Random Matrix Theory for Modern Machine Learning: New Intuitions, Improved Methods, and Beyond: Part 1

CIMI Thematic School "Models & Methods for High-dimensional Inference and Learning"

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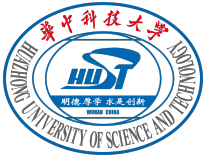
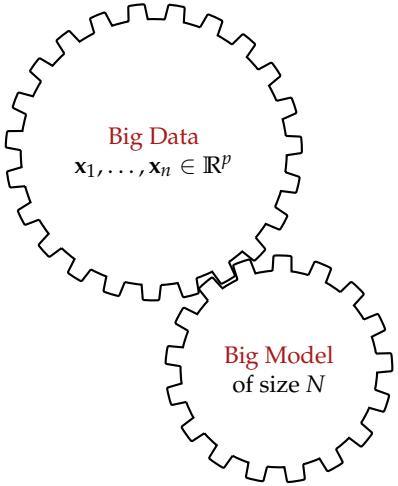


Schedule of the mini-course

1. **Part 1**: Motivation and Mathematical Background (concentration, resolvent-based approach to eigenspectral analysis, high-dimensional linearization, etc.)
2. **Part 2**: Four Ways to Characterize Sample Covariance Matrices and Some More Random Matrix Models (Wigner semicircle law, generalized sample covariance model, and separable covariance model)

Outline

Motivation: understanding large-dimensional machine learning



- **Big Data era**: exploit large n, p, N
- counterintuitive phenomena different from classical asymptotics statistics
- complete change of understanding of many methods in statistics and machine learning (ML)
- **Random Matrix Theory (RMT)** provides the tools!

Sample covariance matrix in the large n, p regime

- **Problem**: estimate covariance $\mathbf{C} \in \mathbb{R}^{p\times p}$ from n data samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ with $\mathbf{x}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$,
- Maximum likelihood sample covariance matrix with entry-wise convergence

$$\hat{\mathbf{C}} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^{\mathsf{T}} \in \mathbb{R}^{p\times p}, \quad [\hat{\mathbf{C}}]_{ij} \to [\mathbf{C}]_{ij}$$

  almost surely as $n \to \infty$: optimal for $n \gg p$ (or, for p "small").

- In the regime $n \sim p$, conventional wisdom breaks down: for $\mathbf{C} = \mathbf{I}_p$ with $n < p$, $\hat{\mathbf{C}}$ has at least $p - n$ zero eigenvalues:

$$\boxed{\|\hat{\mathbf{C}} - \mathbf{C}\| \not\to 0, \quad n, p \to \infty} \Rightarrow \text{ eigenvalue mismatch and not consistent!}$$

- due to **loss of matrix norm "equivalence"**: $\|\mathbf{A}\|_{\max} \leq \|\mathbf{A}\| \leq p\|\mathbf{A}\|_{\max}$ for $\mathbf{A} \in \mathbb{R}^{p\times p}$ and $\|\mathbf{A}\|_{\max} \equiv \max_{ij} |\mathbf{A}_{ij}|$.

When is one in the random matrix regime? Almost always!

What about $n = 100p$? For $\mathbf{C} = \mathbf{I}_p$, as $n, p \to \infty$ with $p/n \to c \in (0, \infty)$: MP law

$$\mu(dx) = (1 - c^{-1})^+ \delta(x) + \frac{1}{2\pi c x} \sqrt{(x - E_-)^+ (E_+ - x)^+} dx$$

where $E_- = (1 - \sqrt{c})^2$, $E_+ = (1 + \sqrt{c})^2$ and $(x)^+ \equiv \max(x, 0)$. Close match!

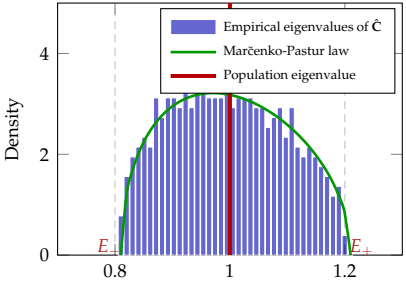


Figure: Eigenvalue distribution of $\hat{\mathbf{C}}$ versus Marčenko-Pastur law, $p = 500$, $n = 50\,000$.

- eigenvalues span on $[E_- = (1 - \sqrt{\mathbf{c}})^2, E_+ = (1 + \sqrt{\mathbf{c}})^2]$.
- for $\mathbf{n = 100p}$, on a range of $\pm\mathbf{2}\sqrt{\mathbf{c}} = \pm\mathbf{0.2}$ around the population eigenvalue **1**.

Noisy linear model

Consider a given set of data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ of size n, composed of the (random) input data $\mathbf{x}_i \in \mathbb{R}^p$ and its corresponding output target $y_i \in \mathbb{R}$, drawn from the following noisy linear model.

Definition (Noisy linear model)

We say a data-target pair $(\mathbf{x}, y) \in \mathbb{R}^p \times \mathbb{R}$ follows a noisy linear model if it satisfies

$$y = \boldsymbol{\beta}_*^\mathsf{T} \mathbf{x} + \epsilon \tag{1}$$

for some deterministic (ground-truth) vector $\boldsymbol{\beta}_* \in \mathbb{R}^p$, and random variable $\epsilon \in \mathbb{R}$ independent of $\mathbf{x} \in \mathbb{R}^p$, with $\mathbb{E}[\epsilon] = 0$ and $\mathrm{Var}[\epsilon] = \sigma^2$.

- aim to find a regressor $\boldsymbol{\beta} \in \mathbb{R}^p$ that best describes the linear relation $y_i \approx \boldsymbol{\beta}^\mathsf{T} \mathbf{x}_i$, by minimizing the ridge-regularized mean squared error (MSE)

$$L(\boldsymbol{\beta}) = \frac{1}{n} \sum_{i=1}^n (y_i - \boldsymbol{\beta}^\mathsf{T} \mathbf{x}_i)^2 + \gamma \|\boldsymbol{\beta}\|^2 = \frac{1}{n} \|\mathbf{X}^\mathsf{T} \boldsymbol{\beta} - \mathbf{y}\|^2 + \gamma \|\boldsymbol{\beta}\|^2 \tag{2}$$

for $\mathbf{y} = [y_1, \ldots, y_n]^\mathsf{T} \in \mathbb{R}^n$, $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{p \times n}$, and some regularization penalty $\gamma \geq 0$

Out-of-sample prediction risk

- unique solution given by

$$\boldsymbol{\beta}_\gamma = \left(\mathbf{X}\mathbf{X}^\mathsf{T} + n\gamma \mathbf{I}_p\right)^{-1}\mathbf{X}\mathbf{y} = \mathbf{X}\left(\mathbf{X}^\mathsf{T}\mathbf{X} + n\gamma \mathbf{I}_n\right)^{-1}\mathbf{y}, \quad \gamma > 0 \tag{3}$$

- in the $\gamma = 0$ setting, the minimum ℓ_2 norm least squares solution

$$\boldsymbol{\beta}_0 = \left(\mathbf{X}\mathbf{X}^\mathsf{T}\right)^{+}\mathbf{X}\mathbf{y} = \mathbf{X}\left(\mathbf{X}^\mathsf{T}\mathbf{X}\right)^{+}\mathbf{y}, \tag{4}$$

  where $(\mathbf{A})^+$ denotes the Moore–Penrose pseudoinverse, also **"ridgeless" least squares solution**.
- statistical quality of $\boldsymbol{\beta}$, as a function of dimensions n, p, noise level σ^2, and the regularization γ
- evaluating the **out-of-sample prediction risk** (or simply, **risk**)

$$R_\mathbf{X}(\boldsymbol{\beta}) = \mathbb{E}[(\boldsymbol{\beta}^\mathsf{T}\hat{\mathbf{x}} - \boldsymbol{\beta}_*^\mathsf{T}\hat{\mathbf{x}})^2 \mid \mathbf{X}] = \underbrace{(\mathbb{E}[\boldsymbol{\beta} \mid \mathbf{X}] - \boldsymbol{\beta}_*)^\mathsf{T}\mathbf{C}(\mathbb{E}[\boldsymbol{\beta} \mid \mathbf{X}] - \boldsymbol{\beta}_*)}_{\equiv B_\mathbf{X}(\boldsymbol{\beta})} + \underbrace{\operatorname{tr}\left(\operatorname{Cov}[\boldsymbol{\beta} \mid \mathbf{X}]\mathbf{C}\right)}_{\equiv V_\mathbf{X}(\boldsymbol{\beta})} \tag{5}$$

  for an independent test data point. We denote $\mathbb{E}[\mathbf{x}_i\mathbf{x}_i^\mathsf{T}] = \mathbf{C}$, and $B_\mathbf{X}(\boldsymbol{\beta}), V_\mathbf{X}(\boldsymbol{\beta})$ the **bias** as well as **variance** of the solution $\boldsymbol{\beta}$.

Objects of interest

$$\boxed{\begin{aligned} B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) &= (\mathbb{E}[\boldsymbol{\beta} \mid \mathbf{X}] - \boldsymbol{\beta}_*)^{\mathsf{T}} \mathbf{C} (\mathbb{E}[\boldsymbol{\beta} \mid \mathbf{X}] - \boldsymbol{\beta}_*) \\ V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) &= \operatorname{tr}\left(\operatorname{Cov}[\boldsymbol{\beta} \mid \mathbf{X}] \mathbf{C}\right). \end{aligned}} \tag{6}$$

- Denote $\boxed{\mathbf{Q}(-\gamma) \equiv (\hat{\mathbf{C}} + \gamma \mathbf{I}_p)^{-1}}$ the resolvent of the SCM $\hat{\mathbf{C}} = \frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{T}}$. Write

$$B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = \boldsymbol{\beta}_*^{\mathsf{T}} \left(\mathbf{I}_p - \mathbf{Q}(-\gamma)\hat{\mathbf{C}}\right) \mathbf{C} \left(\mathbf{I}_p - \mathbf{Q}(-\gamma)\hat{\mathbf{C}}\right) \boldsymbol{\beta}_*, \quad V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = \frac{\sigma^2}{n} \operatorname{tr}\left(\mathbf{Q}(-\gamma)\hat{\mathbf{C}}\mathbf{Q}(-\gamma)\mathbf{C}\right). \tag{7}$$

- For $\gamma > 0$, one has $\mathbf{I}_p - \mathbf{Q}(-\gamma)\hat{\mathbf{C}} = \mathbf{I}_p - \mathbf{Q}(-\gamma)(\hat{\mathbf{C}} + \gamma\mathbf{I}_p - \gamma\mathbf{I}_p) = \gamma\mathbf{Q}(-\gamma)$, so that

$$B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = \gamma^2 \boldsymbol{\beta}_*^{\mathsf{T}} \mathbf{Q}^2(-\gamma) \boldsymbol{\beta}_* = \boxed{-\gamma^2 \frac{\partial \boldsymbol{\beta}_*^{\mathsf{T}} \mathbf{Q}(-\gamma) \boldsymbol{\beta}_*}{\partial \gamma}} \tag{8}$$

$$V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = \sigma^2 \left(\frac{1}{n} \operatorname{tr} \mathbf{Q}(-\gamma) - \frac{\gamma}{n} \operatorname{tr} \mathbf{Q}^2(-\gamma)\right) = \boxed{\sigma^2 \left(\frac{1}{n} \operatorname{tr} \mathbf{Q}(-\gamma) + \frac{\gamma}{n} \frac{\partial \operatorname{tr} \mathbf{Q}(-\gamma)}{\partial \gamma}\right)} \tag{9}$$

  where we used the fact that $\mathbf{C} = \mathbf{I}_p$ and $\partial \mathbf{Q}(-\gamma)/\partial\gamma = -\mathbf{Q}^2(-\gamma)$.
- suffice to evaluate quadratic and trace forms of the random resolvent matrix $\mathbf{Q}(-\gamma)$.

Numerical results

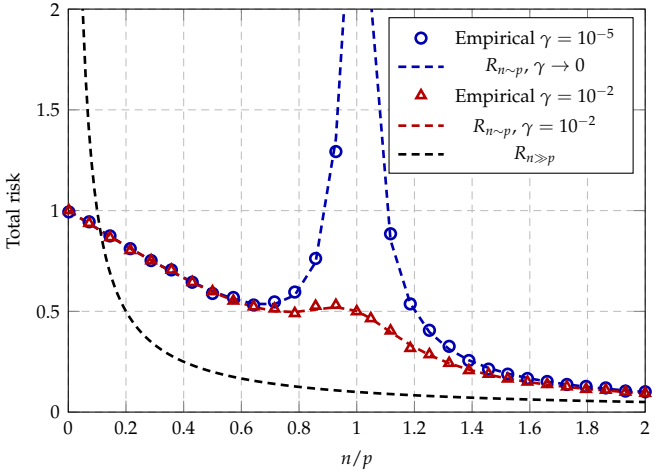


Figure: Out-of-sample risk $R_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) = B_{\mathbf{X}}(\boldsymbol{\beta}_\gamma) + V_{\mathbf{X}}(\boldsymbol{\beta}_\gamma)$ of the ridge regression solution $\boldsymbol{\beta}_\gamma$ as a function of the dimension ratio n/p, for fixed $p = 512$, $\|\boldsymbol{\beta}_*\| = 1$, and different regularization penalty $\gamma = 10^{-2}$ and $\gamma = 10^{-5}$, Gaussian $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$ and $\varepsilon \sim \mathcal{N}(0, \sigma^2 = 0.1)$.

