Neural Tangent Kernels

CPSC 532D: Modern Statistical Learning Theory

30 ~~28~~ November 2022

cs.ubc.ca/~dsuth/532D/22w1/

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:
  - Behaviour of deep nets converges to kernel ridge regression with the **neural tangent kernel**

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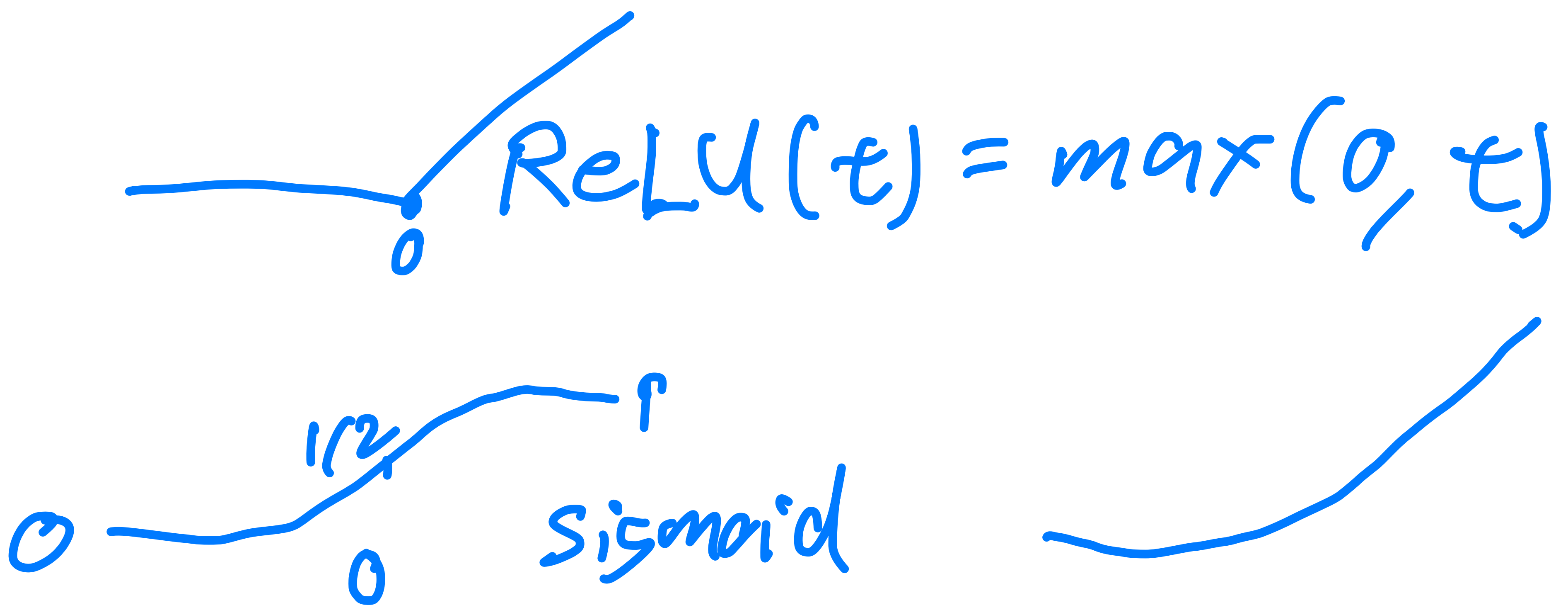

