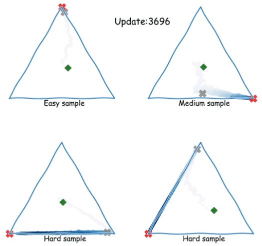
Local Learning Dynamics Help Explain (Post-)Training Behaviour

Danica J. Sutherland (she)
University of British Columbia (UBC) / Alberta Machine Intelligence Institute (Amii)

Knowl. dist. analysis
[ICLR-22]



Yi Ren
Shangmin Guo

Finetuning analysis
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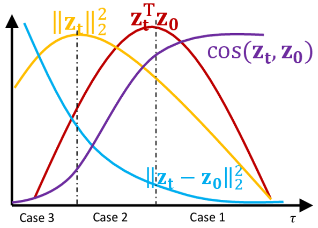

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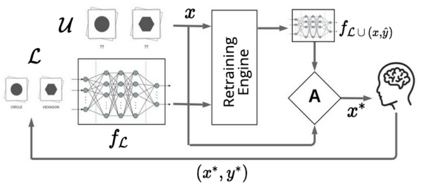
Active learning
[NeurIPS-22]



M. Amin Mohamadi
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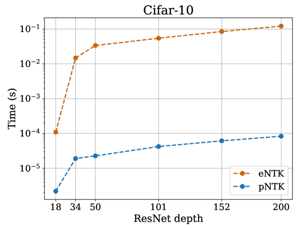
Pseudo-NTK
[ICML-23]



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DPO/etc analysis
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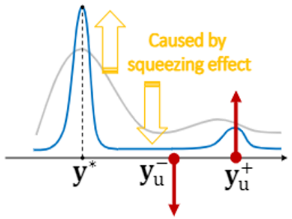
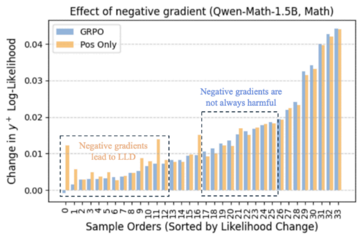


Yi Ren

GRPO analysis+fix
[arXiv]



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Penn – June 2025

HTML version

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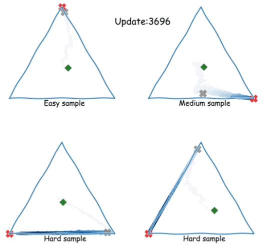

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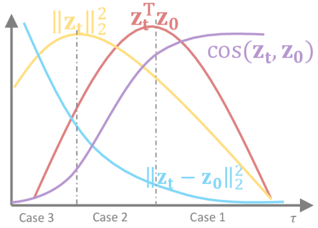

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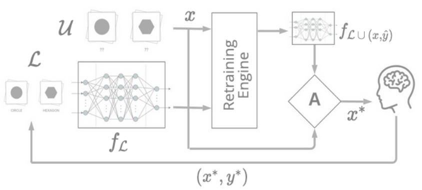

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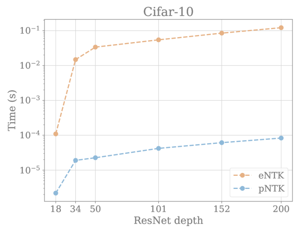

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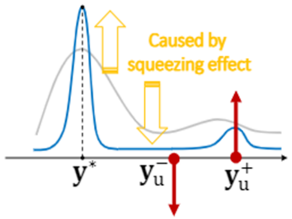

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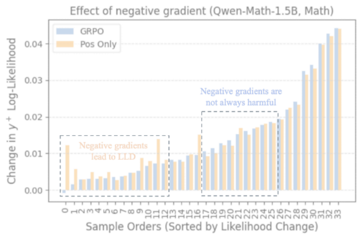

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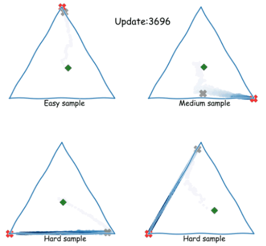

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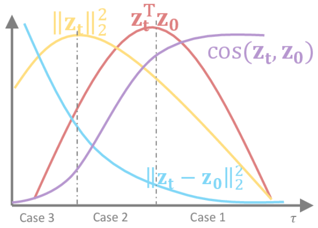

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Active
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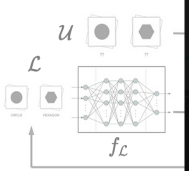

M. Amin
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Yi (Joshua) Ren

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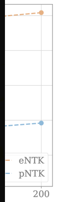

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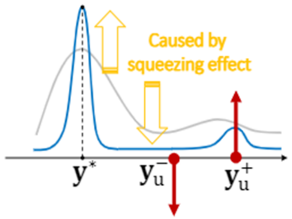

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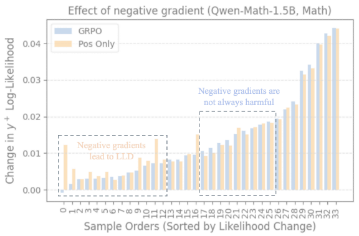

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- Language models (e.g. GPT-2)
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r/learnprogramming • 7 yr. ago
RobotWizardz

Why on people on stack overflow so rude?

Honestly everytime I go to ask a question I'm scared that I'll be met with an overwhelming amount of negatives and comments telling me my questions are stupid it seems very hostile / scary. I'm

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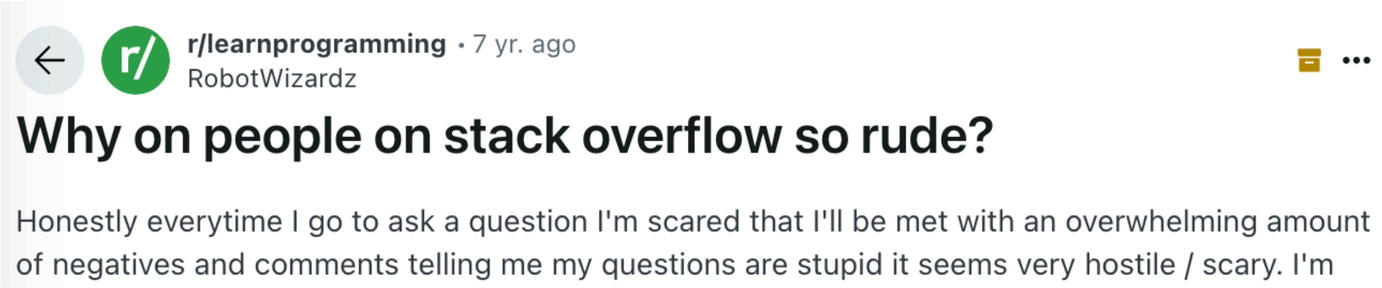

- Turning a language model into a chatbot (e.g. ChatGPT):
  - Run "supervised fine-tuning" on a dataset of chatbot-like interactions
  - Run "preference optimization": given prompt x, say A, not B

Surprises in LLM post-training

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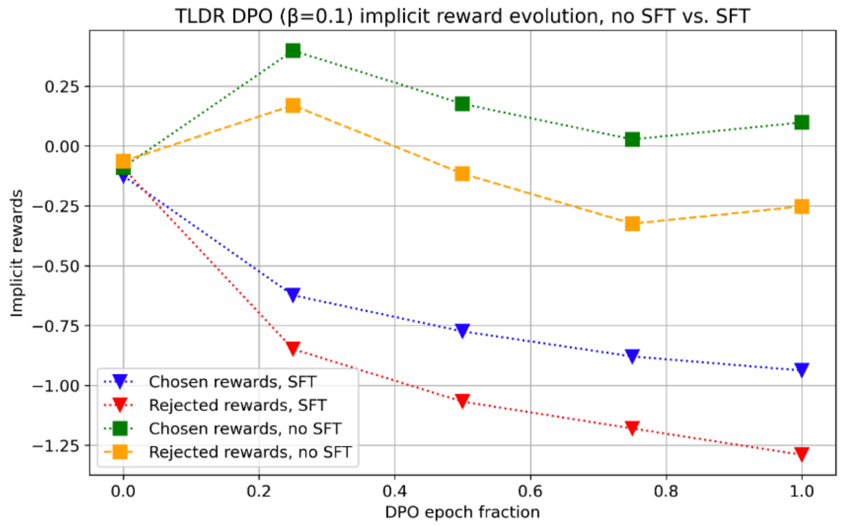

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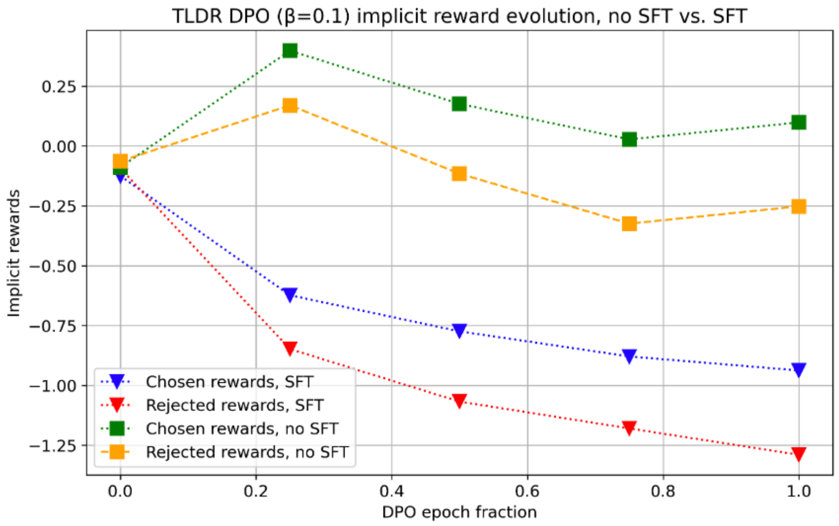

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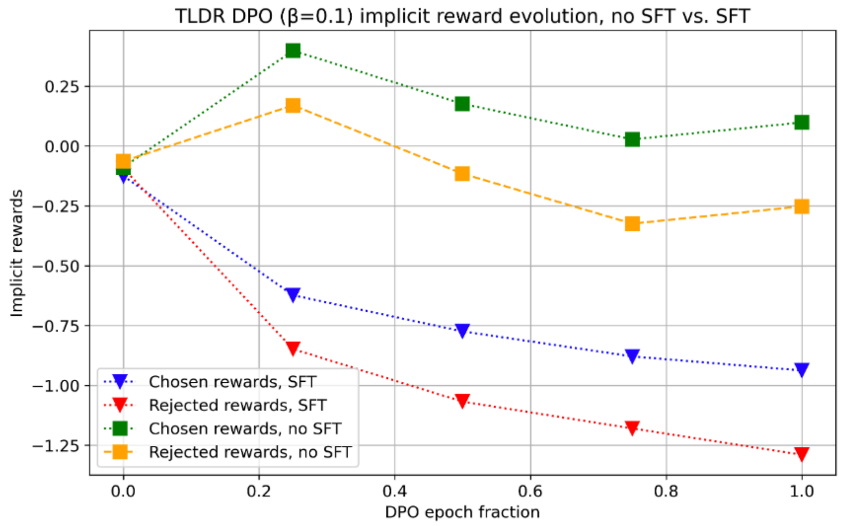

- Even in the best case, "too much" DPO hurts [RHPF CoLM-24]
- Makes B way less likely, but eventually, model almost always says some C
- There are some workarounds, but...why?

Learning dynamics

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    - Also been called "local elasticity" [HS ICLR-20]

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- $\mathcal{G}_t(x_i, y_i) = \nabla_{\mathbf{z}} \mathcal{L}(x_i, y_i)\big|_{\mathbf{z}_t}$: how much do I need to change my x_i prediction?
  - For square loss with $\sigma(\mathbf{z}) = \mathbf{z}$, $\mathcal{G}_t = \mathbf{f}_t(x_i) - y_i$: how wrong was I before?
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- $\mathcal{A}_t(\tilde{x}) = \nabla_{\mathbf{z}} \sigma(\mathbf{z}_t)$ just "converts" prediction changes
  - If $\sigma(\mathbf{z}) = \mathbf{z}$, $\mathcal{A}_t$ is the identity; if $\sigma = \log \mathrm{Softmax}$, $\mathcal{A}_t = \mathbf{I}_k - \mathbf{1}_k\, \pi_t(\tilde{x})^\mathsf{T}$

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- $\mathcal{K}_t(\tilde{x}, x_i) = (\nabla_{\mathbf{w}} \mathbf{z}(\tilde{x})\big|_{\mathbf{w}_t})(\nabla_{\mathbf{w}} \mathbf{z}(x_i)\big|_{\mathbf{w}_t})^\mathsf{T}$ is $k \times k$ empirical neural tangent kernel of $\mathbf{z}$

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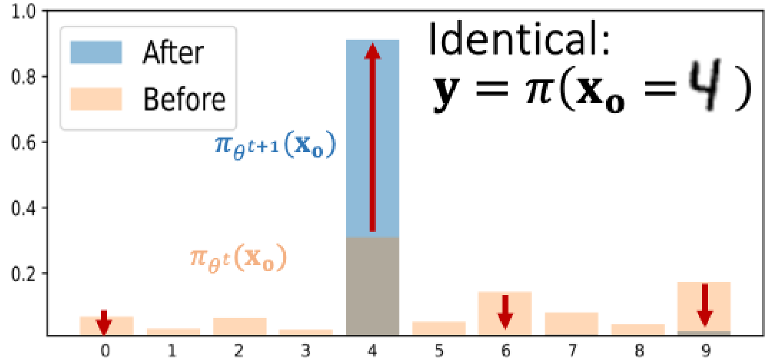
$$\mathbf{f}_{t+1}(\tilde{x}) - \mathbf{f}_t(\tilde{x}) = -\eta\, \mathcal{A}_t(\tilde{x})\, \mathcal{K}_t(\tilde{x}, x_i)\, \mathcal{G}_t(x_i, y_i) + \mathcal{O}(\eta^2)$$