Linear model trained with gradient descent

- Consider again minimizing the following loss function to obtain the linear model parameter $\boldsymbol{\beta}$:

$$L(\boldsymbol{\beta}) = \frac{1}{2n}\sum_{i=1}^{n}(y_i - \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i)^2 + \frac{\gamma}{2}\|\boldsymbol{\beta}\|^2 = \frac{1}{2n}\|\mathbf{X}^\mathsf{T}\boldsymbol{\beta} - \mathbf{y}\|^2 + \frac{\gamma}{2}\|\boldsymbol{\beta}\|^2 \tag{10}$$

- but this time using gradient descent with infinitely small step size (i.e., gradient flow)

$$\frac{d\boldsymbol{\beta}(t)}{dt} = -\frac{\partial L(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} \Rightarrow \boldsymbol{\beta}(t) = e^{-(\hat{\mathbf{C}}+\gamma\mathbf{I}_p)t}\boldsymbol{\beta}(0) + \left(\mathbf{I}_p - e^{-(\hat{\mathbf{C}}+\gamma\mathbf{I}_p)t}\right)\boldsymbol{\beta}_{RR}, \tag{11}$$

  where we recall $\hat{\mathbf{C}} = \frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$ the SCM and denote $\boldsymbol{\beta}_{\mathrm{RR}} = \left(\hat{\mathbf{C}} + \gamma\mathbf{I}_p\right)^{-1}\frac{1}{n}\mathbf{X}\mathbf{y}$ is the ridge regression solution (that corresponds to $\boldsymbol{\beta}(t)$ as $t \to \infty$)
- understand the interplay between **training dynamics** and **generalization performance**
- slightly more involved eigenspectral functional of $\hat{\mathbf{C}}$
- as well shall see below, writes as (complex counter) integration of the resolvent $\boxed{\mathbf{Q}(z) = (\hat{\mathbf{C}} - z\mathbf{I}_p)^{-1}}$

Some numerical results

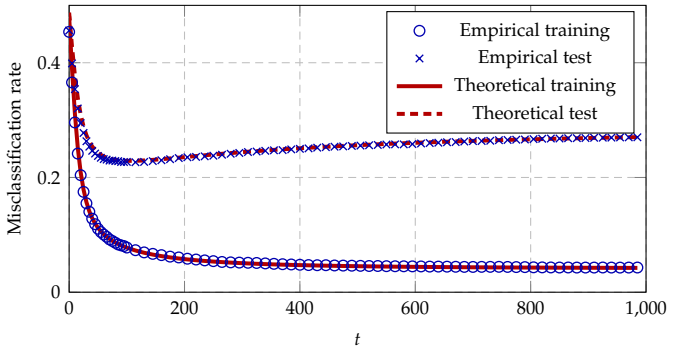


Figure: Training and test misclassification rates of a linear network as a function of the gradient descent training time t, for $p = 256$, $n = 512$, $\gamma = 0$, $\alpha = 10^{-2}$, $\sigma^2 = 0.1$ and $\boldsymbol{\mu} = [-\mathbf{1}_{p/2}, \mathbf{1}_{p/2}]/\sqrt{p}$. Empirical results averaged over 50 runs.

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

$$\frac{1}{n}\sum_{i=1}^{n} x_i \to \mu, \tag{12}$$

  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

$$\sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)\right) \to \mathcal{N}(0, \sigma^2), \tag{13}$$

  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

$$[\mathbf{W}]_{ij} \sim \mathcal{N}(0, N^{-1}). \tag{14}$$

```
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

$$[\mathbf{W}]_{ij} \sim \mathcal{N}(0, 2N^{-1}). \tag{15}$$

```
torch.nn.init.kaiming_normal_
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- derivation based on **forward propagation**
- similar considerations for CNN, RNN, ResNet, etc.

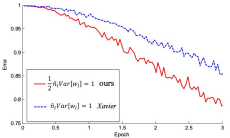


Figure 2. The convergence of a **22-layer** large model (B in Table 3). The x-axis is the number of training epochs. The y-axis is the top-1 error of 3,000 random val samples, evaluated on the center crop. We use ReLU as the activation for both cases. Both our initialization (red) and "Xavier" (blue)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

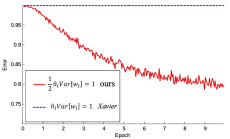


Figure 3. The convergence of a **30-layer** small model (see the main text). We use ReLU as the activation for both cases. Our initialization (red) is able to make it converge. But "Xavier" (blue) [7] completely stalls - we also verify that its gradients are all diminishing. It does not converge even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

$$\boxed{\mathbf{h}_i^{(1)} = \frac{1}{N^{a_1}\sqrt{p}}\mathbf{W}^{(1)}\mathbf{x}_i, \quad \mathbf{h}_i^{(\ell)} = \frac{1}{N^{a_\ell}}\mathbf{W}^{(\ell)}\sigma_\ell\left(\mathbf{h}_i^{(\ell-1)}\right)} \quad i \in \{1, \ldots, n\} \tag{16}$$

- 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

$$\frac{d\boldsymbol{\theta}}{dt} = -\eta\frac{\partial L(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \eta\frac{1}{n}\sum_{i=1}^n \Delta_i \frac{\partial f_{\boldsymbol{\theta}}(\mathbf{x}_i)}{\partial \boldsymbol{\theta}}, \quad \Delta_i \equiv -\frac{\partial L(f_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i)}{\partial f_{\boldsymbol{\theta}}(\mathbf{x}_i)}, \tag{17}$$

  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 $W_{ij}^{(1)} \sim \mathcal{N}(0, N^{-b_1})$

[1]This part is majorly borrowed from the Lecture Notes on Infinite-Width Limits of Neural Networks, by Cengiz Pehlevan and Blake Bordelon, *Princeton Machine Learning Theory Summer School*, 2023.

Appropriate scaling of large and deep NNs

Settings:

- **scaling of NN model**: $\mathbf{h}_i^{(1)} = \frac{1}{N^{a_1}\sqrt{p}}\mathbf{W}^{(1)}\mathbf{x}_i$, $\mathbf{h}_i^{(\ell)} = \frac{1}{N^{a_\ell}}\mathbf{W}^{(\ell)}\sigma_\ell\left(\mathbf{h}_i^{(\ell-1)}\right)$, $f_{\boldsymbol{\theta}}(\mathbf{x}_i) = \frac{1}{\gamma N^{a_L}}\left(\mathbf{w}^{(L)}\right)^\intercal \sigma_\ell\left(\mathbf{h}_i^{(\ell-1)}\right)$
- **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 $\mathbf{h}^{(1)}$: $\mathbb{E}[\mathbf{h}_i^{(1)}] = \mathbf{0}$, $\mathbb{E}[\mathbf{h}_i^{(1)}(\mathbf{h}_j^{(1)})^\intercal]_{kq} = \delta_{kq}N^{-(2a_1+b_1)} \cdot \frac{1}{p}\mathbf{x}_i^\intercal\mathbf{x}_j$; 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 $\boldsymbol{\Phi}^{(\ell)} \in \mathbb{R}^{n\times n}, \Phi_{ij}^{(\ell)} = \frac{1}{N}\sigma(\mathbf{h}_i^{(\ell)})^\intercal\sigma(\mathbf{h}_j^{(\ell)})$
   - 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 $\boxed{2a_\ell + c = 1, \ell \in \{2, \ldots, L\}}$

Appropriate scaling of large and deep NNs

Settings:

- **scaling of NN model**: $\mathbf{h}_i^{(1)} = \frac{1}{N^{a_1}\sqrt{p}}\mathbf{W}^{(1)}\mathbf{x}_i$, $\mathbf{h}_i^{(\ell)} = \frac{1}{N^{a_\ell}}\mathbf{W}^{(\ell)}\sigma_\ell\left(\mathbf{h}_i^{(\ell-1)}\right)$, $f_{\boldsymbol{\theta}}(\mathbf{x}_i) = \frac{1}{\gamma N^{a_L}}\left(\mathbf{w}^{(L)}\right)^\top \sigma_\ell\left(\mathbf{h}_i^{(\ell-1)}\right)$
- **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:

$$\boxed{d = 1/2, c = 1, a_\ell = 0, b_\ell = 1, a_1 = -1/2, b_1 = 1} \tag{18}$$

- 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

[2] Blake Bordelon et al. "Depthwise Hyperparameter Transfer in Residual Networks: Dynamics and Scaling Limit". In: *The Twelfth International Conference on Learning Representations*. Oct. 2023

Some experiments on muP and µTransfer

Show some simulations!

Some experiments on muP and µTransfer

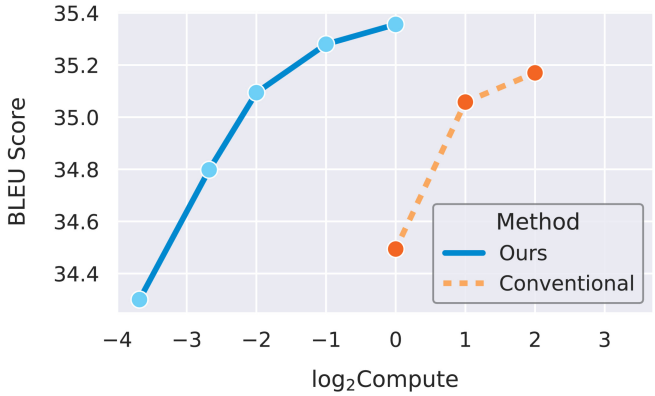


Figure: Comparison µTransfer, which transfers tuned hyperparameters from a small proxy model, with directly tuning the large target model, on IWSLT14 De-En, a machine translation dataset.

Take-away of this section

- sample covariance matrix $\hat{\mathbf{C}}$ have different behavior in the large n, p regime
- loss of matrix norm "equivalence" for large matrices $\|\mathbf{A}\|_{\max} \leq \|\mathbf{A}\| \leq p\|\mathbf{A}\|_{\max}$ for $\mathbf{A} \in \mathbb{R}^{p\times p}$ and $\|\mathbf{A}\|_{\max} \equiv \max_{ij} |\mathbf{A}_{ij}|$
- evaluation of linear regression model trained with gradient descent involves **eigenspectral functionals** of SCM, **RMT** provides **an analytic answer**
- further allows better **understanding and scaling** of large and deep neural networks

Summary: analyze and optimize large-scale ML models

Definition (High-dimensional Equivalent)

For a random matrix $\mathbf{X} \in \mathbb{R}^{p\times n}$ and a (possibly) nonlinear model of interest $f(\mathbf{X})$ of $\mathbf{X}$ for some $f\colon \mathbb{R}^{p\times n} \to \mathbb{R}^{p\times n}$, we are interested in the behavior of the scalar observation $g(f(\mathbf{X}))$ of the random model $f(\mathbf{X})$, via the observation map $g\colon \mathbb{R}^{p\times n} \to \mathbb{R}$.
We say that $\bar{\mathbf{X}}_f$ (which may be deterministic or random) is an High-dimensional Equivalent for the random model $f(\mathbf{X})$ with respect to the observation map g if we have, with probability at least $1-\delta(p,n)$ that

$$\left| \frac{g(f(\mathbf{X})) - g(\mathbf{X}_f)}{g(f(\mathbf{X}))} \right| \leq \varepsilon(n,p), \tag{19}$$

for some non-negative functions $\varepsilon(n,p)$ and $\delta(n,p)$ that decrease to zero as $n,p \to \infty$.

Summary: analyze and optimize large-scale ML models

Analyze and Optimize Large-scale ML model $f(\mathbf{X}, \mathbf{\Theta})$

Objective: Evaluation of $f(\mathbf{X}, \mathbf{\Theta})$ via Performance Metric $g(\cdot)$

Technical Challenge 1 High-dimensionality in $\mathbf{X}, \mathbf{\Theta}$	**Key Idea 1** Concentration of $g(f(\mathbf{X}, \mathbf{\Theta})) \simeq \mathbb{E}[g(f(\mathbf{X}, \mathbf{\Theta}))]$
Technical Challenge 2 Analysis of Eigen-functional	**Key Idea 2** Leave-one-out + complex analysis
Technical Challenge 3 Non-linearity in ML model	**Key Idea 3** High-dimensional linearization of $f(\mathbf{X}, \mathbf{\Theta})$

Characterization of scalar random variables: from moments to tails

Definition (Moments and moment generating function, MGF)

For a scalar random variable x defined on some probability space $(\Omega, \mathcal{F}, \mathbb{P})$, we denote

- $\mathbb{E}[x]$ the *expectation* of x;
- $\mathrm{Var}[x] = \mathbb{E}[(x - \mathbb{E}[x])^2]$ the *variance* of x;
- for $p > 0$, $\mathbb{E}[x^p]$ the p^{th} *moment* of x, and $\mathbb{E}[|x|^p]$ the p^{th} *absolute moment*;
- for $\lambda \in \mathbb{R}$, $M_x(\lambda) = \mathbb{E}[e^{\lambda x}] = \sum_{p=0}^{\infty} \frac{\lambda^p}{p!} \mathbb{E}[x^p]$ the *moment generating function (MGF)* of x.

Lemma (Moments versus tails)

For a scalar random variable x and fixed $p > 0$, we have

1. $\mathbb{E}[|x|^p] = \int_0^{\infty} p t^{p-1} \mathbb{P}(|x| \geq t)\, dt$
2. $\mathbb{P}(|x| \geq t) \leq \exp(-\lambda t) M_{|x|}(\lambda)$, *for $t > 0$ and MGF $M_{|x|}(\lambda)$ of $|x|$*

Definition (Sub-gaussian and sub-exponential distributions)

For a standard Gaussian random variable $x \sim \mathcal{N}(0,1)$, its law given by $\mu(dt) = \frac{1}{\sqrt{2\pi}} \exp(-t^2/2)$, so that $\mathbb{P}(x \geq X) = \mu([X,\infty)) = \frac{1}{\sqrt{2\pi}} \int_X^\infty \exp(-t^2/2)\, dt \leq \exp(-X^2/2)$.

