sphere (spin class models)
- Haeffele et al.'15,16: overparameterized tensor factorization models, every local optima are global optima
- Kawaguchi'16: linear networks have no poor local optima
- Bruna et al.'16,17: simple sublevel set topology of multilinear regression, with group symmetry, and some nonlinear networks
- Chaudhari et al'17: Moreau envelope of empirical risk
- Pennington & Bahri'17: Hessian Analysis using Random Matrix Theory

A Dream: All Critical Point = Global Optima?

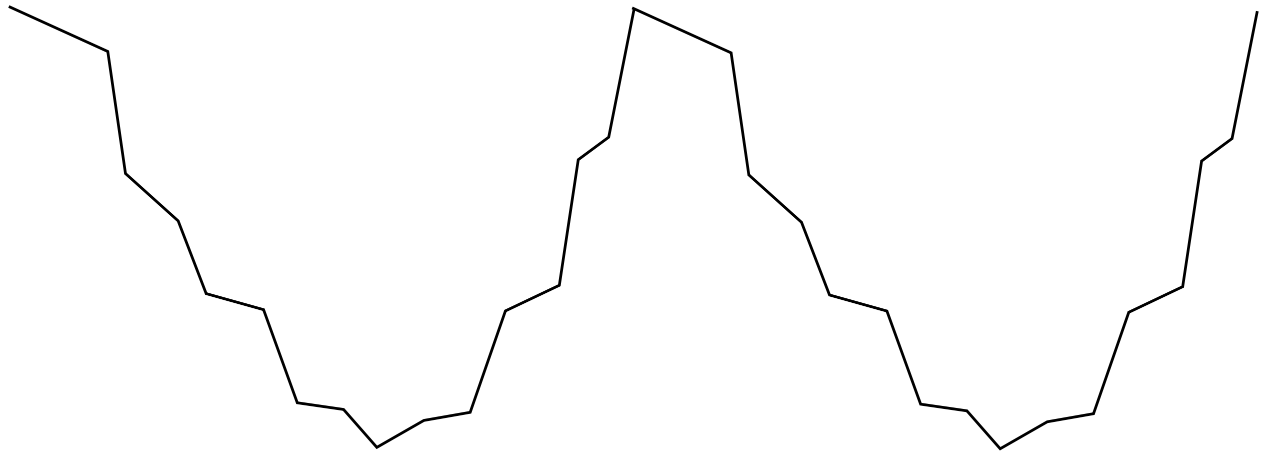
- Models from Statistical physics have been considered as possible approximations [Dauphin et al.'14, Choromanska et al.'15, Segun et al.'15]
- Tensor factorization models capture some of the non convexity essence [Anandukar et al'15, Cohen et al. '15, Haeffele et al.'15]
- [Shafran and Shamir,'15] studies bassins of attraction in neural networks in the overparametrized regime.
- [Soudry'16, Song et al'16] study Empirical Risk Minimization in two-layer ReLU networks, also in the over-parametrized regime.
- [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.

Nonconvexity vs. Gradient Descent



- We can perturb any convex function in such a way it is no longer convex, but such that gradient descent still converges.
- E.g. quasi-convex functions.

Symmetry and Group Invariance



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

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

Linear Networks

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

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

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

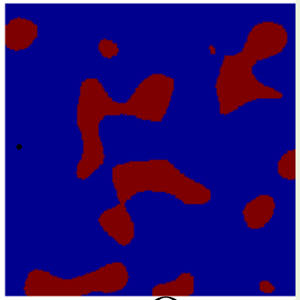
Theorem: [Kawaguchi'16] If $\Sigma = \mathbb{E}(XX^T)$ and $\mathbb{E}(XY^T)$ are full-rank and Σ has distinct eigenvalues, then $E(\Theta)$ has no poor local minima.

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

Toplogy of Nonconvex Landscape

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

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



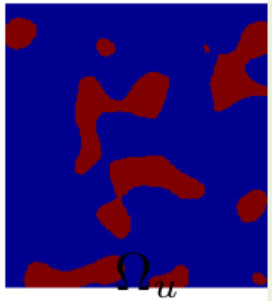
Ω_u

- A first notion we address is about the topology of the level sets .

