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

Motivation: do we (still) need math and theory in modern ML?

- **Math has helped a lot in the past**: from Kepler's laws of planetary motion to Newton and calculus
- **AI is doing great**: there is a bit math (in defining problems and computing), but hardly analytic
- for modern AI: **intuition, data, and computation** seem the most important, NOT analytic math theory
- **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)

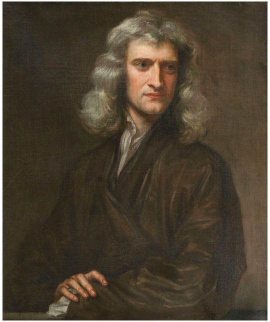


Figure: Portrait of Newton at 46, 1689.

Scaling of sum of independent random variables: LLN and CLT

- **Strong law of large numbers (LLN)**: for a sequence of i.i.d. random variables $x_1, \ldots, x_n$ with the same expectation $\mathbb{E}[x_i] = \mu < \infty$, we have
$$\frac{1}{n}\sum_{i=1}^{n} x_i \to \mu, \tag{1}$$
almost surely as $n \to \infty$.
- **Central limit theorem (CLT)**: for a sequence of i.i.d. random variables $x_1, \ldots, x_n$ with the same expectation $\mathbb{E}[x_i] = \mu$ and variance $\mathrm{Var}[x_i] = \sigma^2 < \infty$, we have
$$\sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)\right) \to \mathcal{N}(0, \sigma^2), \tag{2}$$
in distribution as $n \to \infty$.

Consequences of LLN and CLT

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 $\frac{1}{n}\sum_{i=1}^{n} x_i$:

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

We have known this a bit in the context of DNN

- DNNs involve linear (i.e., weights) and nonlinear (i.e., activation) transformation
- **Xavier initialization** [GB10]: for sigmoid-type activation, randomly initialize a weight matrix $\mathbf{W} \in \mathbb{R}^{N \times N}$ having N neurons as

$$[\mathbf{W}]_{ij} \sim \mathcal{N}(0, N^{-1}). \tag{3}$$

```
torch.nn.init.xavier_normal_
```

- **He initialization** [He+15]: for ReLU-type activation, randomly initialize a weight matrix $\mathbf{W} \in \mathbb{R}^{N \times N}$ having N neurons as

$$[\mathbf{W}]_{ij} \sim \mathcal{N}(0, 2N^{-1}). \tag{4}$$

```
torch.nn.init.kaiming_normal_
```

- derivation based on **forward propagation**
- similar considerations for CNN, RNN, ResNet, etc.

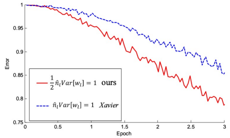


Figure 2. The convergence of a **22-layer** large model (B in Table 3). The x-axis is the number of training epochs. The y-axis is the top-1 error of 3,000 random val samples, evaluated on the center crop. We use ReLU as the activation for both cases. Both our initialization (red) and "*Xavier*" (blue)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

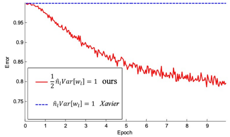


Figure 3. The convergence of a **30-layer** small model (see the main text). We use ReLU as the activation for both cases. Our initialization (red) is able to make it converge. But "*Xavier*" (blue) [7] completely stalls - we also verify that its gradients are all diminishing. It does not converge even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

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

Let us say more on the appropriate scaling of large and deep NNs

Setup and Notations:

- supervised training of an L-layer multi-layer perceptrons (MLP) with full batch gradient flow
- input data $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^p$, denote pre-activation vectors $\mathbf{h}_i^{(\ell)} \in \mathbb{R}^N$ at layer $\ell \in \{1, \ldots, L\}$ as

$$\boxed{\mathbf{h}_i^{(1)} = \frac{1}{N^{a_1}\sqrt{p}} \mathbf{W}^{(1)} \mathbf{x}_i, \quad \mathbf{h}_i^{(\ell)} = \frac{1}{N^{a_\ell}} \mathbf{W}^{(\ell)} \sigma_\ell \left(\mathbf{h}_i^{(\ell-1)} \right)} \quad i \in \{1, \ldots, n\} \tag{5}$$