- $\mathcal{G}_t(x_i, y_i) = \nabla_{\mathbf{z}} \mathcal{L}(x_i, y_i)\big|_{\mathbf{z}_t}$: how much do I need to change my x_i prediction?
  - For square loss with $\sigma(\mathbf{z}) = \mathbf{z}$, $\mathcal{G}_t = \mathbf{f}_t(x_i) - y_i$: how wrong was I before?
  - For cross-entropy on logits, $\mathcal{G}_t = \mathrm{Softmax}(\mathbf{z}_t(x_i))_{y_i} - e_{y_i}$: how wrong was I before?
- $\mathcal{A}_t(\tilde{x}) = \nabla_{\mathbf{z}} \sigma(\mathbf{z}_t)$ just "converts" prediction changes
  - If $\sigma(\mathbf{z}) = \mathbf{z}$, $\mathcal{A}_t$ is the identity; if $\sigma = \log \mathrm{Softmax}$, $\mathcal{A}_t = \mathbf{I}_k - \mathbf{1}_k\, \pi_t(\tilde{x})^\mathsf{T}$
- $\mathcal{K}_t(\tilde{x}, x_i) = (\nabla_{\mathbf{w}} \mathbf{z}(\tilde{x})|_{\mathbf{w}_t})(\nabla_{\mathbf{w}} \mathbf{z}(x_i)|_{\mathbf{w}_t})^\mathsf{T}$ is $k \times k$ empirical neural tangent kernel of $\mathbf{z}$
  - If x_i, $\tilde{x}$ are "dissimilar" (small eNTK), stepping on (x_i, y_i) barely changes $\tilde{x}$ prediction
  - If x_i, $\tilde{x}$ are "similar" (large eNTK), makes $\tilde{x}$ prediction more like y_i

Example: learning dynamics on MNIST

$$\log \pi_{t+1}(\tilde{x}) - \log \pi_t(\tilde{x}) \approx -\eta \mathcal{A}_t(\tilde{x}) \mathcal{K}_t(\tilde{x}, x_i) \mathcal{G}_t(x_i, y_i)$$



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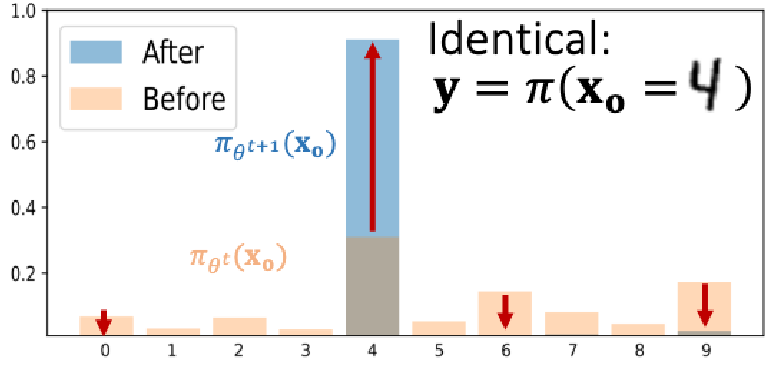

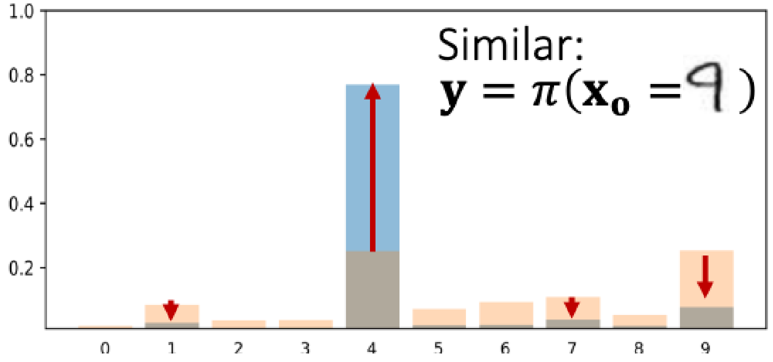

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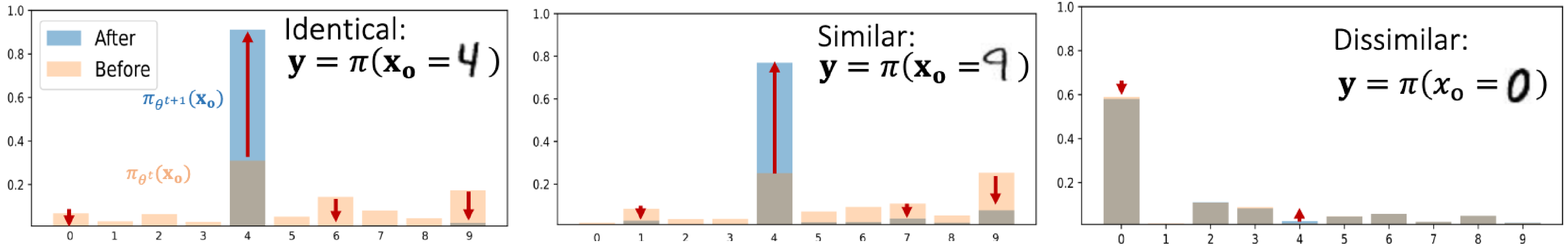

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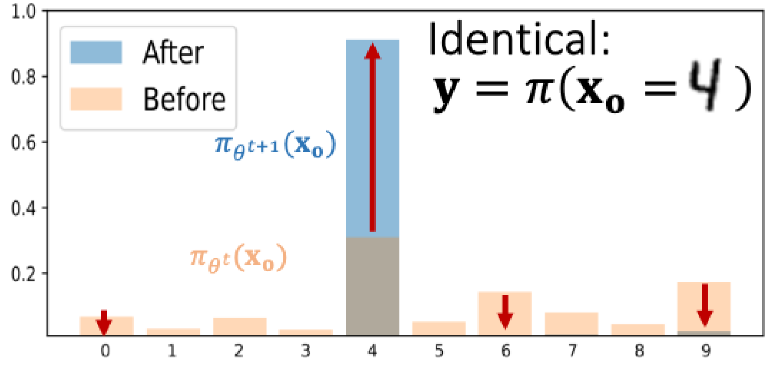

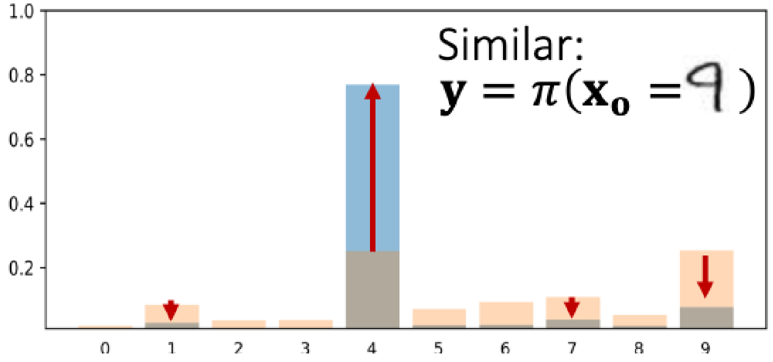

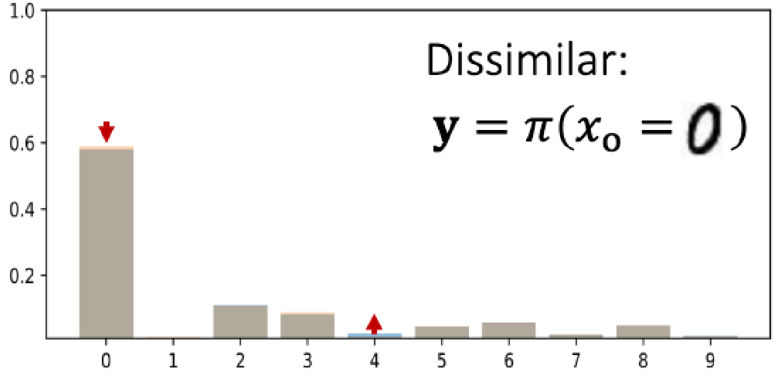

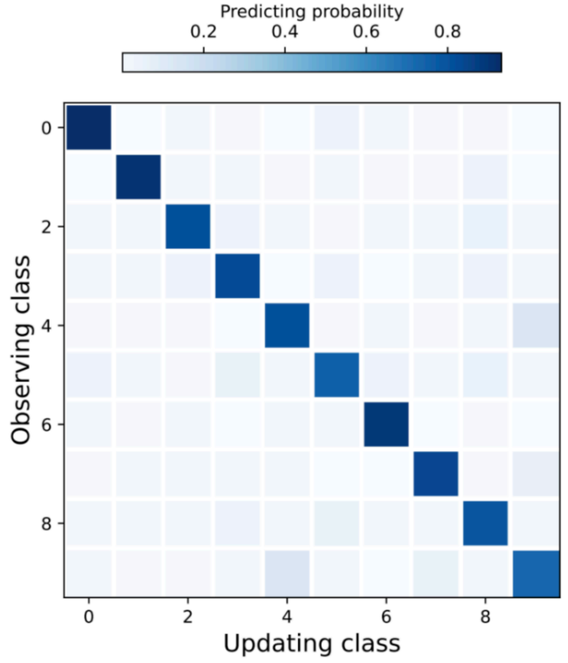

But wait...aren't NTKs an unrealistic approximation?

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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

A quick aside: the “NTK regime” and infinite limits

- Full-batch GD:

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- Observation II: As f becomes "infinitely wide" with any usual architecture+init* [Yang 2019], $\mathcal{K}_0(x_1, x_2) \xrightarrow{a.s.} \mathrm{NTK}(x_1, x_2)$, 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], …

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  - 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]

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- Workaround: track some informative possible responses
  - The dataset responses, rephrases, similar strings with different meanings
  - Irrelevant responses in training set, random sentences...

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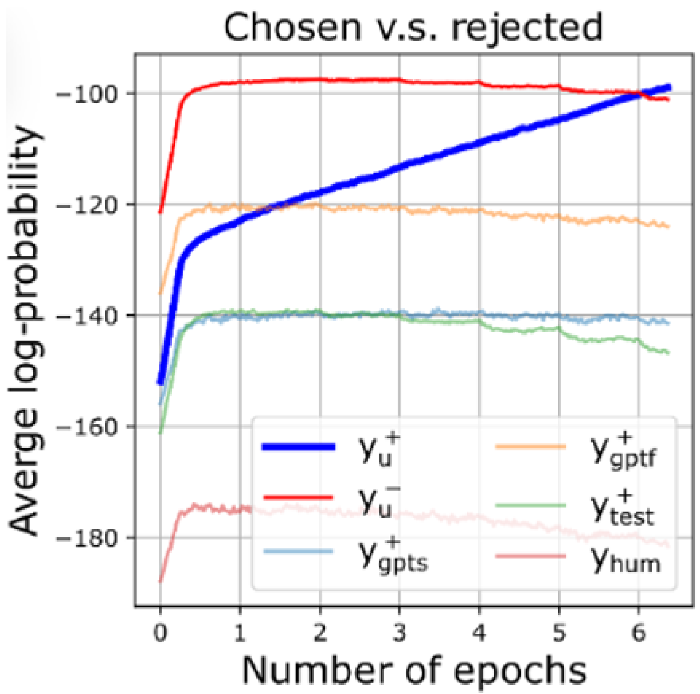

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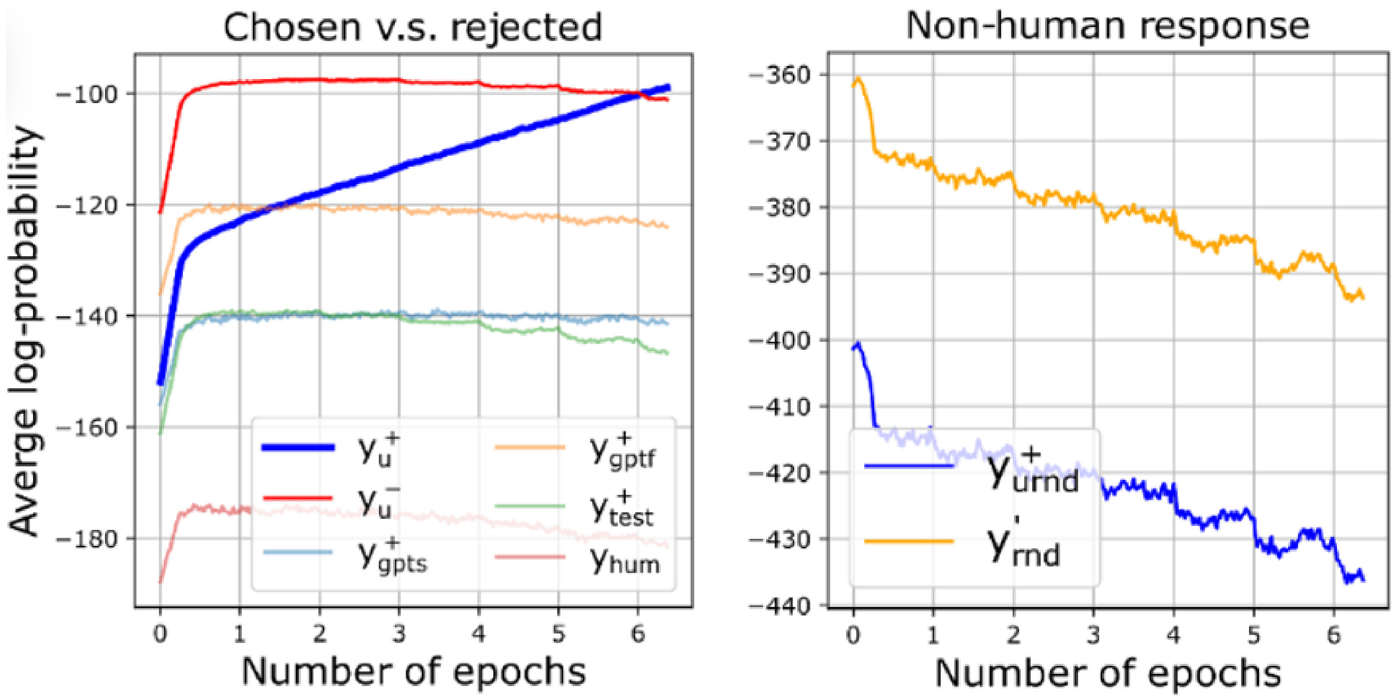