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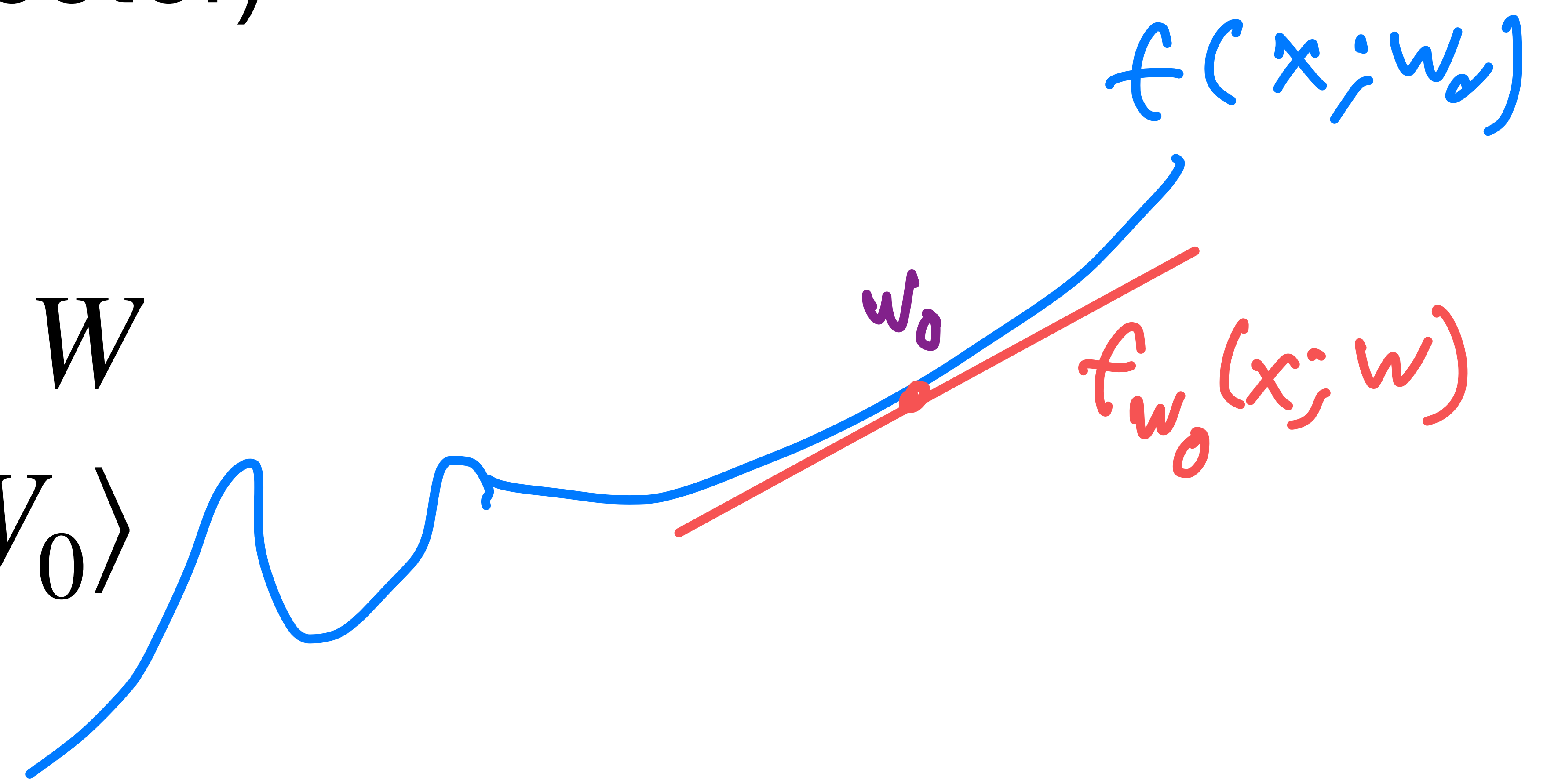

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  - We'll see that, for large m and random W_0, $f \approx f_{W_0}$ through training

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\end{aligned}$$

$\mathrm{ReLU}(t) = \max(0,t)$

$= t\,\mathbb{1}(t>0)$

$\mathrm{ReLU}'(t) = \begin{cases} 1 & \text{if } t>0 \\ 0 & \text{if } t\leq 0 \end{cases}$

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We'll see shortly that $f - f_{W_0}$ *shrinks* as m grows

