Neural Tangent Kernels (+ etc) CPSC 532S: Modern Statistical Learning Theory 23 March 2022 cs.ubc.ca/~dsuth/532S/22/

Admin

- - Whole assignment now due **Monday**
- A4 will be posted soon, due Friday the 8th (last day of term)
 - Yes, the same day as the project report; usual late policy
- Project scope:
 - I'm just looking for signs that you've read and understood the papers
 - If you're doing a lit review: ~3-4 papers is the expected amount
 - Talk about how the settings / conclusions relate to each other, what they leave open, etc
 - about when they hold / don't

• A3 Q1 is broken, to be replaced (with something as similar as possible) tonight

An "extension" can absolutely just be poking at the assumptions and talking

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- What's the optimization error for SGD/similar?

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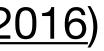
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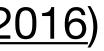
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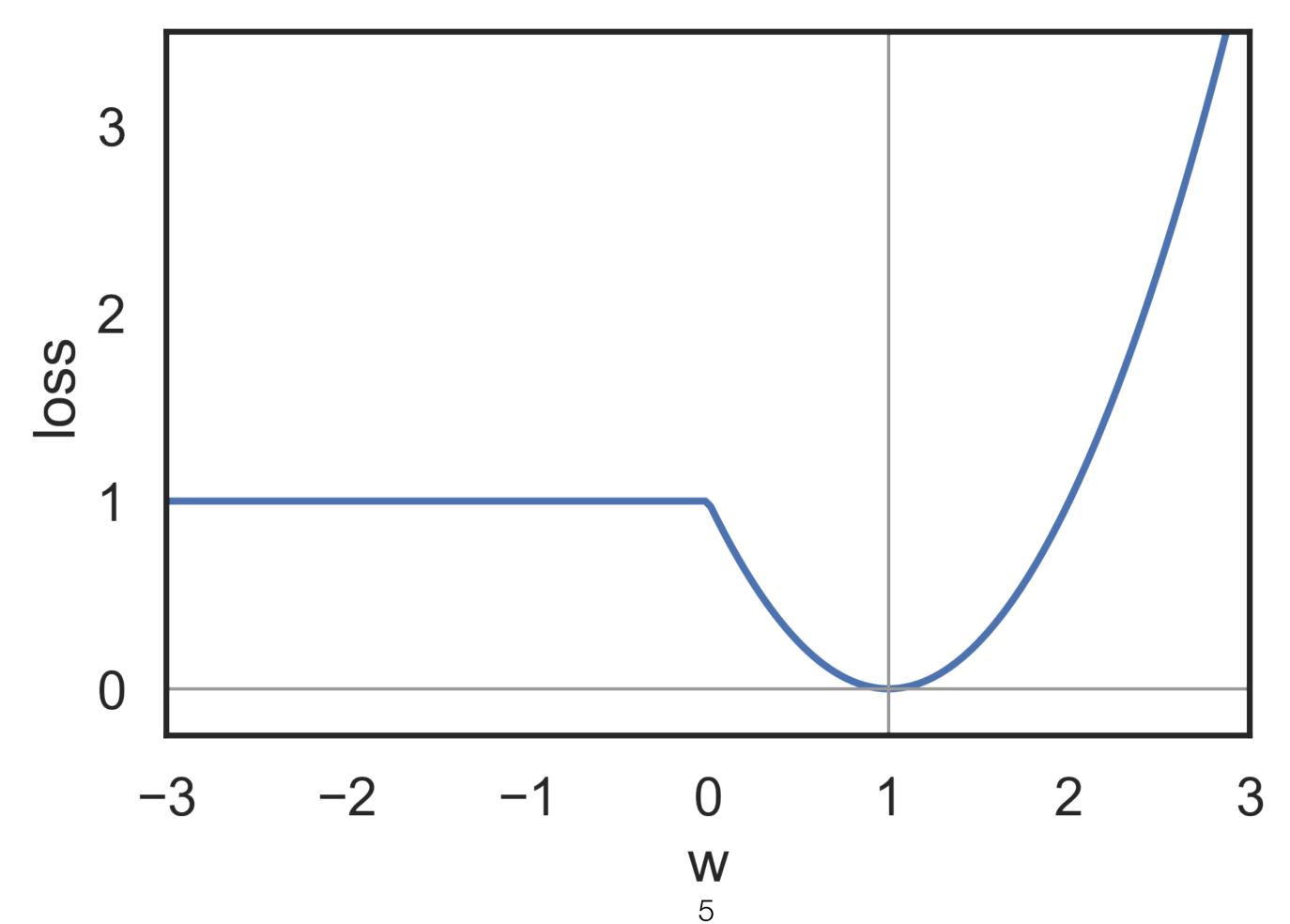