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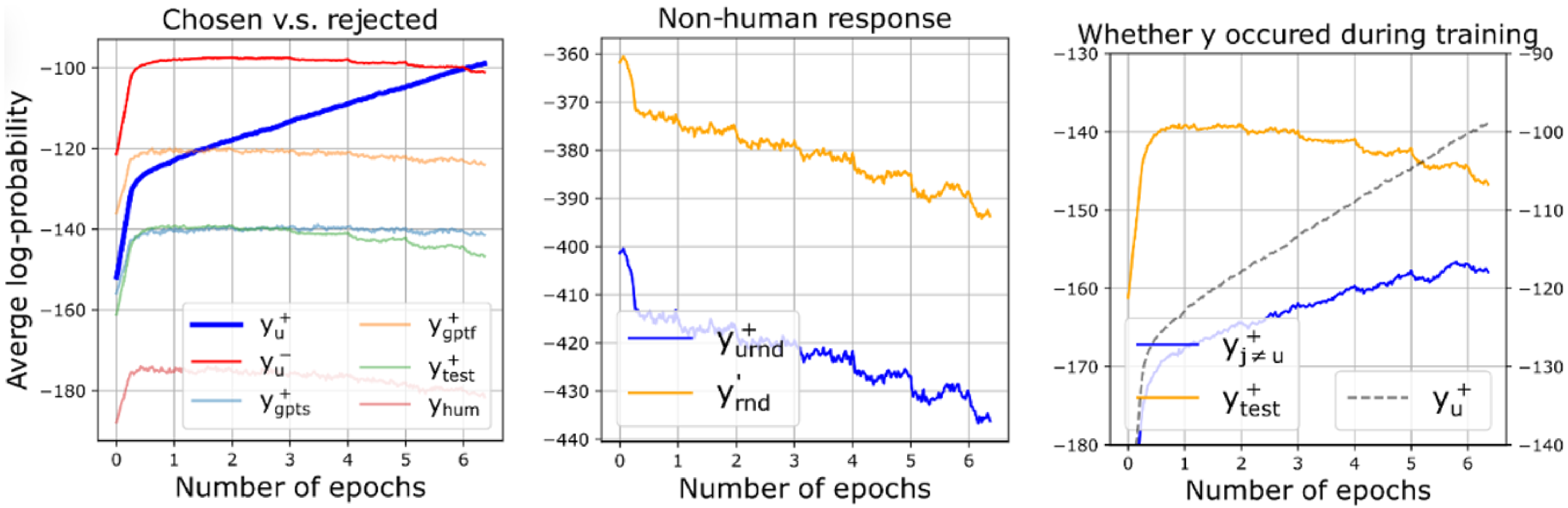
- Also makes answers to different questions more likely…one form of hallucination?



Direct Preference Optimization (DPO)

$$\mathcal{L}_t^{\mathrm{DPO}}(x_i, y_i^+, y_i^-) = \log \sigma \left(\beta \left[\log \frac{\pi_t(y_i^+ \mid x_i)}{\pi_{\mathrm{ref}}(y_i^+ \mid x_i)} - \log \frac{\pi_t(y_i^- \mid x_i)}{\pi_{\mathrm{ref}}(y_i^- \mid x_i)} \right] \right)$$

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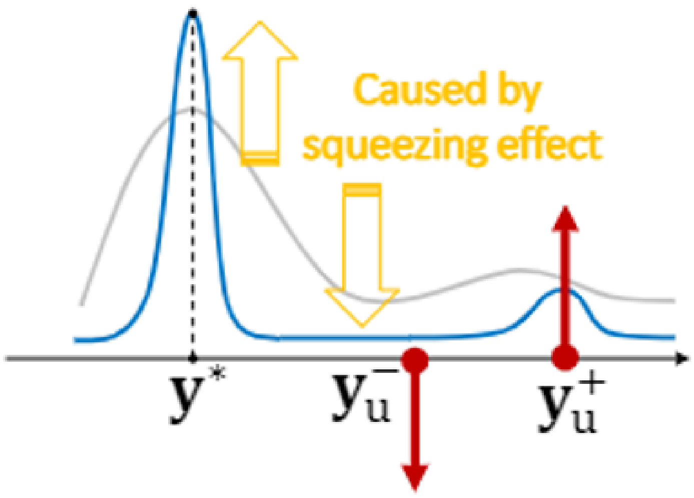
This negative gradient can do really weird things:



Negative gradients and the squeezing effect

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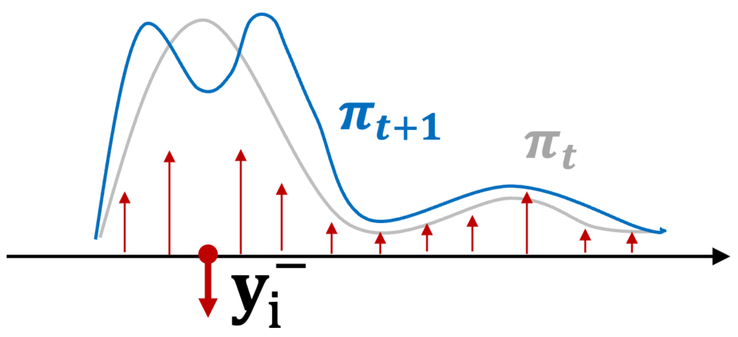

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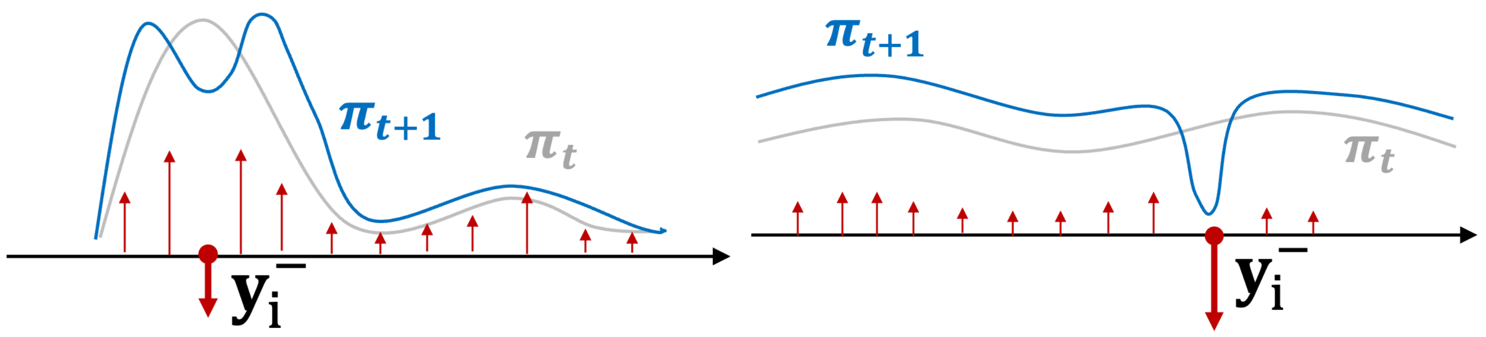
$$\pi(y \mid x) = \frac{\exp(z(x)_y)}{\exp(z(x)_y) + \exp(z(x)_{y^*}) + \ldots}$$

- To decrease $\log \pi((y_i^-)_m \mid [\chi_i^-]_{:m})$, decrease numerator and increase denominator



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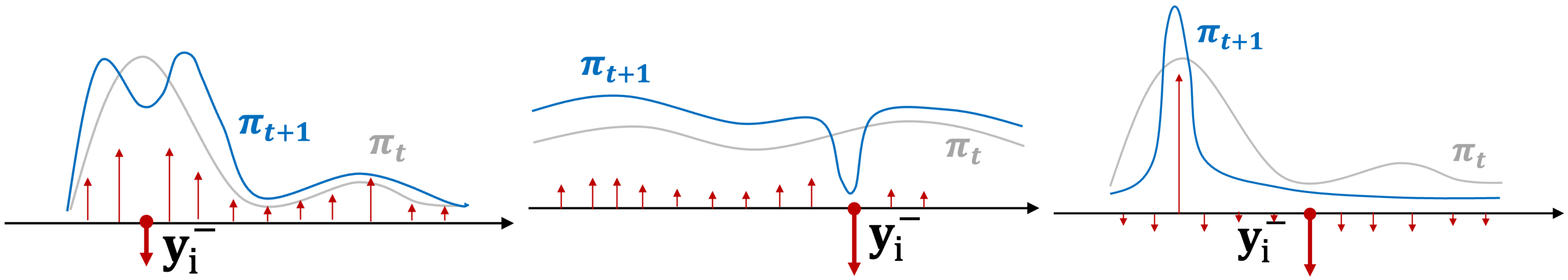

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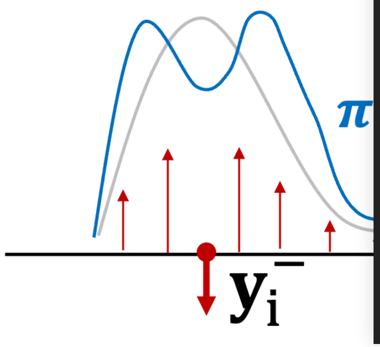
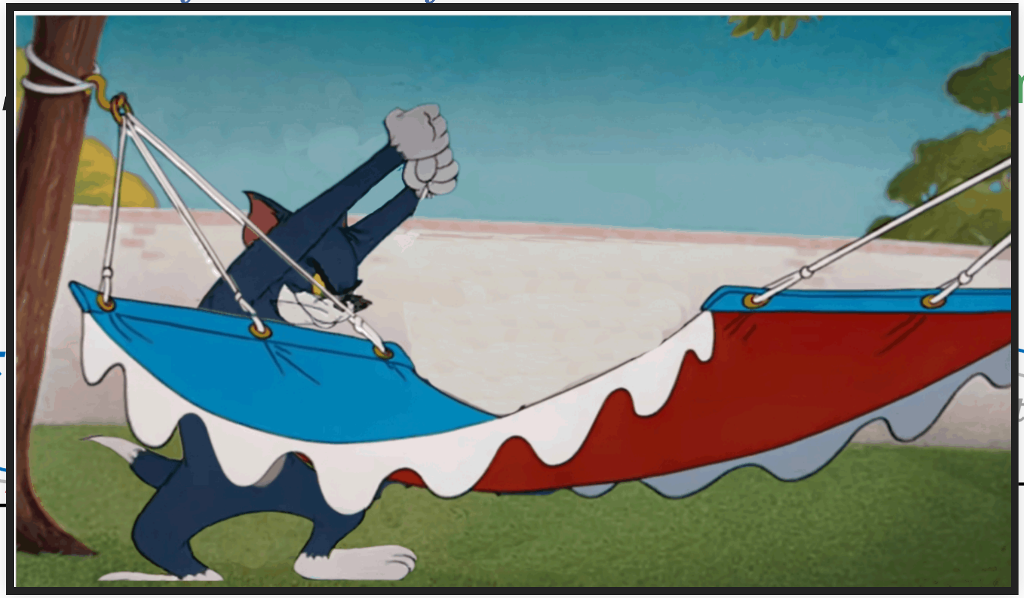
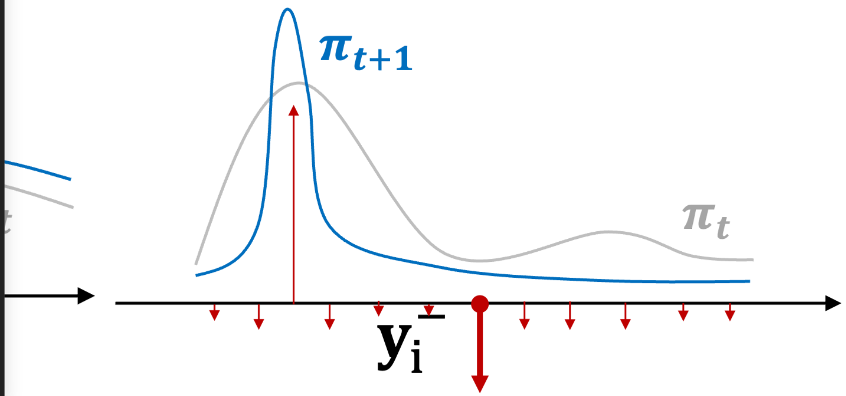
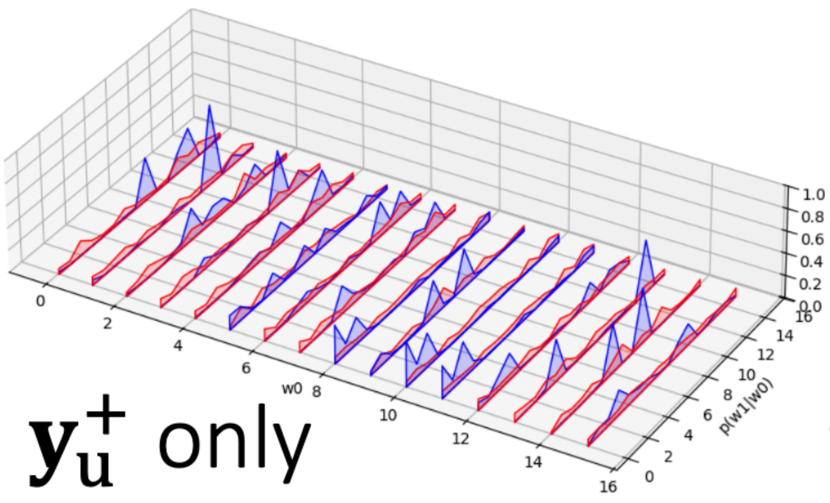
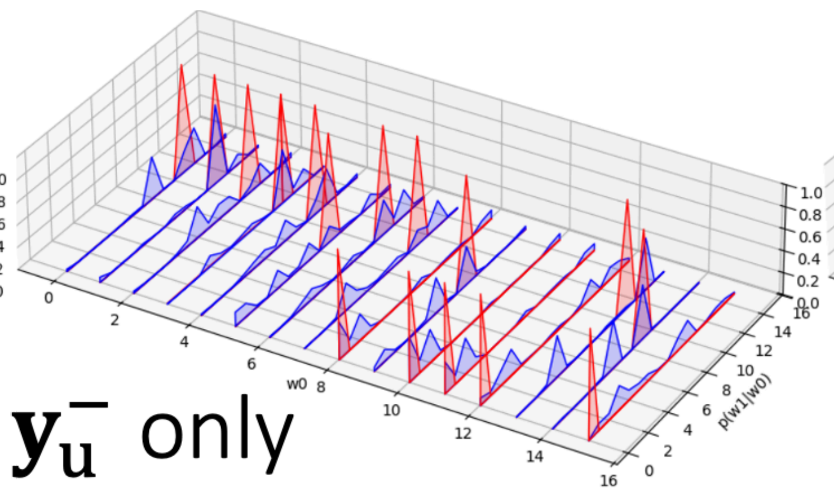