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Linearization quality

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

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$$= x^\top x' \left[\frac{1}{m} \sum_{j=1}^{m} a_j^2 \sigma'(w_{0,j}^\top x) \sigma'(w_{0,j}^\top x') \right] \xrightarrow{m \to \infty} x^\top x' \, \mathbb{E}_w \left[\sigma'(w^\top x) \, \sigma'(w^\top x') \right]$$

if $|a_j| = 1$

arccos kernel

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

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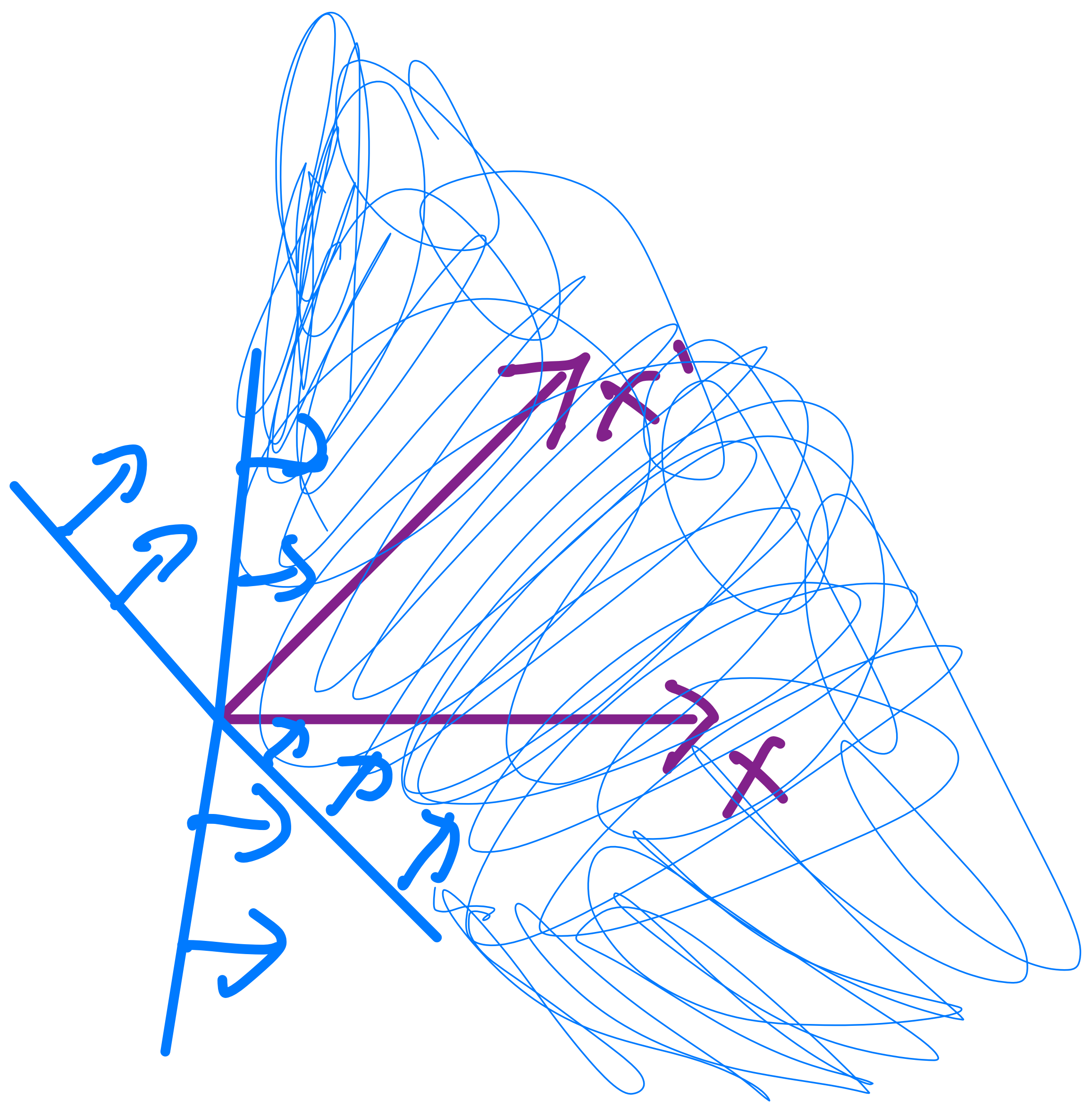

