A Defense of (Empirical) Neural Tangent Kernels

Danica J. Sutherland (she)

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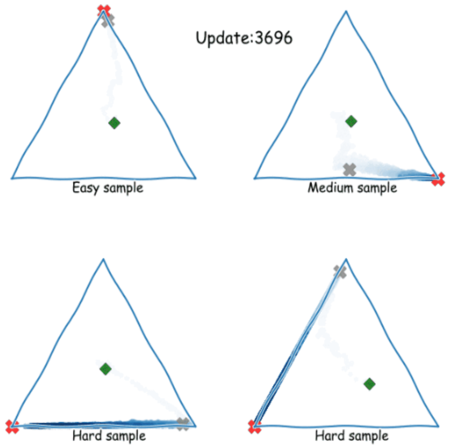
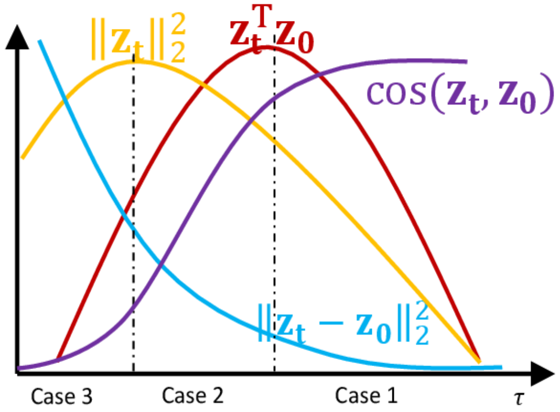
“Zig-zagging” [ICLR-22]



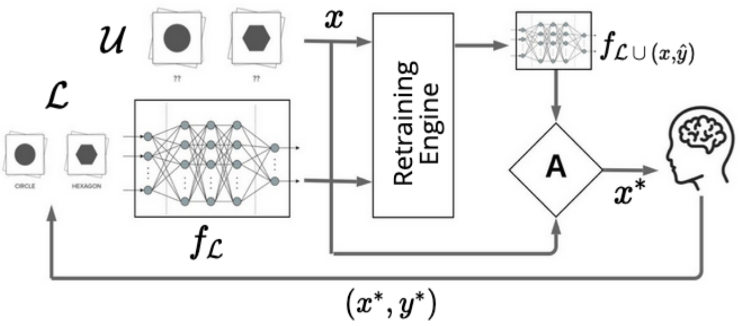
Yi Ren
Shangmin Guo

Finetuning [ICLR-23]



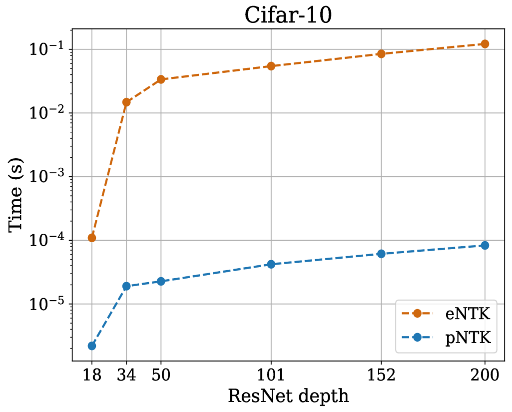
Yi Ren
Shangmin Guo
Wonho Bae

Active learning [NeurIPS-22]



Mohamad Amin Mohamadi
Wonho Bae

Pseudo-NTK [new!]

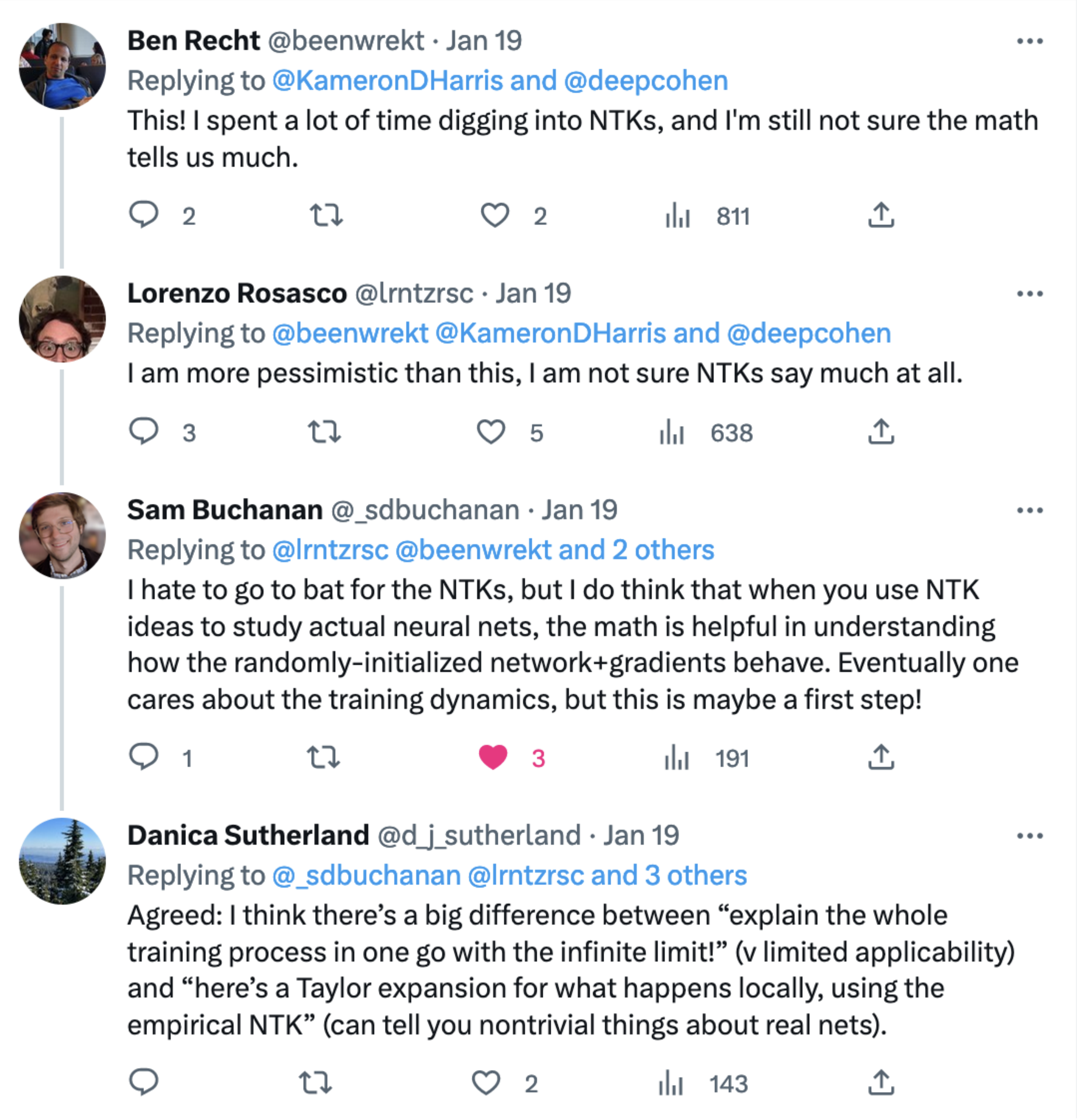


Mohamad Amin Mohamadi
Wonho Bae

University of Michigan AI Seminar - March 23, 2023

HTML version

(A lot of) this talk in a tweet:



Ben Recht @beenwrekt · Jan 19
Replying to @KameronDHarris and @deepcohen
This! I spent a lot of time digging into NTKs, and I'm still not sure the math tells us much.
2 2 811

Lorenzo Rosasco @lrntzrsc · Jan 19
Replying to @beenwrekt @KameronDHarris and @deepcohen
I am more pessimistic than this, I am not sure NTKs say much at all.
3 5 638

Sam Buchanan @_sdbuchanan · Jan 19
Replying to @lrntzrsc @beenwrekt and 2 others
I hate to go to bat for the NTKs, but I do think that when you use NTK ideas to study actual neural nets, the math is helpful in understanding how the randomly-initialized network+gradients behave. Eventually one cares about the training dynamics, but this is maybe a first step!
1 3 191

Danica Sutherland @d_j_sutherland · Jan 19
Replying to @_sdbuchanan @lrntzrsc and 3 others
Agreed: I think there’s a big difference between “explain the whole training process in one go with the infinite limit!” (v limited applicability) and “here’s a Taylor expansion for what happens locally, using the empirical NTK” (can tell you nontrivial things about real nets).
2 143

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- $\ell'_y(\hat{y}) = \hat{y} - y$ for square loss, $\hat{y}_y - \log \sum_{j=1}^{k} \exp(\hat{y}_j)$ for cross-entropy

- Full-batch GD:

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- Observation II: As f becomes "infinitely wide" with any usual architecture+init* [Yang 2019], $\mathrm{eNTK}_{\mathbf{w}_0}(x_1, x_2) \xrightarrow{a.s.} \mathrm{NTK}(x_1, x_2)$, independent of the random $\mathbf{w}_0$

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  - Good results in statistical testing [Jia+ 2021], dataset distillation [Nguyen+ 2021], clustering for active learning batch queries [Holzmüller+ 2022], …

But (infinite) NTKs aren't “the answer”

- Computational expense:
  - Poor scaling for large-data problems: typically n^2 memory and n^2 to n^3 computation
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    - Internal activations in the networks don't change much [Chizat+ 2019] [Yang/Hu 2021]
  - We now know many problems where gradient descent on an NN $\gg$ *any* kernel method
    - Cases where GD error $\to 0$, any kernel is *barely* better than random [Malach+ 2021]

What can we learn from empirical NTKs?

