## Guarantees for fitting NNs with GD

## ECE826 Lecture 10:

## Contents

- Going deeper on PL
- No bad local minima
- It's all about the Jacobian
- Brief overview of NTK/large overparameterization

# Minimizing the Empirical Risk • The empirical cost function that we have access to $\min_{h \in \mathcal{H}} \left( R_{S}[h] = \frac{1}{n} \sum_{i=1}^{n} \ell(h(x_{i}); y_{i}) \right)$

how fast?

• The answer must depend on: 1) *n*, the sample size 2)  $\mathcal{H}$ , the hypothesis class and loss function 3)  $\mathcal{D}$ , the data distribution 4) the optimization algorithm that outputs our classifier

### • <u>Question</u>: Can we approximate the solution to this minimization? If so



# Last time: PL is good

## SGD/GD on general non convex functions?

### Theorem

# SGD with step-size $\gamma = \frac{R}{\beta L^2 T}$ satisfy

Proof:

$$\begin{split} \min_{k \in [T]} \mathbb{E} \|\nabla f(w_k)\|^2 &\leq 2\sqrt{\frac{R\beta L^2}{T}} \\ f(w_{k+1}) - f(w_k) - \langle \nabla f(w_k), w_{k+1} - w_k \rangle \leq \frac{\beta}{2} \|w_k - w_{k+1}\|^2 \\ \mathbb{E} f(w_{k+1}) - \mathbb{E} f(w_k) + \gamma \langle \nabla f(w_k), \nabla f_{s_k}(w_k) \rangle \leq \frac{\beta}{2} \|\gamma \nabla f_{s_k}(w_k)\|^2 \end{split}$$

 $\square || \vee / (W_{l_r}) ||$ 

This is a very slow rate, that is very conservative. Makes sense!

 $\gamma L p$ 

JUVKJ

It also doesn't tell us anything about the quality of the solution that SGD finds

Let f(w) be a  $\beta$ -smooth function with L-bounded stoch gradients (i.e.,  $\mathbb{E}_i \|\nabla f_i(w)\| \leq L$ ). Then, the gradients of



## GD on Polyak-Łojasiewicz functions

Theorem

Let f(w) be a  $\beta$ -smooth,  $\mu$ -PL function (i.e.,  $\| \nabla_w L(w) \|$ Then, GD with with step-size  $\gamma = \frac{1}{r}$  satisfies  $f(w_k) - f^* \leq$ R  $f(w_{k+1}) - f(w_k)$ Proof:  $\leq -\gamma \|\nabla f(w_k)\|$ much faster rate < when is PL satisfied?  $\implies \overline{f(w_{k+1})} - \overline{f(w_k)} - f^* \le -\frac{1}{\beta} \|\nabla f(w_k)\| = \frac{1}{\beta} \|\nabla f$  $f(w_{k+1}) - f^* \le -\frac{\mu}{\beta}(f(w_k) - f^*) - (f^* - f(w_k))$  $f(w_{k+1}) - f^* \le \left(1 - \frac{\mu}{\beta}\right)(f(w_k) - f^*)$ 

$$w) \parallel^2 \ge \mu(L(w) - L^*).$$

$$\left(1-\frac{\mu}{\beta}\right)^k \left(f(w_0)-f^*\right)$$

$$0 \le \langle \nabla f(w_k), w_{k+1} - w_k \rangle + \frac{p}{2} \|w_k - w_{k+1}\|^2$$

$$\| \|^{2} + \frac{\beta}{2\beta^{2}} \| \nabla f(w_{k}) \|^{2}$$

$$\|w_{k}^{2}\|^{2} \leq -\frac{\mu}{\beta}(f(w_{k}) - f^{*}) - f^{*}$$

### Loss landscapes and optimization in over-parameterized non-linear systems and neural networks

Chaoyue Liu<sup>a</sup>, Libin Zhu<sup>b,c</sup>, and Mikhail Belkin<sup>c</sup>

<sup>a</sup>Department of Computer Science and Engineering, The Ohio State University <sup>b</sup>Department of Computer Science and Engineering, University of California, San Diego <sup>c</sup>Halicioğlu Data Science Institute, University of California, San Diego