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This kernel is universal on $\{x \in \mathbb{R}^{d+1} : \|x\| = 1,\, x_{d+1} = 1/\sqrt{2}\}$

Non-ReLU, multi-layer version

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- The big remaining result:
  - Training f for square loss $\approx$ kernel ridge(less) 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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- 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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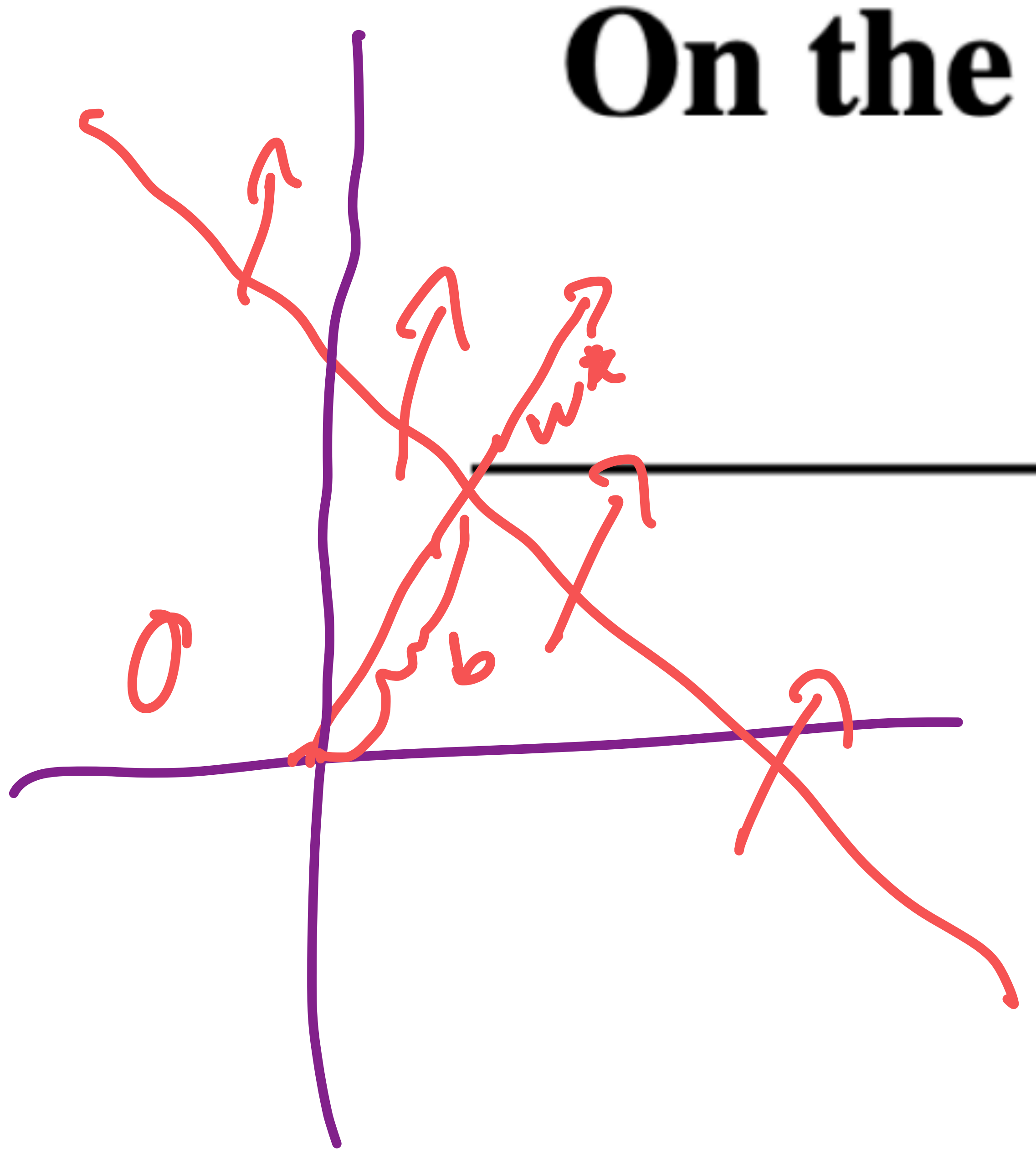
  - Can be practically useful in some settings
  - Probably a building block for whatever comes next