- We say y is a *sub-gaussian random variable* if it has a tail that decays *as fast as* standard Gaussian random variables, that is
$$\mathbb{P}\left(|y| \geq t\right) \leq \exp(-t^2/\sigma_{\mathcal{N}}^2), \tag{20}$$
for some $\sigma_{\mathcal{N}} > 0$ (known as the *sub-gaussian norm* of y) for all $t > 0$.
- We can define a *sub-exponential random variable* z similarly via $\mathbb{P}(|z| \geq t) \leq \exp(-t/\sigma_{\mathcal{N}})$.

- for a sub-gaussian random variable x of mean $\mu = \mathbb{E}[x]$ and sub-gaussian norm $\sigma_{\mathcal{N}}$ that
$$\mathbb{P}\left(|x - \mu| \geq t\sigma_{\mathcal{N}}\right) \leq \exp(-t^2), \tag{21}$$
for all $t > 0$, in which the sub-gaussian norm $\sigma_{\mathcal{N}}$ of x acts as a scale parameter (that is similar, in spirit, to the variance parameter of Gaussian distribution).

A collection of scalar random variables: from LLN to CLT

For a collection of independent and identically distributed (i.i.d.) random variables $x_1, \ldots, x_n$ of mean μ and variance σ^2, we have, by independence, that

$$\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n} x_i\right] = \mu, \quad \mathrm{Var}\left[\frac{1}{n}\sum_{i=1}^{n} x_i\right] = \frac{1}{n^2}\sum_{i=1}^{n}\mathrm{Var}[x_i] = \frac{\sigma^2}{n}. \tag{22}$$

- for μ, σ^2 do *not* scale with n, the (random) sample mean strongly concentrates around its expectation μ.

Theorem (Weak and strong law of large numbers, LLN)

For a sequence of i.i.d. random variables $x_1, \ldots, x_n$ with finite expectation $\mathbb{E}[x_i] = \mu < \infty$, we have that the sample mean

$$\frac{1}{n}\sum_{i=1}^{n} x_i \to \mu, \tag{23}$$

*in probability/almost surely as $n \to \infty$, known as the **weak law/strong of large numbers (LLN)**.*

Theorem (Central limit theorem, CLT)

For a sequence of i.i.d. random variables $x_1, \ldots, x_n$ with $\mathbb{E}[x_i] = \mu$ and $\mathrm{Var}[x_i] = \sigma^2$, we have, for every $t \in \mathbb{R}$ that

$$\mathbb{P}\left(\frac{1}{\sigma\sqrt{n}}\sum_{i=1}^{n}(x_i - \mu) \geq t\right) \to \frac{1}{\sqrt{2\pi}}\int_t^\infty e^{-x^2/2}\,dx \tag{24}$$

as $n \to \infty$. That is, as $n \to \infty$, the random variable $\frac{1}{\sigma\sqrt{n}}\sum_{i=1}^{n}(x_i - \mu) \to \mathcal{N}(0,1)$ in distribution.

Remark (Unified form of LLN and CLT)

The results of LLN and CLT can be compactly written as $\frac{1}{n}\sum_{i=1}^{n} x_i \simeq \underbrace{\mu}_{O(1)} + \underbrace{\mathcal{N}(0,1)\cdot\sigma/\sqrt{n}}_{O(n^{-1/2})}$, as $n \to \infty$, for μ, σ both of order $O(1)$.

(i) In the first order (of magnitude $O(1)$), it has an asymptotically deterministic behavior around the expectation μ; and

(ii) in the second order (of magnitude $O(n^{-1/2})$), it strongly concentrates around this deterministic quantity with a universal Gaussian fluctuation, regardless of the distribution of the component of x_i.

Concentration of random vectors in high dimensions?

- "concentration" for a random vector $\mathbf{x} \in \mathbb{R}^n$?

Observation (Random vectors do not "concentrate" around their means)

For two *independent* random vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, having i.i.d. entries with zero mean and unit variance (that is, $\mu = 0$ and $\sigma = 1$), we have that

$$\mathbb{E}[\|\mathbf{x} - \mathbf{0}\|_2^2] = \mathbb{E}[\mathbf{x}^\mathsf{T}\mathbf{x}] = \mathrm{tr}(\mathbb{E}[\mathbf{x}\mathbf{x}^\mathsf{T}]) = n, \tag{25}$$

and further by independence that

$$\mathbb{E}[\|\mathbf{x} - \mathbf{y}\|_2^2] = \mathbb{E}[\mathbf{x}^\mathsf{T}\mathbf{x} + \mathbf{y}^\mathsf{T}\mathbf{y}] = 2n. \tag{26}$$

- the origin $\mathbf{0}$ (and *mean* of $\mathbf{x}$) is always, in expectation, at the midpoint of two independent draws of random vectors in $\mathbb{R}^n$
- any random vector $\mathbf{x} \in \mathbb{R}^n$ with n large is not close to its mean
- $\mathbf{x}$ does not itself "concentrate" around any n-dimensional deterministic vector in any traditional sense.

Numerical illustration

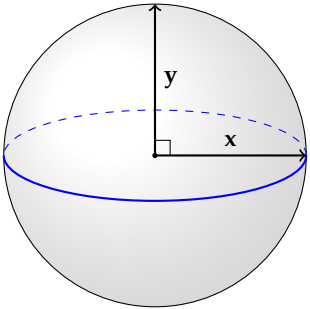


Figure: Visualization of "non-concentration" behavior of large-dimensional random vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.

- In spite of this, from the LLN and CLT one expects that some types of "observations" of $\mathbf{x} \in \mathbb{R}^n$ (e.g., averages over all the entries of $\mathbf{x}$, to retrieve the sample mean), must concentrate in some sense for n large
- we "interpret" the sample mean as a linear scalar observation of a vector $\mathbf{x} \in \mathbb{R}^n$.

Remark (Sample mean as a linear scalar observation)

Let $\mathbf{x} \in \mathbb{R}^n$ be a random vector having i.i.d. entries, then the sample mean of the entries of $\mathbf{x}$ can be rewritten as the following linear scalar observation $f\colon \mathbb{R}^n \to \mathbb{R}$ of $\mathbf{x}$ defined as

$$f(\mathbf{x}) = \mathbf{1}_n^{\mathsf{T}}\mathbf{x}/n = \frac{1}{n}\sum_{i=1}^{n} x_i, \text{ or } f(\cdot) = \mathbf{1}_n^{\mathsf{T}}(\cdot)/n. \tag{27}$$

- LLN and CLT are nothing but asymptotic characterization of the concentration behavior of the linear scalar observation $f(\mathbf{x})$ of the random vector $\mathbf{x} \in \mathbb{R}^n$
- we can say things non-asymptotically as well, under two different assumptions on the tail of $\mathbf{x}$.
  - (i) are only assumed to have finite variance σ^2 (but nothing on its tail behavior or higher-order moments); and
  - (ii) have sub-gaussian tails with sub-gaussian norm $\sigma_{\mathcal{N}}$.

Table: Different types of characterizations of the linear scalar observation $f(\mathbf{x}) = \mathbf{x}^\mathsf{T}\mathbf{1}_n/n$ for $\mathbf{x} \in \mathbb{R}^n$, having i.i.d. entries with mean $\mathbb{E}[x_i] = \mu$ and variance σ^2 or sub-gaussian norm $\sigma_{\mathcal{N}}$.

	First-order behavior	Second-order behavior
Asymptotic	$f(\mathbf{x}) \to \mu$ via Law of Large Numbers	$\frac{\sqrt{n}}{\sigma}(f(\mathbf{x}) - \mu) \to \mathcal{N}(0,1)$ in law Central Limit Theorem
Non-asymptotic under finite variance	$\mathbb{E}[f(\mathbf{x})] = \mu$	$\mathbb{P}\left(\lvert f(\mathbf{x}) - \mu\rvert \geq t\sigma/\sqrt{n}\right) \leq t^{-2}$ via Chebyshev's inequality
Non-asymptotic under sub-gaussianity	$\mathbb{E}[f(\mathbf{x})] = \mu$	$\mathbb{P}\left(\lvert f(\mathbf{x}) - \mu\rvert \geq t\sigma_{\mathcal{N}}/\sqrt{n}\right) \leq \exp(-Ct^2)$ via sub-gaussian tail bound

Remark (Concentration of scalar observation of large random vectors)

A random vector $\mathbf{x} \in \mathbb{R}^n$, when "observed" via the linear scalar observation $f(\mathbf{x}) = \mathbf{1}_n^\mathsf{T}\mathbf{x}/n$:

$$f(\mathbf{x}) \simeq \underbrace{\mu}_{O(1)} + \underbrace{X/\sqrt{n}}_{O(n^{-1/2})}, \tag{28}$$

for n large, with some random X of order $O(1)$ that:

(i-i) has a tail that decays (at least) as t^{-2}, for finite n and $\mathbf{x}$ having entries of bounded variance;

(i-ii) has a sub-gaussian tail (at least) as $\exp(-t^2)$, for finite n and $\mathbf{x}$ having sub-gaussian entries;

(ii) has a precise Gaussian tail *independent* of the law of (the entries of) $\mathbf{x}$, but in the limit of $n \to \infty$ via CLT.

Lipschitz, quadratic concentration, and beyond

The concentration properties extend beyond the specific *linear* observation, $f(\mathbf{x}) = \mathbf{1}_n^\mathsf{T}\mathbf{x}/n$, to many types of (possibly) nonlinear observations.

Definition (Scalar observation maps)

For random vector $\mathbf{x} \in \mathbb{R}^n$, we say $f(\mathbf{x}) \in \mathbb{R}$ is a scalar observation of $\mathbf{x}$ with observation map $f\colon \mathbb{R}^n \to \mathbb{R}$.

Table: Different types of scalar observations $f(\mathbf{x})$ of random vector $\mathbf{x} \in \mathbb{R}^n$, having independent entries.

	Scalar observation	Characterization
Linear	sample mean $f(\mathbf{x}) = \mathbf{1}_n^\mathsf{T}\mathbf{x}/n$, and $f(\mathbf{x}) = \mathbf{a}^\mathsf{T}\mathbf{x}$ for $\mathbf{a} \in \mathbb{R}^n$	Table in last slide
Lipschitz	$f(\mathbf{x})$ for a Lipschitz map $f\colon \mathbb{R}^n \to \mathbb{R}$	Lipschitz concentration
Quadratic form	$f(\mathbf{x}) = \mathbf{x}^\mathsf{T}\mathbf{A}\mathbf{x}$ for some $\mathbf{A} \in \mathbb{R}^{n\times n}$	Hanson–Wright inequality
Nonlinear quadratic form	$f(\mathbf{x}) = \sigma(\mathbf{x}^\mathsf{T}\mathbf{Y})\mathbf{A}\sigma(\mathbf{Y}^\mathsf{T}\mathbf{x})$ for entry-wise $\sigma\colon \mathbb{R} \to \mathbb{R}$, $\mathbf{A} \in \mathbb{R}^{n\times n}$ and $\mathbf{Y} \in \mathbb{R}^{p\times n}$	Nonlinear quadratic concentration, of direct use in NN

Theorem (Concentration of Lipschitz map of Gaussian random vectors, [Ver18, Theorem 5.2.2])

For a standard Gaussian random vector $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$ *and a Lipschitz function* $f\colon \mathbb{R}^n \to \mathbb{R}$ *that satisfies* $|f(\mathbf{y}_1) - f(\mathbf{y}_2)| \leq K_f \|\mathbf{y}_1 - \mathbf{y}_2\|_2$ *for any* $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^n$*, we have, for all* $t > 0$ *that*

$$\mathbb{P}\left(|f(\mathbf{x}) - \mathbb{E}[f(\mathbf{x})]| \geq t\right) \leq \exp(-Ct^2/K_f^2), \tag{29}$$

for some universal constant $C > 0$*, with* $K_f > 0$ *known as the Lipschitz constant of* f*.*

Remark (Concentration of Lipschitz observation of large random vectors)

The Lipschitz scalar observations $f(\mathbf{x})$ *of the random vector* $\mathbf{x} \in \mathbb{R}^n$ *behave as*

$$f(\mathbf{x}) \simeq \underbrace{\mathbb{E}[f(\mathbf{x})]}_{O(1)} + \underbrace{K_f}_{O(n^{-1/2})}, \tag{30}$$

for n *large, where* K_f *is the Lipschitz constant of* f *that is, in general, of order* $O(n^{-1/2})$ *for* $\mathbb{E}[f(\mathbf{x})] = O(1)$*, for example for* $f(\mathbf{x}) = \mathbf{x}^\mathsf{T}\mathbf{1}_n/n$*.*

[3] Roman Vershynin. *High-Dimensional Probability: An Introduction with Applications in Data Science.* Cambridge Series in Statistical and

Concentration of quadratic forms

- intuitively expect that non-Lipschitz observation $f(\mathbf{x})$ still concentrates in some way, but "less so"

Theorem (Hanson–Wright inequality for quadratic forms, [Ver18, Theorem 6.2.1])

For a random vector $\mathbf{x} \in \mathbb{R}^n$ having independent, zero-mean, unit-variance, sub-gaussian entries with sub-gaussian norm bounded by $\sigma_{\mathcal{N}}$, and deterministic matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, we have, for every $t > 0$, that

$$\mathbb{P}\left(\left|\mathbf{x}^{\mathsf{T}}\mathbf{A}\mathbf{x} - \operatorname{tr}\mathbf{A}\right| \geq t\right) \leq \exp\left(-\frac{C}{\sigma_{\mathcal{N}}^2}\min\left(\frac{t^2}{\sigma_{\mathcal{N}}^2\|\mathbf{A}\|_F^2}, \frac{t}{\|\mathbf{A}\|_2}\right)\right), \tag{31}$$

for some universal constant $C > 0$.