May 28, 2021

### A Convergence Theory for Deep Learning via Over-Parameterization



### Overparameterized Nonlinear Learning: Gradient Descent Takes the Shortest Path?

Samet Oymak<sup>\*</sup> and Mahdi Soltanolkotabi<sup>†</sup>



Simon S. Du<sup>\*1</sup> Jason D. Lee<sup>\*2</sup> Haochuan Li<sup>\*34</sup> Liwei Wang<sup>\*54</sup> Xiyu Zhai<sup>\*6</sup>





PL-like conditions and old elin neighborhoods around initialization/optima.



PL in Nonlinear Least Squares

### Nonlinear least squares W The gradient of the loss is equal to $\nabla_w \|h(X;w) - y\|^2 = [\nabla_w h(X;w)](h(X;w) - y)$

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- Let us refer to  $J(w) = \nabla_w h(X; w) \in \mathbb{R}^{d \times n}$  as the Jacobian of the predictions
- Note that again  $\left\| \nabla_{w} L(w) \right\|^{2} = \left\| J(w)(h(X;w) - y) \right\|$

Nonlinear least squares

$$\| ^{2} \geq 4\lambda_{\min}(J(w)^{T}J(w)) \| h(X;w) - y \| ^{2}$$

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$$\| \|^2 \ge 4\lambda_{\min}(J(w)^T J(w)) \| h(X;w) - y \|^2$$

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Non-linear least squares where min rank(J(w(w)) = n are PL in  $\mathcal{W}$  $w \in \mathcal{W}$ 

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### Most modern DL theory work tries to show that the above is indeed the case

Nonlinear least squares

$$\left\| \right\|^{2} \ge 4\lambda_{\min}(J(w)^{T}J(w)) \left\| h(X;w) - y \right\|^{2}$$

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Non-linear least squares where min rank(J(w(w)) = n are PL in  $\mathcal{W}$  $w \in \mathcal{M}$ 



### PL in Neural Networks?

### No bad local minima almost always?

### No bad local minima: Data independent training error guarantees for multilayer neural networks

Daniel Soudry

Department of Statistics Columbia University New York, NY 10027, USA daniel.soudry@gmail.com Yair Carmon Department of Electrical Engineering Stanford University Stanford, CA 94305, USA yairc@stanford.edu

### No bad local minima: Data independent training error guarantees for multilayer neural networks

Daniel Soudry Department of Statistics Columbia University New York, NY 10027, USA daniel.soudry@gmail.com

Yair Carmon Department of Electrical Engineering Stanford University Stanford, CA 94305, USA yairc@stanford.edu

Theorem (informal): For I-hidden layer nets rank(J(w)) = n almost surely for leaky-ReLU networks, if  $d_0 \cdot d_1 \ge n$ For L-hidden layer nets rank(J(w)) = n a.s., if params. of last layer  $\geq n$ 



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Most modern DL theory work tries to show that the above is indeed the case





More examples

## I-layer linear Neural Networks

Let us assume we have a 1-layer linear network. The prediction of this network is given as  $h(W; x) = \langle v, Wx \rangle$ 

### reminder: $\left\| \nabla_{w} L(w) \right\|^{2} \ge 4\lambda_{\min}(J(w)^{T}J(w)) \left\| h(X;w) - y \right\|$

- The Jacobian is equal to  $J(w) = \nabla_w h(W, x) = \begin{bmatrix} v_1 x_1 \\ \vdots \\ v_k x_1 \end{bmatrix}$
- Note that  $J(w) = v \otimes X$  and we know that  $rank(J(w)) = rank(v) \cdot rank(X) = rank(X)$
- •Hence, if the matrix of data points is full rank n, then the cost function is PL.





assume output edges are all fixed

$$\begin{bmatrix} v_1 x_2 & \dots & v_1 x_n \\ \vdots & \dots & \vdots \\ v_1 & v_k x_2 & \dots & v_k x_n \end{bmatrix} \in \mathbb{R}^{kd \times n}$$

