Identifying good directions to escape the NTK regime and efficiently learn low-degree plus sparse polynomials Eshaan Nichani¹, Yu Bai², and Jason D. Lee¹ NeurIPS 2022

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Optimization

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Couple to convex problem \bullet





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Generalization



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Q: Can we encourage each neuron to move further and escape the NTK regime? **Does this allow us to break NTK sample complexity lower bounds?**

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• 2-layer neural network of width m: $f(x; \mathbf{W}) = m^{-1/2} a^T \sigma(\mathbf{W}x)$, where $a \in \mathbb{R}^m, \mathbf{W} \in \mathbb{R}^{m \times d}$.

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Feature map $\phi : \mathbb{R}^{d} \to \mathbb{R}^{ma}$

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Goal #1: Regularize to prevent movement in small eigenvalue directions.



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Lemma (informal): Eigenspectrum of Σ can be partitioned into 3 groups:

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Goal #2: Move in Q_3 directions, but minimally in Q_2 directions.

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$$\sum_{n=1}^{N} + \frac{1}{2} \left(\mathbf{W} - \mathbf{W}_{0} \right)^{T} \nabla_{\mathbf{W}}^{2} f(x; \mathbf{W}_{0}) (\mathbf{W} - \mathbf{W}_{0})$$
QuadNTK

expansion:

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NTK is minimax optimal for dense polynomials, QuadNTK can learn sparse polynomials. **Question:** Can we jointly use **both** terms to learn a larger class of functions?

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• $f_{\leq k}$ is dense degree k polynomial (low-degree term)

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- We obtain better sample complexity than either NTK or QuadNTK on their own \Longrightarrow best of both worlds!

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4. Generalization

Small regularized training loss implies small population loss.

Experiments

 $f_L + f_Q$ trained on a degree 2 signal with $d^{1.5}$ samples

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 - How does the QuadNTK relate to feature learning?

Thanks for Listening!

References:

[1] Sanjeev Arora, Simon S. Du, Wei Hu, Zhiyuan Li, Ruslan Salakhutdinov, and Ruosong Wang. On exact computation with an infinitely wide neural net. In Advances in Neural Information Processing Systems (NeurIPS), 2019. [2] Behrooz Ghorbani, Song Mei, Theodor Misiakiewicz, and Andrea Montanari. Linearized two-layers neural networks in high dimension. The Annals of Statistics, 49:1029-1054, 2021 [3] Andrea Montanari and Yiqiao Zhong. The interpolation phase transition in neural networks: Memorization and generalization under lazy training, 2020. URL https://arxiv.org/ abs/2007.12826. [4] Yu Bai and Jason D. Lee. Beyond linearization: On quadratic and higher-order approximation of wide neural networks. In International Conference on Learning

Representations (ICLR), 2020.