- depending on the interplay between the "range" t and the deterministic matrix $\mathbf{A}$, the random quadratic form $\mathbf{x}^{\mathsf{T}}\mathbf{A}\mathbf{x}$ swings between a sub-gaussian ($\exp(-t^2)$) and a sub-exponential ($\exp(-t)$) tail

Remark (Concentration of Euclidean norm of large random vectors)

It follows that the squared Euclidean norm $\|\mathbf{x}\|_2^2$, as a (non-Lipschitz) quadratic observation of $\mathbf{x} \in \mathbb{R}^n$, behaves as

$$\frac{1}{n}\|\mathbf{x}\|_2^2 \simeq 1 + O(n^{-1/2}), \quad n \gg 1. \tag{32}$$

Concentration of nonlinear quadratic forms

- nonlinear quadratic forms $\frac{1}{n} f(\mathbf{x}^\mathsf{T}\mathbf{Y})\mathbf{A} f(\mathbf{Y}^\mathsf{T}\mathbf{x})$ for Gaussian $\mathbf{x} \in \mathbb{R}^p$ and deterministic $\mathbf{A} \in \mathbb{R}^{n\times n}, \mathbf{Y} \in \mathbb{R}^{p\times n}$

Theorem (Concentration of nonlinear quadratic forms, [LLC18, Lemma 1])

For a standard Gaussian random vector $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$ and deterministic $\mathbf{A} \in \mathbb{R}^{n\times n}, \mathbf{Y} \in \mathbb{R}^{p\times n}$ such that $\|\mathbf{A}\|_2 \le 1, \|\mathbf{Y}\|_2 = 1$, we have, for Lipschitz function $f : \mathbb{R} \to \mathbb{R}$ with Lipschitz constant K_f and any $t > 0$ that

$$\mathbb{P}\left(\left| \frac{1}{n} f(\mathbf{x}^\mathsf{T}\mathbf{Y})\mathbf{A} f(\mathbf{Y}^\mathsf{T}\mathbf{x}) - \frac{1}{n} \operatorname{tr} \mathbf{A}\mathbf{K}_f(\mathbf{Y}) \right| \ge \frac{t}{\sqrt{n}} \right) \le \exp\left(-\frac{C}{K_f^2} \min\left(\frac{t^2}{(|f(0)| + K_f\sqrt{p/n})^2}, \sqrt{n}t \right) \right), \tag{33}$$

with $\mathbf{K}_f(\mathbf{Y}) = \mathbb{E}_\mathbf{x}[f(\mathbf{Y}^\mathsf{T}\mathbf{x}) f(\mathbf{x}^\mathsf{T}\mathbf{Y})] \in \mathbb{R}^{n\times n}$, for some universal constant $C > 0$.

- a nonlinear extension of the Hanson–Wright inequality (consider, e.g., $\mathbf{Y} = \mathbf{I}_n$ with $p = n$)

Remark (Concentration of nonlinear quadratic form observation of large random vectors):

$$\frac{1}{n} f(\mathbf{x}^\mathsf{T}\mathbf{Y})\mathbf{A} f(\mathbf{Y}^\mathsf{T}\mathbf{x}) \simeq \frac{1}{n} \operatorname{tr} \mathbf{A}\mathbf{K}_f(\mathbf{Y}) + O(n^{-1/2}), \tag{34}$$

for n large, with $\max\{f(0), K_f, p/n\} = O(1)$, and similar first and second order behavior as above.

[4] Cosme Louart, Zhenyu Liao, and Romain Couillet. "A random matrix approach to neural networks". In: *Annals of Applied Probability* 28.2 (2018), pp. 1190–1248

Take-away of this section

- high-dimensional random vectors are **not** "concentrating", but orthogonal
- scalar observation $f(\mathbf{x})$ of large random vector $\mathbf{x}$ **does concentrate**: linear, Lipschitz, quadratic form, and nonlinear quadratic forms, etc.
- same holds for random matrices, leads to **Deterministic Equivalent** for random matrices with respect to observation $g(\cdot)$

Definition (**High-dimensional Deterministic Equivalent**)

We say that $\bar{\mathbf{Q}} \in \mathbb{R}^{p\times p}$ is an $(\varepsilon_1, \varepsilon_2, \delta)$-**Deterministic Equivalent** for the symmetric random matrix $\mathbf{Q} \in \mathbb{R}^{p\times p}$ if, for a deterministic matrix $\mathbf{A} \in \mathbb{R}^{p\times p}$ and vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^p$ of unit norms (spectral and Euclidean, respectively), we have, with probability at least $1-\delta(p)$ that

$$\left|\frac{1}{p}\operatorname{tr}\mathbf{A}(\mathbf{Q}-\bar{\mathbf{Q}})\right| \leq \varepsilon_1(p), \quad \left|\mathbf{a}^{\mathsf{T}}(\mathbf{Q}-\bar{\mathbf{Q}})\mathbf{b}\right| \leq \varepsilon_2(p), \tag{35}$$

for some non-negative functions $\varepsilon_1(p), \varepsilon_2(p)$ and $\delta(p)$ that decrease to zero as $p \to \infty$. To denote this relation, we use the notation

$$\mathbf{Q} \overset{\varepsilon_1,\varepsilon_2,\delta}{\longleftrightarrow} \bar{\mathbf{Q}}, \text{ or simply } \mathbf{Q} \leftrightarrow \bar{\mathbf{Q}}. \tag{36}$$

A quick recap on linear algebra: matrices

Definition (Matrix inner product and Frobenius norm)

Given matrices $\mathbf{X}, \mathbf{Y} \in \mathbb{R}^{m \times n}$,

- $\mathrm{tr}(\mathbf{X}^\mathsf{T}\mathbf{Y}) = \sum_{i=1}^{n} [\mathbf{X}^\mathsf{T}\mathbf{Y}]_{ii} = \sum_{i=1}^{n}\sum_{j=1}^{m} X_{ji}Y_{ji}$ is the matrix inner product between $\mathbf{X}$ and $\mathbf{Y}$, where $\mathrm{tr}(\mathbf{A})$ is the trace of $\mathbf{A}$; and
- $\|\mathbf{X}\|_F^2 = \mathrm{tr}(\mathbf{X}^\mathsf{T}\mathbf{X}) = \sum_{i=1}^{n} [\mathbf{X}^\mathsf{T}\mathbf{X}]_{ii} = \sum_{i=1}^{n}\sum_{j=1}^{m} X_{ji}^2$ denotes the (squared) Frobenius norm of $\mathbf{X}$, which is also the sum of the squared entries of $\mathbf{X}$.

Definition (Matrix norm)

For $\mathbf{X} \in \mathbb{R}^{p \times n}$, the following "entry-wise" extension of the p-norms of vectors.

1. matrix Frobenius norm $\|\mathbf{X}\|_F = \sqrt{\sum_{i,j} X_{ij}^2} = \|\mathrm{vec}(\mathbf{X})\|_2$ that extends the vector ℓ_2 Euclidean norm; and
2. matrix maximum norm $\|\mathbf{X}\|_{\max} = \max_{i,j} |X_{ij}| = \|\mathrm{vec}(\mathbf{X})\|_\infty$ that extends the vector ℓ_∞ norm.

and also matrix norm induced by vectors: $\|\mathbf{X}\|_p \equiv \sup_{\|\mathbf{v}\|_p = 1} \|\mathbf{X}\mathbf{v}\|_p$.

- taking $p = 2$ is the spectral norm: $\|\mathbf{X}\|_2 = \sqrt{\lambda_{\max}(\mathbf{X}\mathbf{X}^\mathsf{T})} = \sigma_{\max}(\mathbf{X})$, with $\lambda_{\max}(\mathbf{X}\mathbf{X}^\mathsf{T})$ and $\sigma_{\max}(\mathbf{X})$ the maximum eigenvalue and singular of $\mathbf{X}\mathbf{X}^\mathsf{T}$ and $\mathbf{X}$, respectively.

Remark (Matrix norm "equivalence")

For a matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$*, one has the following*

1. $\|\mathbf{A}\|_2 \leq \|\mathbf{A}\|_F \leq \sqrt{\operatorname{rank}(\mathbf{A})} \cdot \|\mathbf{A}\|_2 \leq \sqrt{\max(m,n)} \cdot \|\mathbf{A}\|_2$*, so that the control of the spectral norm via the Frobenius norm can be particularly loose for matrices of large rank; and*
2. $\|\mathbf{A}\|_{\max} \leq \|\mathbf{A}\|_2 \leq \sqrt{mn} \cdot \|\mathbf{A}\|_{\max}$*, with* $\|\mathbf{A}\|_{\max} \equiv \max_{i,j} |A_{ij}|$ *the max norm of* $\mathbf{A}$*, so that the max and spectral norm can be significantly different for matrices of large size.*

- matrix norm "equivalence" holds only up to **dimensional factors** (e.g., rank and size)

Definition (Eigen-decomposition of symmetric matrices)

A symmetric real matrix $\mathbf{X} \in \mathbb{R}^{n\times n}$ admits the following eigen-decomposition

$$\mathbf{X} = \mathbf{U}_{\mathbf{X}}\mathbf{\Lambda}_{\mathbf{X}}\mathbf{U}_{\mathbf{X}}^{\mathsf{T}} = \sum_{i=1}^{n} \lambda_i(\mathbf{X})\mathbf{u}_i\mathbf{u}_i^{\mathsf{T}}, \tag{37}$$

for diagonal $\mathbf{\Lambda}_{\mathbf{X}} = \operatorname{diag}\{\lambda_i(\mathbf{X})\}_{i=1}^{n}$ containing $\lambda_1(\mathbf{X}), \ldots, \lambda_n(\mathbf{X})$ the real eigenvalues of $\mathbf{X}$, and orthonormal $\mathbf{U}_{\mathbf{X}} = [\mathbf{u}_1, \ldots, \mathbf{u}_n] \in \mathbb{R}^{n\times n}$ containing the corresponding eigenvectors. In particular,

$$\mathbf{X}\mathbf{u}_i = \lambda_i(\mathbf{X})\mathbf{u}_i. \tag{38}$$

- interested in a single eigenvalue of a symmetric real matrix, $\mathbf{X} \in \mathbb{R}^{n\times n}$, one may either resort to the eigenvalue-eigenvector equation in (38) or the determinant equation $\det(\mathbf{X} - \lambda\mathbf{I}_n) = 0$
- classical RMT is interested in the *joint* behavior of all eigenvalues $\lambda_1(\mathbf{X}), \ldots, \lambda_n(\mathbf{X})$, e.g., the (empirical) eigenvalue distribution of $\mathbf{X}$

Definition (Empirical Spectral Distribution, ESD)

For a real symmetric matrix $\mathbf{X} \in \mathbb{R}^{n\times n}$, the *empirical spectral distribution (ESD)* or *empirical spectral measure* $\mu_{\mathbf{X}}$ of $\mathbf{X}$ is defined as the normalized counting measure of the eigenvalues $\lambda_1(\mathbf{X}), \ldots, \lambda_n(\mathbf{X})$ of $\mathbf{X}$,

$$\mu_{\mathbf{X}} \equiv \frac{1}{n}\sum_{i=1}^{n} \delta_{\lambda_i(\mathbf{X})}, \tag{39}$$

where δ_x represents the Dirac measure at x. Since $\int \mu_{\mathbf{X}}(dx) = 1$, the spectral measure $\mu_{\mathbf{X}}$ of a matrix $\mathbf{X} \in \mathbb{R}^{n\times n}$ (which may be random or not) is a probability measure.

- $\int t\mu_{\mathbf{X}}(dt) = \frac{1}{n}\sum_{i=1}^{n} \lambda_i(\mathbf{X})$ is the first moment of $\mu_{\mathbf{X}}$, and gives the average of all eigenvalues of $\mathbf{X}$; and
- $\int t^2\mu_{\mathbf{X}}(dt) = \frac{1}{n}\sum_{i=1}^{n} \lambda_i^2(\mathbf{X})$ is the second moment of $\mu_{\mathbf{X}}$, so that $\int t^2\mu_{\mathbf{X}}(dt) - \left(\int t\mu_{\mathbf{X}}(dt)\right)^2$ gives the variance of the eigenvalues of $\mathbf{X}$.

A unified spectral analysis approach via the resolvent

- **Note**: here everything hold deterministically, not necessarily random **yet**
- combined with **Deterministic Equivalent** and concentration, gives the whole picture

Definition (Resolvent)

For a symmetric matrix $\mathbf{X} \in \mathbb{R}^{p\times p}$, the resolvent $\mathbf{Q}_{\mathbf{X}}(z)$ of $\mathbf{X}$ is defined, for $z \in \mathbb{C}$ not an eigenvalue of $\mathbf{X}$, as

$$\mathbf{Q}_{\mathbf{X}}(z) \equiv \left(\mathbf{X} - z\mathbf{I}_p\right)^{-1}. \tag{40}$$

Proposition (Properties of resolvent)

For $\mathbf{Q}_{\mathbf{X}}(z)$ the resolvent of a symmetric matrix $\mathbf{X} \in \mathbb{R}^{p\times p}$ with ESD $\mu_{\mathbf{X}}$ with supported on $\mathrm{supp}(\mu_{\mathbf{X}})$, then

(i) $\mathbf{Q}_{\mathbf{X}}(z)$ is complex analytic on its domain of definition $\mathbb{C} \setminus \mathrm{supp}(\mu_{\mathbf{X}})$;

(ii) it is bounded in the sense that $\|\mathbf{Q}_{\mathbf{X}}(z)\|_2 \leq 1/\operatorname{dist}(z, \mathrm{supp}(\mu_{\mathbf{X}}))$;

(iii) $x \mapsto \mathbf{Q}_{\mathbf{X}}(x)$ for $x \in \mathbb{R} \setminus \mathrm{supp}(\mu_{\mathbf{X}})$ is an increasing matrix-valued function with respect to symmetric matrix partial ordering (i.e., $\mathbf{A} \succeq \mathbf{B}$ whenever $\mathbf{z}^\mathsf{T}(\mathbf{A} - \mathbf{B})\mathbf{z} \geq 0$ for all $\mathbf{z}$).