In this talk:

- As a theoretical-ish tool for local understanding:
  - Fine-grained explanation for early stopping in knowledge distillation
  - How you should fine-tune models
- As a practical tool for approximating “lookahead” in active learning
- Plus: efficiently approximating eNTKs for large output dimensions k, with guarantees

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Better supervisory signal implies better learning

- Classification: target is $L_P(f) = \mathbb{E}_{(x,y)}\, \ell_y(f(x)) = \mathbb{E}_x\, \mathbb{E}_{y|x}\, \ell_y(f(x))$

- Normally: see $\{(x_i, y_i)\}$, minimize

$$L(f) = \frac{1}{N} \sum_{i=1}^{N} \ell_{y_i}(f(x_i))$$

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- Potentially better scheme: see $\{(x_i, p_i^{tar})\}$, minimize $L^{tar}(f) = \frac{1}{N}\sum_{i=1}^{N} p_i^{tar} \cdot \vec{\ell}(f(x_i))$

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$$L(f) = \frac{1}{N}\sum_{i=1}^{N} \ell_{y_i}(f(x_i)) = \frac{1}{N}\sum_{i=1}^{N}\sum_{c=1}^{k} \mathbb{I}(y_i = c)\ell_c(f(x_i)) = \frac{1}{N}\sum_{i=1}^{n} e_{y_i} \cdot \vec{\ell}(f(x_i))$$

- Potentially better scheme: see $\{(x_i, p_i^{tar})\}$, minimize $L^{tar}(f) = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} p_i^{tar} \cdot \vec{\ell}(f(x_i))$
  - Can reduce variance if $p_i^{tar} \approx p_i^*$, the true conditional probabilities

Better supervisory signal implies better learning

- Classification: target is $L_P(f) = \mathbb{E}_{(x,y)}\, \ell_y(f(x)) = \mathbb{E}_x\, \mathbb{E}_{y|x}\, \ell_y(f(x))$
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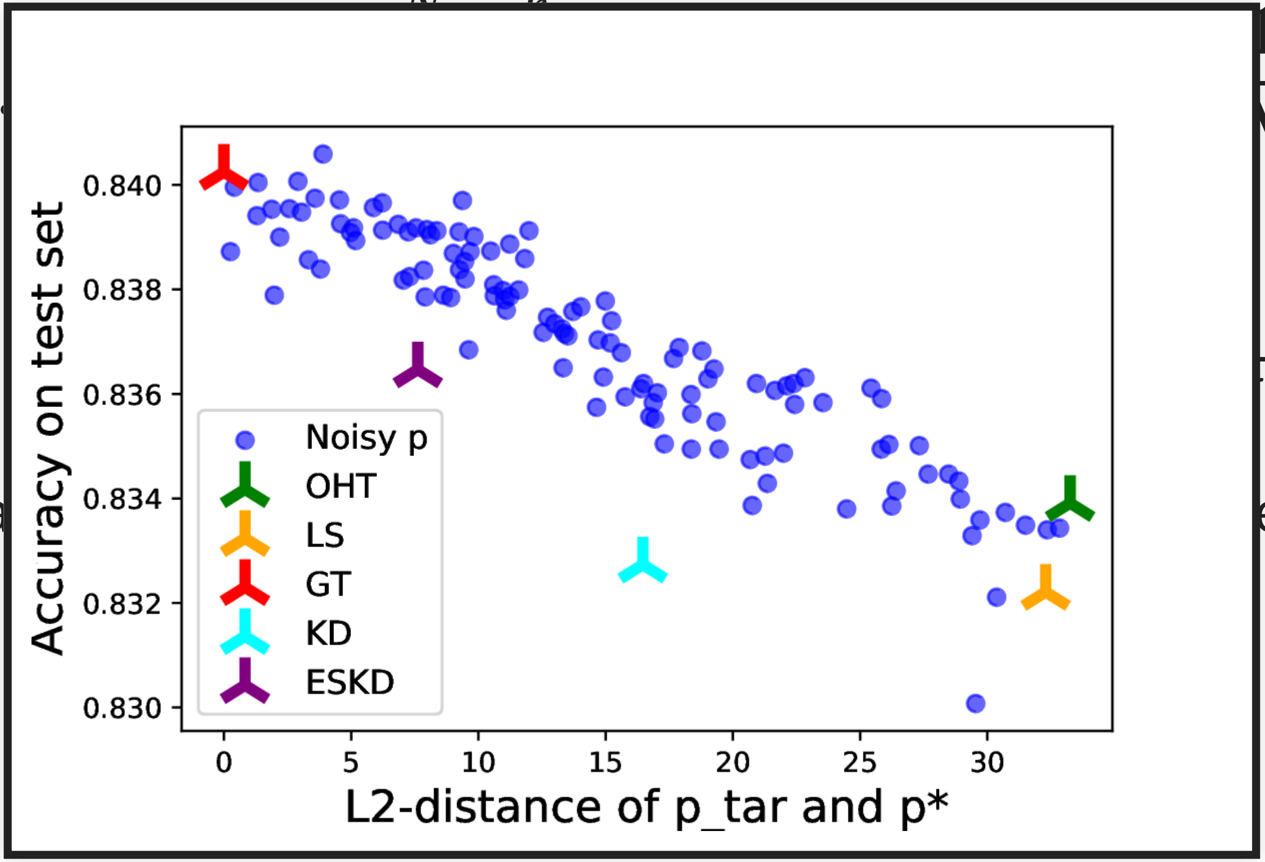

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  - Can reduce varia ... es

Knowledge distillation

- Process:
  - Train a teacher $f^{teacher}$ on $\{(x_i, y_i)\}$ with standard ERM, $L(f)$
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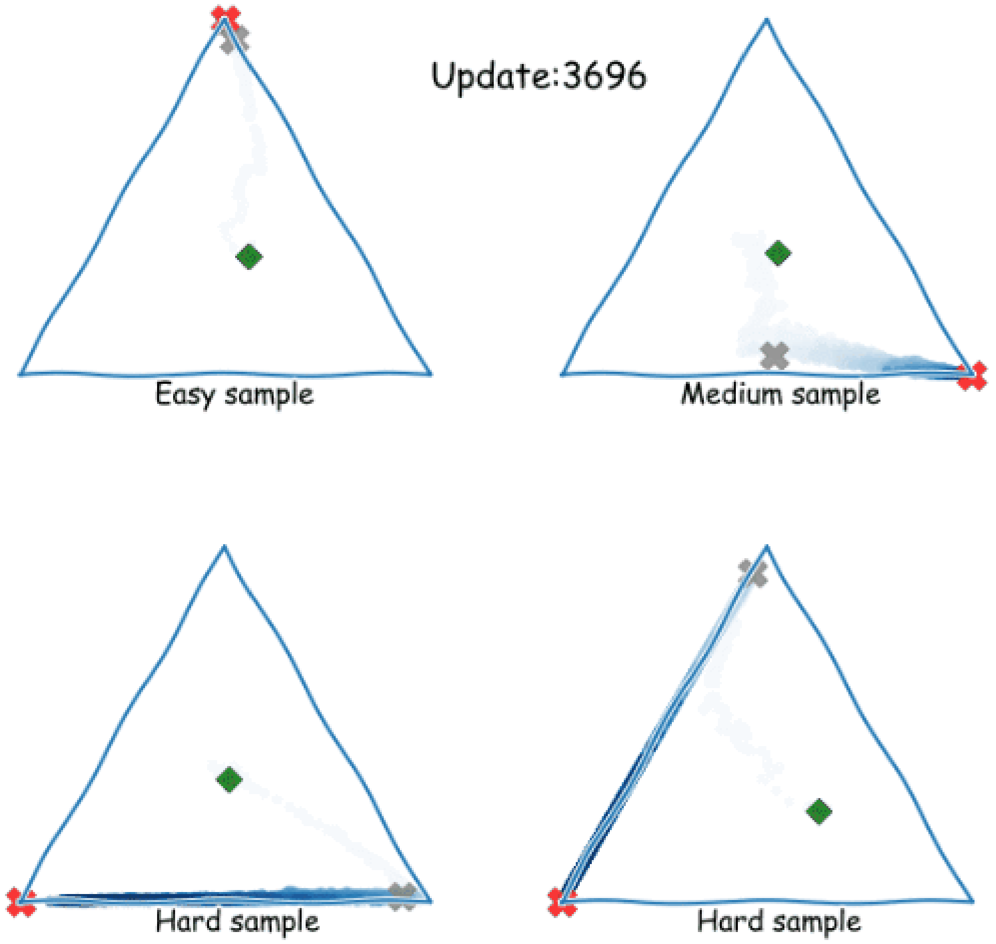
- But why would that be?

