Random Matrix Theory for Machine Learning

Part 1: Motivating Questions and Building Blocks

Fabian Pedregosa[1], Courtney Paquette[1,2], Tom Trogdon[3], Jeffrey Pennington[1]

[1] Google Research, [2] McGill University, [3] University of Washington

https://random-matrix-learning.github.io

About this tutorial

Objective:

- Applications of *Random Matrix Theory* (RMT) in Machine Learning.
- Proof techniques in RMT

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Structure:

1. Motivating Questions and Building Blocks, *Fabian Pedregosa*
2. Introduction to Random Matrix Theory, *Courtney Paquette*
3. Analysis of Numerical Algorithms, *Tom Trogdon*
4. The Mystery of Generalization: Why Does Deep Learning Work?, *Jeffrey Pennington*

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What is a Random Matrix?

A *random matrix* is a matrix whose entries are random variables, not necessarily independent.

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Example

Realization of a random matrix:

$$Z = \begin{bmatrix} 1.066 & 0.908 & 1.026 & -0.294 & 0.879 \\ 0.908 & -1.794 & 0.596 & -1.014 & -0.103 \\ 1.026 & 0.596 & -0.246 & 0.968 & 0.750 \\ -0.294 & -1.014 & 0.968 & 0.184 & 0.812 \\ 0.879 & -0.103 & 0.750 & 0.812 & 0.210 \end{bmatrix}$$

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Goal of Random Matrix Theory is to understand their

- eigenvalues
- eigenvectors
- norms
- singular values
- singular vectors
- ...

Where do Random Matrices Come From?

1928: Eigenvalues of Normal Covariance Matrices

THE GENERALISED PRODUCT MOMENT DISTRIBUTION IN SAMPLES FROM A NORMAL MULTIVARIATE POPULATION.

By JOHN WISHART, M.A., B.Sc. Statistical Department, Rothamsted Experimental Station.

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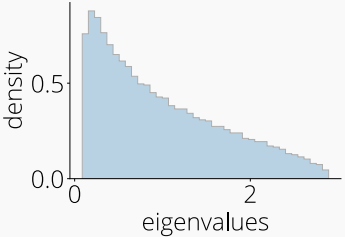

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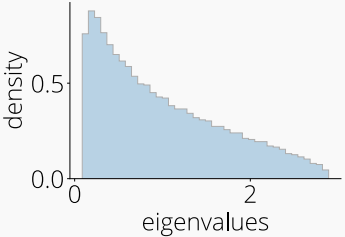
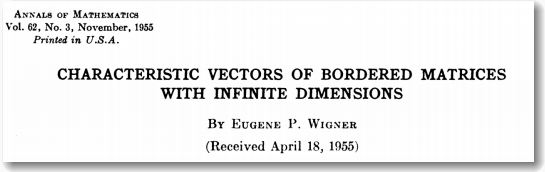


$$W = XX^\top, X_{ij} \sim \mathcal{N}(0,1)$$

$$p(\lambda_1, \ldots, \lambda_N) \propto e^{-\frac{1}{2}\sum_i \lambda_i} \prod \lambda_i^{(n-p-1)/2} \prod_{i<j} |\lambda_i - \lambda_j|$$

1955: Random Symmetric Matrices



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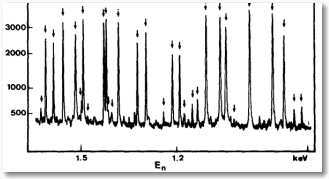
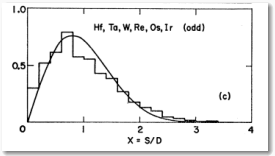
CHARACTERISTIC VECTORS OF BORDERED MATRICES WITH INFINITE DIMENSIONS

BY EUGENE P. WIGNER

(Received April 18, 1955)

Eugene Wigner



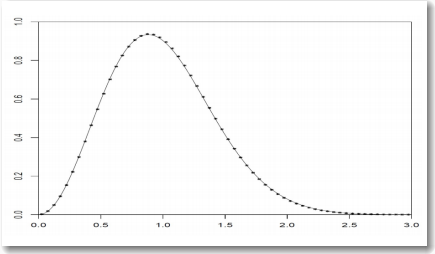


Energy levels of heavy nuclei, compared with the random matrix theory prediction.