On the Power and Limitations of Random Features for Understanding Neural Networks

Gilad Yehudai **Ohad Shamir**
Weizmann Institute of Science
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- Roughly: there is a $w^* \in \mathbb{R}^d$ with $\|w^*\| = d^2$, $b^* \in \mathbb{R}$ s.t.
  - if $\mathbb{E}_{x \sim \mathcal{N}(0,I)}\left[(f(x) - \mathbf{ReLU}(\langle w^*, x\rangle + b^*))^2\right] \leq \frac{1}{50}$,
  - then $\|f\|_{\mathrm{NTK}} \geq \exp(\Omega(d))$
- and if f's init is isotropic, true for any w^* with $\|w^*\| = d^2$
- But GD learns this (at linear rate) with $\mathbf{poly}(d)$ samples

for $x \sim \mathcal{N}(0,I)$
$y = \mathrm{ReLU}(\langle w^*, x\rangle + b^*)$
$L_D^{sq}(f) =$

Quantifying the Benefit of Using Differentiable Learning over Tangent Kernels

Eran Malach Hebrew University of Jerusalem eran.malach@mail.huji.ac.il
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Nathan Srebro Toyota Technological Institute at Chicago nati@ttic.edu
Collaboration on the Theoretical Foundations of Deep Learning (deepfoundations.ai)

<table>
<tr><th colspan="2"></th><th>NTK at same Initialization</th><th>NTK at alternate randomized Initialization</th><th>NTK of arbitrary model or even an arbitrary Kernel</th></tr>
<tr><td colspan="2">GD with unbiased initialization ($\forall_x f_{\theta_0}(x) = 0$) ensures small error</td><td>▸ NTK edge $\geq \text{poly}^{-1}$ (Thm. 1)
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</table>

Making Look-Ahead Active Learning Strategies Feasible with Neural Tangent Kernels

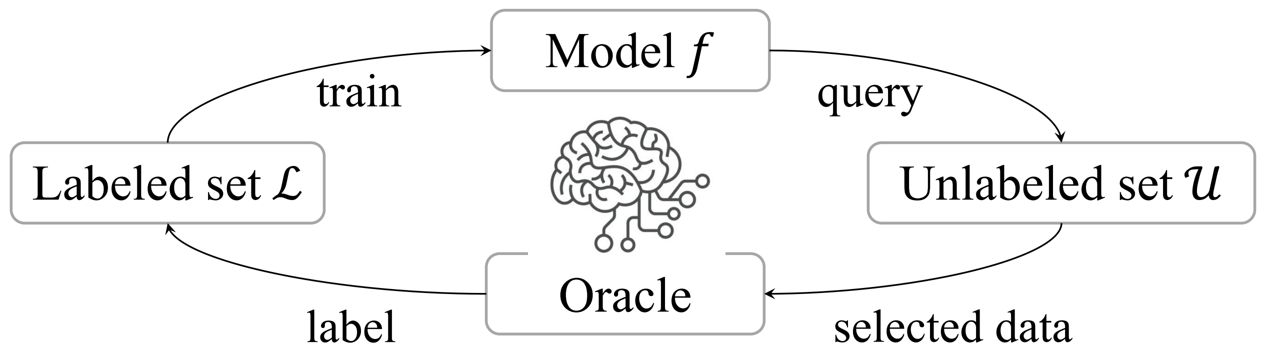
Mohamad Amin Mohamad*, Wonho Bae*, Danica J. Sutherland