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Bad local minima in ReLU nets

 $h(x) = \operatorname{ReLU}(wx)$ (reals to reals), square loss, S = ((1,1)):



Sub-Optimal Local Minima Exist for Neural Networks with Almost All Non-Linear Activations

Tian Ding* Dawei Li[†] Ruoyu Sun [‡]

Nov 4, 2019

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- Implicit in these papers:
 - neural tangent kernel

• Behaviour of deep nets converges to kernel ridge regression with the



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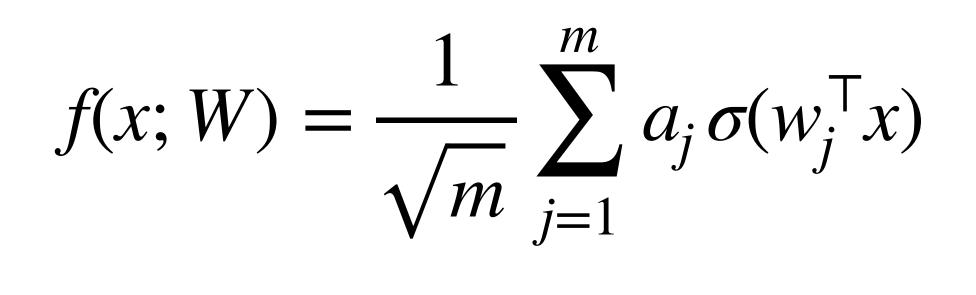
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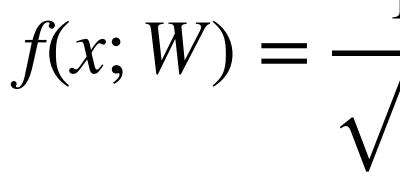
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 - Approximates behaviour of f as we change W; nonlinear in x• We'll see that, for large *m* and random $W_0, f \approx f_{W_0}$ through training



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= 0 for ReLU

 $= \frac{1}{\sqrt{m}} \sum_{i=1}^{m} a_{i} \left(\left[\sigma(w_{0,j}^{\mathsf{T}} x) - \sigma'(w_{0,j}) w_{0,j}^{\mathsf{T}} x \right] + \sigma'(w_{0,j}) w_{j}^{\mathsf{T}} x \right)$

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We'll see shortly that $f - f_0$ shrinks as *m* grows

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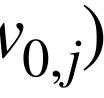
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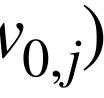


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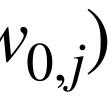


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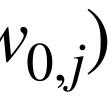
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$$\leq \frac{1}{\sqrt{m}} \sum_{j=1}^{m} \frac{1}{2} \beta (w_j^{\mathsf{T}} x - w_{0,j}^{\mathsf{T}} x)^2$$

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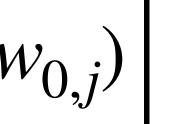
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 $|\sigma(r) - \sigma(s) - \sigma'(s)(r-s)|$

$$\begin{split} \left| f(x;W) - f_{W_0}(x;W) \right| &\leq \frac{1}{\sqrt{m}} \sum_{j=1}^m |a_j| \left| \sigma(w_j^\top x) - \sigma(w_{0,j}^\top x$$