A unified spectral analysis approach via the resolvent

- for real z, the resolvent $\mathbf{Q}_{\mathbf{X}}(z)$ is nothing but a regularized inverse of $\mathbf{X}$
- when interested in the eigenvalues and eigenvectors of $\mathbf{X} \in \mathbb{R}^{p \times p}$, consider the eigenvalue and eigenvector equation

$$\mathbf{X}\mathbf{v} = \lambda \mathbf{v} \Leftrightarrow (\mathbf{X} - \lambda \mathbf{I}_p)\mathbf{v} = \mathbf{0}, \quad \lambda \in \mathbb{R}, \mathbf{v} \in \mathbb{R}^p, \tag{41}$$

  for an eigenvalue-eigenvector pair $(\lambda, \mathbf{v})$ of $\mathbf{X}$ with $\mathbf{v} \neq \mathbf{0}$
- again a linear system, but solving for a pair of eigenvalue and eigenvector $(\lambda, \mathbf{v})$ for which the inverse/resolvent $(\mathbf{X} - \lambda \mathbf{I}_p)^{-1}$ does not exist
- while seemingly less convenient at first sight, turns out to be very efficient in providing a unified assess to general spectral functionals of $\mathbf{X}$, by taking z to be complex and exploiting tools from **complex analysis**

Theorem (Cauchy's integral formula)

For $\Gamma \subset \mathbb{C}$ a positively (i.e., counterclockwise) oriented simple closed curve and a complex function $f(z)$ analytic in a region containing Γ and its inside, then

(i) *if $z_0 \in \mathbb{C}$ is enclosed by Γ, $f(z_0) = -\frac{1}{2\pi i} \oint_\Gamma \frac{f(z)}{z_0 - z} dz$;*

(ii) *if not, $\frac{1}{2\pi i} \oint_\Gamma \frac{f(z)}{z_0 - z} dz = 0$.*

$$(\mathbf{X} - \lambda \mathbf{I}_p)\mathbf{v} = \mathbf{0} \Rightarrow \mathbf{Q}_{\mathbf{X}}(z) = (\mathbf{X} - z\mathbf{I}_n)^{-1} \tag{42}$$

- let $\mathbf{X} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\mathsf{T}$ be the spectral decomposition of $\mathbf{X}$, with $\mathbf{\Lambda} = \{\lambda_i(\mathbf{X})\}_{i=1}^p$ eigenvalues and $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_p] \in \mathbb{R}^{p \times p}$ the associated eigenvectors, then

$$\mathbf{Q}(z) = \mathbf{U}(\mathbf{\Lambda} - z\mathbf{I}_p)^{-1}\mathbf{U}^\mathsf{T} = \sum_{i=1}^{p} \frac{\mathbf{u}_i \mathbf{u}_i^\mathsf{T}}{\lambda_i(\mathbf{X}) - z}. \tag{43}$$

- thus, same eigenspace as $\mathbf{X}$, but maps the eigenvalues $\lambda_i(\mathbf{X})$ of $\mathbf{X}$ to $1/(\lambda_i(\mathbf{X}) - z)$.

Applying Cauchy's integral formula to the resolvent matrix $\mathbf{Q}_{\mathbf{X}}(z)$ allows one to (somewhat magically!) assess the **eigenvalue** and **eigenvector** behavior of $\mathbf{X}$:

- characterize the eigenvalues of $\mathbf{X}$, one needs to determine a $z \in \mathbb{R}$ such that $\mathbf{Q}_{\mathbf{X}}(z)$ does *not* exist.
- can be done by directly calling the Cauchy's integral formula, which allows to determine the value of a (sufficiently nice) function f at a point of interest $z_0 \in \mathbb{R}$, by integrating its "inverse" $g_f(z) = f(z)/(z_0 - z)$ on the complex plane.
- this "inverse" $g_f(z)$ is akin to the resolvent and does not, *by design*, exist at the point of interest z_0.
- in the following example, we compare the two approaches of

(i) **directly solving** the determinantal equation; and
(ii) use resolvent + Cauchy's integral formula.

A resolvent approach to spectral analysis: an example

Consider the following two-by-two real symmetric random matrix

$$\mathbf{X} = \begin{bmatrix} x_1 & x_2 \\ x_2 & x_3 \end{bmatrix} \in \mathbb{R}^{2\times 2}, \tag{44}$$

for (say independent) random variables x_1, x_2, x_3. For $\lambda_1(\mathbf{X})$ and $\lambda_2(\mathbf{X})$ the two (random) eigenvalues of $\mathbf{X}$ with associated (random) eigenvectors $\mathbf{u}_1(\mathbf{X}), \mathbf{u}_2(\mathbf{X}) \in \mathbb{R}^2$, we are interested in

$$f_{\mathbf{X}} = \mathbb{E}\left[f(\lambda_1(\mathbf{X})) + f(\lambda_2(\mathbf{X}))\right], \qquad g_{i,\mathbf{X}} = \mathbf{a}^\mathsf{T}\mathbb{E}[\mathbf{u}_i(\mathbf{X})\mathbf{u}_i(\mathbf{X})^\mathsf{T}]\mathbf{b},\ i \in \{1,2\}, \tag{45}$$

for some function $f\colon \mathbb{R} \to \mathbb{R}$ and deterministic $\mathbf{a}, \mathbf{b} \in \mathbb{R}^2$.

(i) **Directly solve** for the eigenvalues from the determinantal equation as

$$0 = \det(\mathbf{X} - \lambda \mathbf{I}_2) \Leftrightarrow \lambda(\mathbf{X}) = \frac{1}{2}\left(x_1 + x_3 \pm \sqrt{(x_1+x_3)^2 - 4(x_1x_3 - x_2^2)}\right), \tag{46}$$

and the associated eigenvectors from $\mathbf{X}\mathbf{u}_i(\mathbf{X}) = \lambda_i(\mathbf{X})\mathbf{u}_i(\mathbf{X})$, $i \in \{1,2\}$. Then compute $f_{\mathbf{X}} = \mathbb{E}\left[f(\lambda_1(\mathbf{X})) + f(\lambda_2(\mathbf{X}))\right]$, $g_{i,\mathbf{X}} = \mathbf{a}^\mathsf{T}\mathbb{E}[\mathbf{u}_i(\mathbf{X})\mathbf{u}_i(\mathbf{X})^\mathsf{T}]\mathbf{b}$

- needs to **re-compute** of the expectation for a different choice of function f and the eigen-pair $(\lambda_1(\mathbf{X}), \mathbf{u}_1(\mathbf{X}))$ or $(\lambda_2(\mathbf{X}), \mathbf{u}_2(\mathbf{X}))$ of interest.

(ii) The **resolvent** approach:

$$\begin{aligned} f_{\mathbf{X}} &= \mathbb{E}\left[f(\lambda_1(\mathbf{X})) + f(\lambda_2(\mathbf{X}))\right] \\ &= \mathbb{E}\left[-\frac{1}{2\pi\imath}\oint_\Gamma \left(\frac{f(z)}{\lambda_1(\mathbf{X})-z} + \frac{f(z)}{\lambda_2(\mathbf{X})-z}\right) dz\right] \\ &= -\frac{1}{2\pi\imath}\oint_\Gamma \mathbb{E}\left[f(z)\,\mathrm{tr}\,\mathbf{Q}_{\mathbf{X}}(z)dz\right] = -\frac{1}{2\pi\imath}\oint_\Gamma f(z)\,\mathrm{tr}\left(\mathbb{E}[\mathbf{Q}_{\mathbf{X}}(z)]\right) dz, \end{aligned}$$

for Γ a positively-oriented contour that circles around both (random) eigenvalues of $\mathbf{X}$.

- a much more **unified approach** to the quantity $f_{\mathbf{X}}$ for different choices of f
- compute the expected resolvent once (which is much simpler in the case of large random matrices)
- then perform **contour integration** with the function f of interest.
- similarly, for $g_{i,\mathbf{X}}$, it follows that

$$g_{i,\mathbf{X}} = \mathbf{a}^\mathsf{T}\mathbb{E}[\mathbf{u}_i(\mathbf{X})\mathbf{u}_i(\mathbf{X})^\mathsf{T}]\mathbf{b} = -\frac{1}{2\pi\imath}\oint_{\Gamma_i} \mathbf{a}^\mathsf{T}\mathbb{E}[\mathbf{Q}_{\mathbf{X}}(z)]\mathbf{b}\,dz \tag{47}$$

for some contour Γ_i that circles around only $\lambda_i(\mathbf{X}), i \in \{1,2\}$

- given the expected resolvent $\mathbb{E}[\mathbf{Q}(z)]$, it suffices to choose the specific contour Γ_i to get the different expressions of $g_{1,\mathbf{X}}$ and $g_{2,\mathbf{X}}$

Resolvent as the core object

Objects of interest	Functionals of resolvent $\mathbf{Q}_{\mathbf{X}}(z)$
ESD $\mu_{\mathbf{X}}$ of $\mathbf{X}$	Stieltjes transform $m_{\mu_{\mathbf{X}}}(z) = \frac{1}{p} \operatorname{tr} \mathbf{Q}_{\mathbf{X}}(z)$
Linear spectral statistics (LSS): $f(\mathbf{X}) \equiv \frac{1}{p} \sum_i f(\lambda_i(\mathbf{X}))$	Integration of trace of $\mathbf{Q}_{\mathbf{X}}(z)$: $-\frac{1}{2\pi i} \oint_\Gamma f(z) \frac{1}{p} \operatorname{tr} \mathbf{Q}_{\mathbf{X}}(z)\, dz$ (via Cauchy's integral)
Projections of eigenvectors $\mathbf{v}^\mathsf{T}\mathbf{u}(\mathbf{X})$ and $\mathbf{v}^\mathsf{T}\mathbf{U}(\mathbf{X})$ onto some given vector $\mathbf{v} \in \mathbb{R}^p$	Bilinear form $\mathbf{v}^\mathsf{T}\mathbf{Q}_{\mathbf{X}}(z)\mathbf{v}$ of $\mathbf{Q}_{\mathbf{X}}$
General matrix functional $F(\mathbf{X}) = \sum_i f(\lambda_i(\mathbf{X}))\mathbf{v}_1^\mathsf{T}\mathbf{u}_i(\mathbf{X})\mathbf{u}_i(\mathbf{X})^\mathsf{T}\mathbf{v}_2$ involving both eigenvalues and eigenvectors	Integration of bilinear form of $\mathbf{Q}_{\mathbf{X}}(z)$: $-\frac{1}{2\pi i} \oint_\Gamma f(z)\mathbf{v}_1^\mathsf{T}\mathbf{Q}_{\mathbf{X}}(z)\mathbf{v}_2\, dz$

Using the resolvent to access eigenvalue distribution

Definition (Resolvent)

For a symmetric matrix $\mathbf{X} \in \mathbb{R}^{p\times p}$, the resolvent $\mathbf{Q}_{\mathbf{X}}(z)$ of $\mathbf{X}$ is defined, for $z \in \mathbb{C}$ not an eigenvalue of $\mathbf{X}$, as

$$\mathbf{Q}_{\mathbf{X}}(z) \equiv \left(\mathbf{X} - z\mathbf{I}_p\right)^{-1}. \tag{48}$$

- let $\mathbf{X} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\mathsf{T}}$ be the spectral decomposition of $\mathbf{X}$, with $\mathbf{\Lambda} = \{\lambda_i(\mathbf{X})\}_{i=1}^{p}$ eigenvalues and $\mathbf{U} = [\mathbf{u}_1, \ldots, \mathbf{u}_p] \in \mathbb{R}^{p\times p}$ the associated eigenvectors, then

$$\mathbf{Q}(z) = \mathbf{U}(\mathbf{\Lambda} - z\mathbf{I}_p)^{-1}\mathbf{U}^{\mathsf{T}} = \sum_{i=1}^{p} \frac{\mathbf{u}_i\mathbf{u}_i^{\mathsf{T}}}{\lambda_i(\mathbf{X}) - z}. \tag{49}$$

- thus, same eigenspace as $\mathbf{X}$, but maps the eigenvalues $\lambda_i(\mathbf{X})$ of $\mathbf{X}$ to $1/(\lambda_i(\mathbf{X}) - z)$.
- eigenvalue of $\mathbf{Q}_{\mathbf{X}}(z)$, and the resolvent matrix itself, must explode as z approaches any eigenvalue of $\mathbf{X}$.
- take the trace $\operatorname{tr}\mathbf{Q}_{\mathbf{X}}(z)$ of $\mathbf{Q}_{\mathbf{X}}(z)$ as the quantity to "locate" the eigenvalues of the matrix $\mathbf{X}$ of interest
- for $\mu_{\mathbf{X}} \equiv \frac{1}{p}\sum_{i=1}^{p}\delta_{\lambda_i(\mathbf{X})}$ the ESD of $\mathbf{X}$,

$$\boxed{\frac{1}{p}\operatorname{tr}\mathbf{Q}(z) = \frac{1}{p}\sum_{i=1}^{p}\frac{1}{\lambda_i(\mathbf{X}) - z} = \int \frac{\mu_{\mathbf{X}}(dt)}{t - z} \equiv m_{\mu_{\mathbf{X}}}(z)}. \tag{50}$$

Definition (Stieltjes transform)

For a real probability measure μ with support $\text{supp}(\mu)$, the *Stieltjes transform* $m_\mu(z)$ is defined, for all $z \in \mathbb{C} \setminus \text{supp}(\mu)$, as

$$m_\mu(z) \equiv \int \frac{\mu(dt)}{t - z}. \tag{51}$$

Proposition (Properties of Stieltjes transform, [HLN07])

For m_μ the Stieltjes transform of a probability measure μ, it holds that

(i) m_μ is complex analytic on its domain of definition $\mathbb{C} \setminus \text{supp}(\mu)$;

(ii) it is bounded $|m_\mu(z)| \leq 1/\operatorname{dist}(z, \text{supp}(\mu))$;

(iii) it is an increasing function on all connected components of its restriction to $\mathbb{R} \setminus \text{supp}(\mu)$ (since $m'_\mu(x) = \int (t-x)^{-2} \mu(dt) > 0$) with $\lim_{x \to \pm\infty} m_\mu(x) = 0$ if $\text{supp}(\mu)$ is bounded; and

(iv) $m_\mu(z) > 0$ for $z < \inf \text{supp}(\mu)$, $m_\mu(z) < 0$ for $z > \sup \text{supp}(\mu)$ and $\Im[z] \cdot \Im[m_\mu(z)] > 0$ if $z \in \mathbb{C} \setminus \mathbb{R}$; and

BTW, for any $\mathbf{u} \in \mathbb{R}^p$ and matrix $\mathbf{A} \in \mathbb{R}^{p \times p}$ so that $\operatorname{tr}(\mathbf{A}) = 1$, $\mathbf{u}^\mathsf{T} \mathbf{Q}_\mathbf{X}(z) \mathbf{u}$, $\operatorname{tr}(\mathbf{A}\mathbf{Q}_\mathbf{X}(z))$ are STs.

