Understanding and Scaling Large and Deep Neural Networks or "Random Matrix Theory for Extremely Large-Scale ML"

@ Shanghai Jiao Tong University

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based on work of G. Yang at xAI, C. Pehlevan at Harvard, J. Pennington at Google, etc.

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Outline

1. Motivation: do we (still) need math and theory for modern ML?
2. Math theory for modern ML: a theoretical perspective
3. Math theory for modern ML: a practical perspective

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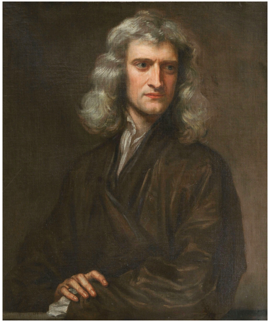

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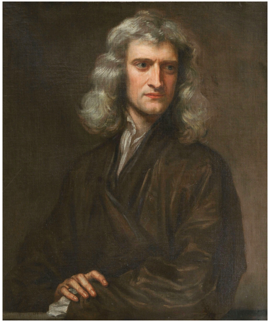

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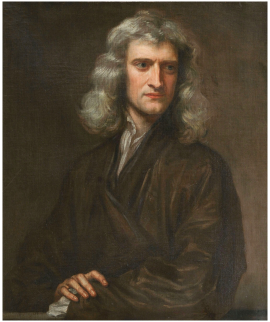

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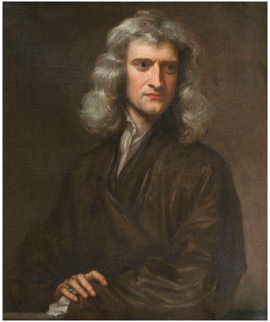
- **In this talk**, convey that math theory is still **important** in the design of large-scale ML models, with the example of **Random Matrix Theory (RMT)** for large and deep neural networks (DNNs)



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Scaling of sum of independent random variables: LLN and CLT

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$$\sqrt{n} \left(\frac{1}{n} \sum_{i=1}^{n} (x_i - \mu) \right) \to \mathcal{N}(0, \sigma^2), \tag{2}$$
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For i.i.d. random variables $x_1, \ldots, x_n$ of zero mean and unit variance, e.g., $x_i \sim \mathcal{N}(0,1)$, we have, for n large, the following scaling laws for the sum $\frac{1}{n} \sum_{i=1}^{n} x_i$:

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- $\frac{1}{n} \sum_{i=1}^{n} x_i \simeq 0$ by LLN; and
- $\frac{1}{\sqrt{n}} \sum_{i=1}^{n} x_i = O(1)$ with high probability by CLT.

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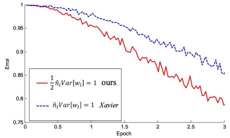

Figure 2. The convergence of a **22-layer** large model (B in Table 3). The x-axis is the number of training epochs. The y-axis is the top-1 error of 3,000 random val samples, evaluated on the center crop. We use ReLU as the activation for both cases. Both our initialization (red) and "*Xavier*" (blue) [7] lead to convergence, but ours starts reducing error earlier.

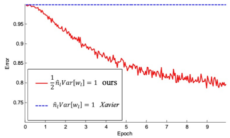

Figure 3. The convergence of a **30-layer** small model (see the main text). We use ReLU as the activation for both cases. Our initialization (red) is able to make it converge. But "*Xavier*" (blue) [7] completely stalls - we also verify that its gradients are all diminishing. It does not converge even given more epochs.

Figure: Numerical results in [He+15] for moderately deep NN.