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The Jacobian is equal to 
$$J(w) = \begin{bmatrix} v_1 \sigma'(\langle w_1, x_1 \rangle) \cdot x_1 & v_2 \sigma'(\langle w_1, x_2 \rangle) \cdot x_2 & \dots & v_k \sigma'(\langle w_1, x_n \rangle) \cdot x_n \\ \vdots & \vdots & \dots & \vdots \\ v_1 \sigma'(\langle w_k, x_1 \rangle) \cdot x_1 & v_2 \sigma'(\langle w_k, x_2 \rangle) \cdot x_2 & \dots & v_k \sigma'(\langle w_k, x_n \rangle) \cdot x_n \end{bmatrix}$$



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Note rank(J(w)) = n if the rank of the data matrix is n.





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Note rank(J(w)) = n if the rank of the data matrix is n.



### assume output edges are all fixed

this would again imply that all local minima = global, but speed of convergence open



What if we only trained the last layer?



### I-layer Neural Networks





• Note that  $\min_{v} \sum_{i} \left( \langle v, \sigma(Wx_i) \rangle - y_i \right)^2$  is equivalent to  $\min_{v} \|Qv - y\|^2$  where  $Q = \left[ \sigma(Wx_1) \dots \sigma(Wx_n) \right]$ 

### I-layer Neural Networks







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- •Training the last layer is a CONVEX problem! Can always fit perfectly as long as Q is full rank

### I-layer Neural Networks





## Is Q full rank?

- Reminder:  $Q = \left[\sigma(Wx_1) \dots \sigma(Wx_n)\right]$ . Note that  $\bullet$  $[QQ^T]_{i,i} = \langle \sigma(Wx_i),$
- What would happen if we took the number of parameters to infinity?

$$\frac{1}{k} \sum_{l=1}^{k} \sigma(w_l x_i) \cdot \sigma(w_l x_l)$$

Theorem (Du et al):

at rank(Q) = rank(QQ<sup>T</sup>) and that  

$$\sigma(Wx_j) \rangle = \sum_{l=1}^k \sigma(w_l x_l) \cdot \sigma(w_l x_j)$$

$$(x_j) \longrightarrow E_w[\sigma(wx_i) \cdot \sigma(wx_j)] = K_{i,j}^\infty$$

For ReLu networks  $K^{\infty}$  is full-rank as long as two input points are not parallel. Moreover,  $K^p$  is very close to  $K^{\infty}$  (hence similar spectral properties) for polynomial overparameterization.





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- Training the last layer is a CONVEX problem! Can always fit perfectly as long as Q is full rank (true for large enough overparameterization and full rank inputs)

Training the last layer, not very interesting? Seems that it doesn't capture much of the non-convex nature of DL?

### I-layer Neural Networks





## L-layer Neural Networks

Let us assume we have a 1-layer linear network



- •Note that  $\min_{v} \sum_{i} \left( \langle v, h(W; x) \rangle y_i \right)^2$  is equivalent to  $\min_{v} \|Qv y\|^2$  where  $Q = \left[ h(w; x_1) \dots h(w; x_n) \right]$
- Training the last layer is a CONVEX problem no matter how deep the net is!)

Training the last layer, not very interesting? Seems that it doesn't capture much of the non-convex nature of DL?



Assume all but last layers are random



## Back to training all the layers

Many recent works show that if the overparameterization is VERY large, then  $h(w;x) \approx h(w_0;x) + \langle w - w_0, \nabla_w h(w_t;x) \rangle$ 

Many recent works show that if the overparameterization is VERY large, then

dynamics

$$y - h(w_k; X) = (I_n -$$

 $h(w; x) \approx h(w_0; x) + \langle w - w_0, \nabla_w h(w_t; x) \rangle$ 

Specifically, the network behaves like a linear classifier and the residual error follows the following

 $\gamma G(k))(y - h(w_k; X))$ 

- Many recent works show that if the overparameterization is VERY large, then
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Specifically, the network behaves like a linear classifier and the residual error follows the following

 $y - h(w_k; X) = (I_n - \gamma G(k))(y - h(w_k; X))$ 

- Many recent works show that if the overparameterization is VERY large, then
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- where  $G(k) = J(w_k)^T J(w_k)$
- When the overparameterization is large then  $||G(k) G(0)|| < \epsilon$ .