Zig-Zagging behaviour in learning



Plots of (three-way) probabilistic predictions: × shows p_i^*, × shows y_i

eNTK explains it

- Let $q_t(\tilde{x}) = \mathrm{softmax}(f_t(\tilde{x})) \in \mathbb{R}^k$; for cross-entropy loss, one SGD step gives us

$$q_{t+1}(\tilde{x}) - q_t(\tilde{x}) = \eta\, \mathcal{A}_t(\tilde{x})\ \mathrm{eNTK}_{\mathbf{w}_t}(\tilde{x}, x_i)\,(p_i^{tar} - q_t(x_i)) + \mathcal{O}(\eta^2)$$

$\mathcal{A}_t(\tilde{x}) = \mathrm{diag}(q_t(\tilde{x})) - q_t(\tilde{x}) q_t(\tilde{x})^\mathsf{T}$ is the covariance of a $\mathrm{Categorical}(q_t(\tilde{x}))$

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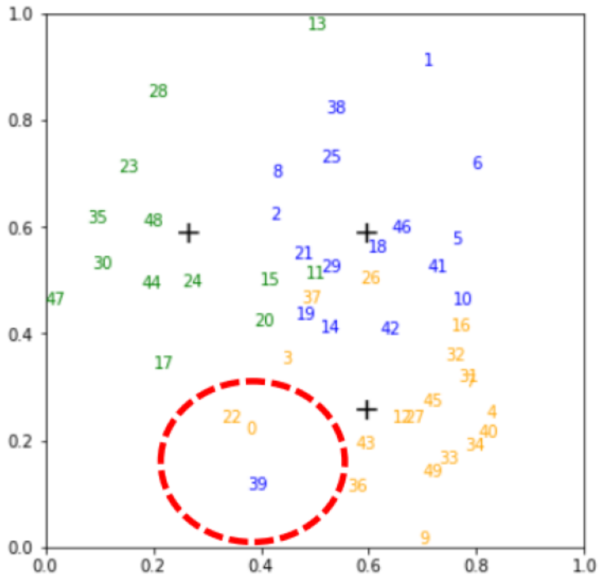

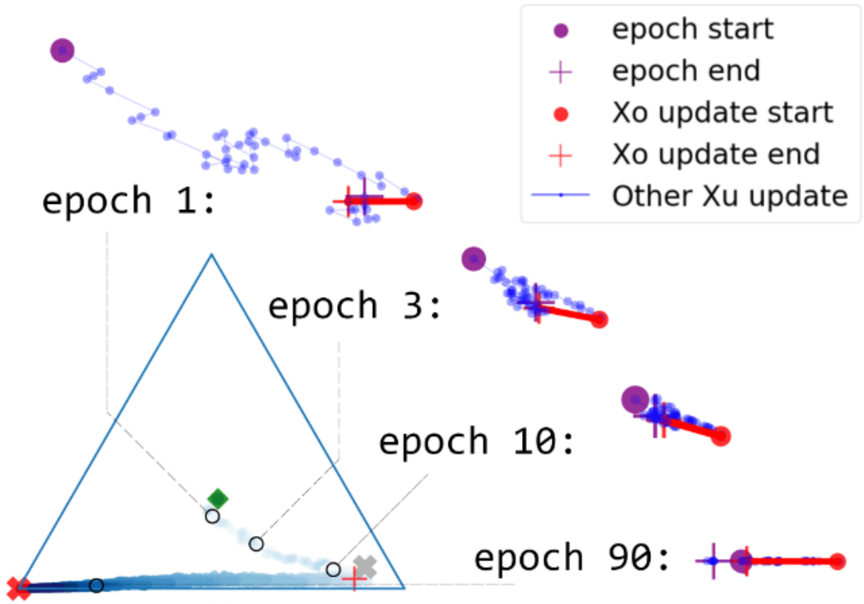

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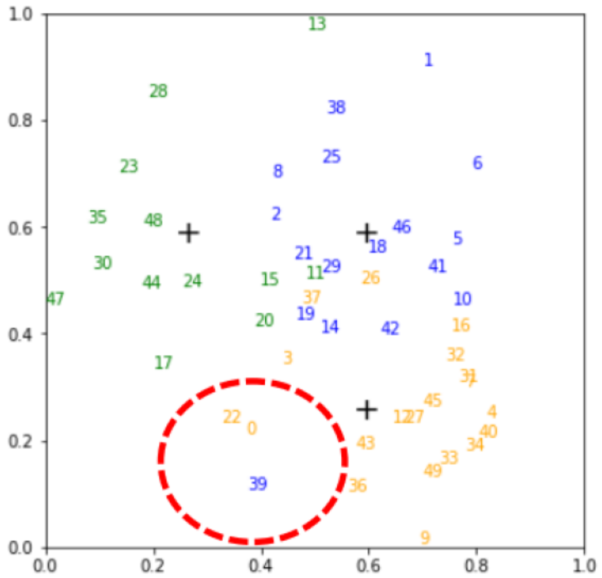

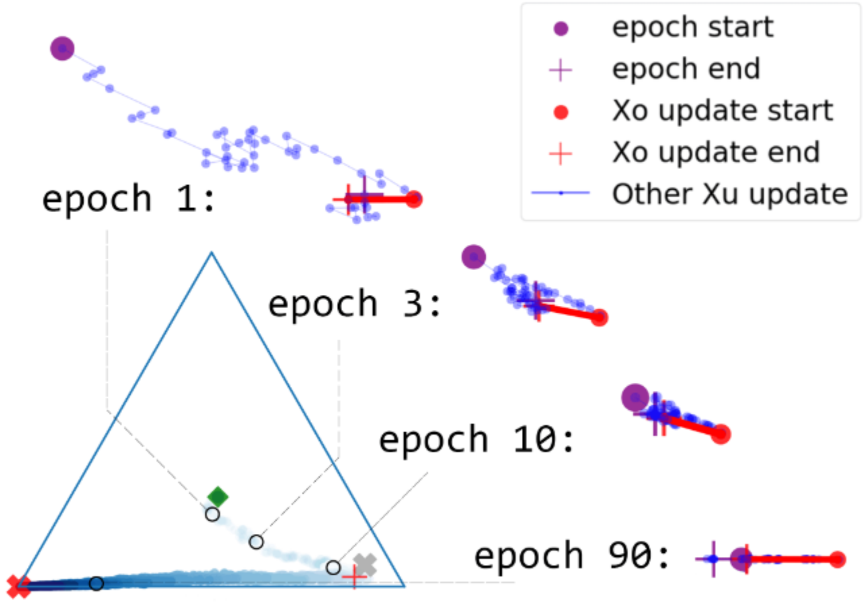

- Improves distillation (esp. with noisy labels) to take moving average of $q_t(x_i)$ as p_i^{tar}

What can we learn from empirical NTKs?

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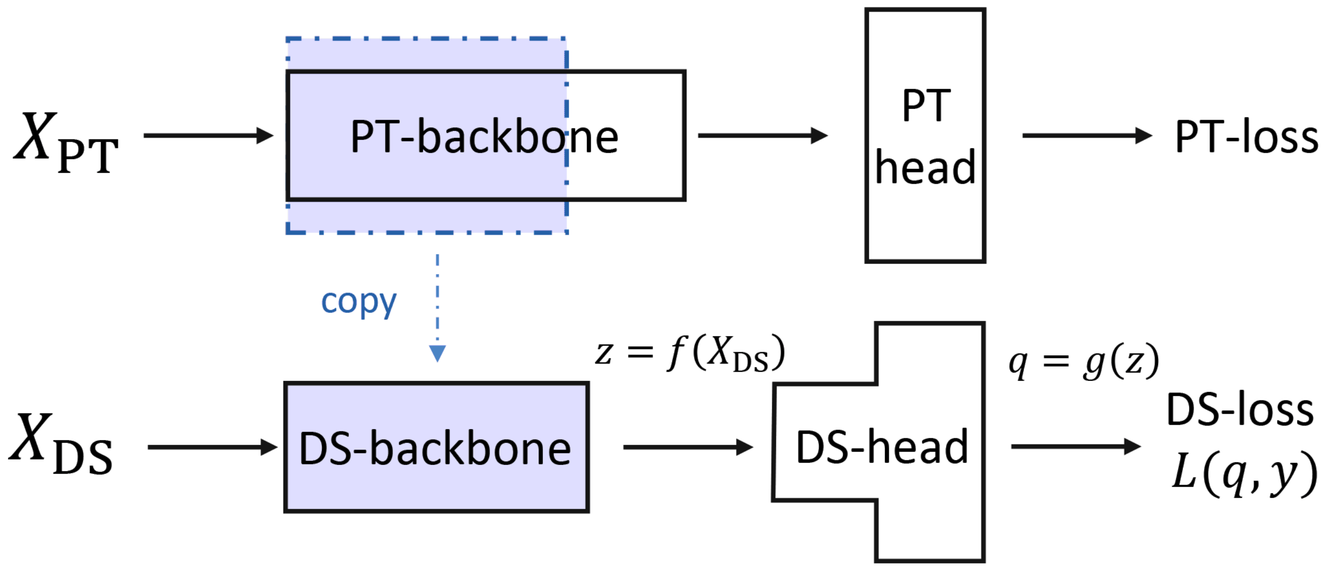
Fine-tuning