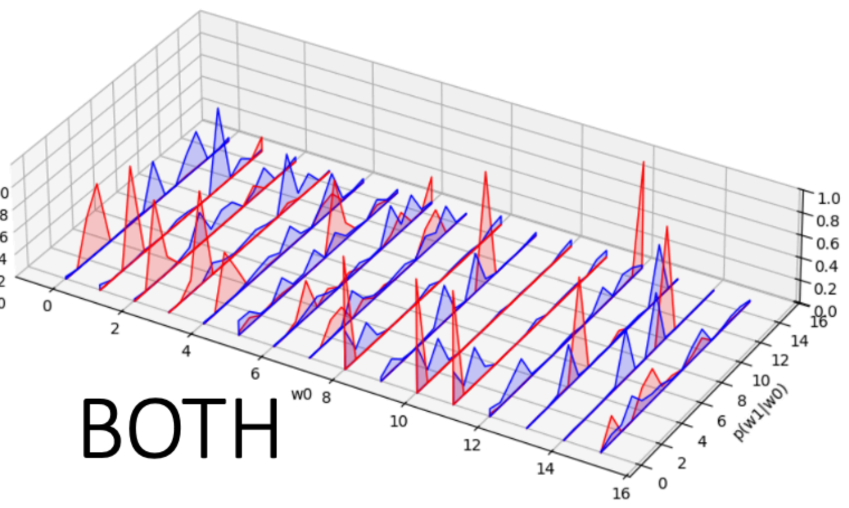




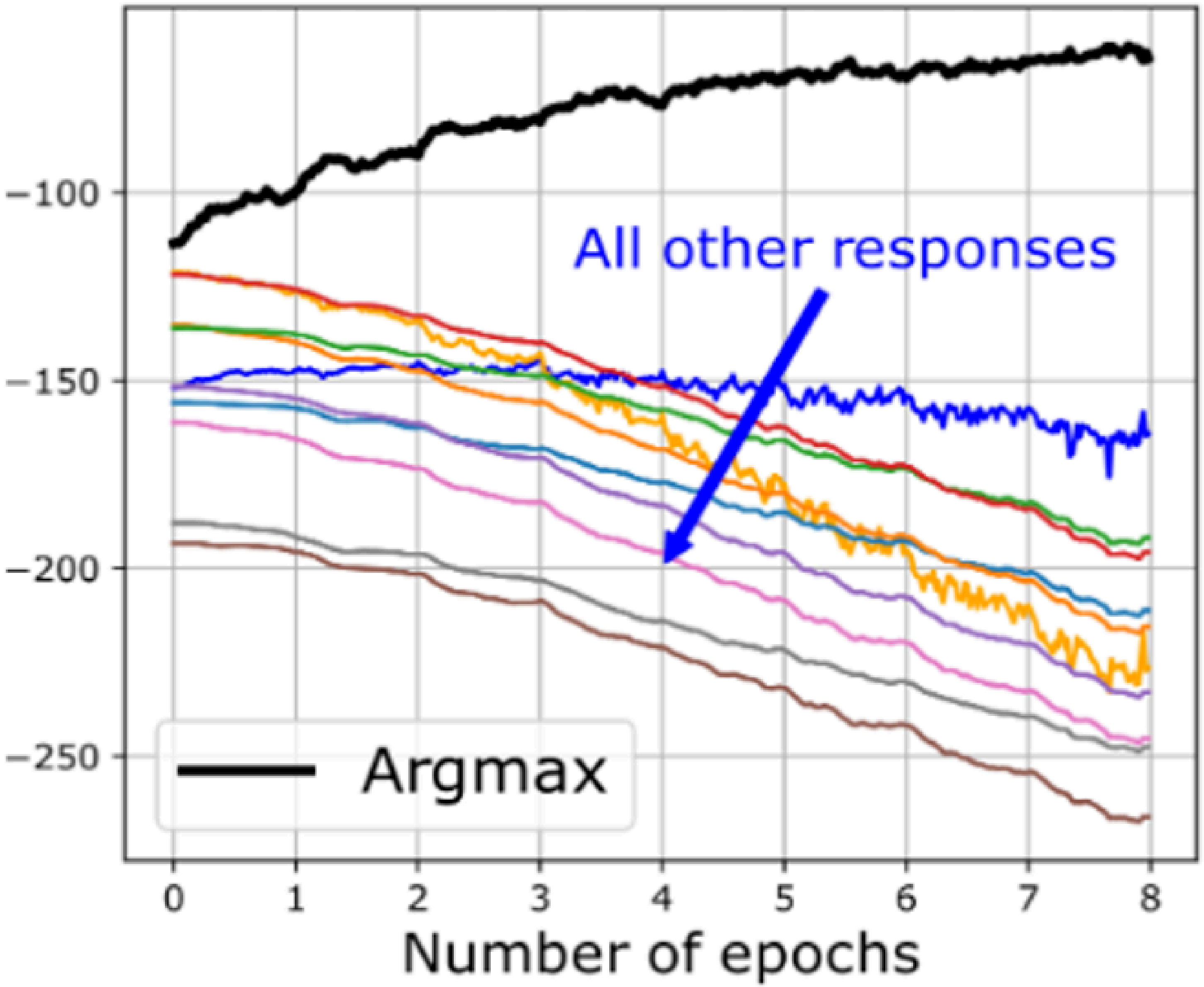
Positive gradients cancel out...*in the positive context*







Squeezing effect accumulates over time



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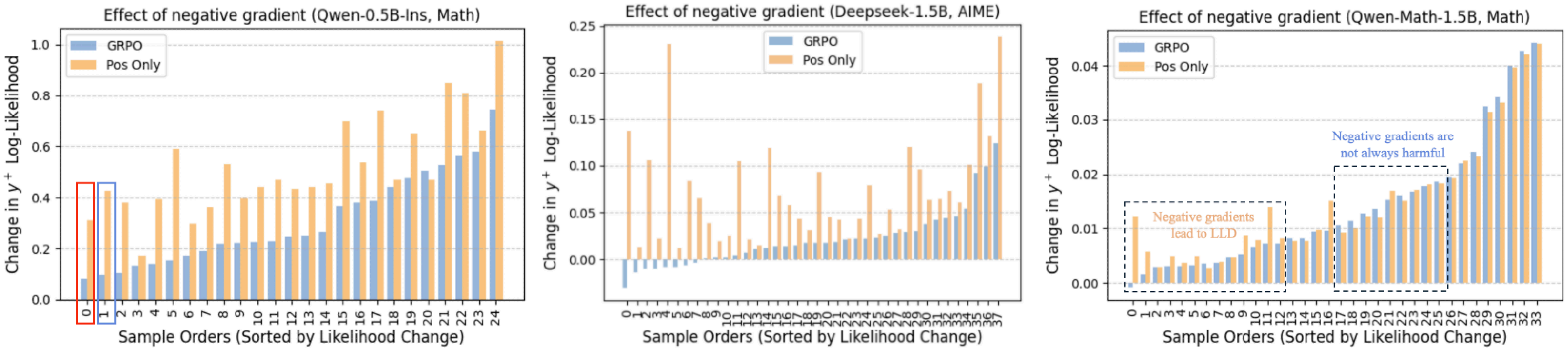
Group Relative Policy Optimization (GRPO) [DeepSeekMath 24]

- Similar to a “group-wise” version of DPO; negative gradients have similar effect!



(a) Qwen-0.5B-Instruct (b) Deepseek-1.5B (c) Qwen-Math-1.5B

Figure 1: We show that negative gradients can lead to small or reduced likelihood change of positive samples in GRPO. The log-likelihood gains achieved by `Pos Only` training (orange) are significantly higher than those from GRPO (blue) for Qwen-0.5B-Ins (a) and Deepseek-1.5B (b). In Qwen-Math-1.5B (c), samples with small or reduced $\Delta(\boldsymbol{x})$ (left) are primarily influenced by negative gradients, as evidenced by their larger $\Delta(\boldsymbol{x})$ in the `Pos Only` setup. However, some samples on the right show smaller $\Delta(\boldsymbol{x})$ than in GRPO, indicating that negative gradients are not always harmful.

Negative token hidden rewards

Down-weight penalties on tokens that are probably okay

Base model + Method	AIME24	AMC	MATH500	Minerva	Olympiad	Avg.
Qwen2.5-Math-1.5B						
Base	3.3	20.0	39.6	7.7	24.9	19.10
GRPO	13.3	57.5	**71.8**	29.0	34.1	41.14
Pos Only	10.0	57.5	70.6	30.1	31.0	39.84
NTHR	**16.7**	**57.5**	70.8	**30.5**	**34.2**	**41.94**
Qwen2.5-0.5B-Ins						
Base	0.0	2.5	33.4	4.4	7.0	9.46
GRPO	0.0	7.5	33.8	**9.2**	8.1	11.72
NTHR	0.0	**10.0**	**36.6**	8.1	**8.6**	**12.66**
Qwen2.5-1.5B-Ins						
Base	0.0	22.5	53.0	19.1	20.7	23.06
GRPO	3.3	32.5	57.2	18.8	**23.0**	26.96
NTHR	**6.7**	**35.0**	**58.8**	**21.0**	20.9	**28.48**
Qwen2.5-Math-1.5B (deepscaler)						
Base	3.3	20.0	39.6	7.7	24.9	19.10
GRPO	10.0	42.5	72.4	**32.4**	**31.9**	37.80
NTHR	**16.7**	**47.5**	**73.2**	29.4	31.4	**39.60**
Qwen2.5-3B						
Base	10.0	37.5	58.6	26.1	24.6	31.36
GRPO	6.7	35.0	**66.6**	31.2	**29.9**	33.88
NTHR	**10.0**	**47.5**	65.6	**31.6**	26.8	**36.30**

Table 2: Results across selected math benchmarks for different Qwen2.5 models and methods. NTHR consistently provides average performance gains on various models.