[5] Walid Hachem, Philippe Loubaton, and Jamal Najim. "Deterministic equivalents for certain functionals of large random matrices". In: *The Annals of Applied Probability* 17.3 (2007), pp. 875–930

Definition (Inverse Stieltjes transform)

For a, b continuity points of the probability measure μ, we have

$$\mu([a,b]) = \frac{1}{\pi} \lim_{y \downarrow 0} \int_a^b \Im \left[m_\mu(x + \imath y) \right] \, dx. \tag{52}$$

Besides, if μ admits a density f at x (i.e., $\mu(x)$ is differentiable in a neighborhood of x and $\lim_{\epsilon \to 0} (2\epsilon)^{-1} \mu([x-\epsilon, x+\epsilon]) = f(x)$),

$$f(x) = \frac{1}{\pi} \lim_{y \downarrow 0} \Im \left[m_\mu(x + \imath y) \right]. \tag{53}$$

Definition (Linear Spectral Statistic, LSS)

For a symmetric matrix $\mathbf{X} \in \mathbb{R}^{p\times p}$, the *linear spectral statistics* (LSS) $f_{\mathbf{X}}$ of $\mathbf{X}$ is defined as the averaged statistics of the eigenvalues $\lambda_1(\mathbf{X}), \ldots, \lambda_p(\mathbf{X})$ of $\mathbf{X}$ via some function $f\colon \mathbb{R} \to \mathbb{R}$, that is

$$f(\mathbf{X}) = \frac{1}{p}\sum_{i=1}^{p} f(\lambda_i(\mathbf{X})). \tag{54}$$

In particular, we have $= \int f(t)\mu_{\mathbf{X}}(dt)$, for $\mu_{\mathbf{X}}$ the ESD of $\mathbf{X}$.

LSS via contour integration: For $\lambda_1(\mathbf{X}), \ldots, \lambda_p(\mathbf{X})$ eigenvalues of a symmetric matrix $\mathbf{X} \in \mathbb{R}^{p\times p}$, some function $f\colon \mathbb{R} \to \mathbb{R}$ that is complex analytic in a compact neighborhood of the support $\mathrm{supp}(\mu_{\mathbf{X}})$ (of the ESD $\mu_{\mathbf{X}}$ of $\mathbf{X}$), then

$$f(\mathbf{X}) = \int f(t)\mu_{\mathbf{X}}(dt) = -\int \frac{1}{2\pi\imath}\oint_{\Gamma} \frac{f(z)\,dz}{t-z}\mu_{\mathbf{X}}(dt) = -\frac{1}{2\pi\imath}\oint_{\Gamma} f(z) m_{\mu_{\mathbf{X}}}(z)\,dz, \tag{55}$$

for *any* contour Γ that encloses $\mathrm{supp}(\mu_{\mathbf{X}})$, i.e., all the eigenvalues $\lambda_i(\mathbf{X})$.

Remark (LSS to retrieve the inverse Stieltjes transform formula):

$$\frac{1}{p}\sum_{\lambda_i(\mathbf{X})\in[a,b]}\delta_{\lambda_i(\mathbf{X})} = -\frac{1}{2\pi\imath}\oint_\Gamma 1_{\Re[z]\in[a-\varepsilon,b+\varepsilon]}(z)m_{\mu_\mathbf{X}}(z)\,dz$$
$$= -\frac{1}{2\pi\imath}\int_{a-\varepsilon_x-\imath\varepsilon_y}^{b+\varepsilon_x-\imath\varepsilon_y} 1_{\Re[z]\in[a-\varepsilon,b+\varepsilon]}(z)m_{\mu_\mathbf{X}}(z)\,dz - \frac{1}{2\pi\imath}\int_{b+\varepsilon_x+\imath\varepsilon_y}^{a-\varepsilon_x+\imath\varepsilon_y} 1_{\Re[z]\in[a-\varepsilon,b+\varepsilon]}(z)m_{\mu_\mathbf{X}}(z)\,dz$$
$$-\frac{1}{2\pi\imath}\int_{a-\varepsilon_x+\imath\varepsilon_y}^{a-\varepsilon_x-\imath\varepsilon_y} 1_{\Re[z]\in[a-\varepsilon,b+\varepsilon]}(z)m_{\mu_\mathbf{X}}(z)\,dz - \frac{1}{2\pi\imath}\int_{b+\varepsilon_x-\imath\varepsilon_y}^{b+\varepsilon_x+\imath\varepsilon_y} 1_{\Re[z]\in[a-\varepsilon,b+\varepsilon]}(z)m_{\mu_\mathbf{X}}(z)\,dz.$$

- Since $\Re[m(x+\imath y)] = \Re[m(x-\imath y)], \Im[m(x+\imath y)] = -\Im[m(x-\imath y)]$;
- we have $\int_{a-\varepsilon_x}^{b+\varepsilon_x} m_{\mu_\mathbf{X}}(x-\imath\varepsilon_y)\,dx + \int_{b+\varepsilon_x}^{a-\varepsilon_x} m_{\mu_\mathbf{X}}(x+\imath\varepsilon_y)dx = -2\imath\int_{a-\varepsilon_x}^{b+\varepsilon_x}\Im[m_{\mu_\mathbf{X}}(x+\imath\varepsilon_y)]\,dx$;
- and consequently $\mu([a,b]) = \frac{1}{p}\sum_{\lambda_i(\mathbf{X})\in[a,b]}\lambda_i(\mathbf{X}) = \frac{1}{\pi}\lim_{\varepsilon_y\downarrow 0}\int_a^b \Im[m_{\mu_\mathbf{X}}(x+\imath\varepsilon_y)]\,dx$.

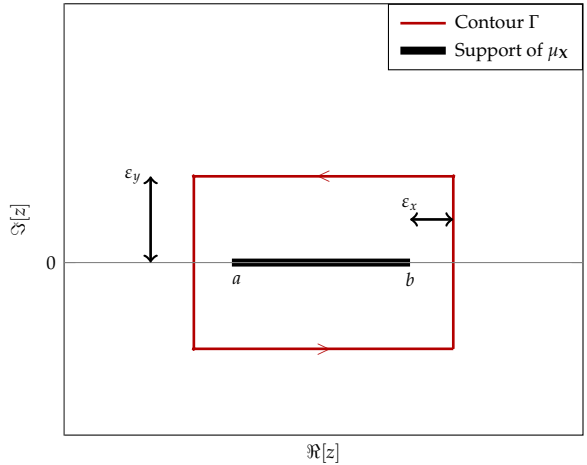


Figure: Illustration of a rectangular contour Γ and support of $\mu_{\mathbf{X}}$ on the complex plane.

Definition (Matrix spectral functionals)

For a symmetric matrix $\mathbf{X} \in \mathbb{R}^{p\times p}$, we say $F\colon \mathbb{R}^{p\times p} \to \mathbb{R}^{p\times p}$ is a matrix spectral functional of $\mathbf{X}$,

$$F(\mathbf{X}) = \sum_{i\in\mathcal{I}\subseteq\{1,\ldots,p\}} f(\lambda_i(\mathbf{X}))\mathbf{u}_i\mathbf{u}_i^\mathsf{T}, \quad \mathbf{X} = \sum_{i=1}^{p} \lambda_i(\mathbf{X})\mathbf{u}_i\mathbf{u}_i^\mathsf{T}. \tag{56}$$

Spectral functional via contour integration: For $\mathbf{X} \in \mathbb{R}^{p\times p}$, resolvent $\mathbf{Q}_\mathbf{X}(z) = (\mathbf{X} - z\mathbf{I}_p)^{-1}$, $z \in \mathbb{C}$, and $f\colon \mathbb{R} \to \mathbb{R}$ analytic in a neighborhood of the contour $\Gamma_\mathcal{I}$ that circles around the eigenvalues $\lambda_i(\mathbf{X})$ of $\mathbf{X}$ with their indices in the set $\mathcal{I} \subseteq \{1,\ldots,p\}$,

$$F(\mathbf{X}) = -\frac{1}{2\pi\imath} \oint_{\Gamma_\mathcal{I}} f(z)\mathbf{Q}_\mathbf{X}(z)\, dz. \tag{57}$$

Example: access to the i-th eigenvector $\mathbf{u}_i$ of $\mathbf{X}$ through

$$\mathbf{u}_i\mathbf{u}_i^\mathsf{T} = -\frac{1}{2\pi\imath} \oint_{\Gamma_{\lambda_i(\mathbf{X})}} \mathbf{Q}_\mathbf{X}(z)\, dz, \tag{58}$$

for $\Gamma_{\lambda_i(\mathbf{X})}$ a contour circling around $\lambda_i(\mathbf{X})$ only, so eigenvector projection $(\mathbf{v}^\mathsf{T}\mathbf{u}_i)^2 = -\frac{1}{2\pi\imath} \oint_{\Gamma_{\lambda_i(\mathbf{X})}} \mathbf{v}^\mathsf{T}\mathbf{Q}_\mathbf{X}(z)\mathbf{v}\, dz$.

Example: training linear model with gradient descent

Note that

$$\begin{aligned}\boldsymbol{\beta}_*^{\mathsf{T}}\boldsymbol{\beta}(t) &= \boldsymbol{\beta}_*^{\mathsf{T}} e^{-t\hat{\mathbf{C}}}\boldsymbol{\beta}(0) + \boldsymbol{\beta}_*^{\mathsf{T}}\left(\mathbf{I}_p - e^{-t\hat{\mathbf{C}}}\right)\boldsymbol{\beta}_{RR} \\ &= \boldsymbol{\beta}_*^{\mathsf{T}} e^{-t\hat{\mathbf{C}}}\boldsymbol{\beta}(0) + \boldsymbol{\beta}_*^{\mathsf{T}}\left(\mathbf{I}_p - e^{-t\hat{\mathbf{C}}}\right)\hat{\mathbf{C}}^{-1}\frac{1}{n}\mathbf{X}y \\ &= -\frac{1}{2\pi\imath}\oint_\Gamma \left(\exp(-tz)\cdot\boldsymbol{\beta}_*^{\mathsf{T}}\mathbf{Q}(z)\boldsymbol{\beta}(0) + \frac{1-\exp(-zt)}{z}\cdot\frac{1}{n}\boldsymbol{\beta}_*^{\mathsf{T}}\mathbf{Q}(z)\mathbf{X}y\right)dz,\end{aligned}$$

for Γ a positively oriented contour that circles around all eigenvalues of $\hat{\mathbf{C}}$, and resolvent

$$\mathbf{Q}(z) = (\hat{\mathbf{C}} - z\mathbf{I}_p)^{-1} = \left(\frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{T}} - z\mathbf{I}_p\right)^{-1}. \tag{59}$$

Take-away messages of this section

- "basic" probability: **concentration** of scalar observations of large random vectors: simple and involved, linear and nonlinear objects
- boils down to **expectation computation/evaluation**
- **same** holds for scalar observations of large random matrices
- linear algebra: matrix norm "equivalence" but up to **dimensional factors**
- **resolvent** (i.e., regularized inverse) naturally appears in eigenvalue/eigenvector assessment
- a unified **resolvent**-based to eigenspectral analysis of (not necessarily random) matrices: Cauchy's integral formula, Stieltjes transform (and its inverse), Linear Spectral Statistic, and generic matrix spectral functionals, etc.