- Pretrain, re-initialize a random head, then adapt to a downstream task. Two phases:
  - Head probing: only update the head $g(z)$
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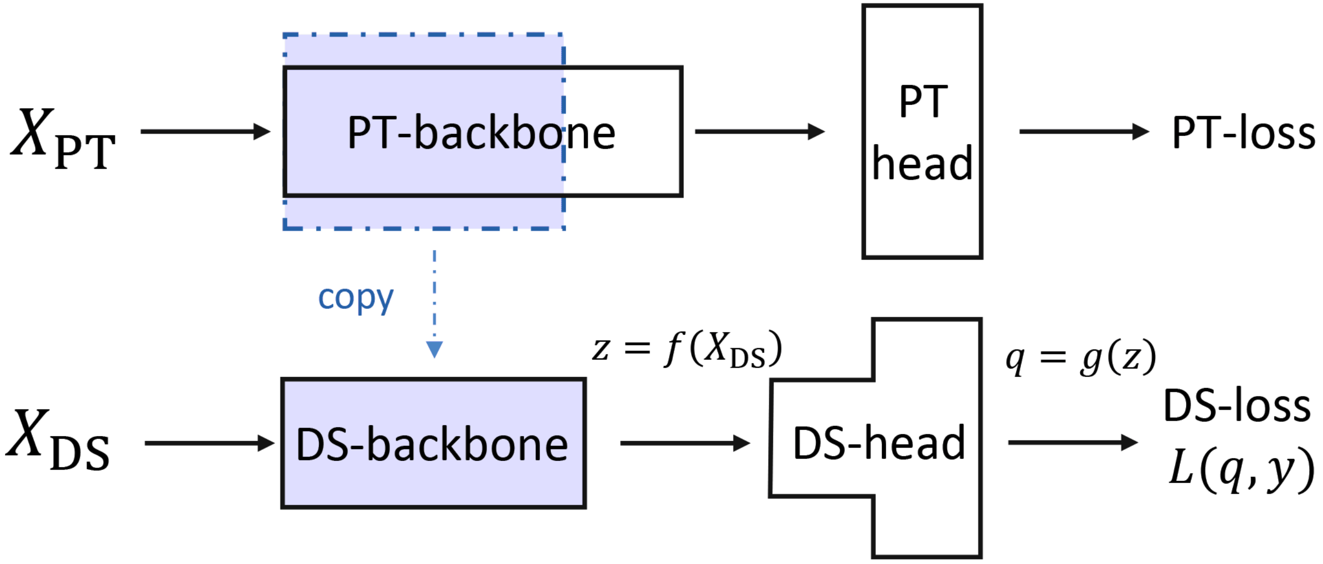

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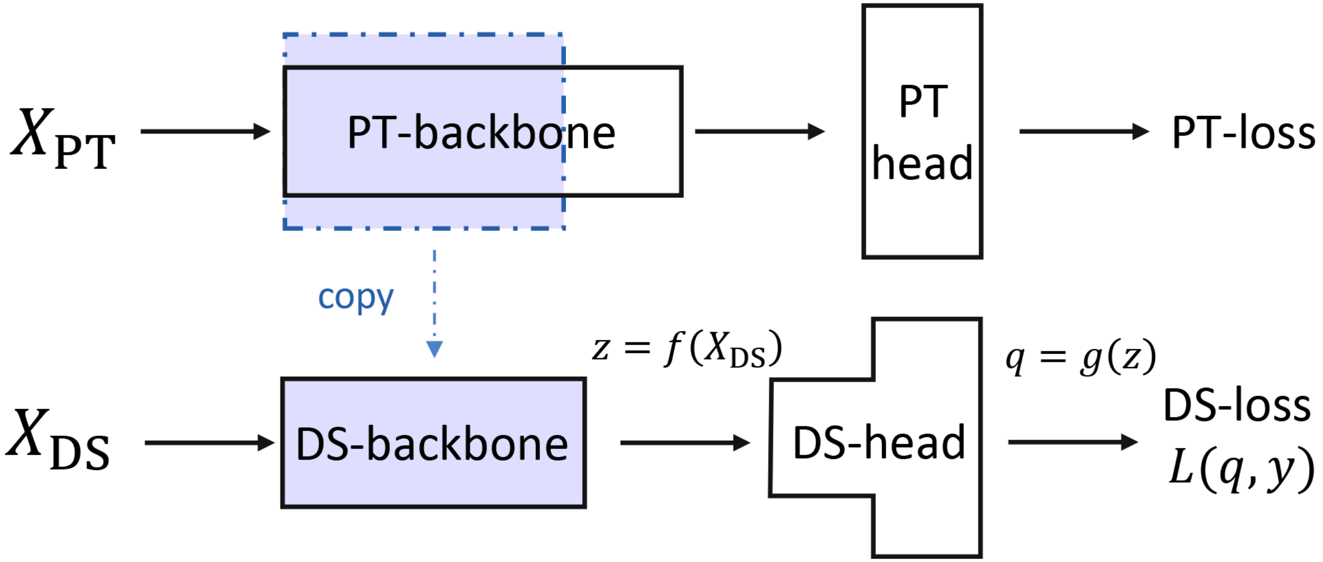

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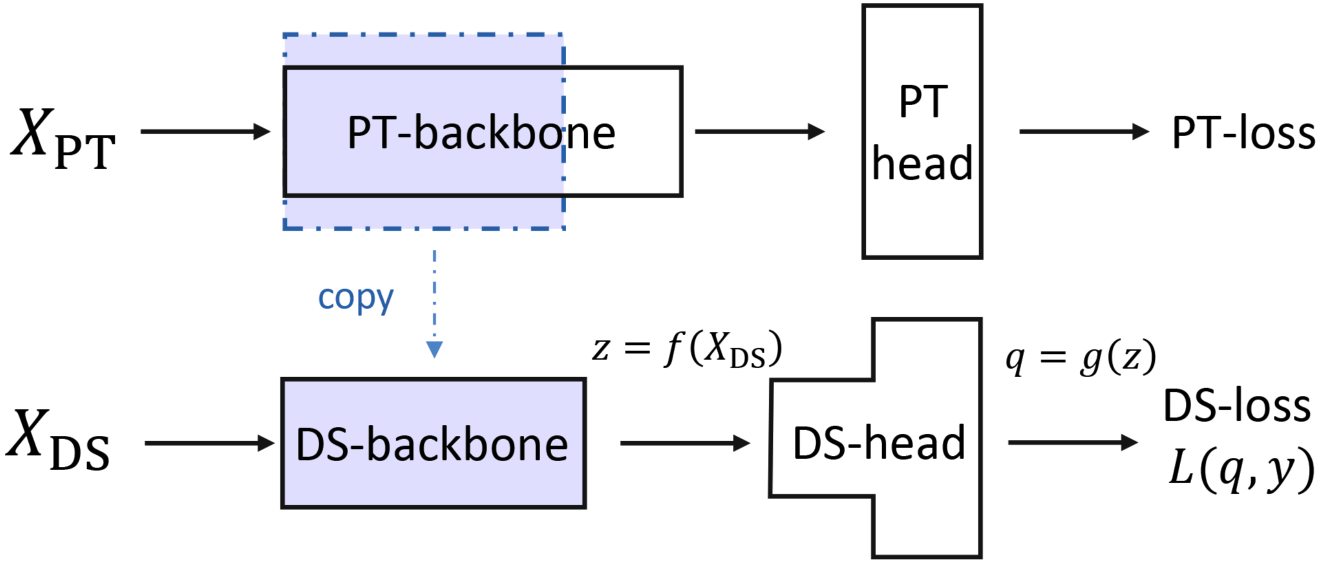

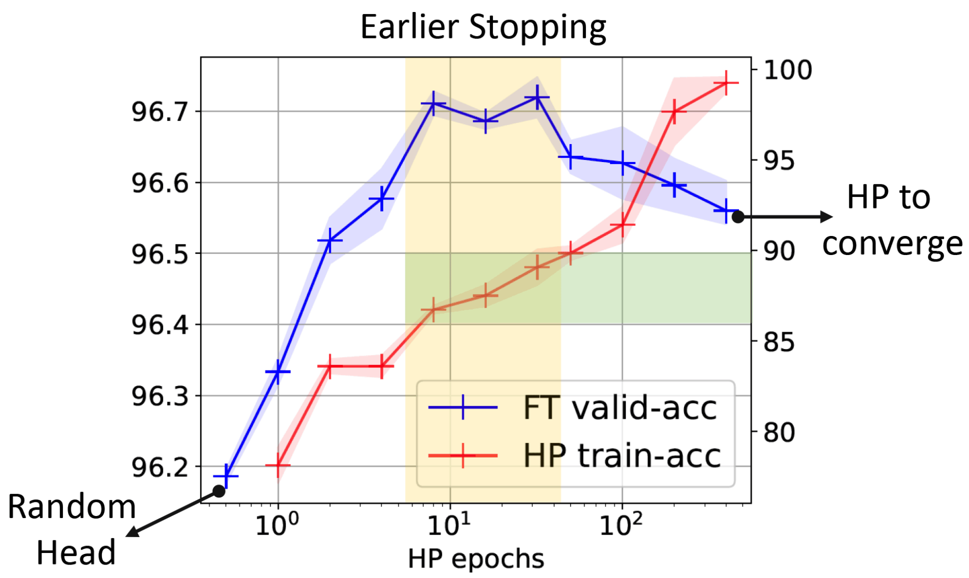

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- If we didn't do any head probing, "direction" is very random, especially if g is rich
- Specializing to simple linear-linear model, can get insights about trends in z
- Recommendations from paper:
  - Early stop during head probing (ideally, try multiple lengths for downstream task)
  - Label smoothing can help; so can more complex heads, but be careful

How good will our fine-tuned features be? [Wei/Hu/Steinhardt 2022]

On Transfer Learning via Linearized Neural Networks

Wesley J. Maddox[*1] **Shuai Tang**[*2] **Pablo Garcia Moreno**[3]
Andrew Gordon Wilson[1] **Andreas Damianou**[3]

[1] New York University, New York, NY
[2] UCSD, San Diego, CA
[3] Amazon, Cambridge, UK

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  - How you should fine-tune models
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Pool-based active learning

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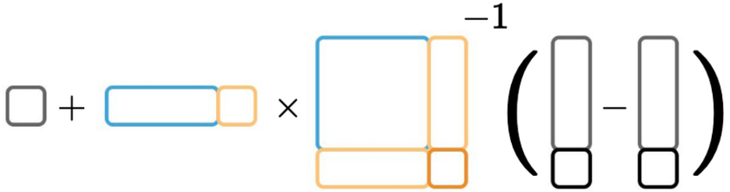
  - Rank-one updates for efficient computation: schema 