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

Simple Topology

- A first notion we address is about the topology of the level sets .
  - In particular, we ask how connected they are, i.e. how many connected components N_u at each energy level u?

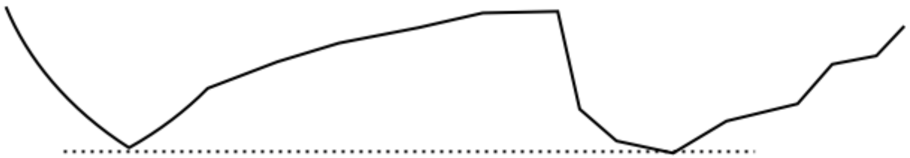


- This is directly related to the question of global minima:

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

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

- We say E is *simple* in that case.
- The converse is clearly not true.



Simple Topology of Linear Networks [Bruna-Freeman'16]

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

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) $E(W_1, W_2) = \mathbb{E}_{(X,Y)\sim P}\|W_2 W_1 X - Y\|^2 + \lambda(\|W_1\|^2 + \|W_2\|^2)$ satisfies $N_u = 1 \ \forall \ u$ if $n_1 > \min(n, m)$.

- We pay extra redundancy price to get simple topology.

Group Symmetries [Bruna-Venturi-Bandiera'17]

- Q: How much extra redundancy are we paying to achieve $N_u = 1$ instead of simply no poor-local minima?

  - In the multilinear case, we don't need $n_k > \min(n, m)$
    - ❖ We do the same analysis in the quotient space defined by the equivalence relationship $W \sim \tilde{W} \Leftrightarrow W = \tilde{W}U \ , \ U \in GL(\mathbb{R}^n) \ .$

Corollary [LBB'17]: The Multilinear regression $\mathbb{E}_{(X,Y)\sim P}\|W_1 \dots W_k X - Y\|^2$ has no poor local minima.

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

Nonlinear ReLU network

- Good behavior is recovered with nonlinear ReLU networks, provided they are sufficiently overparametrized:
- Setup: two-layer ReLU network:
$$\Phi(X;\Theta) = W_2\rho(W_1 X)\ ,\ \rho(z) = \max(0,z). W_1 \in \mathbb{R}^{m\times n}, W_2 \in \mathbb{R}^m$$

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

- Overparametrisation "wipes-out" local minima (and group symmetries).
- The bound is cursed by dimensionality, ie exponential in n .
- *Open question:* polynomial rate using Taylor decomp of $\rho(z)$?

Better Optimization Algorithms?

- Backpropagation Algorithm (made popular by Rumelhart-Hinton-Williams' 1986) as stochastic gradient descent is equivalent to Larangian Multiplier method with gradient descent on weights (prox-linear)
  - Used in control theory (dynamic programming) in 1960s
- It suffers from vanishing of gradients due to the chain rule of gradient map