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Better supervisory signal implies better learning

- Classification: target is $\mathcal{L}_P = \mathbb{E}_{(x,y)}\,\mathcal{L}(x,y) = \mathbb{E}_x\,\mathbb{E}_{y|x}\,\ell_y(f(x))$
- Normally: see $\{(x_i, y_i)\}$, minimize

$$\mathcal{L}_{\mathbf{X},\mathbf{y}} = \frac{1}{N}\sum_{i=1}^{N} \ell_{y_i}(f(x_i))$$

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  - Can reduce variance if $p_i^{tar} \approx p_i^*$, the true conditional probabilities

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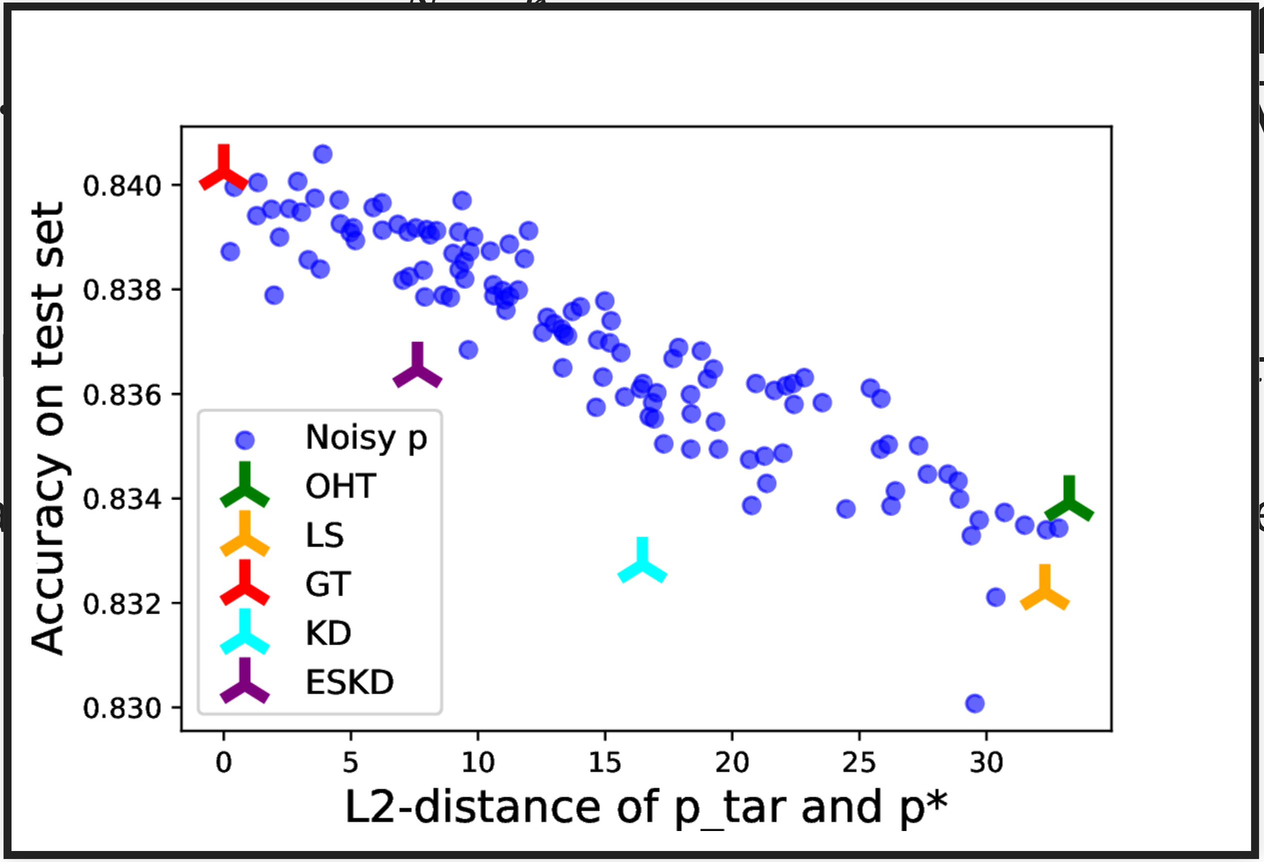

Knowledge distillation

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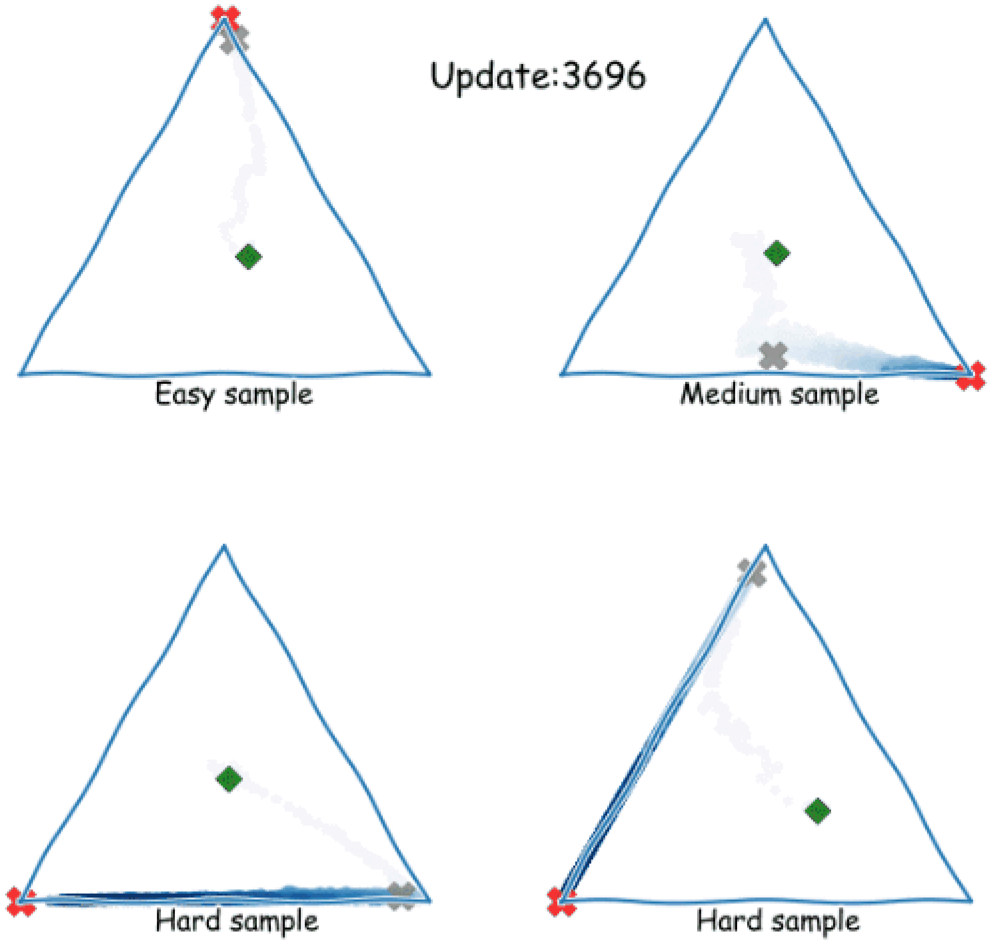
- But why would that be?

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

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

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

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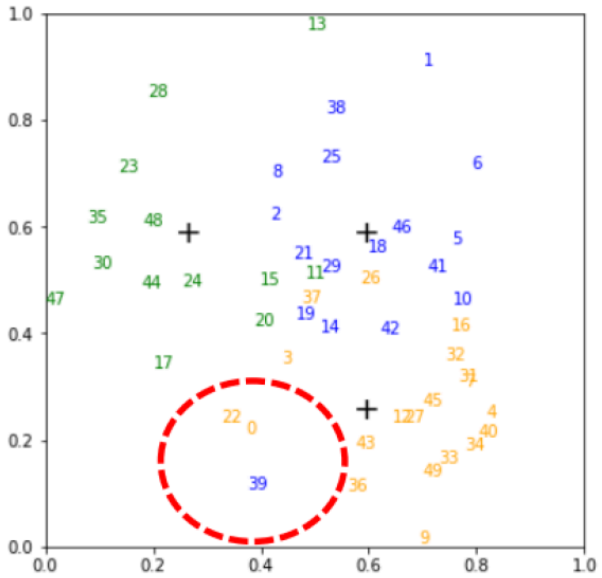

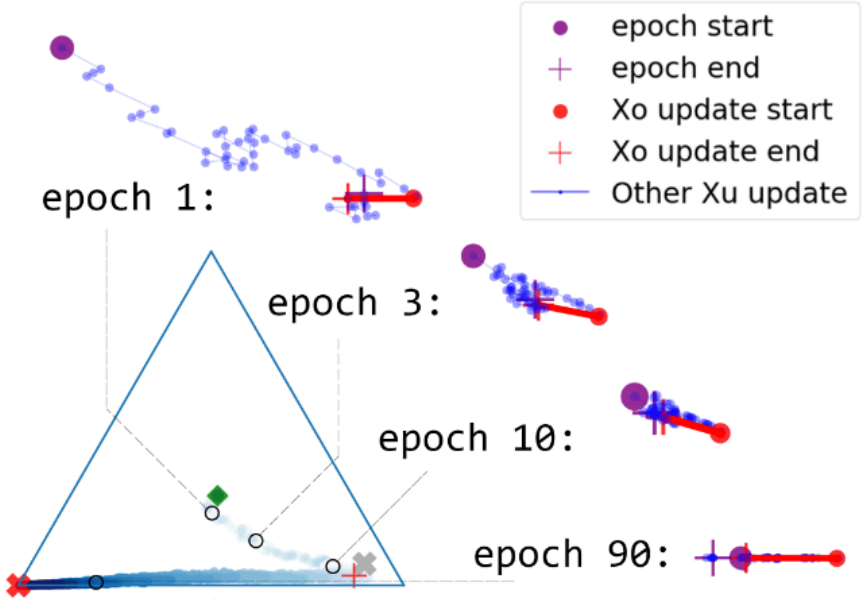

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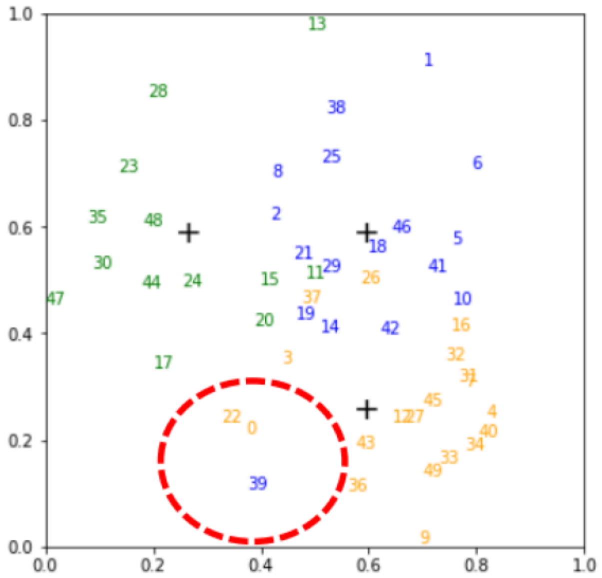

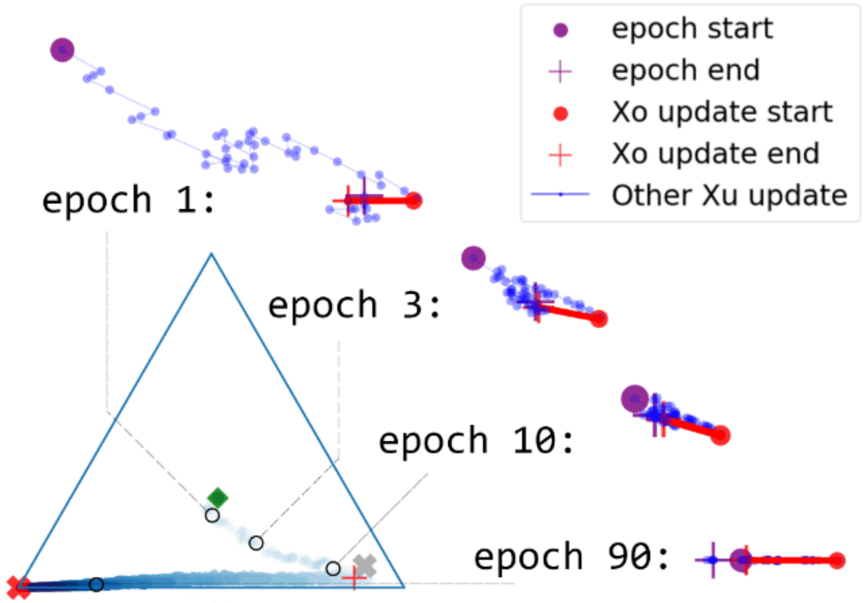

- Improves distillation (esp. with noisy labels) to take moving average of $q_t(x_i)$ as p_i^{tar}

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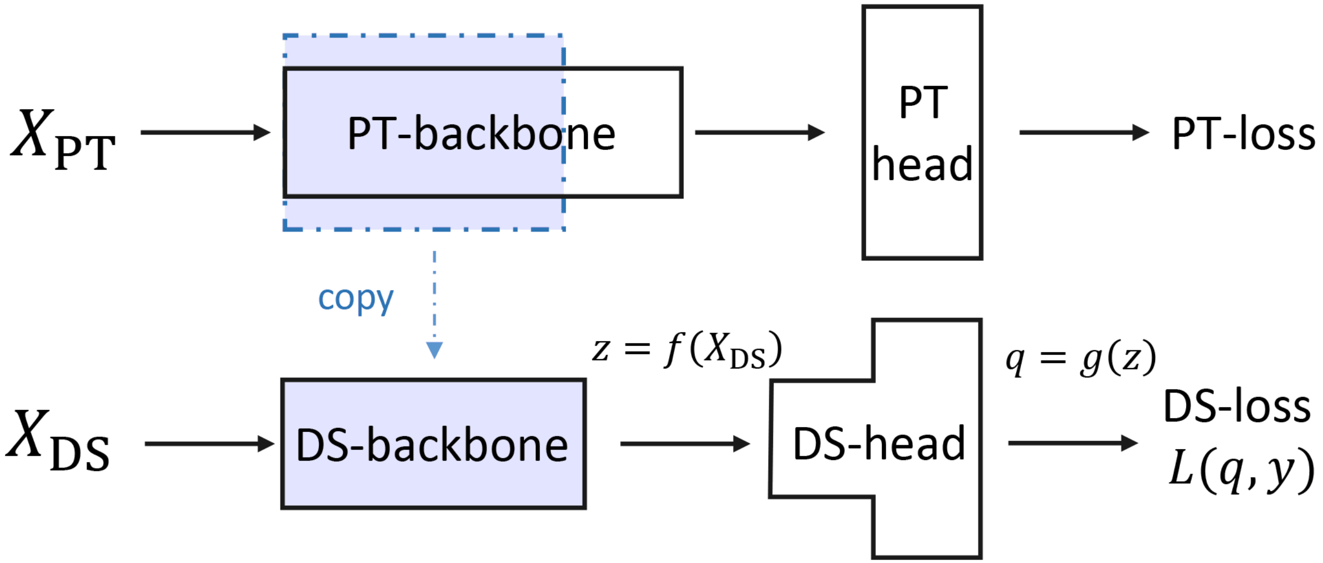
Fine-tuning