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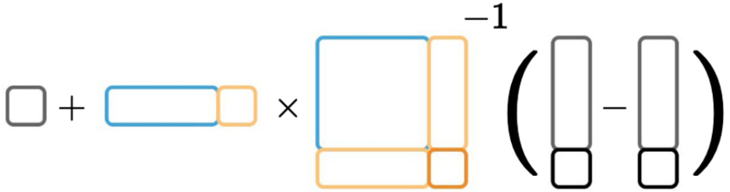
  - Rank-one updates for efficient computation: schema 

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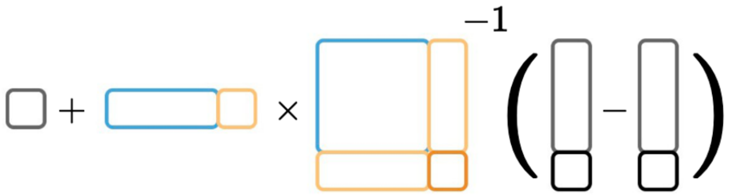
  - Rank-one updates for efficient computation: schema 

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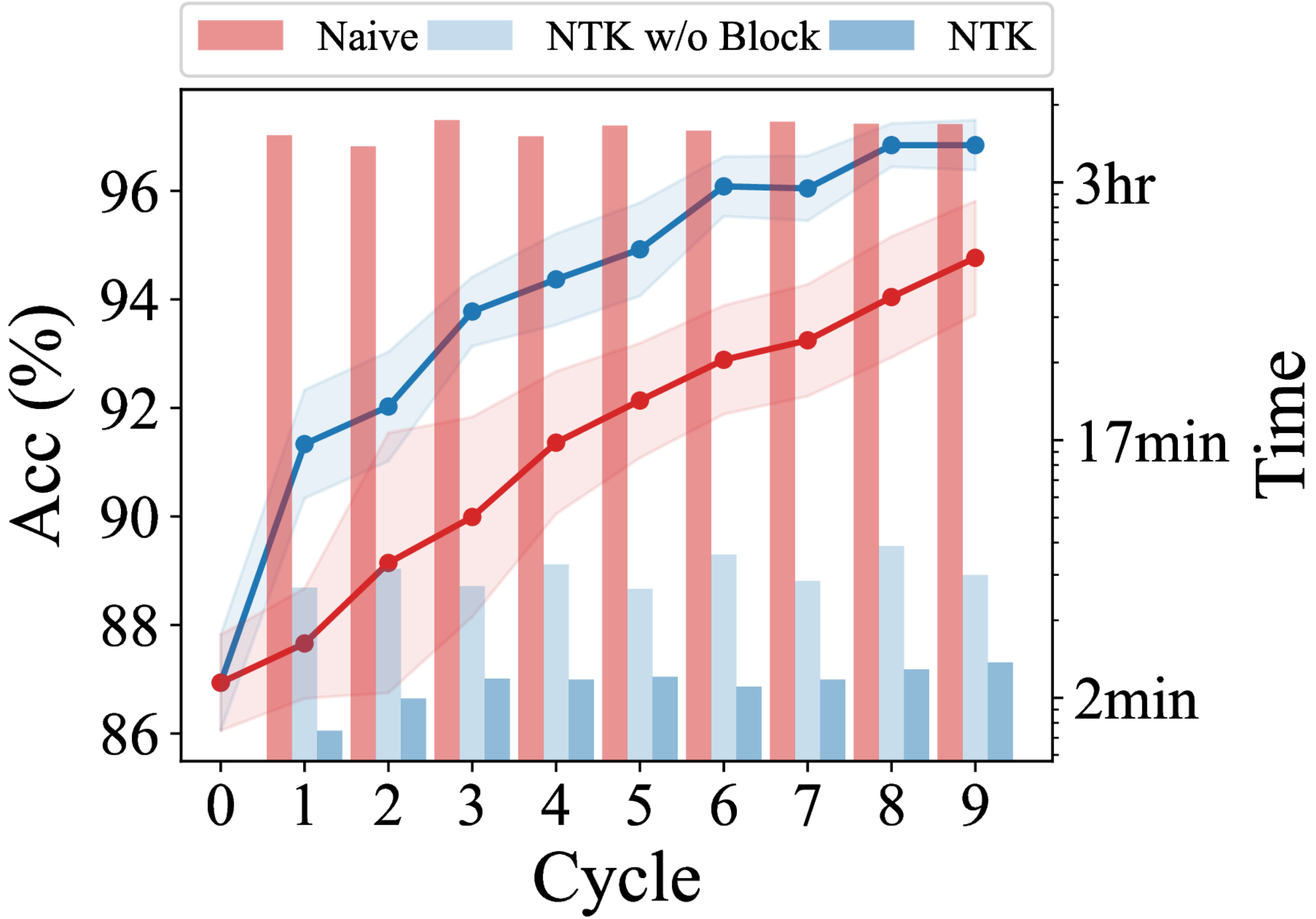
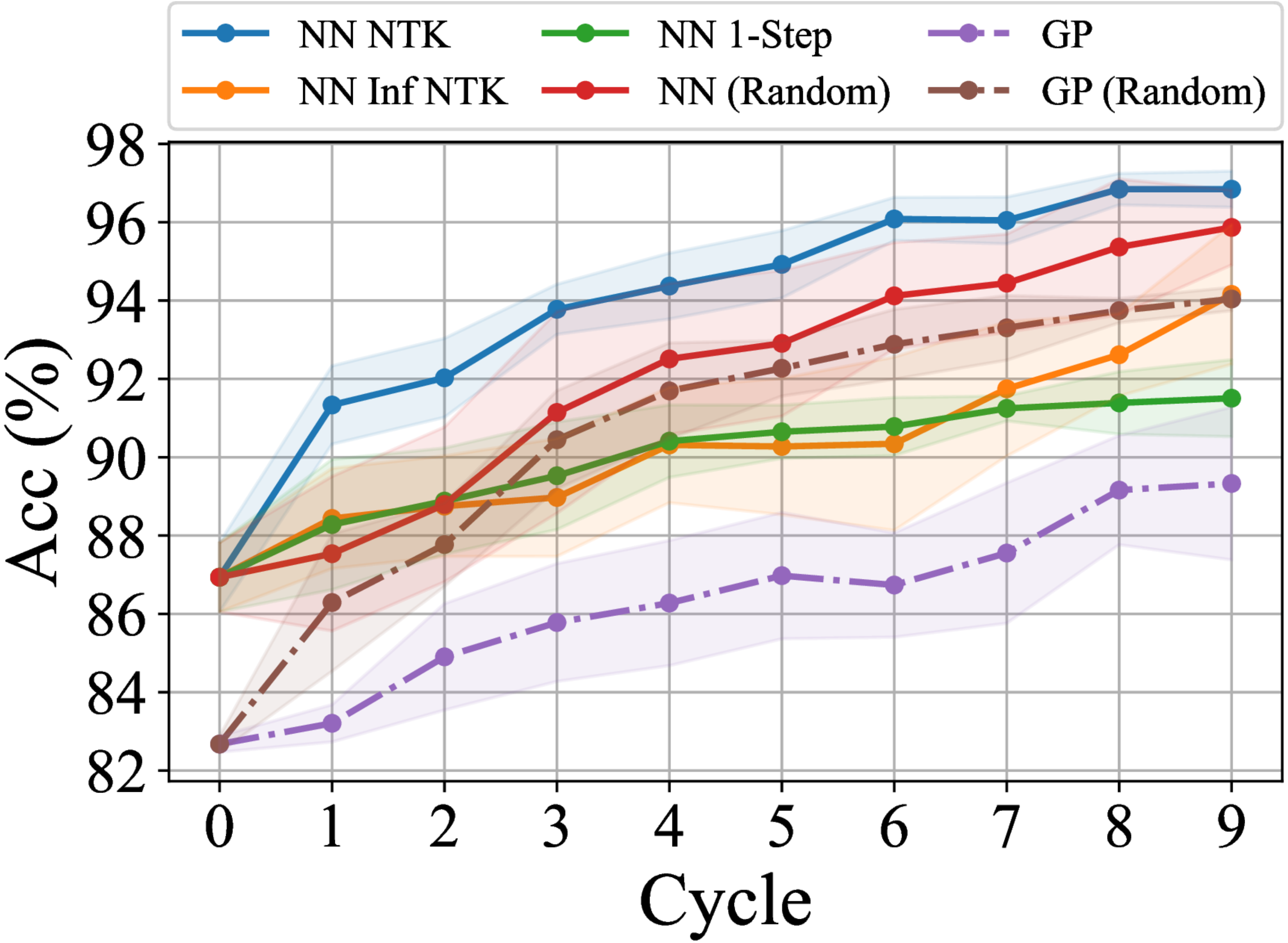
- Local approximation with eNTK “should” work much more broadly than “NTK regime”