- scalar output $\boxed{f_{\boldsymbol{\theta}}(\mathbf{x}_i) = \frac{1}{\gamma N^{a_L}} \left(\mathbf{w}^{(L)} \right)^{\mathsf{T}} \sigma_\ell \left(\mathbf{h}_i^{(\ell-1)} \right)}$ for trainable parameters $\boldsymbol{\theta} = \{ \mathbf{W}^{(1)}, \ldots, \mathbf{w}^{(L)} \}$.
- for a training set $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, train the above DNN on the loss function $L(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^n L(f_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i)$, with full-batch gradient flow

$$\frac{d\boldsymbol{\theta}}{dt} = -\eta \frac{\partial L(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \eta \frac{1}{n} \sum_{i=1}^n \Delta_i \frac{\partial f_{\boldsymbol{\theta}}(\mathbf{x}_i)}{\partial \boldsymbol{\theta}}, \quad \Delta_i \equiv -\frac{\partial L(f_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i)}{\partial f_{\boldsymbol{\theta}}(\mathbf{x}_i)}, \tag{6}$$

  learning rate $\boxed{\eta = \eta_0 \gamma^2 N^{-c}}$ and **feature learning parameter** $\boxed{\gamma = \gamma_0 N^d}$ for $\eta_0 = \Theta(1)$ and $\gamma_0 = \Theta(1)$
- **initialization scaling scheme**: $\boxed{w_i^{(L)} \sim \mathcal{N}(0, N^{-b_L}), W_{ij}^{(\ell)} \sim \mathcal{N}(0, N^{-b_\ell})}$ and $W_{ij}^{(1)} \sim \mathcal{N}(0, N^{-b_1})$

Appropriate scaling of large and deep NNs

Settings:

- **scaling of NN model**: $\mathbf{h}_i^{(1)} = \frac{1}{N^{a_1}\sqrt{p}} \mathbf{W}^{(1)} \mathbf{x}_i$, $\mathbf{h}_i^{(\ell)} = \frac{1}{N^{a_\ell}} \mathbf{W}^{(\ell)} \sigma_\ell \left(\mathbf{h}_i^{(\ell-1)} \right)$, $f_{\boldsymbol{\theta}}(\mathbf{x}_i) = \frac{1}{\gamma N^{a_L}} \left(\mathbf{w}^{(L)} \right)^\mathsf{T} \sigma_\ell \left(\mathbf{h}_i^{(\ell-1)} \right)$
- **initialization scaling**: $w_i^{(L)} \sim \mathcal{N}(0, N^{-b_L})$, $W_{ij}^{(\ell)} \sim \mathcal{N}(0, N^{-b_\ell})$, and $W_{ij}^{(1)} \sim \mathcal{N}(0, N^{-b_1})$
- **trained under full-batch gradient flow**: $\frac{d\boldsymbol{\theta}}{dt} = -\eta \frac{\partial L(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \eta \frac{1}{n} \sum_{i=1}^n \Delta_i \frac{\partial f_{\boldsymbol{\theta}}(\mathbf{x}_i)}{\partial \boldsymbol{\theta}}$ of learning rate $\eta = \eta_0 \gamma^2 N^{-c}$ and feature learning parameter $\gamma = \gamma_0 N^d$ for $\eta_0 = \Theta(1)$ and $\gamma_0 = \Theta(1)$

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 $\mathbf{\Phi}^{(\ell)} \in \mathbb{R}^{n \times n}$, $\Phi_{ij}^{(\ell)} = \frac{1}{N} \sigma(\mathbf{h}_i^{(\ell)})^\mathsf{T} \sigma(\mathbf{h}_j^{(\ell)})$
   - under the condition of $\Theta(1)$ pre-activation, it can be shown that in the $N \to \infty$ limit that the pre-activations are **Gaussian process** of zero mean, and covariance given by the (expected) conjugate kernel
   - for $\partial_t f_{\boldsymbol{\theta}}(\cdot) = \Theta(1)$, we get $\boxed{2a_1 + c = 0}$ and $\boxed{2a_\ell + c = 1, \ell \in \{2, \ldots, L\}}$
   - include **classical "mean-field" parameterization** (with $c = 0$, $a_1 = 0$, and $a_\ell = 1/2$) as special case

Appropriate scaling of large and deep NNs

Settings:

- **scaling of NN model**: $\mathbf{h}_i^{(1)} = \frac{1}{N^{a_1}\sqrt{p}} \mathbf{W}^{(1)} \mathbf{x}_i$, $\mathbf{h}_i^{(\ell)} = \frac{1}{N^{a_\ell}} \mathbf{W}^{(\ell)} \sigma_\ell \left(\mathbf{h}_i^{(\ell-1)} \right)$, $f_{\boldsymbol{\theta}}(\mathbf{x}_i) = \frac{1}{\gamma N^{a_L}} \left(\mathbf{w}^{(L)} \right)^\mathsf{T} \sigma_\ell \left(\mathbf{h}_i^{(\ell-1)} \right)$
- **initialization scaling**: $w_i^{(L)} \sim \mathcal{N}(0, N^{-b_L})$, $W_{ij}^{(\ell)} \sim \mathcal{N}(0, N^{-b_\ell})$, and $W_{ij}^{(1)} \sim \mathcal{N}(0, N^{-b_1})$
- **trained under full-batch gradient flow**: $\frac{d\boldsymbol{\theta}}{dt} = -\eta \frac{\partial L(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \eta \frac{1}{n} \sum_{i=1}^n \Delta_i \frac{\partial f_{\boldsymbol{\theta}}(\mathbf{x}_i)}{\partial \boldsymbol{\theta}}$ of learning rate $\eta = \eta_0 \gamma^2 N^{-c}$ and feature learning parameter $\gamma = \gamma_0 N^d$ for $\eta_0 = \Theta(1)$ and $\gamma_0 = \Theta(1)$

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

3. **features evolve in $\Theta(1)$ time**:
   - by $\partial_t \mathbf{h}_i^{(\ell)} = \Theta(1)$ we have $2a_1 + c - d + 1/2 = 0$, recall that $2a_1 + c = 0$, this is $d = 1/2$, similarly $2a_\ell + c - d - 1/2 = 0$ so that $\boxed{d = 1/2}$
   - in fact, any $d < 1/2$ leads to kernel behavior, and $d = 0$ the **NTK parameterization**

- if further demand raw learning rate $\eta = \Theta(1)$, then parameterization is unique:

$$\boxed{d = 1/2, c = 1, a_\ell = 0, b_\ell = 1, a_1 = -1/2, b_1 = 1} \tag{7}$$

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

What is good about this appropriate scaling

- well, things (e.g., DNN pre-activation, evolution of prediction and feature/pre-activation with respect to time) do not scale with the network width N
- BTW, in the case of **ResNet**, a scaling scheme of a similar type can be obtained by considering the infinitely deep $L \to \infty$ limit [Bor+23]
- idea of **maximal update parameterization (muP)** for **hyperparameter transfer** in large models (G. Yang)
- in muP, "narrow" and wide neural networks **share the same set of optimal hyperparameters**, e.g., optimal learning rate (and decay), cross-entropy temperature, initialization scale, regularization, etc.
- one can tune the large model **by just tuning a tiny version** of it and copying over the hyperparameters

Some experiments on muP and μTransfer

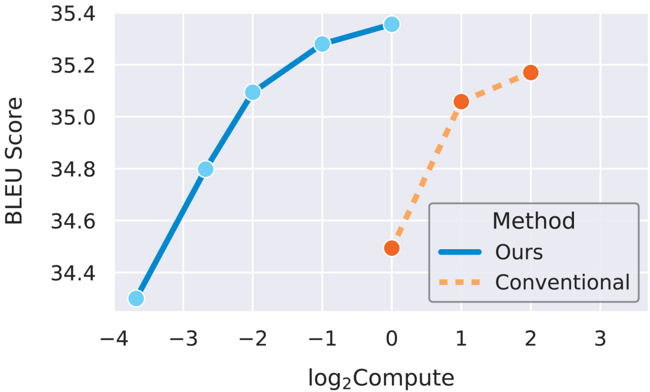


Figure: Comparison μTransfer, which transfers tuned hyperparameters from a small proxy model, with directly tuning the large target model, on IWSLT14 De-En, a machine translation dataset.

Take-away

Take-away messages:

- math/statistics tells a lot about how to scale things, like LLN and CLT
- rather elementary calculus allow to understand the **proper scaling** of large-scale DNN models: for now, **not widely known**
- can be (arguably) applied to transfer optimal hyperparameter design for extremely large-scale models

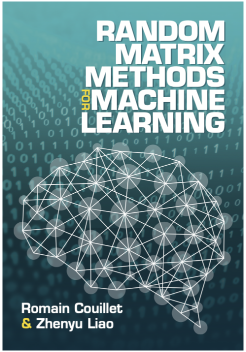
References:

- 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

RMT for machine learning: from theory to practice!

Random matrix theory (RMT) for machine learning:

- **change of intuition** from small to large dimensional learning paradigm!
- **better understanding** of existing methods: why they work if they do, and what the issue is if they do not
- **improved novel methods** with performance guarantee!



- book *"Random Matrix Methods for Machine Learning"*
- by Romain Couillet and **Zhenyu Liao**
- Cambridge University Press, 2022
- a pre-production version of the book and exercise solutions at `https://zhenyu-liao.github.io/book/`
- MATLAB and Python codes to reproduce all figures at `https://github.com/Zhenyu-LIAO/RMT4ML`

Thank you! Q & A?