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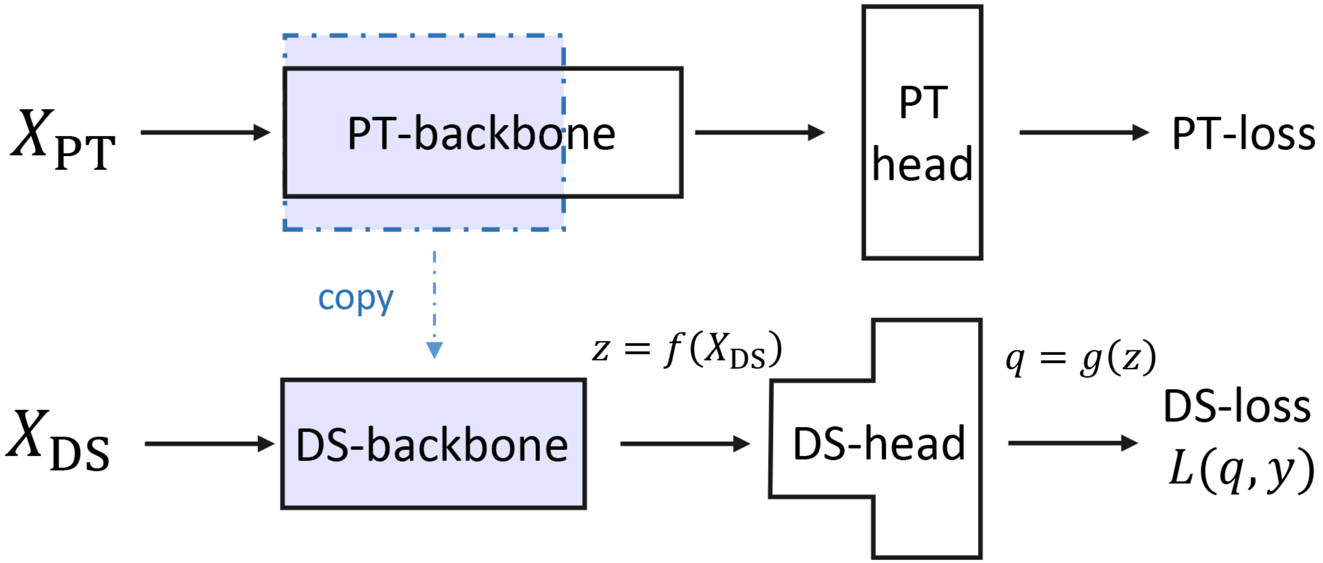

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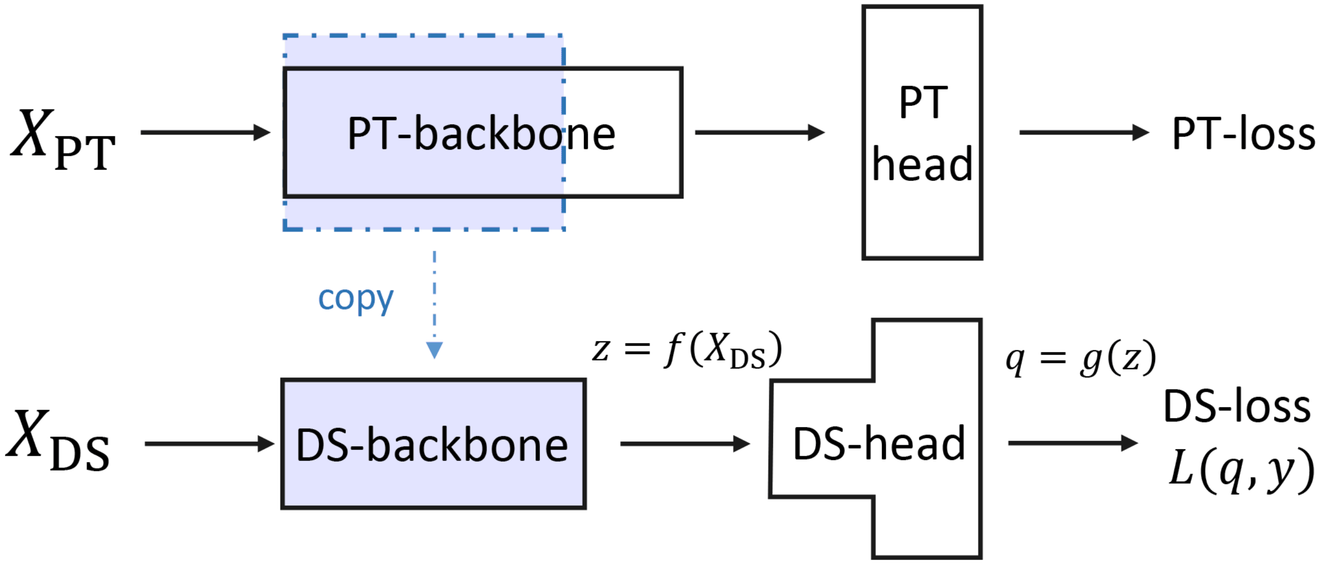

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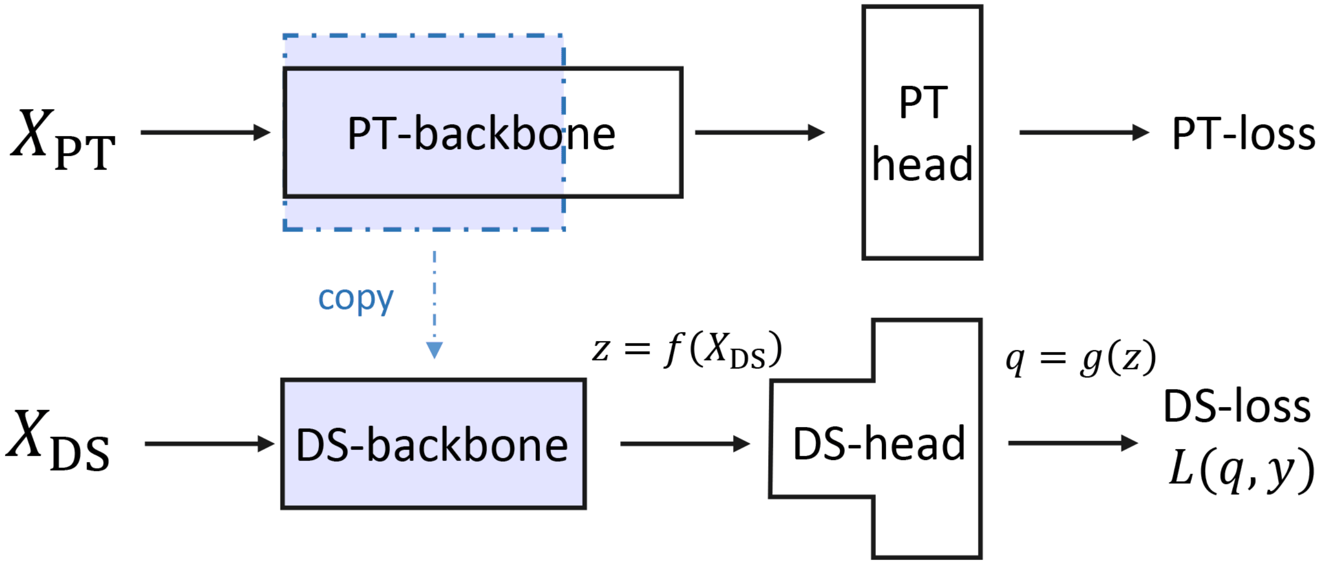

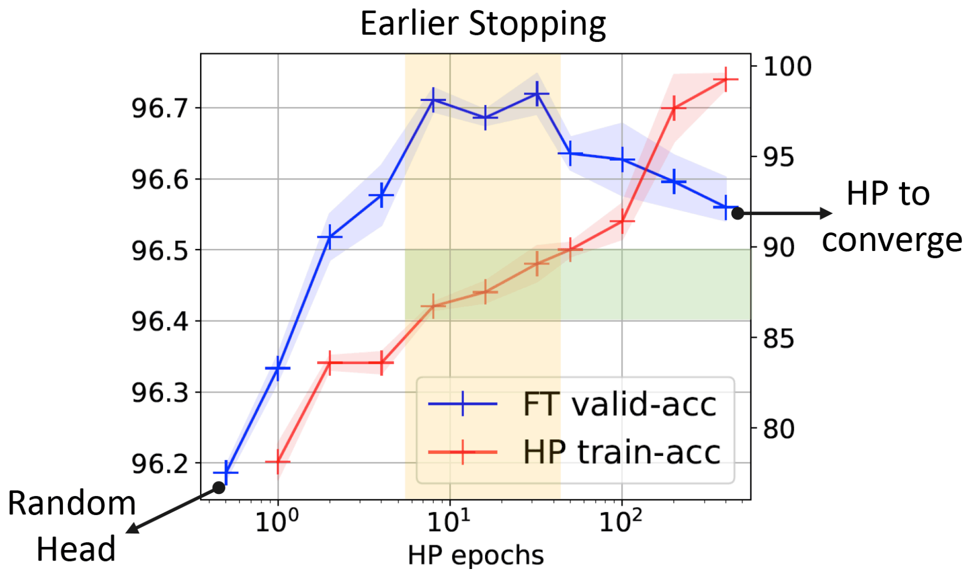

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How much do we change our features?

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- 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]

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Approximate retraining with local linearization

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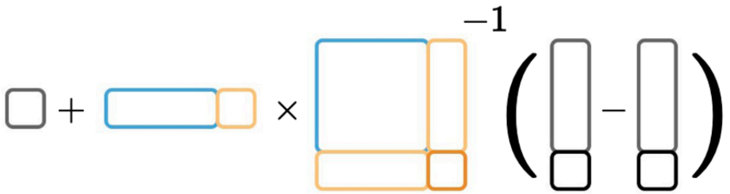
  - Rank-one updates for efficient computation: schema 

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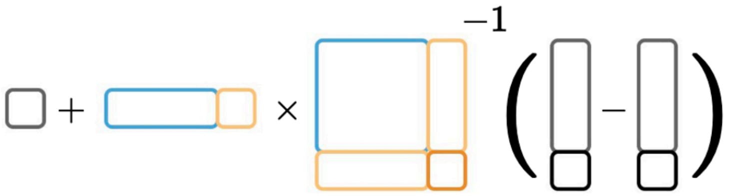
  - Rank-one updates for efficient computation: schema 

- We prove this is exact for infinitely wide networks
  - $f_0 \rightarrow f_{\mathcal{L}} \rightarrow f_{\mathcal{L}\cup\{(x_i,y_i)\}}$ agrees with direct $f_0 \rightarrow f_{\mathcal{L}\cup\{(x_i,y_i)\}}$

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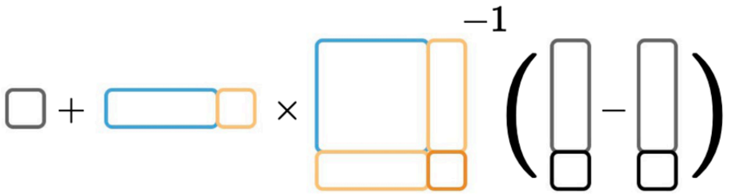
  - Rank-one updates for efficient computation: schema 