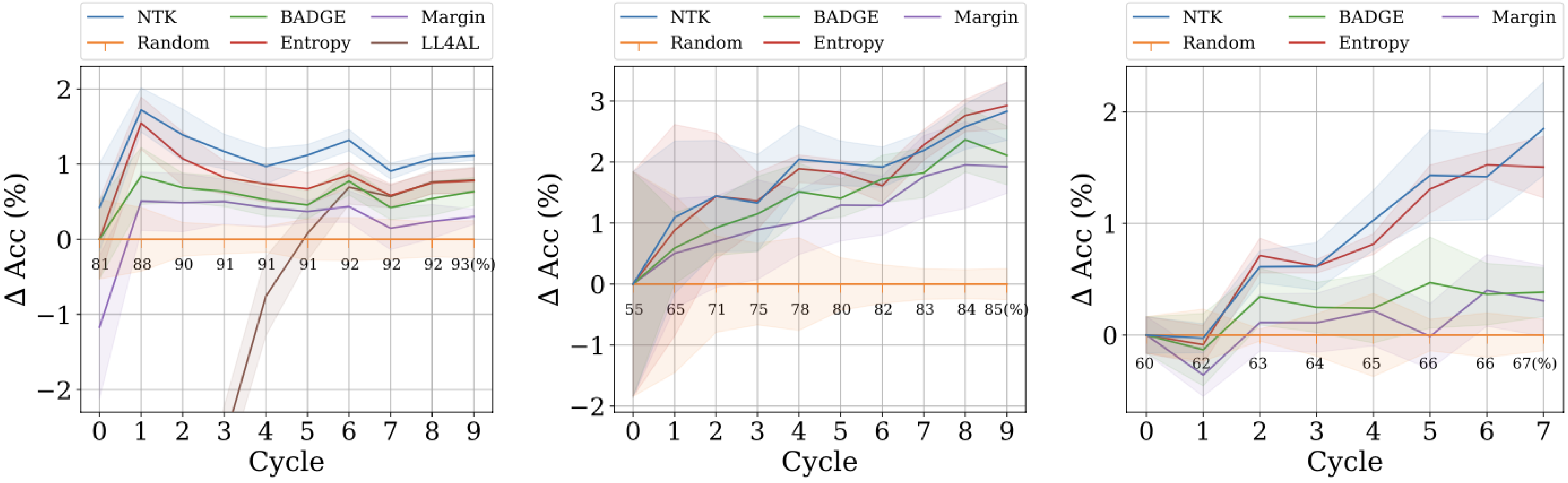
Much faster than SGD



Much more effective than infinite NTK and one-step SGD



Matches/beats state of the art



(a) SVHN: 1-layer WideResNet (b) CIFAR10: 2-layer WideResNet (c) CIFAR100: ResNet18

Figure 2: Comparison of the-state-of-the-art active learning methods on various benchmark datasets. Vertical axis shows difference from random acquisition, whose accuracy is shown in text.

Downside: usually more computationally expensive (especially memory)

Enables new interaction modes

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- But actually, we know that $\mathbb{E}_{\mathbf{w}}\, \mathrm{eNTK}_{\mathbf{w}}(x_1, x_2)$ is diagonal for most architectures
  - Let $\mathrm{pNTK}_{\mathbf{w}}(x_1, x_2) = \underbrace{[\nabla_{\mathbf{w}} f_1(x_1)]}_{1 \times p} \underbrace{[\nabla_{\mathbf{w}} f_1(x_2)]^{\mathsf{T}}}_{p \times 1}$.

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  - Can also use "sum of logits" $\frac{1}{\sqrt{k}} \sum_{j=1}^{k} f_j$ instead of just "first logit" f_1
- Lots of work (including above) has used pNTK instead of eNTK
  - Often without saying anything; sometimes doesn't seem like they know they're doing it

Approximating empirical NTKs

- I hid something from you on active learning (and Wei/Hu/Steinhardt fine-tuning) results...
- With k classes, $\mathrm{eNTK}(\mathbf{X}, \mathbf{X}) \in \mathbb{R}^{kN \times kN}$ – potentially very big
- But actually, we know that $\mathbb{E}_{\mathbf{w}}\, \mathrm{eNTK}_{\mathbf{w}}(x_1, x_2)$ is diagonal for most architectures
  - Let $\mathrm{pNTK}_{\mathbf{w}}(x_1, x_2) = \underbrace{[\nabla_{\mathbf{w}} f_1(x_1)]}_{1\times p}\underbrace{[\nabla_{\mathbf{w}} f_1(x_2))^{\mathsf{T}}}_{p\times 1}$.

  $\mathbb{E}_{\mathbf{w}}\, \mathrm{eNTK}_{\mathbf{w}}(x_1, x_2) = \mathbb{E}_{w}[\mathrm{pNTK}_{\mathbf{w}}(x_1, x_2)] I_k$. $\mathrm{pNTK}(\mathbf{X}, \mathbf{X}) \in \mathbb{R}^{N \times N}$ (no k!)

  - Can also use "sum of logits" $\frac{1}{\sqrt{k}} \sum_{j=1}^{k} f_j$ instead of just "first logit" f_1
- Lots of work (including above) has used pNTK instead of eNTK
  - Often without saying anything; sometimes doesn't seem like they know they're doing it
- Can we justify this more rigorously?

pNTK motivation

- Say $f(x) = V\phi(x)$, $\phi(x) \in \mathbb{R}^h$, and $V \in \mathbb{R}^{k \times h}$ has rows $v_j \in \mathbb{R}^h$ with iid entries

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$$\mathrm{eNTK}_{\mathbf{w}}(x_1, x_2)_{jj'} = v_j^\mathsf{T}\, \mathrm{eNTK}^{\phi}_{\mathbf{w}\setminus V}(x_1, x_2)\, v_{j'} + \mathbb{I}(j = j')\phi(x_1)^\mathsf{T} \phi(x_2)$$

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- We want to bound difference $\mathrm{eNTK}(x_1, x_2) - \mathrm{pNTK}(x_1, x_2) I_k$

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  - Want $v_1^\mathsf{T} A v_1$ and $v_j^\mathsf{T} A v_j$ to be close, and $v_j^\mathsf{T} A v_{j'}$ small, for random v and fixed A

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$$\begin{aligned} \mathrm{eNTK}_{\mathbf{w}}(x_1, x_2)_{jj'} &= v_j^\mathsf{T}\, \mathrm{eNTK}^{\phi}_{\mathbf{w}\setminus V}(x_1, x_2)\, v_{j'} + \mathbb{I}(j = j')\phi(x_1)^\mathsf{T}\phi(x_2) \\ \mathrm{pNTK}_{\mathbf{w}}(x_1, x_2) &= v_1^\mathsf{T}\, \mathrm{eNTK}^{\phi}_{\mathbf{w}\setminus V}(x_1, x_2)\, v_1 + \phi(x_1)^\mathsf{T}\phi(x_2) \end{aligned}$$

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  - Want $v_1^\mathsf{T} A v_1$ and $v_j^\mathsf{T} A v_j$ to be close, and $v_j^\mathsf{T} A v_{j'}$ small, for random v and fixed A
  - Using Hanson-Wright: $\dfrac{\lVert \mathrm{eNTK} - \mathrm{pNTK}\, I \rVert_F}{\lVert \mathrm{eNTK} \rVert_F} \le \dfrac{\lVert \mathrm{eNTK}^{\phi} \rVert_F + 4\sqrt{h}}{\mathrm{Tr}(\mathrm{eNTK}^{\phi})} k \log \dfrac{2k^2}{\delta}$

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  - Using Hanson-Wright: $\dfrac{\|\mathrm{eNTK} - \mathrm{pNTK}\, I\|_F}{\|\mathrm{eNTK}\|_F} \le \dfrac{\left\|\mathrm{eNTK}^\phi\right\|_F + 4\sqrt{h}}{\mathrm{Tr}(\mathrm{eNTK}^\phi)} k \log \dfrac{2k^2}{\delta}$
  - Fully-connected ReLU nets at init., fan-in mode: numerator $\mathcal{O}(h\sqrt{h})$, denom $\Theta(h^2)$

pNTK's Frobenius error

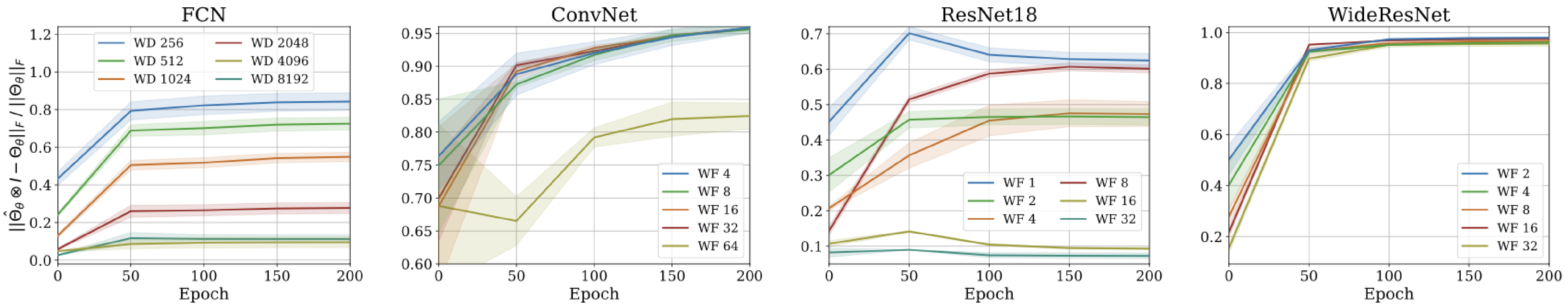

Figure 3: Evaluating the **relative difference of Frobenius norm of** $\Theta_\theta(\mathcal{D}, \mathcal{D})$ **and** $\hat{\Theta}_\theta(\mathcal{D}, \mathcal{D}) \otimes I_O$ at initialization and throughout training, based on $\mathcal{D}$ being 1000 random points from CIFAR-10. Wider nets have more similar $\|\Theta_\theta\|_F$ and $\|\hat{\Theta}_\theta \otimes I_O\|_F$ at initialization.