Two different scaling regimes

Example (Nonlinear objects in two scaling regimes)

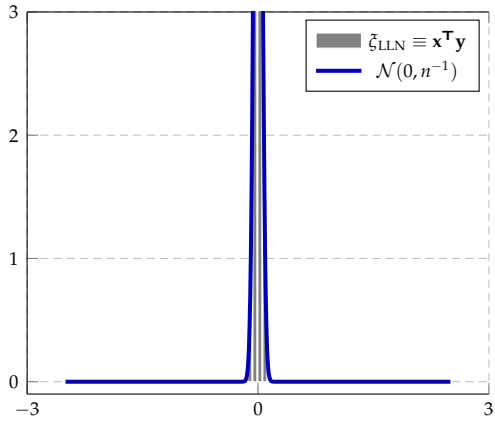
Let $\mathbf{x} \in \mathbb{R}^n$ be a random vector so that $\sqrt{n}\mathbf{x}$ has i.i.d. standard Gaussian entries with zero mean and unit variance, and $\mathbf{y} \in \mathbb{R}^n$ be a deterministic vector of unit norm $\|\mathbf{y}\| = 1$; and consider the following two families of nonlinear objects of interest with a nonlinear function f acting on different regimes:

(i) **LLN regime**: here we are interested in $f(\|\mathbf{x}\|^2)$ and $f(\mathbf{x}^\mathsf{T}\mathbf{y})$; and

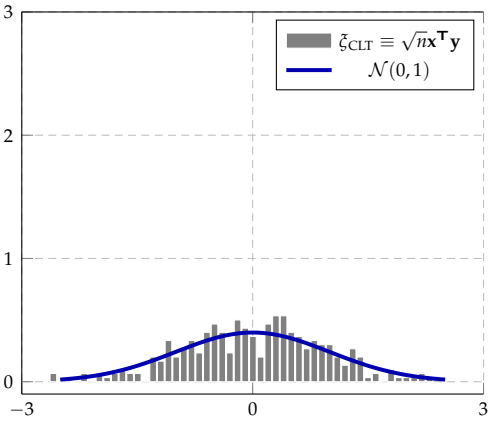
(ii) **CLT regime**: here we are interested in $f(\sqrt{n}(\|\mathbf{x}\|^2 - 1))$ and $f(\sqrt{n} \cdot \mathbf{x}^\mathsf{T}\mathbf{y})$.

- the (strong) **law of large numbers (LLN)** implies that
$$\|\mathbf{x}\|^2 \to \mathbb{E}[\mathbf{x}^\mathsf{T}\mathbf{x}] = 1 \text{ and } \mathbf{x}^\mathsf{T}\mathbf{y} \to \mathbb{E}[\mathbf{x}^\mathsf{T}\mathbf{y}] = 0$$
almost surely as $n \to \infty$; and
- the **central limit theorem (CLT)** implies that
$$\sqrt{n}(\|\mathbf{x}\|^2 - 1) \to \mathcal{N}(0, 2) \text{ and } \sqrt{n} \cdot \mathbf{x}^\mathsf{T}\mathbf{y} \to \mathcal{N}(0, 1)$$
in law as $n \to \infty$
- leads to the more compact form, for n large,
$$\|\mathbf{x}\|^2 \simeq 1 + \mathcal{N}(0, 2)/\sqrt{n} \text{ and } \mathbf{x}^\mathsf{T}\mathbf{y} \simeq 0 + \mathcal{N}(0, 1)/\sqrt{n}. \tag{60}$$

Illustration of the two scaling regime



(a) LLN regime



(b) CLT regime

Figure: Illustrations of random variables in LLN (**left**) and CLT (**right**) regime, with $n = 500$.

Two different scaling regimes and their corresponding linearization

Table: Comparison between two different high-dimensional linearization approaches.

Scaling regime	LLN type	CLT type
Object of interest	$f(\xi)$ for (almost) deterministic $\xi = \tau + o(1)$	$f(\xi)$ for random ξ, e.g., $\xi \sim \mathcal{N}(0, 1)$
Linearization technique	Taylor expansion	Orthogonal polynomial
Smoothness of f	Locally smooth f	Possibly non-smooth f

Theorem (Taylor's theorem for deterministic single-variable functions)

Let $f\colon \mathbb{R} \to \mathbb{R}$ be a function that is at least k times continuously differentiable in a neighborhood of a given point $\tau \in \mathbb{R}$. Then, there exists a function $h_k\colon \mathbb{R} \to \mathbb{R}$ such that

$$f(x) = f(\tau) + f'(x-\tau) + \frac{f''(\tau)}{2}(x-\tau)^2 + \ldots + \frac{f^{(k)}(\tau)}{k!}(x-\tau)^k + h_k(x)(x-\tau)^k, \tag{61}$$

with $\lim_{x\to\tau} h_k(x) = 0$ so that $h_k(x)(x-\tau)^k = o(|x-\tau|^k)$ as $x \to \tau$.

What makes the Taylor expansion approach work for random nonlinear functions $f(x)$?

- **Smoothness.** nonlinear f should be smooth, at least in the neighborhood of the point τ of interest, so that the derivatives $f'(\tau), f''(\tau), \ldots$ make sense.
- **Concentration.** variable of interest x is sufficiently close to (or, concentrates around, when being random) the point τ so that the higher orders terms are neglectable

Proposition (Taylor expansion of high-dimensional random functions in the LLN regime)

For random variable $\xi = \|\mathbf{x}\|^2$ with $\sqrt{n}\mathbf{x} \in \mathbb{R}^n$ having i.i.d. standard Gaussian entries, in the LLN regime, it follows from LLN and CLT that $\|\mathbf{x}\|^2 - 1 = O(n^{-1/2})$ with high probability for n large, so that one can apply Taylor theorem to write

$$f(\|\mathbf{x}\|^2) = f(1) + f'(1) \underbrace{(\|\mathbf{x}\|^2 - 1)}_{O(n^{-1/2})} + \frac{1}{2} f''(1) \underbrace{(\|\mathbf{x}\|^2 - 1)^2}_{O(n^{-1})} + O(n^{-3/2}), \tag{62}$$

with high probability. Similarly,

$$f(\mathbf{x}^\mathsf{T}\mathbf{y}) = f(0) + f'(0) \underbrace{\mathbf{x}^\mathsf{T}\mathbf{y}}_{O(n^{-1/2})} + \frac{1}{2} f''(0) \underbrace{(\mathbf{x}^\mathsf{T}\mathbf{y})^2}_{O(n^{-1})} + O(n^{-3/2}), \tag{63}$$

again as a consequence of $\sqrt{n} \cdot \mathbf{x}^\mathsf{T}\mathbf{y} \xrightarrow{d} \mathcal{N}(0,1)$ in distribution as $n \to \infty$, where the orders $O(n^{-\ell})$ hold with high probability for n large.

A functional analysis perspective of expectation of nonlinear random function

- Consider the following functional analysis perspective of the expectation $\mathbb{E}[f(\xi)]$
- For a random variable ξ following some law μ, the expectation $\mathbb{E}[f(\xi)]$ of the nonlinear transformation $f(\xi)$ can be expresses as

$$\mathbb{E}_{\xi\sim\mu}[f(\xi)] = \int f(t)\mu(dt). \tag{64}$$

- In the case of Euclidean space, the canonical vectors $\mathbf{e}_1, \ldots, \mathbf{e}_n$ form an orthonormal basis of $\mathbb{R}^n$; and thus any vector $\mathbf{x}$ living in the Euclidean space $\mathbb{R}^n$ can be decomposed as

$$\mathbf{x} = \sum_{i=1}^{n} (\mathbf{x}^\mathsf{T}\mathbf{e}_i)\mathbf{e}_i = \sum_{i=1}^{n} x_i\mathbf{e}_i, \tag{65}$$

  with the inner product $\mathbf{x}^\mathsf{T}\mathbf{e}_i = x_i$ the ith coordinate of $\mathbf{x}$.
- A similar result holds more generally, e.g., or a function f living in some (infinite dimensional) function space, can be decomposed into the sum of "orthonormal" basis functions, weighted by the projection (i.e., inner product) of f onto these basis functions

Definition (Orthogonal polynomials and orthogonal polynomial expansion)

For a probability measure μ, define the inner product

$$\langle f, g \rangle \equiv \int f(\xi) g(\xi) \mu(d\xi) = \mathbb{E}[f(\xi) g(\xi)], \tag{66}$$

for $\xi \sim \mu$. We say that $\{P_\ell(\xi), \ell \geq 0\}$ is a family of orthogonal polynomials with respect to this inner product, obtained by the Gram-Schmidt procedure on the monomials $\{1, \xi, \xi^2, \ldots\}$, with $P_0(\xi) = 1$, where P_ℓ is a polynomial function of degree ℓ that satisfies

$$\langle P_{\ell_1}, P_{\ell_2} \rangle = \mathbb{E}[P_{\ell_1}(\xi) P_{\ell_2}(\xi)] = \delta_{\ell_1 = \ell_2}. \tag{67}$$

Then, for any function $f \in L^2(\mu)$, the orthogonal polynomial expansion of f is

$$f(\xi) \sim \sum_{\ell=0}^{\infty} a_\ell P_\ell(\xi), \quad a_\ell = \int f(\xi) P_\ell(\xi) \mu(d\xi) \tag{68}$$

- denote "$f \sim \sum_{l=0}^{\infty} a_\ell P_\ell$" to denote that $\|f - \sum_{\ell=0}^{L} a_\ell P_\ell\|_\mu \to 0$ as $L \to \infty$ with $\|f\|_\mu^2 = \langle f, f \rangle$, or equivalently $\int \left(f(\xi) - \sum_{\ell=0}^{L} a_\ell P_\ell(\xi)\right)^2 \mu(d\xi) = \mathbb{E}\left[\left(f(\xi) - \sum_{\ell=0}^{L} a_\ell P_\ell(\xi)\right)^2\right] \to 0$.

Theorem (Hermite polynomial decomposition)

For $\xi \in \mathbb{R}$, the ℓ^{th} order normalized Hermite polynomial, denoted $P_\ell(\xi)$, is given by given by

$$P_0(\xi) = 1, \text{ and } P_\ell(\xi) = \frac{(-1)^\ell}{\sqrt{\ell!}} e^{\frac{\xi^2}{2}} \frac{d^n}{d\xi^n}\left(e^{-\frac{\xi^2}{2}}\right), \text{ for } \ell \geq 1. \tag{69}$$

and the family of (normalized) Hermite polynomials

(i) *being orthogonal polynomials and (as the name implies) are orthonormal with respect the standard Gaussian measure: $\int P_m(\xi)P_n(\xi)\mu(d\xi) = \delta_{nm}$, for $\mu(dt) = \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} dt$ the standard Gaussian measure; and*

(ii) *form an orthonormal basis of $L^2(\mu)$, the Hilbert space consist of all square-integrable functions with respect to the inner product $\langle f, g\rangle \equiv \int f(\xi)g(\xi)\mu(d\xi)$, and that one can formally expand any $f \in L^2(\mu)$ as*

$$f(\xi) \sim \sum_{\ell=0}^{\infty} a_{\ell,f} P_\ell(\xi), \quad a_{\ell,f} = \int f(\xi)P_\ell(\xi)\mu(d\xi) = \mathbb{E}[f(\xi)P_\ell(\xi)], \tag{70}$$

where we use '$f \sim \sum_{\ell=0}^{\infty} a_{\ell,f} P_\ell$' for standard Gaussian $\xi \sim \mathcal{N}(0,1)$. The coefficients $a_{\ell,f}$s are generalized moments of the standard Gaussian measure μ involving f, and we have

$$a_{0,f} = \mathbb{E}_{\xi\sim\mathcal{N}(0,1)}[f(\xi)], \quad a_{1,f} = \mathbb{E}[\xi f(\xi)], \quad \sqrt{2}a_{2,f} = \mathbb{E}[\xi^2 f(\xi)] - a_{0,f}, \quad \nu_f = \mathbb{E}[f^2(\xi)] = \sum_{\ell=0} a_{\ell,f}^2. \tag{71}$$

Numerical illustration of Hermite polynomials

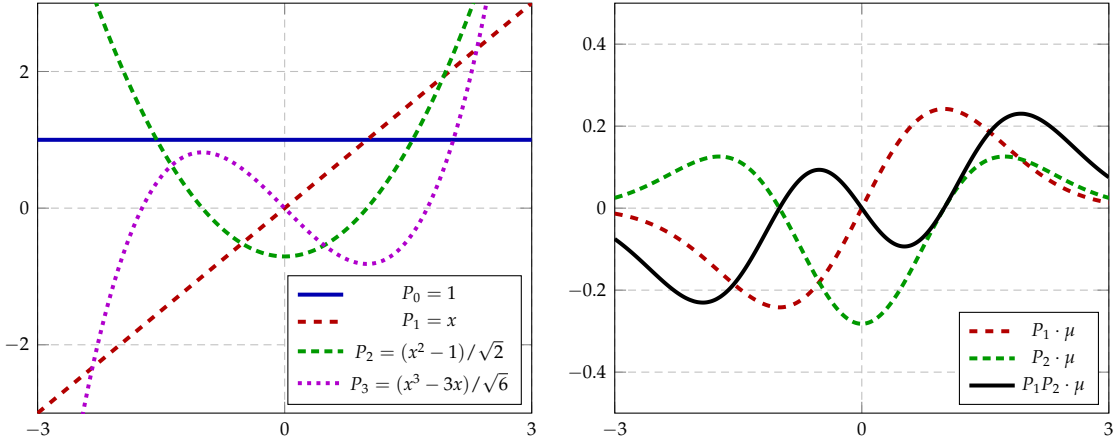


Figure: Illustration of the first four Hermite polynomials (**left**) and of the first- and second-order Hermite polynomial (P_1 and P_2) weighted by the Gaussian mixture $\mu(dx) = \exp(-x^2/2)/\sqrt{2\pi}$ (**right**).