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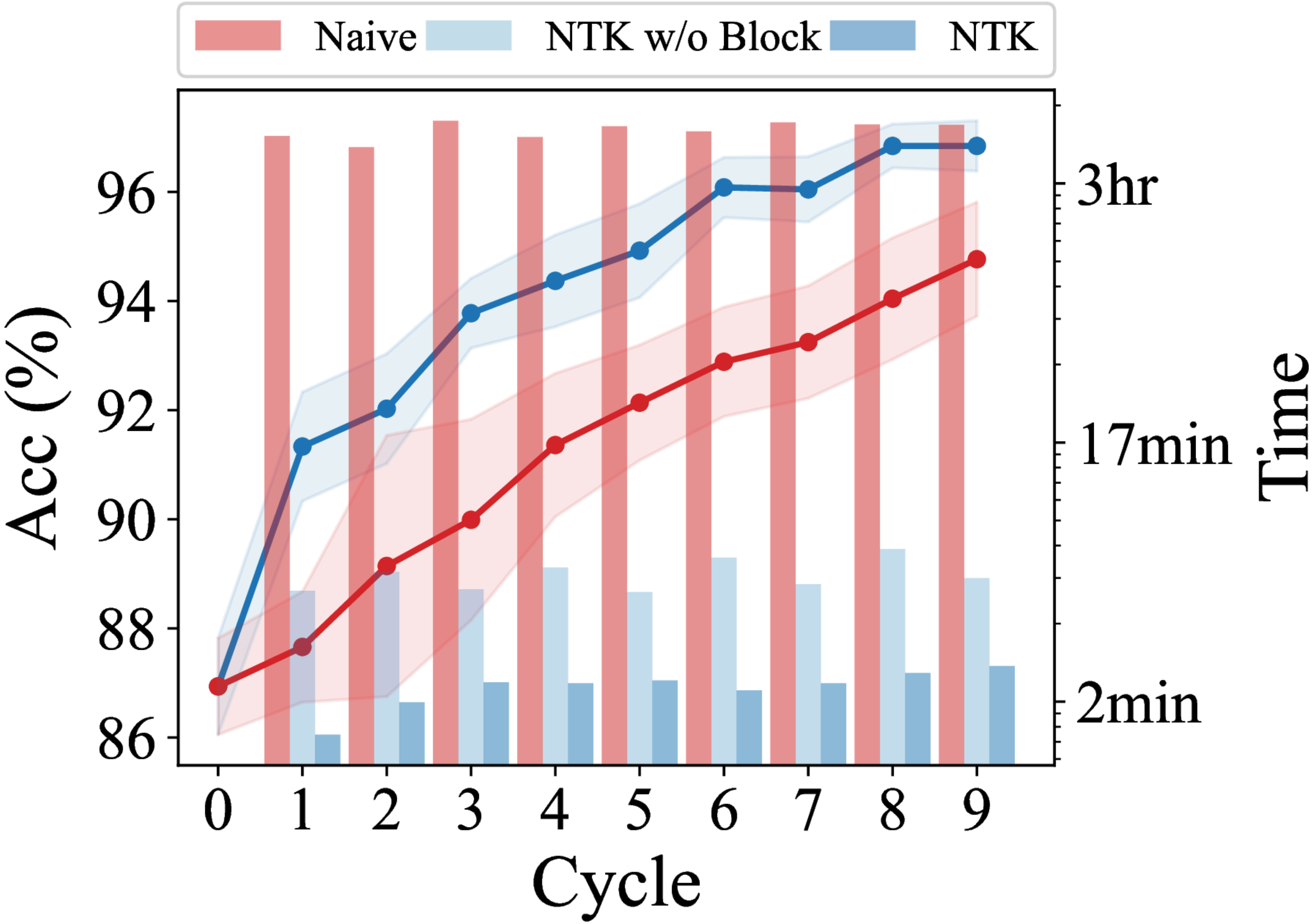
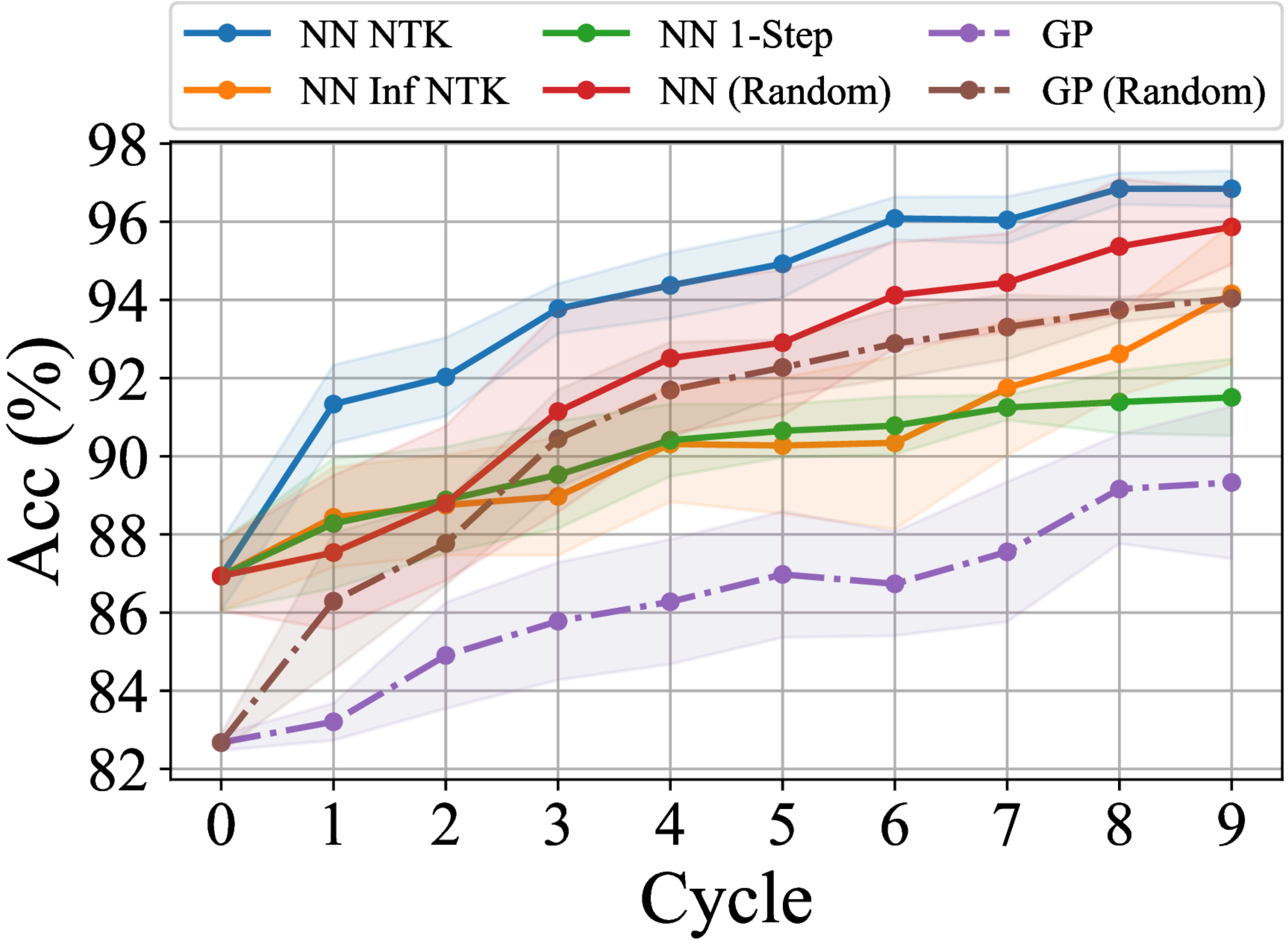
- Local approximation with eNTK “should” work much more broadly than “NTK regime”

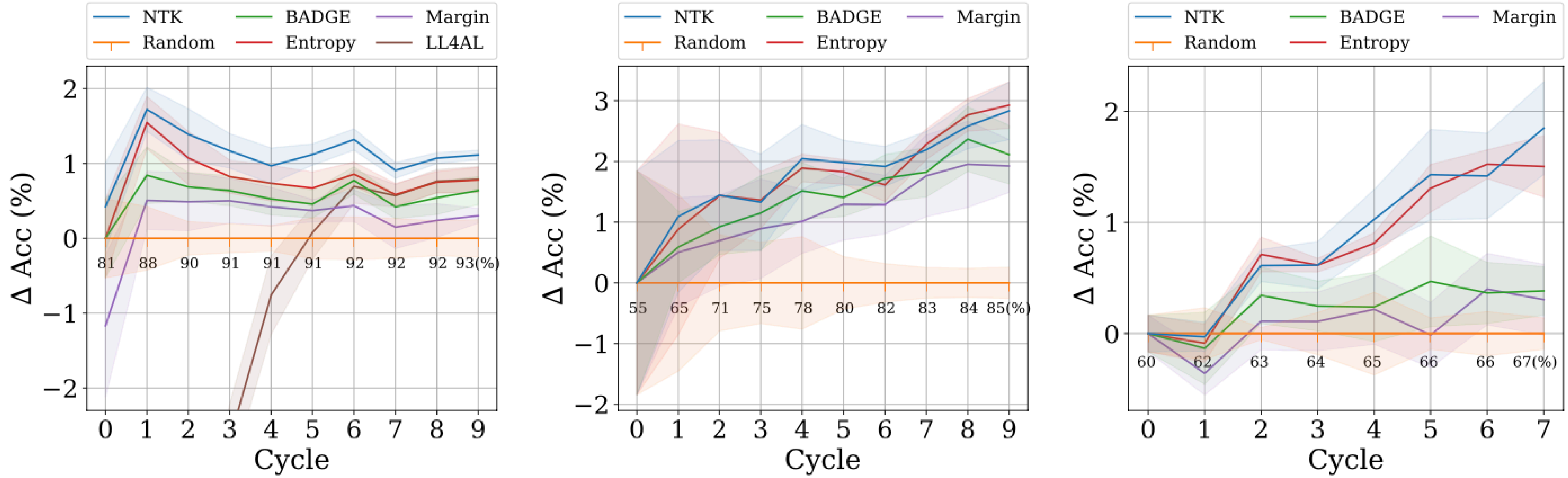
Much faster than SGD



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

What can we learn from empirical NTKs?

- As a theoretical tool for local understanding:
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  - Why GRPO does weird stuff + how to fix
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  - 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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- Lots of work (including above) has used pNTK instead of $\mathcal{K}$
  - 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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  - Fully-connected ReLU nets at init., fan-in mode: numerator $\mathcal{O}(h\sqrt{h})$, denom $\Theta(h^2)$

pNTK's Frobenius error

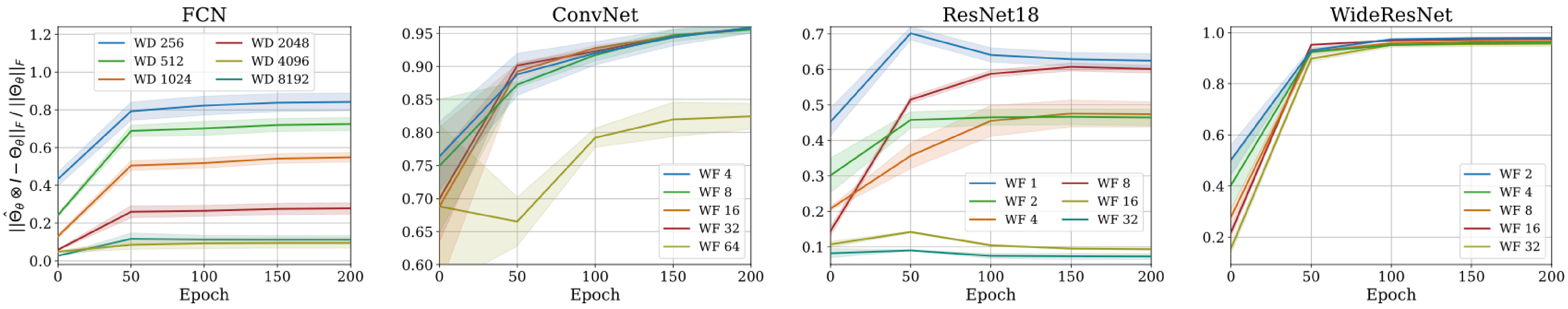

Figure 3: Evaluating the **relative difference of Frobenius norm of** $\Theta_\theta(\mathcal{D}, \mathcal{D})$ **and** $\hat{\Theta}_\theta(\mathcal{D}, \mathcal{D}) \otimes I_O$ at initialization and throughout training, based on $\mathcal{D}$ being 1000 random points from CIFAR-10. Wider nets have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

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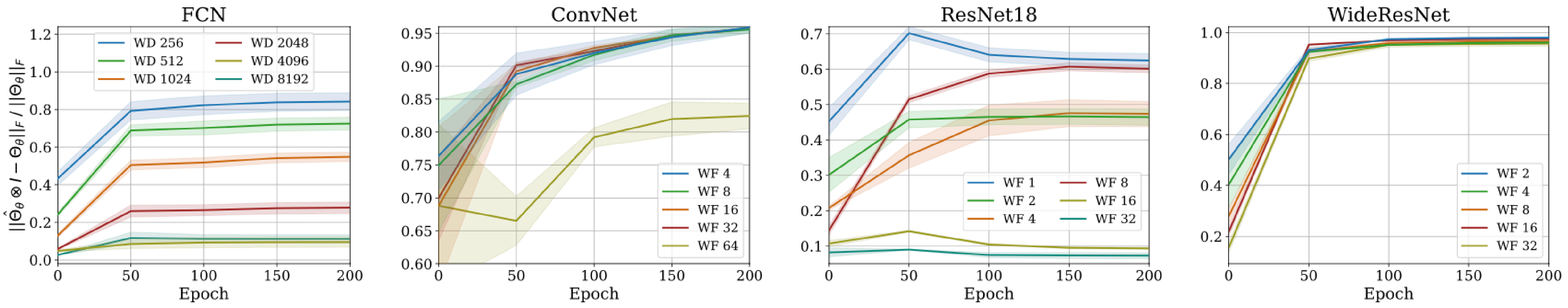

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Same kind of theorem / empirical results for largest eigenvalue,
and empirical results for $\lambda_{\min}$, condition number

Kernel regression with pNTK

- Reshape things to handle prediction appropriately:

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

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

Kernel regression with pNTK

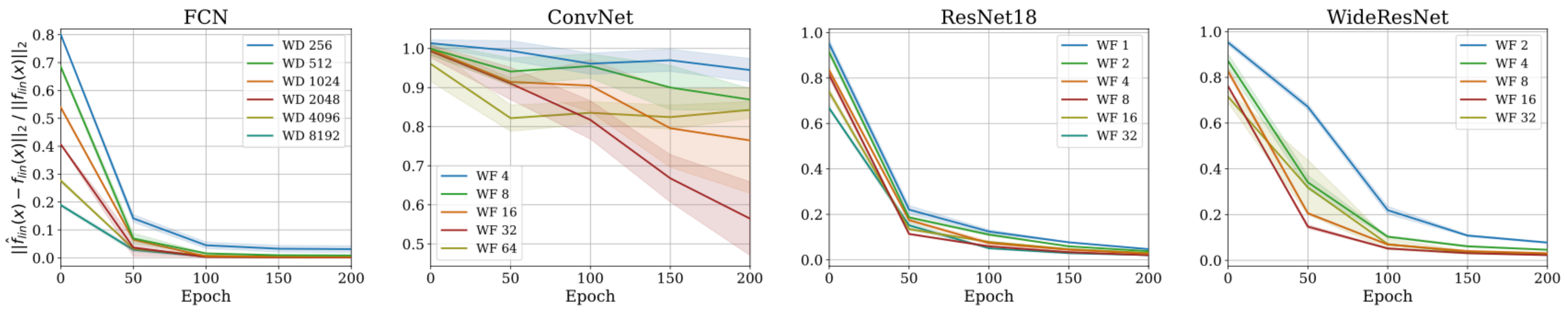


Figure 7: The **relative difference of kernel regression outputs**, (4) and (5), when training on $|\mathcal{D}| = 1000$ random CIFAR-10 points and testing on $|\mathcal{X}| = 500$. For wider NNs, the relative difference in $\hat{f}^{lin}(\mathcal{X})$ and $f^{lin}(\mathcal{X})$ decreases at initialization.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