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$$\begin{aligned} |\sigma(r) - \sigma(s) - \sigma'(s)(r-s)| &= \left| \int_{r}^{s} \sigma''(z)(s-z) dz \right| \le \frac{\beta}{2} (r-s)^{2} \\ \left| f(x;W) - f_{W_{0}}(x;W) \right| \le \frac{1}{\sqrt{m}} \sum_{j=1}^{m} |a_{j}| \left| \sigma(w_{j}^{\top}x) - \sigma(w_{0,j}^{\top}x) - \sigma'(w_{0,j}^{\top}x)x^{\top}(w_{j}-w_{0,j}^{\top}x) + \frac{1}{2\sqrt{m}} \sum_{j=1}^{m} \frac{1}{2} \beta(w_{j}^{\top}x - w_{0,j}^{\top}x)^{2} \le \frac{\beta}{2\sqrt{m}} \sum_{j=1}^{m} ||w_{j} - w_{0,j}||^{2} ||x||^{2} \le \frac{\beta}{2\sqrt{m}} ||W - W_{0,j}||^{2} ||W - W_{0,j}||W - W_{0,j}||W - W_{0,j}||^{2} ||W - W_{0,j}||W -$$

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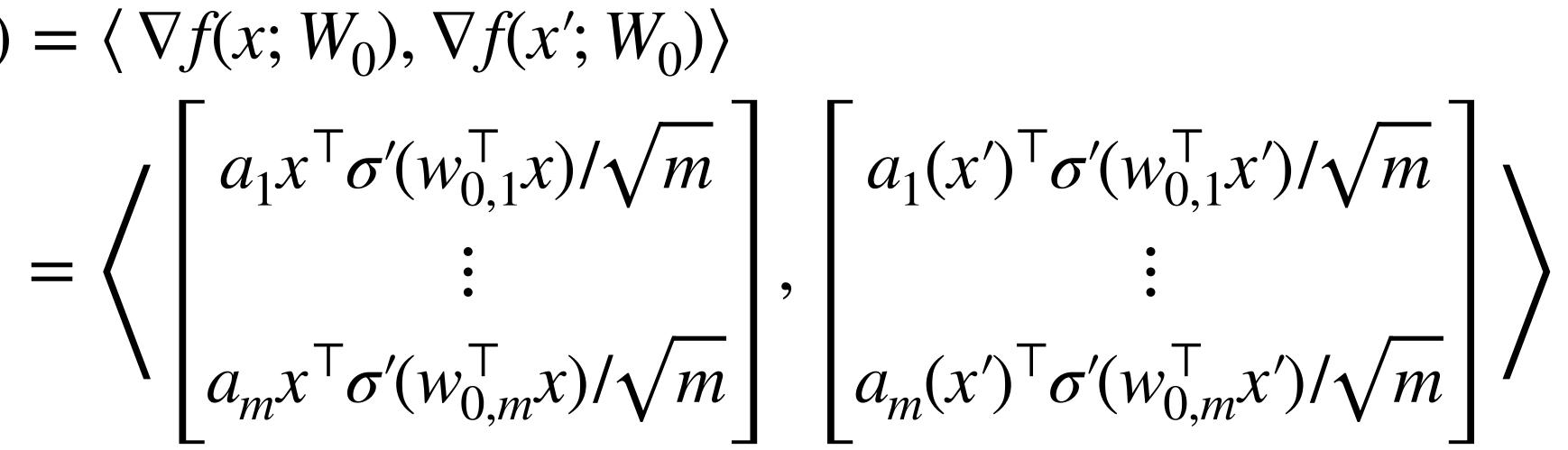
Can do multi-layer versions, but approximation degrades with depth