Virtual Github ArXiv

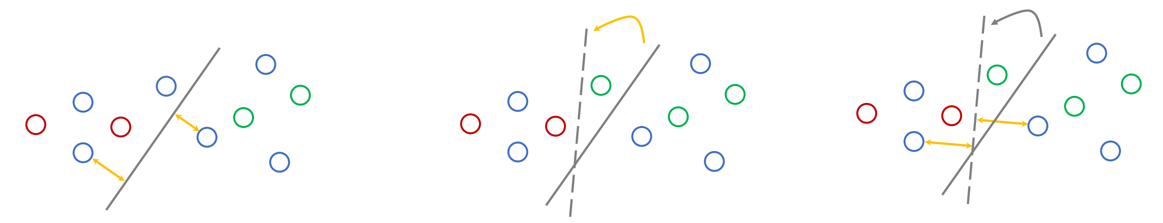
Overview

- Look-ahead active learning strategies: "what would my model do if I saw this label for this point"?
- Too expensive for neural nets
  …unless you use an NTK approximation!
- Outperform existing look-ahead strategies and matches/beats SOTA in pool-based active learning

Preliminary: Active Learning



Acquisition Functions – Selection of Data



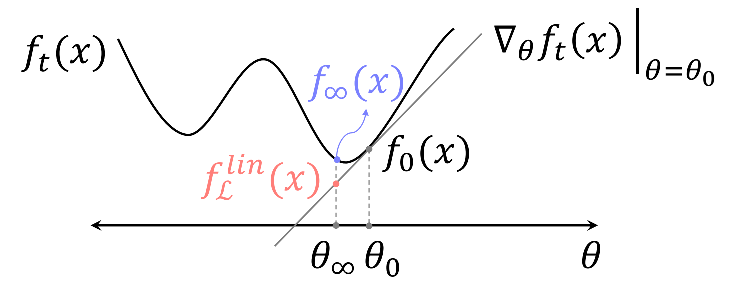
➜ Only look-ahead strategies consider the interaction of the updated model on unseen data [1]

Problems of Look-Ahead Strategies

- Measure the relationship between $f_{\mathcal{L}}$ and $f_{\mathcal{L}^+}$
  e.g. L2-distance: $\|f_{\mathcal{L}}(x) - f_{\mathcal{L}^+}(x)\|_2$
  where $\mathcal{L}^+ = \mathcal{L} \cup \{(x_i, y_i)\}$ with a candidate data (x_i, y_i)
- Infeasible to compute $f_{\mathcal{L}^+}$ for every candidate $(x_i, y_i) \in \mathcal{U}$
- Only special model classes have been available,
  e.g. Naïve Bayes, Gaussian Processes

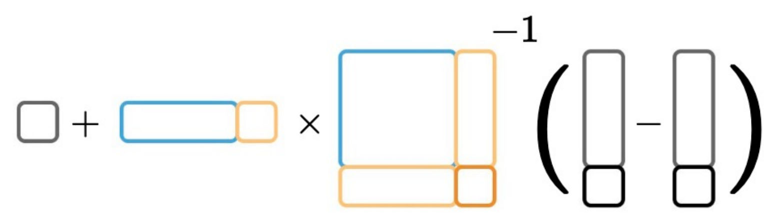
➜ Can we make it feasible for neural networks?