Hermite polynomial "expansion" in the CLT regime

Proposition (Hermite polynomial "expansion" in the CLT regime)

For random variable $\xi_{\mathrm{CLT}} = \sqrt{n} \cdot (\|\mathbf{x}\|^2 - 1)$ *with* $\sqrt{n}\mathbf{x} \in \mathbb{R}^n$ *having i.i.d. standard Gaussian entries, in the CLT regime, it follows from the CLT that* $\xi_{\mathrm{CLT}} \sim \mathcal{N}(0,1)$ *in the* $n \to \infty$ *limit, so that one can write*

$$\mathbb{E}[f(\sqrt{n} \cdot (\|\mathbf{x}\|^2 - 1))] = \mathbb{E}_{\xi \sim \mathcal{N}(0,1)}[f(\xi)] + o(1) = a_{0,f} + o(1), \tag{72}$$

as $n \to \infty$*; and similarly*

$$\mathbb{E}[f(\sqrt{n} \cdot \mathbf{x}^\mathsf{T}\mathbf{y})] = \mathbb{E}_{\xi \sim \mathcal{N}(0,1)}[f(\xi)] + o(1) = a_{0,f} + o(1). \tag{73}$$

- looks **not** extremely insightful
- makes a lot more sense for scalar nonlinear observations of random vectors and random matrices, e.g., $\mathbf{K} = f(\mathbf{X}^\mathsf{T}\mathbf{X}/\sqrt{p})/\sqrt{p} - \mathrm{diag}(\cdot)$, for random matrix $\mathbf{X} \in \mathbb{R}^{p \times n}$

Example (Nonlinear behaviors of tanh in two scaling regimes)

Consider the hyperbolic tangent function $f(t) = \tanh(t)$. This nonlinear function is "close" to different quadratic functions in *different* regimes of interest. More precisely, we have the following.

(i) **In the LLN regime**, we have

$$\tanh(\xi_{\text{LLN}}) \simeq g(\xi_{\text{LLN}}),$$

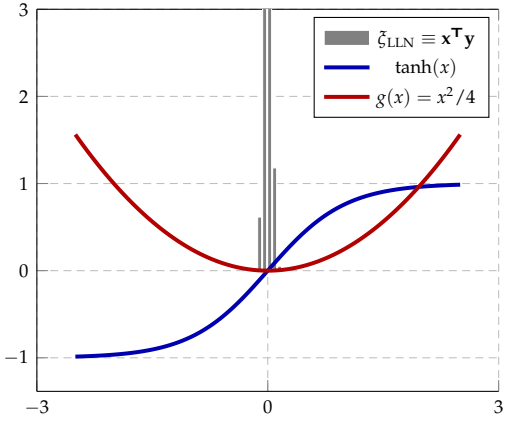
with $g(t) = t^2/4$. This is as a consequence of $\tanh(x) = g(x) = 0$. In particular, $\mathbb{E}[\tanh(\xi_{\text{LLN}})] \simeq \mathbb{E}[g(\xi_{\text{LLN}})]$.

(ii) **In the CLT regime**, we have

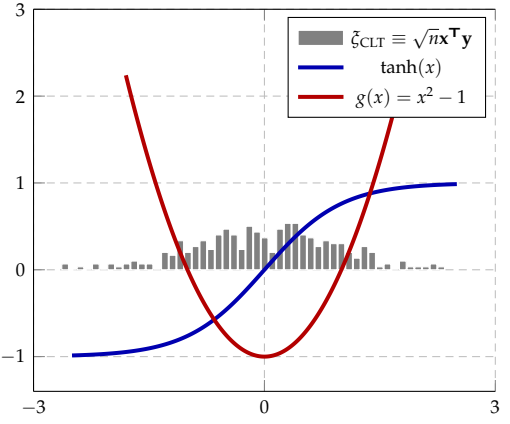
$$\mathbb{E}[\tanh(\xi_{\text{LLN}})] = \mathbb{E}[g(\xi_{\text{LLN}})]$$

in expectation, with now $g(t) = t^2 - 1$, i.e., with a different function. This is a consequence of the fact that their zeroth-order Hermite coefficient $a_0 = 0$.

Numerical illustration of two high-dimensional linearization technique



(a) LLN regime



(b) CLT regime

Figure: Different behavior of nonlinear $f(\xi_{\text{LLN}})$ and $f(\xi_{\text{CLT}})$ for $f(t) = \tanh(t)$ in the LLN and CLT regime, with $n = 500$. We have in particular $\tanh(\xi_{\text{LLN}}) \simeq g(\xi_{\text{LLN}})$ in the LLN regime and $\mathbb{E}[\tanh(\xi_{\text{CLT}})] = \mathbb{E}[g(\xi_{\text{CLT}})]$ in the CLT regime with *different* g.

Definition (High-dimensional Linear Equivalent)

For a random vector $\mathbf{x} \in \mathbb{R}^n$, its nonlinear transformation $f(\mathbf{x}) \in \mathbb{R}^n$ is obtained by applying $f\colon \mathbb{R} \to \mathbb{R}$ entry-wise on $\mathbf{x}$. Consider $g(f(\mathbf{x}))$ a scalar observation of $f(\mathbf{x})$ via observation function $g\colon \mathbb{R}^n \to \mathbb{R}$, we say that the random vector $\tilde{\mathbf{x}}_f$ (defined on an extended probability space if necessary) is an (ε, δ)-Linear Equivalent to $f(\mathbf{x})$ if, with probability at least $1 - \delta(n)$ that

$$\left| g(f(\mathbf{x})) - g(\tilde{\mathbf{x}}_f) \right| \leq \varepsilon(n), \tag{74}$$

for some non-negative functions $\varepsilon(n)$ and $\delta(n)$ that decrease to zero as $n \to \infty$. This, in the limit of $n \to \infty$, leads to

$$g(f(\mathbf{x})) - g(\tilde{\mathbf{x}}_f) \to 0, \tag{75}$$

in probability or almost surely for the observation function $g(\cdot)$, and we denote

$$f(\mathbf{x}) \overset{g}{\leftrightarrow} \tilde{\mathbf{x}}_f. \tag{76}$$

And similarly for a random matrix $\mathbf{X} \in \mathbb{R}^{p \times n}$.

Example: Nonlinear random vectors in two scaling regimes

Example (Nonlinear random vectors in two scaling regimes)

Let $\mathbf{X} \in \mathbb{R}^{p \times n}$ be a *random* matrix so that $\sqrt{n}\mathbf{X}$ has i.i.d. standard Gaussian entries with zero mean and unit variance, and $\mathbf{y} \in \mathbb{R}^n, \boldsymbol{\alpha} \in \mathbb{R}^p$ be *deterministic* vectors of unit norm such that $\|\mathbf{y}\| = 1$ and $\|\boldsymbol{\alpha}\| = 1$; consider the following two families of *scalar* observations of *nonlinear* random vectors with observation function $g\colon \mathbb{R}^p \to \mathbb{R}$ and a nonlinear function f acting on different regimes:

(i) **LLN regime**: $g(f(\mathbf{X}\mathbf{y})) = \frac{1}{\sqrt{n}}\boldsymbol{\alpha}^\mathsf{T} f(\mathbf{X}\mathbf{y})$; and

(ii) **CLT regime**: $g(f(\sqrt{n} \cdot \mathbf{X}\mathbf{y})) = \frac{1}{\sqrt{n}}\boldsymbol{\alpha}^\mathsf{T} f(\sqrt{n} \cdot \mathbf{X}\mathbf{y})$.

Proposition (Taylor expansion of nonlinear random vector in the LLN regime)

Let $\mathbf{X} \in \mathbb{R}^{p\times n}$ be a random matrix so that $\sqrt{n}\mathbf{X}$ has i.i.d. standard Gaussian entries with zero mean and unit variance, and $\mathbf{y} \in \mathbb{R}^n, \boldsymbol{\alpha} \in \mathbb{R}^p$ be deterministic vectors of unit norm such that $\|\mathbf{y}\| = 1$ and $\|\boldsymbol{\alpha}\| = 1$, in the LLN regime, the following Linear Equivalent holds

$$f(\mathbf{X}\mathbf{y}) \overset{g}{\leftrightarrow} \underbrace{f(0)\cdot \mathbf{1}_p}_{O_{\|\cdot\|_\infty}(1)} + \underbrace{f'(0)\cdot \mathbf{X}\mathbf{y}}_{O_{\|\cdot\|_\infty}(n^{-1/2})}, \tag{77}$$

for the scalar observation function $g(\cdot) = \boldsymbol{\alpha}^\mathsf{T}(\cdot)/\sqrt{n}$, up to some approximation error $\varepsilon = O(n^{-1})$.

Proposition (Hermite polynomial expansion in the CLT regime.)

Let $\mathbf{X} \in \mathbb{R}^{p\times n}$ be a random matrix so that $\sqrt{n}\mathbf{X}$ has i.i.d. standard Gaussian entries with zero mean and unit variance, and $\mathbf{y} \in \mathbb{R}^n, \boldsymbol{\alpha} \in \mathbb{R}^p$ be deterministic vectors of unit norm such that $\|\mathbf{y}\| = 1$ and $\|\boldsymbol{\alpha}\| = 1$, in the CLT regime, if the nonlinear $f : \mathbb{R} \to \mathbb{R}$ and $g(\cdot) = \boldsymbol{\alpha}^\mathsf{T}(\cdot)/\sqrt{n}$ are such that $g(f(\sqrt{n}\mathbf{X}\mathbf{y}))$ strongly concentrates, i.e.,

$$g(f(\sqrt{n}\mathbf{X}\mathbf{y})) = \frac{1}{\sqrt{n}}\boldsymbol{\alpha}^\mathsf{T} f(\sqrt{n}\mathbf{X}\mathbf{y}) = \frac{1}{\sqrt{n}}\mathbb{E}[\boldsymbol{\alpha}^\mathsf{T} f(\sqrt{n}\mathbf{X}\mathbf{y})] + \varepsilon(n,p), \tag{78}$$

with high probability for n, p large, so $f(\sqrt{n}\mathbf{X}\mathbf{y}) \overset{g}{\leftrightarrow} a_{0,f}\cdot \mathbf{1}_p$, for the observation function $g(\cdot) = \boldsymbol{\alpha}^\mathsf{T}(\cdot)/\sqrt{n}$.

An additional example in the CLT regime

Example (Hermite polynomial expansion in the CLT regime)

Under the same notations and settings as above but for random observation function

$$g(\cdot) = \frac{1}{\sqrt{n}} \mathbf{y}^\mathsf{T} \mathbf{X}^\mathsf{T} (\cdot), \tag{79}$$

that is assumed to strongly concentrate around its expectation up to some $\varepsilon(n,p)$ for n,p large, then, the following Linear Equivalent holds

$$f(\sqrt{n}\mathbf{X}\mathbf{y}) \overset{g}{\leftrightarrow} a_{1,f} \cdot \sqrt{n}\mathbf{X}\mathbf{y}, \tag{80}$$

up to some approximation error $\varepsilon(n,p)$.

- we also have $f(\sqrt{n}\mathbf{X}\mathbf{y}) \overset{g}{\leftrightarrow} a_{1,f} \cdot \sqrt{n}\mathbf{X}\mathbf{y} + \mathbf{z}$, and Linear Equivalents are not unique
- in some cases we care joint behavior of multiple observation functions, etc.

An additional example of joint behavior in the CLT regime

Example (Hermite polynomial expansion in the CLT regime: joint behavior)

Consider random vector $\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$ having i.i.d. standard Gaussian entries, and nonlinear random vector $f(\mathbf{x})$ with nonlinear $f\colon \mathbb{R} \to \mathbb{R}$ applied entry-wise on $\mathbf{x}$, in the CLT regime. Then, for the *joint* behavior of the two *scalar* observation of $f(\mathbf{x})$,

$$(g_1(f(\mathbf{x})), g_2(f(\mathbf{x}))) = \left(\frac{1}{p} \mathbf{x}^\mathsf{T} f(\mathbf{x}), \frac{1}{p} f(\mathbf{x})^\mathsf{T} f(\mathbf{x}) \right), \tag{81}$$

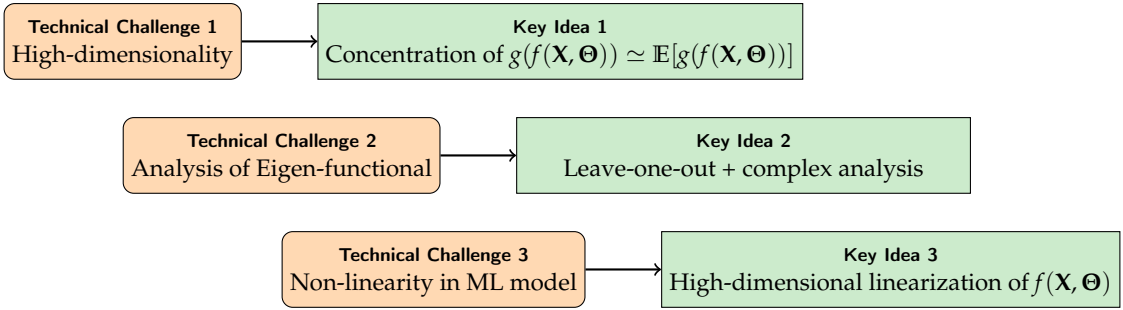
the following asymptotic equivalent linear model holds

$$f(\mathbf{x}) \overset{(g_1, g_2)}{\leftrightarrow} a_{0,f} \cdot \mathbf{1}_p + a_{1,f} \cdot \mathbf{x} + \sqrt{\nu_f - a_{0,f}^2 - a_{1,f}^2} \cdot \mathbf{z}, \tag{82}$$

with $a_{0,f}, a_{1,f}, \nu_f$ the Hermite coefficients of f, and standard Gaussian random vector $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$ that is *independent* of $\mathbf{x}$.

Take-away messages of this section

- two different scaling regimes: LLN versus CLT
- high-dimensional linearizations of nonlinear random functions via **Taylor Expansion** and **Orthogonal Polynomial**
- Taylor Expansion can be performed in a close-to-deterministic fashion
- Orthogonal Polynomial is more tricky and depends on the form of the observation map



Thank you! Q & A?