 $h(w;x) \approx h(w_0;x) + \langle w - w_0, \nabla_w h(w_t;x) \rangle$ 

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- Many recent works show that if the overparameterization is VERY large, then
- dynamics
- where  $G(k) = J(w_k)^T J(w_k)$
- When the overparameterization is large then  $||G(k) G(0)|| < \epsilon$ .
- Moreover G(0) is shown to have a non-zero minimum eigenvalue, so that

 $h(w;x) \approx h(w_0;x) + \langle w - w_0, \nabla_w h(w_t;x) \rangle$ 

Specifically, the network behaves like a linear classifier and the residual error follows the following

 $y - h(w_k; X) = (I_n - \gamma G(k))(y - h(w_k; X))$ 

 $\|y - h(w_k; X)\| \lesssim (1 - \gamma \lambda_p)^k \|y - h(w_k; X)\|$ 

### Theorem (Du et al): 2) 3)

### For width = O(poly(n)) then the NNs+squared loss = PL close to init

For width = O(poly(n)) then the loss function becomes PL around the initial set of weights. GD doesn't move far from init even if run for ever. OPT is close to int GD converges in poly-time to OPT.



Current theoretical SOTA

### **Subquadratic Overparameterization for Shallow Neural Networks**



**Thomas Pethick**<sup>1</sup>

### something odd.

CLL=convex and Lipschitz loss, SD=separable data. Depth Algorithm Setting Activ Re GD on layer 1 2 QL Re GD on layer LLCLL Re SD 2 GD SD and QL Re 2 GD LGD SD and QL Re QL GD Sm 2

Ali Ramezani-Kebrya<sup>1\*</sup>

Armin Eftekhari<sup>2†</sup>

Volkan Cevher<sup>1</sup>

Table 1: Scaling with the number of training data in the overparameterization regime. QL=quadratic loss,

vation	Scaling	Reference
eLU	$ ilde{\Omega}(n^2)$	Oymak and Soltanolkotabi [38]
eLU	$ ilde{\Omega}(n)$	Kawaguchi and Huang [21]
eLU	$ ilde{\Omega}(n^2)$	Song and Yang [39]
eLU	$ ilde{\Omega}(n^6)$	Du et al. [12]
eLU	$\Omega(n^8L^{12})$	Zou and Gu [44]
nooth	$ ilde{\Omega}(n^{rac{3}{2}})$	This paper

A curious observation on fitting the data

### **Small ReLU networks are powerful memorizers:** a tight analysis of memorization capacity

**Chulhee Yun** MIT Cambridge, MA 02139 chulheey@mit.edu

Suvrit Sra MIT

Cambridge, MA 02139 suvrit@mit.edu

Theorem:

Any data set of size n can be memorized by a 3-layer ReLU neural network with O(n) weights.

### These constructions can be made in linear time. Yet SGD on the same arch needs so much more larger overarm. Why??

Ali Jadbabaie MIT Cambridge, MA 02139 jadbabai@mit.edu

But somehow SGD does more than just that...

### Rethinking Generalization [Zhang et al. ICLR17]



Figure 1: Fitting random labels and random pixels on CIFAR10. (a) shows the training loss of various experiment settings decaying with the training steps. (b) shows the relative convergence time with different label corruption ratio. (c) shows the test error (also the generalization error since training error is 0) under different label corruptions.

Overparameterized, SGD-trained models :
I. Can fit even completely random labels (
2. Yet, generalize well

### Open Question: How can this be?

- Maybe every model that fits the training data generalizes (no bad global minima)
- Maybe SGD "can avoid" bad global minima (implicit regularization)?



### Possible Explanations

More on this next time.

### Open Problem for projects

- Understanding the effects of overparameterization
- Deep vs wide networks (width helps in theory, depth in practice).
- Understanding when/if memorization hurts

# reading list

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