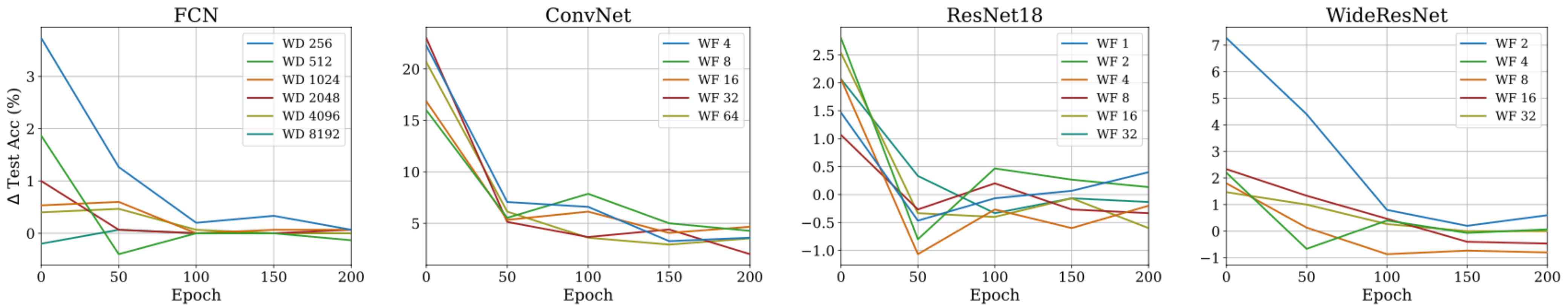


Figure 8: **Using pNTK in kernel regression** (as in Figure 7) **almost always achieves a higher test accuracy than using eNTK.** Wider NNs and trained nets have more similar prediction accuracies of $\hat{f}^{lin}$ and f^{lin} at initialization. Again, the difference between these two continues to vanish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

pNTK speed-up

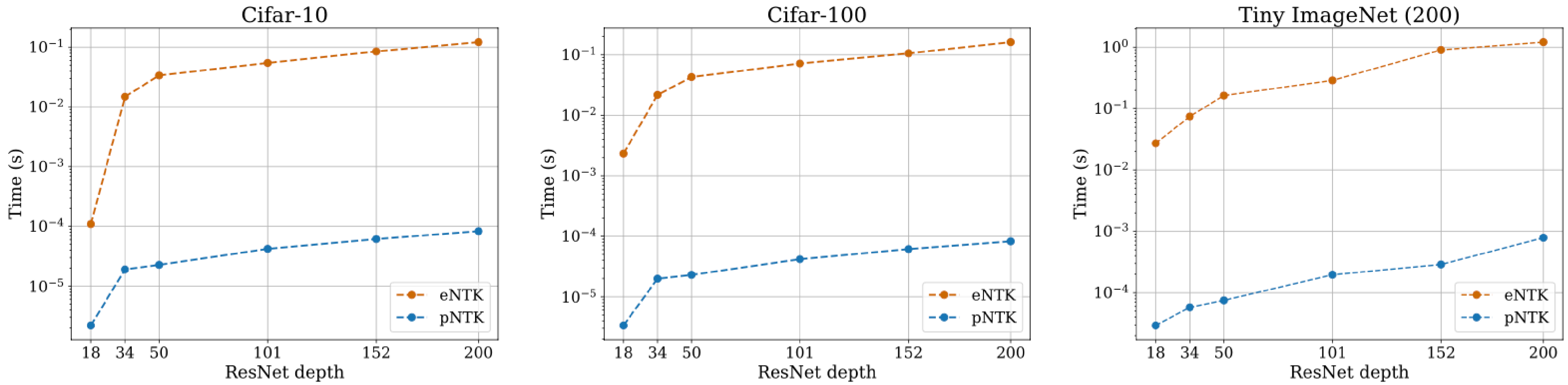
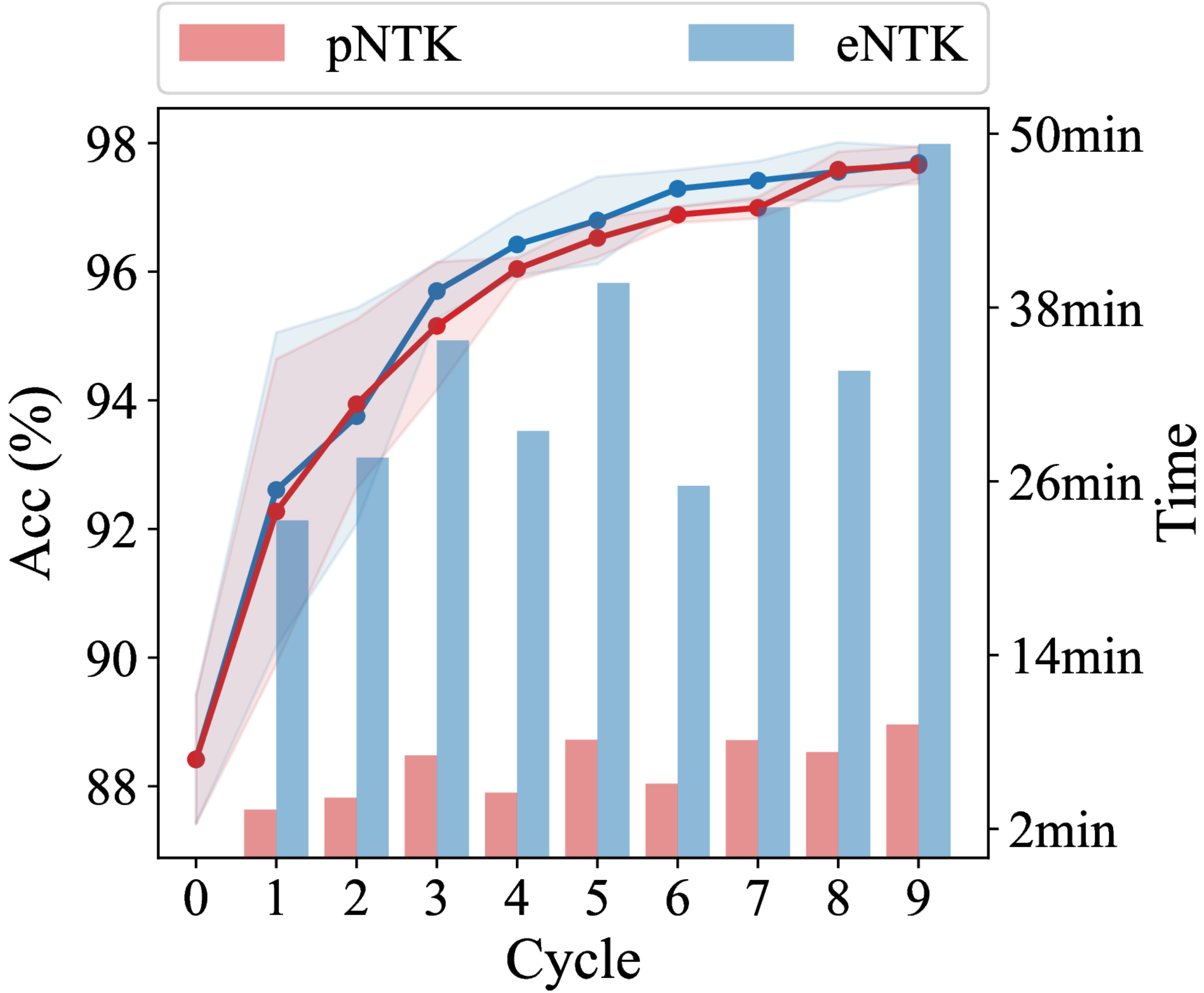


Figure 1: **Wall-clock time to evaluate the eNTK and pNTK** for one pair of inputs, across datasets and ResNet depths.

pNTK speed-up on active learning task



pNTK for full CIFAR-10 regression

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

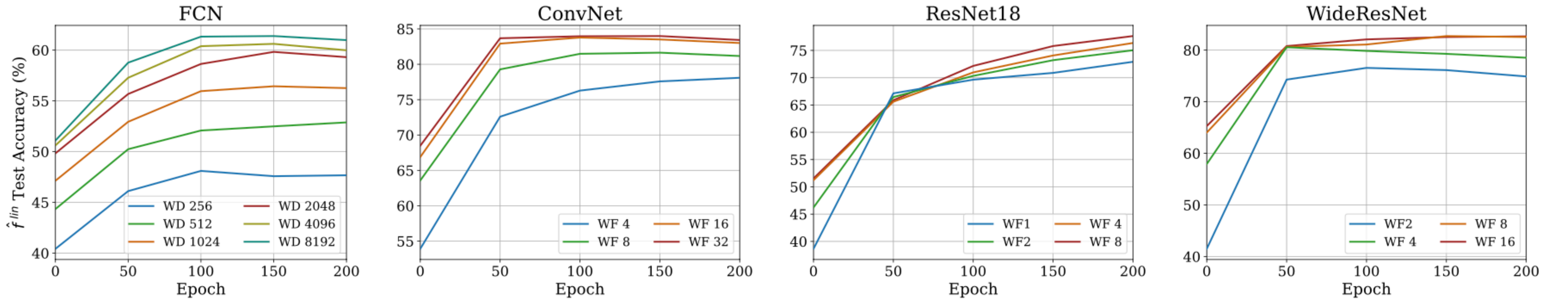


Figure 9: Evaluating the **test accuracy of kernel regression predictions using pNTK as in (5) on the full CIFAR-10 dataset**. As the NN's width grows, the test accuracy of $\hat{f}^{lin}$ also improves, but eventually saturates with the growing width. Using trained weights in computation of pNTK results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

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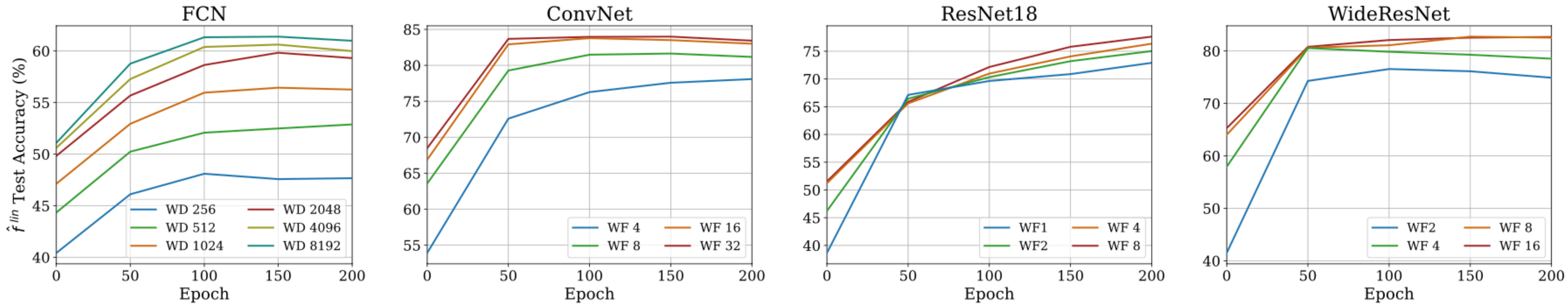

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- Worse than infinite NTK for FCN/ConvNet (where they can be computed, if you try hard)

pNTK for full CIFAR-10 regression

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

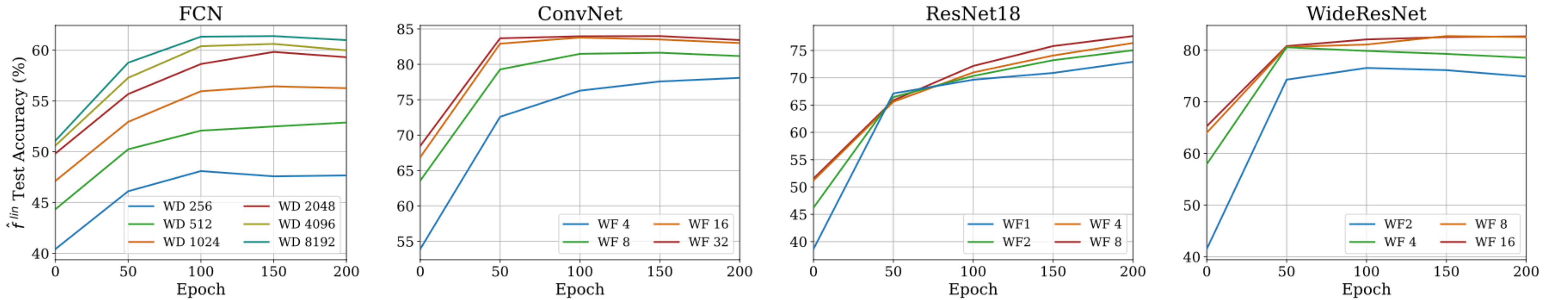

Figure 9: Evaluating the **test accuracy of kernel regression predictions using pNTK as in (5) on the full CIFAR-10 dataset**. As the NN's width grows, the test accuracy of $\hat{f}^{lin}$ also improves, but eventually saturates with the growing width. Using trained weights in computation of pNTK results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

- 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

Ren, S. Learning dynamics of LLM Finetuning

Deng, Ren, M. Li, S., X. Li, Thrampoulidis On the Effect of Negative Gradient in Group Relative Deep Reinforcement Optimization

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