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Objective: for large p, N, achieve **appropriate scaling** on (a, b, c, d) so that

1. **pre-activations $\mathbf{h}^{(\ell)}$ have $\Theta(1)$ entries**:
   - computing the 1st and 2nd moments of $\mathbf{h}^{(1)}$: $\mathbb{E}[\mathbf{h}_i^{(1)}] = \mathbf{0}$, $\mathbb{E}[\mathbf{h}_i^{(1)} (\mathbf{h}_j^{(1)})^\mathsf{T}]_{kq} = \delta_{kq} N^{-(2a_1+b_1)} \cdot \frac{1}{p} \mathbf{x}_i^\mathsf{T} \mathbf{x}_j$; then of $\mathbf{h}^{(\ell)}$
   - we get $\boxed{2a_1 + b_1 = 1}$ and similarly $\boxed{2a_\ell + b_\ell = 1, \ell \in \{1, \ldots, L\}}$
2. **network prediction evolve in $\Theta(1)$ time**:
   - define **feature/conjugate kernel** as the Gram matrix at layer ℓ as $\boldsymbol{\Phi}^{(\ell)} \in \mathbb{R}^{n \times n}$, $\Phi_{ij}^{(\ell)} = \frac{1}{N} \sigma(\mathbf{h}_i^{(\ell)})^\mathsf{T} \sigma(\mathbf{h}_j^{(\ell)})$

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- this is equivalent to the muP parameterization in [YH21]

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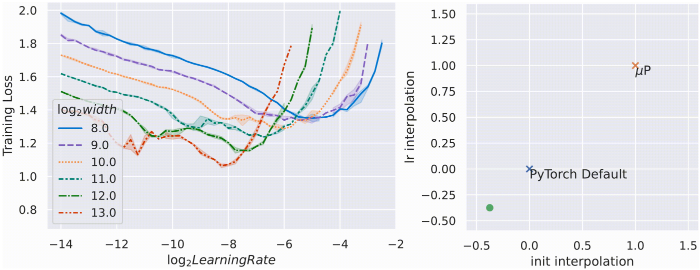
Some experiments on muP and μTransfer



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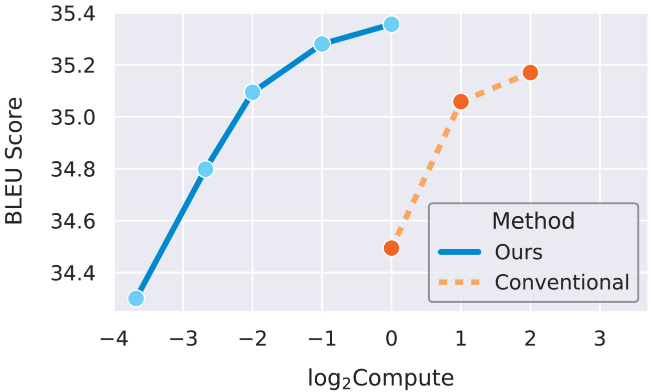

Figure: Comparison μTransfer, which transfers tuned hyperparameters from a small proxy model, with directly tuning the large target model, on IWSLT14 De-En, a machine translation dataset.

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References:

- Tuning GPT-3 on a Single GPU Tensor Programs V, blog by G. Yang. `https://decentdescent.org/tp5.html`
- Cengiz Pehlevan and Blake Bordelon, Lecture Notes on Infinite-Width Limits of Neural Networks, *Princeton Machine Learning Theory Summer School*, 2023.
- Greg Yang and Edward J. Hu. "Tensor Programs IV: Feature Learning in Infinite-Width Neural Networks". In: *Proceedings of the 38th International Conference on Machine Learning*. PMLR, July 2021, pp. 11727–11737

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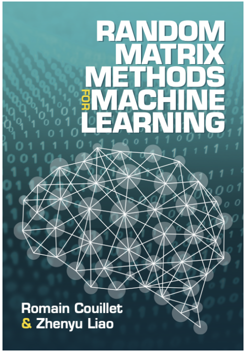

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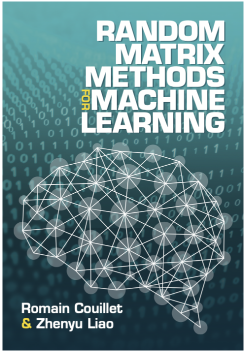

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