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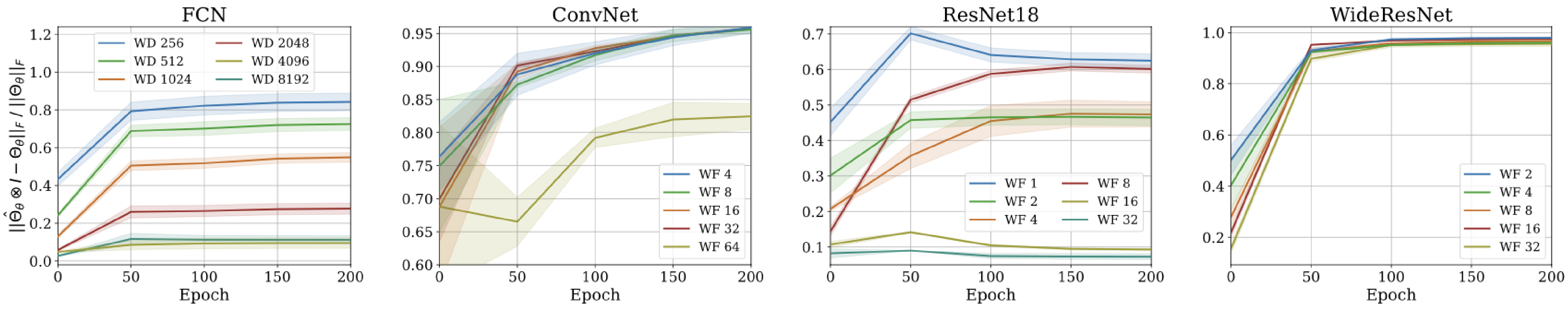

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Same kind of theorem / empirical results for largest eigenvalue,
and empirical results for $\lambda_{\min}$, condition number

Kernel regression with pNTK

- Reshape things to handle prediction appropriately:

$$\underbrace{f_{\text{eNTK}}(\tilde{x})}_{k\times 1} = \underbrace{f_0(\tilde{x})}_{k\times 1} + \underbrace{\text{eNTK}_{\mathbf{w}_0}(\tilde{x}, \mathbf{X})}_{k\times kN} \underbrace{\text{eNTK}_{\mathbf{w}_0}(\mathbf{X}, \mathbf{X})^{-1}}_{kN\times kN} \underbrace{(\mathbf{y} - f_0(\mathbf{X}))}_{kN\times 1}$$

$$\underbrace{f_{\text{pNTK}}(\tilde{x})}_{k\times 1} = \underbrace{f_0(\tilde{x})}_{k\times 1} + \left(\underbrace{\text{pNTK}_{\mathbf{w}_0}(\tilde{x}, \mathbf{X})}_{1\times N} \underbrace{\text{pNTK}_{\mathbf{w}_0}(\mathbf{X}, \mathbf{X})^{-1}}_{N\times N} \underbrace{(\mathbf{y} - f_0(\mathbf{X}))}_{N\times k}\right)^{\mathsf{T}}$$

- We have $\|f_{\text{eNTK}}(\tilde{x}) - f_{\text{pNTK}}(\tilde{x})\| = \mathcal{O}(\frac{1}{\sqrt{h}})$ again
  - If we add regularization, need to “scale” λ between the two

Kernel regression with pNTK

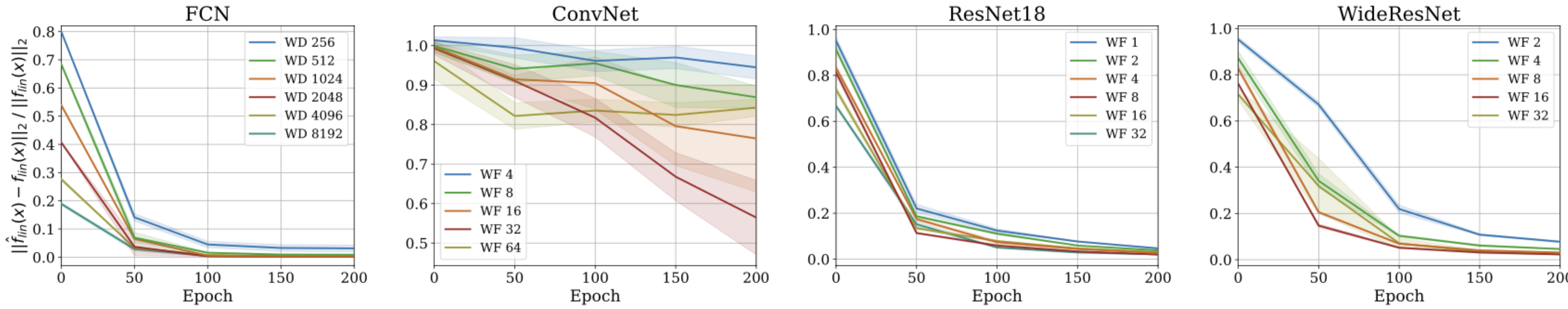


Figure 7: The **relative difference of kernel regression outputs**, (4) and (5), when training on $|\mathcal{D}| = 1000$ random CIFAR-10 points and testing on $|\mathcal{X}| = 500$. For wider NNs, the relative difference in $\hat{f}^{lin}(\mathcal{X})$ and $f^{lin}(\mathcal{X})$ decreases at initialization. Surprisingly, the difference between these two continues to quickly vanish while training the network.

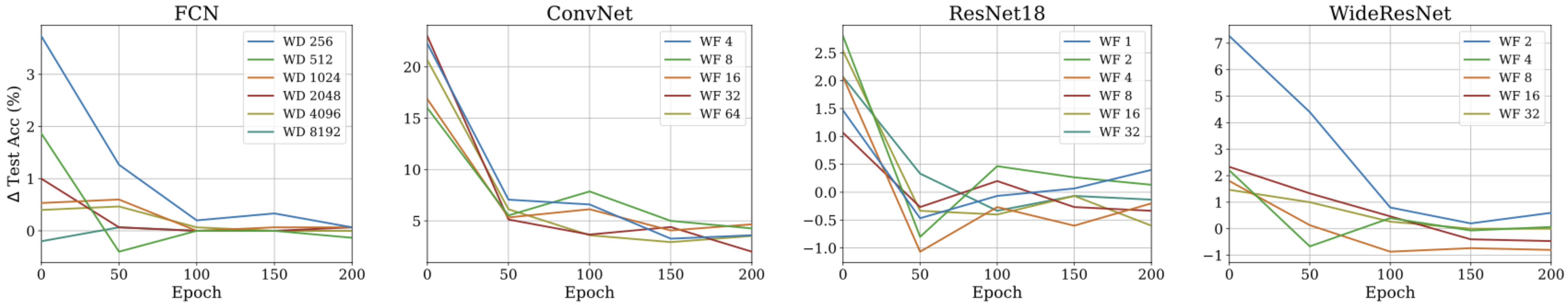


Figure 8: **Using pNTK in kernel regression** (as in Figure 7) **almost always achieves a higher test accuracy than using eNTK.** Wider NNs and trained nets have more similar prediction accuracies of $\hat{f}^{lin}$ and f^{lin} at initialization. Again, the difference between these two continues to vanish throughout the training process using SGD.