Local Approximation of Functions



- Approx. of $f_\infty(x)$ (trained for $t \to \infty$) in a closed form [2],
  $$f_{\mathcal{L}}^{lin}(x) = f_0(x) + \Theta_0(x, \mathcal{X})\Theta_0(\mathcal{X}, \mathcal{X})^{-1}(\mathcal{Y} - f_0(\mathcal{X}))$$
- Bounded as $\sup_t \left\| f_t(x) - f_t^{lin}(x) \right\|_2 = \mathcal{O}\left(\frac{1}{\sqrt{width}}\right)$

NTK Approx. for Look-Ahead Strategies

- For any Look-Ahead strategies e.g. Most Likely Model Output Change (MLMOC),
  $$A_{MLMOC} = \sum_{x \in \mathcal{U}} \|f_{\mathcal{L}}(x) - f_{\mathcal{L}^+}(x)\|_2$$
  approximate $f_{\mathcal{L}^+}(x)$ as,
  $$f_{\mathcal{L}^+}(x) \approx f_{\mathcal{L}^+}^{lin}(x)$$
  $$= f_{\mathcal{L}}(x) + \Theta_{\mathcal{L}}(x, \mathcal{X}^+)\Theta_{\mathcal{L}}(\mathcal{X}^+, \mathcal{X}^+)^{-1}(\mathcal{Y}^+ - f_{\mathcal{L}}(\mathcal{X}^+))$$
- Visually, $f_{\mathcal{L}^+}^{lin}(x) =$ 

➜ Can be computed even faster using block computation

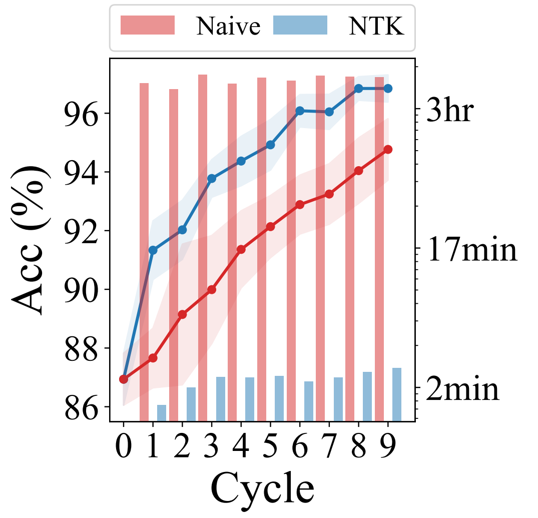
- Approximation of re-training (above) is no more than augmenting kernels, which is justified by **Theorem 3.1**
- (Informal) $S_1 \subseteq S_2 \ldots \subseteq S_C$ denote C datasets. Then, as the width of a network $\to \infty$, $f_{S_C}(x) = f_{S_1, S_2, \ldots, S_C}(x)$

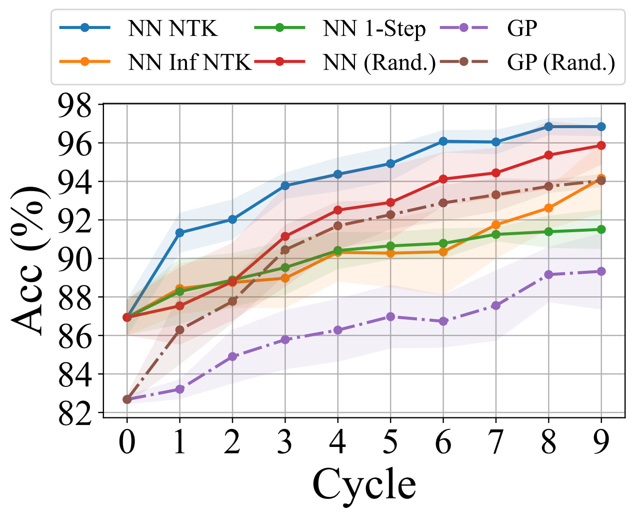
Reference

[1] Freytag et al., Selecting Influential Examples: Active Learning with Expected Model Output Changes, ECCV 2014.

[2] Lee et al., Wide Neural Networks of Any Depth Evolve as Linear Models Under Gradient Descent, NeurIPS 2019.