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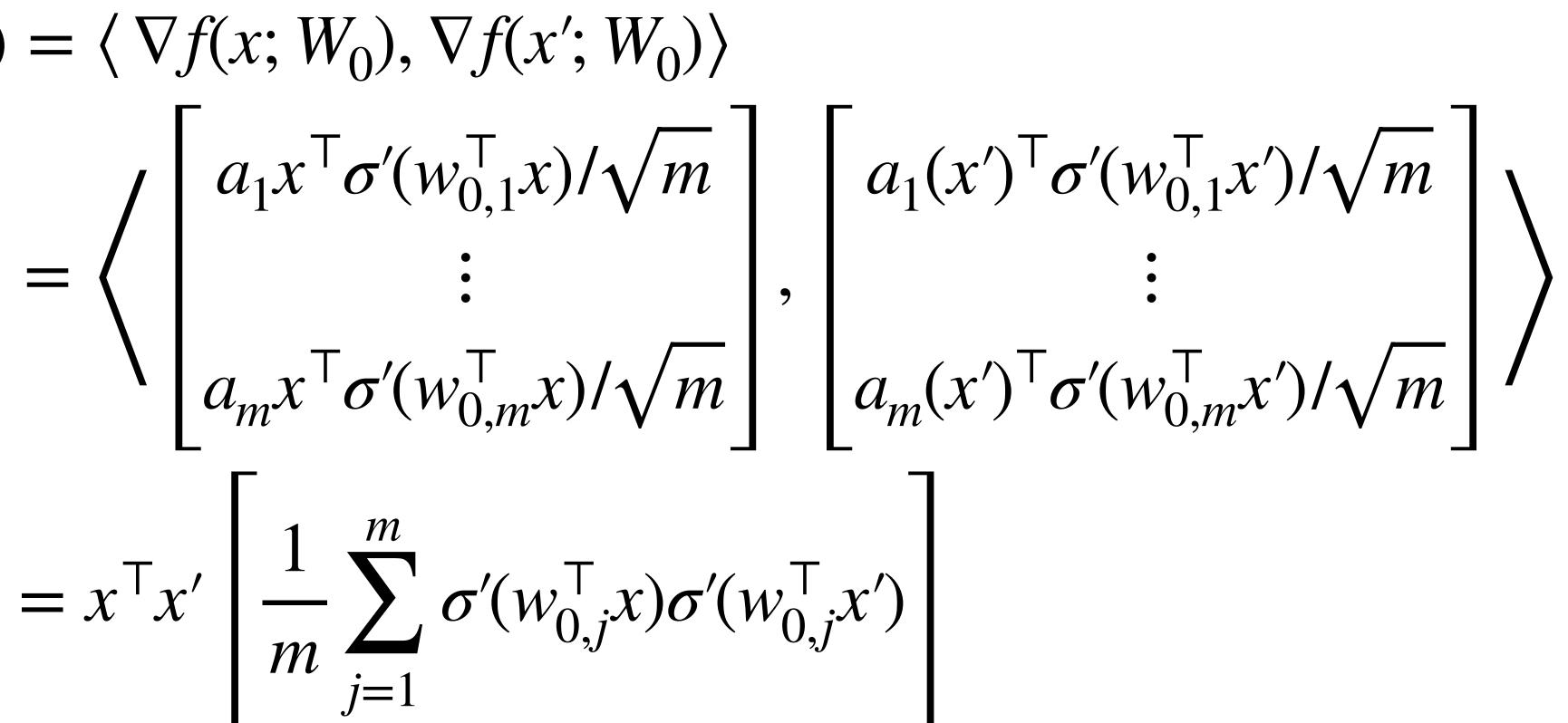
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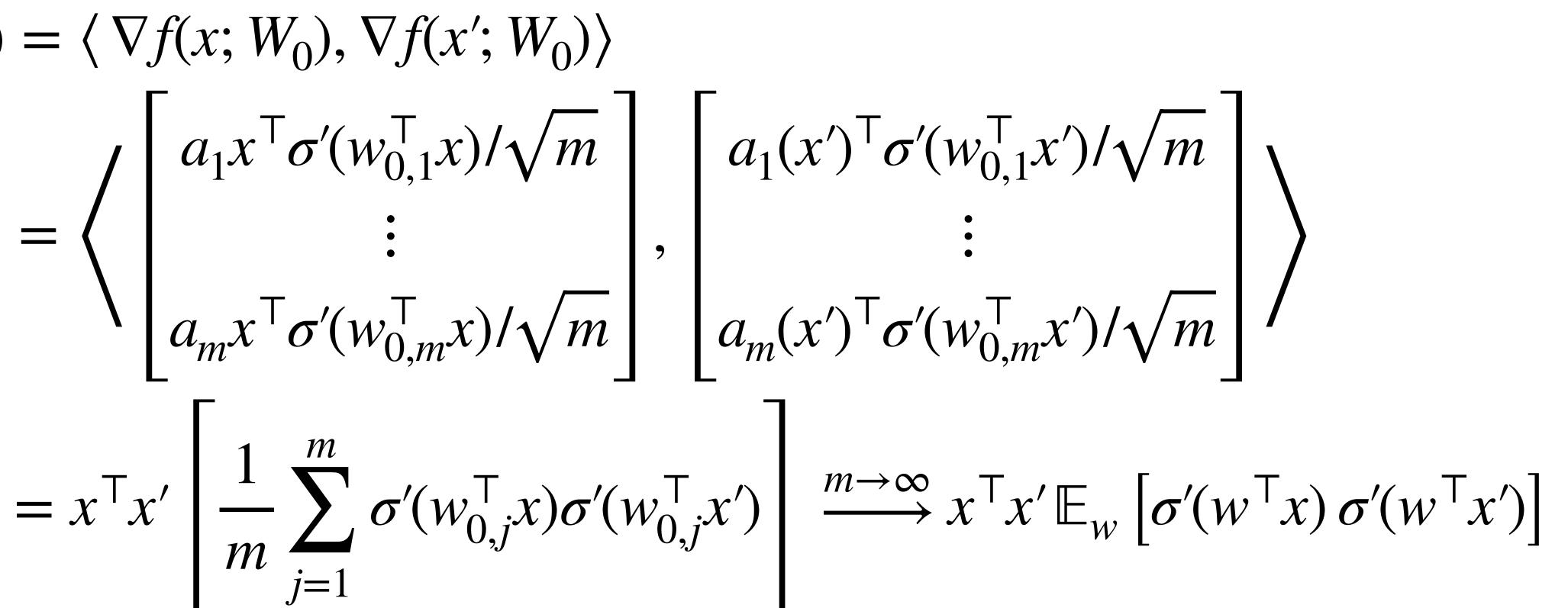
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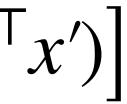