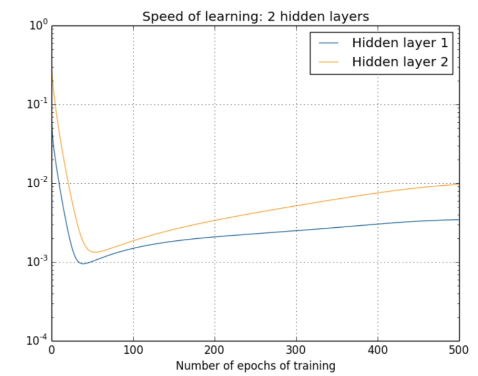
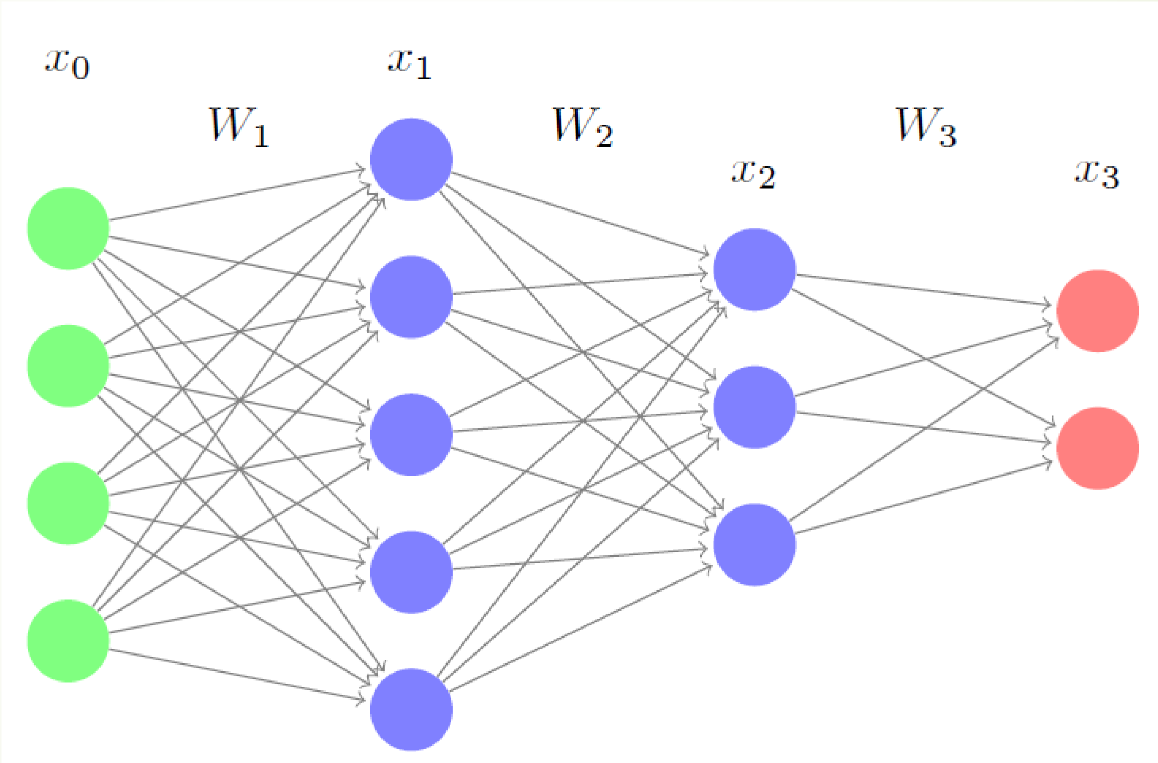


Figure: BP on MNIST[2]: Two hidden layers, speed of learning

Multi-Layer Perceptron (MLP)



Forward Pass

- Cascade of repeated [linear operation followed by coordinatewise nonlinearity]'s
- Nonlinearities: sigmoid, hyperbolic tangent, (recently) ReLU.

Algorithm 1 Forward pass

Input: x_0
Output: x_L

1: **for** $\ell = 1$ to L **do**
2: $\quad x_\ell = f_\ell(W_\ell x_{\ell-1} + b_\ell)$
3: **end for**

Stochastic Gradient Descent Training

- Training examples $\{x_0^i\}_{i=1}^n$ and labels $\{y^i\}_{i=1}^n$
- Output of the network $\{x_L^i\}_{i=1}^m$
- Objective

$$J(\{W_l\}, \{b_l\}) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{2}\|y^i - x_L^i\|_2^2 \tag{1}$$

- Gradient descent

$$W_l = W_l - \eta\frac{\partial J}{\partial W_l}$$

$$b_l = b_l - \eta\frac{\partial J}{\partial b_l}$$

In practice: use Stochastic Gradient Descent (SGD)

Backward Propagation as Lagrangian Multiplier (LeCun'88)

Given n training examples $(I_i, y_i) \equiv$ (input,target) and L layers

- Constrained optimization

$$\begin{aligned} \min_{W,x} \quad & \textstyle\sum_{i=1}^{n} \|x_i(L) - y_i\|_2 \\ \text{subject to} \quad & x_i(\ell) = f_\ell\Big[W_\ell x_i\,(\ell-1)\Big], \\ & i = 1, \ldots, n, \quad \ell = 1, \ldots, L,\ x_i(0) = I_i \end{aligned}$$