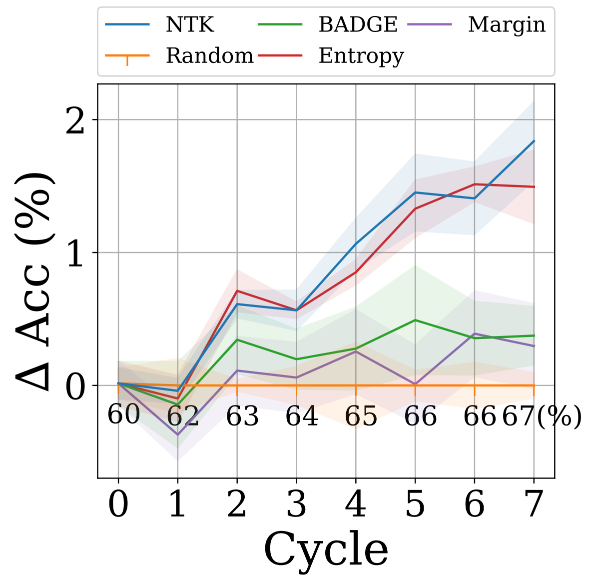
Comparison of Look-Ahead Models



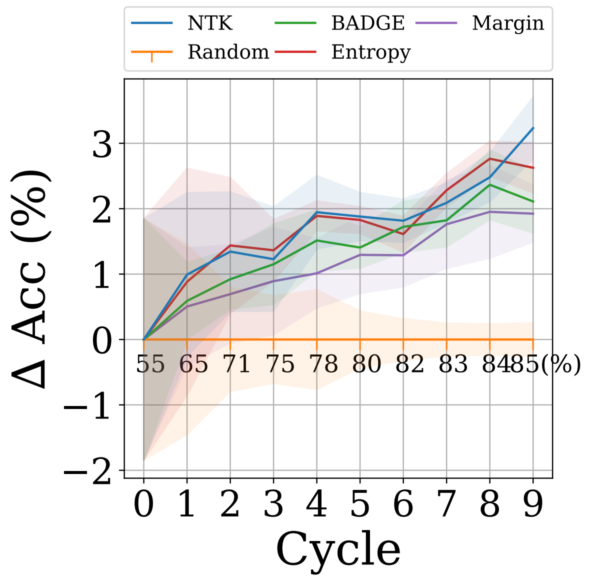


- Performs better and 100 times faster than Naïve
- Outperforms other look-ahead methods – inf. NTK, 1-step approx. of re-training, NTK-based Gaussian Processes

Comparison with State-of-the-art



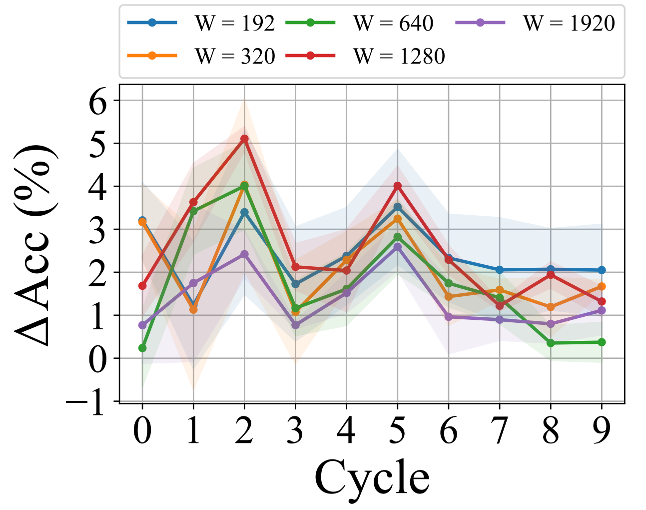
CIFAR10: 2-layer WideResNet



CIFAR100: ResNet18

- Comparable to the SOTA on many datasets including CIFAR10 and 100 with various neural net architectures

Additional Experiments



- Generally robust to the width and look-ahead acquisition functions
- Can be extended to **sequential query strategy** (not available in previous active learning methods)