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arccos kernel

For $||x|| = 1 = ||x'||, \mathbb{E}_w[\sigma'(w^{\top}x)\sigma'(w^{\top}x')] = \frac{1}{2} - \frac{1}{2\pi} \arccos(x^{\top}x'):$

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This kernel is universal on $\{x \in \mathbb{R}^{d+1} : ||x|| = 1, x_{d+1} = 1/\sqrt{2}\}$

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 - Training f for square loss \approx kernel ridge regression with k

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If $k_{SS}^{(w_t)} = k_{SS}$ is constant over time, exact same dynamics as kernel (ridgeless) regression

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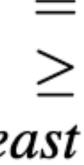
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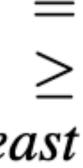
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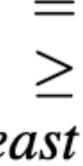
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- gradients are close throughout training => final result is close
- Scales network so that initialization has $f_S \approx 0$

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 - Proof actually needs infinite width but only really shows for finite time t



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- Telgarsky section 8 gives a simplified proof, but it's a little bit WIP

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• AFAIK, the main (only?) proofs that GD optimizes deep networks reasonably

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 - Can be practically useful in some settings

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• AFAIK, the main (only?) proofs that GD optimizes deep networks reasonably

• No.

- Real neural net optimization isn't in "the NTK regime" • NTK regime doesn't allow for feature learning – the kernel doesn't change... There are problems where NNs provably do better than any kernel method
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 - AFAIK, the main (only?) proofs that GD optimizes deep networks reasonably • Can be practically useful in some settings
 - Probably a building block for whatever comes next