pNTK speed-up

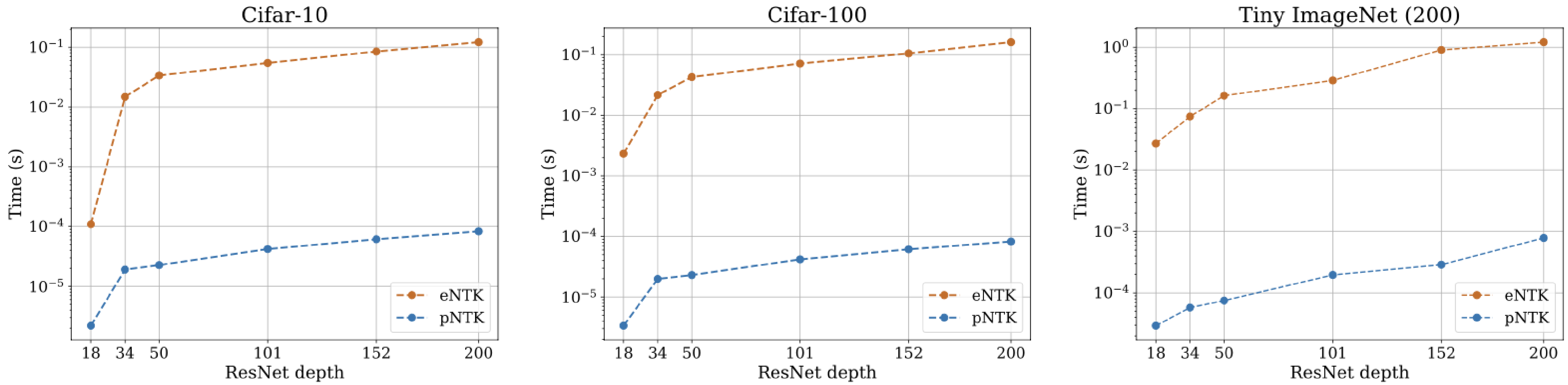
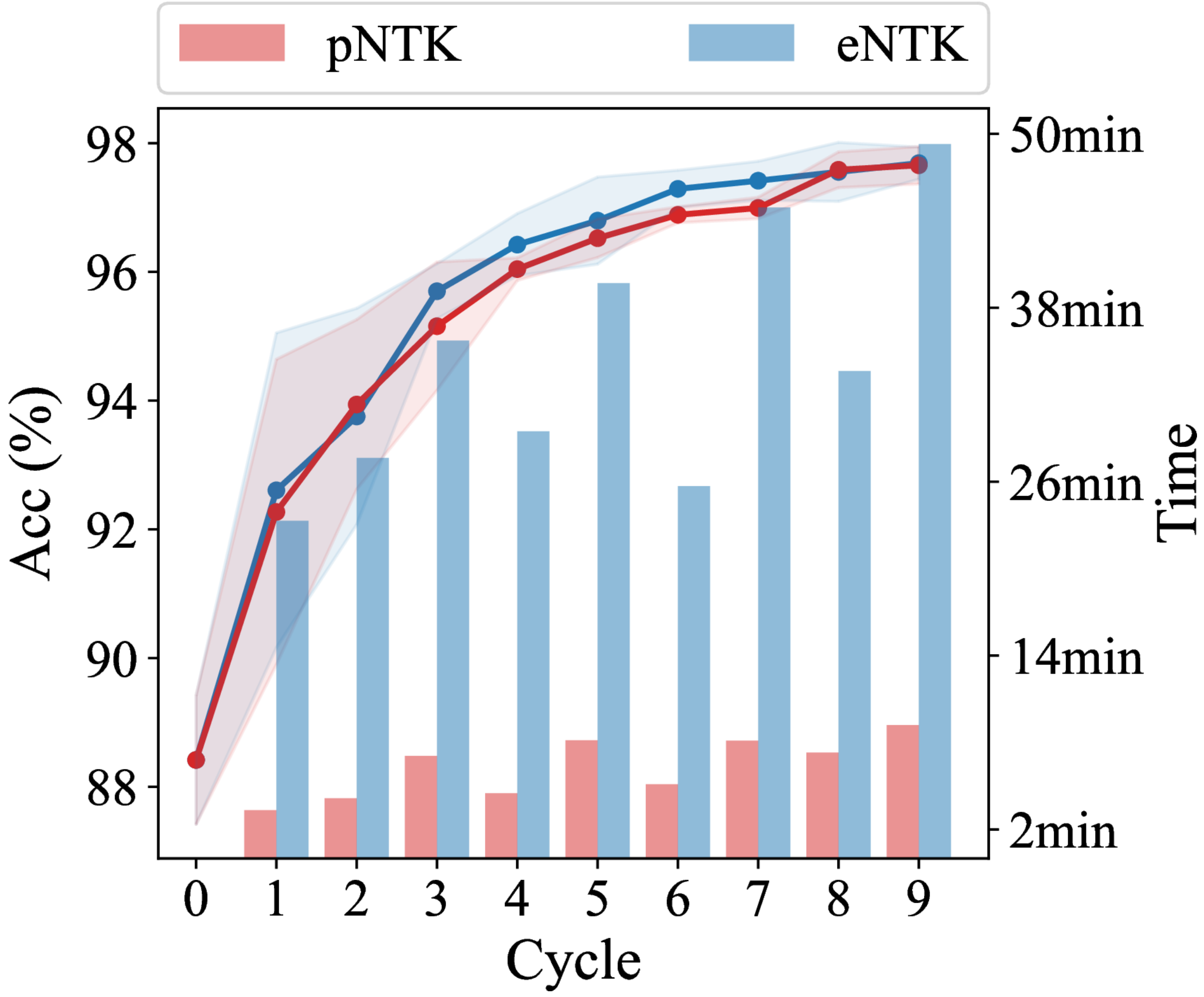


Figure 1: **Wall-clock time to evaluate the eNTK and pNTK** for one pair of inputs, across datasets and ResNet depths.

pNTK speed-up on active learning task



pNTK for full CIFAR-10 regression

- $\mathrm{eNTK}(\mathbf{X}, \mathbf{X})$ on CIFAR-10: 1.8 terabytes of memory
- $\mathrm{pNTK}(\mathbf{X}, \mathbf{X})$ on CIFAR-10: 18 gigabytes of memory

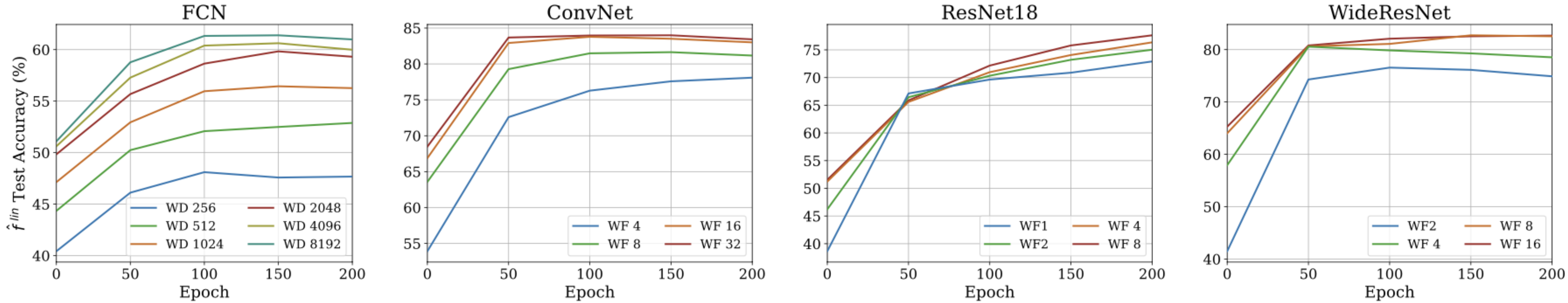


Figure 9: Evaluating the **test accuracy of kernel regression predictions using pNTK as in (5) on the full CIFAR-10 dataset**. As the NN's width grows, the test accuracy of $\hat{f}^{lin}$ also improves, but eventually saturates with the growing width. Using trained weights in computation of pNTK results in improved test accuracy of $\hat{f}^{lin}$.

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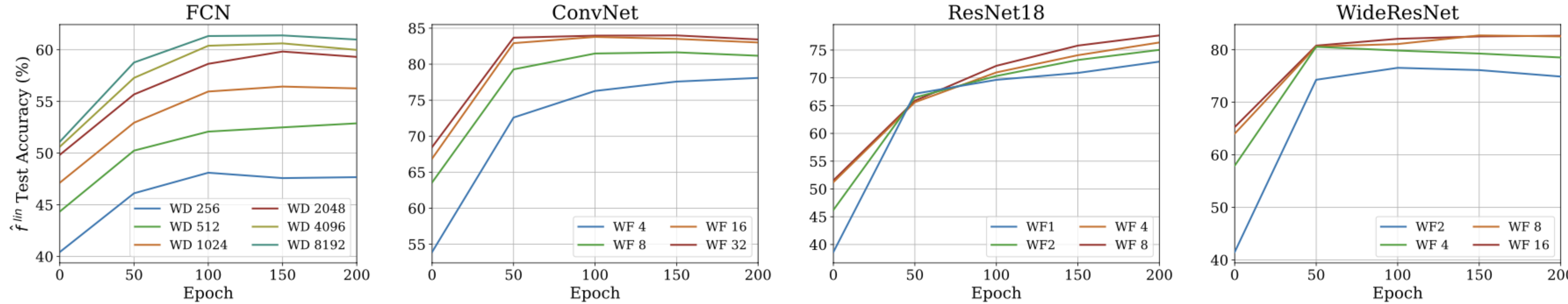

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- Worse than infinite NTK for FCN/ConvNet (where they can be computed, if you try hard)

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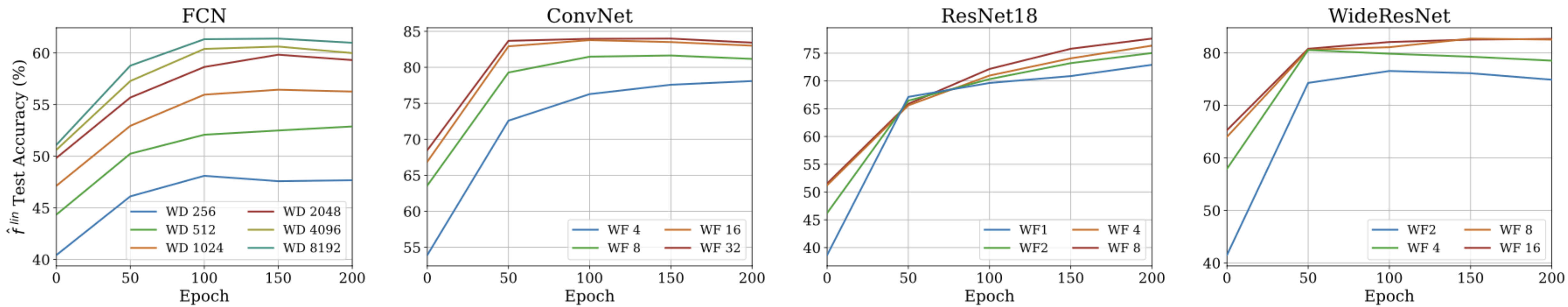

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- Worse than infinite NTK for FCN/ConvNet (where they can be computed, if you try hard)
- Way worse than SGD

Recap

eNTK is a good tool for intuitive understanding of the learning process

Ren, Guo, S. Better Supervisory Signals by Observing Learning Paths

Ren, Guo, Bae, S. How to prepare your task head for finetuning

eNTK is practically very effective at “lookahead” for active learning

Mohamadi*, Bae*, S. Making Look-Ahead Active Learning Strategies Feasible with Neural Tangent Kernels

You should probably use pNTK instead of eNTK for high-dim output problems:

Mohamadi, Bae, S. A Fast, Well-Founded Approximation to the Empirical Neural Tangent Kernel