- Lagrangian formulation (Unconstrained)

$$\min_{W,x,B} \mathcal{L}(W, x, B)$$

$$\mathcal{L}(W, x, B) = \textstyle\sum_{i=1}^{n} \Big\{ \|x_i(L) - y_i\|_2^2 + \textstyle\sum_{\ell=1}^{L} B_i(\ell)^T \Big(x_i(\ell) - f_\ell\Big[W_\ell x_i\,(\ell-1)\Big]\Big) \Big\}$$

http://yann.lecun.com/exdb/publis/pdf/lecun-88.pdf

BP derivation

- $\frac{\partial \mathcal{L}}{\partial B}$

Forward pass

$$x_i(\ell) = f_\ell\Big[\underbrace{W_\ell x_i\,(\ell-1)}_{A_i(\ell)}\Big] \quad \ell = 1, \ldots, L, \quad i = 1, \ldots, n$$

- $\frac{\partial \mathcal{L}}{\partial x}$, $z_\ell = [\nabla f_\ell] B(\ell)$

Backward (adjoint) pass

$$z(L) = 2\nabla f_L\Big[A_i(L)\Big]\,(y_i - x_i(L))$$

$$z_i(\ell) = \nabla f_\ell\Big[A_i(\ell)\Big] W_{\ell+1}^T z_i(\ell+1) \quad \ell = 0, \ldots, L-1$$

- $W \leftarrow W + \lambda \frac{\partial \mathcal{L}}{\partial W}$

Weight update

$$W_\ell \leftarrow W_\ell + \lambda \sum_{i=1}^{n} z_i(\ell) x_i^T(\ell-1)$$

Batch Normalization

Algorithm 2 Batch normalization [Ioffe and Szegedy, 2015]

Input: Values of x over minibatch $x_1 \dots x_B$, where x is a certain channel in a certain feature vector

Output: Normalized, scaled and shifted values $y_1 \dots y_B$

1: $\mu = \frac{1}{B}\sum_{b=1}^{B} x_b$

2: $\sigma^2 = \frac{1}{B}\sum_{b=1}^{B}(x_b - \mu)^2$

3: $\hat{x}_b = \frac{x_b - \mu}{\sqrt{\sigma^2+\epsilon}}$

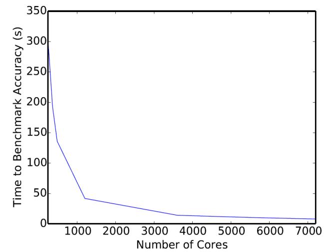
4: $y_b = \gamma\hat{x}_b + \beta$

- Accelerates training and makes initialization less sensitive
- Zero mean and unit variance feature vectors

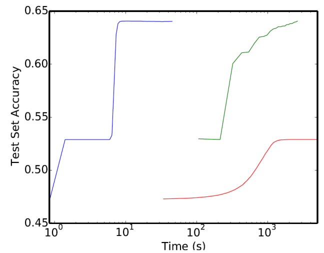
Alternative: (Augmented) Lagrangian Multiplier with Block Coordinate Descent

- ADMM-type: Taylor et al. ICML 2016
- Proximal Propagation, to appear in ICLR 2018
- BCD with zero Lagrangian multiplier: Zhang et al. NIPS 2017
- Discrete EMSA of PMP: **Qianxiao LI** et al 2017, talk on Monday in IAS workshop
  - No-vanshing gradients and parallelizable
- Some convergence theory: preliminary results on ADMM+BCD with **Jinshan Zeng, Shaobo Lin, and Tsz Kit Lau et al.**

Experiment results on Higgs dataset from Taylor et al'16



(a) **Time required for ADMM to reach 64% test accuracy when parallelized over varying levels of cores.** L-BFGS on a GPU required 181 seconds, and conjugate gradients required 44 minutes. SGD never reached 64% accuracy.



(b) **Test set predictive accuracy as a function of time** for ADMM on 7200 cores (blue), conjugate gradients (green), and SGD (red). Note the x-axis is scaled logarithmically.

Thank you!