Source: [Rosenzweig and Porter, 1960]

Model for high-dimensional phenomena

- Number Theory [Montgomery, 1973, Keating, 1993].
- Graph Theory [Erdos and Rényi, 1960].
- Finance [Bouchaud and Potters, 2009].
- Wireless communication [Tulino et al., 2004]
- Machine Learning ...

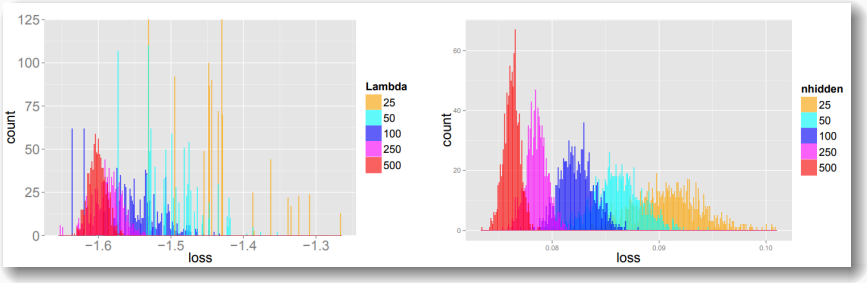


Distribution function of gaps between eigenvalues compared with histogram of gaps between ζ zeros. Source: [Odlyzko, 1987]

Spin Glass model of the Loss Landscape

Early: [Amit et al., 1985, Gardner and Derrida, 1988, Dotsenko, 1995]

Late: [Dauphin et al., 2014, Sagun et al., 2014, Choromanska et al., 2015, Baity-Jesi et al., 2018]



Loss study through spin-glass model. Scaled test losses for the spin-glass (left) and the neural network (right). Source: Choromanska et al. [2015] *The Loss Surfaces of Multilayer Networks*.

Random Matrices in Machine Learning: Loss Landscape

New methods and software[1,2,3] to compute Hessian eigenvalues of large models [Ghorbani et al., 2019, Yao et al., 2020, Papyan, 2020]

[1] *https://github.com/amirgholami/PyHessian*
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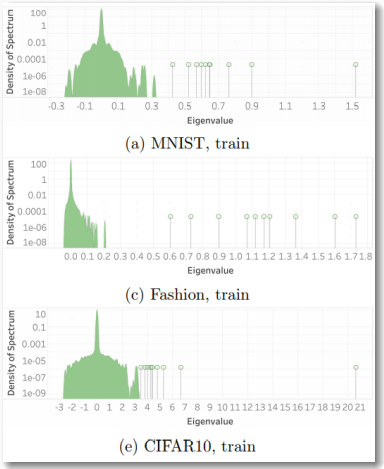
[3] *https://github.com/deep-lab/DeepnetHessian*



Source: [Papyan, 2020]

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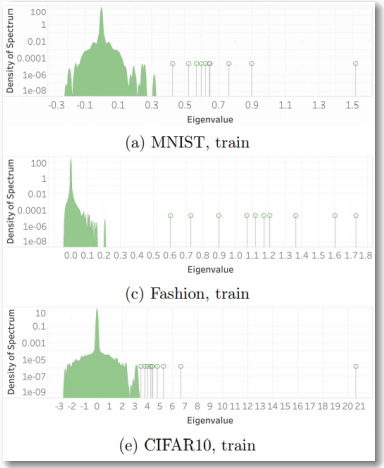
RMT model for the Hessian still an open problem [Liao and Mahoney, 2021, Baskerville et al., 2021] ...

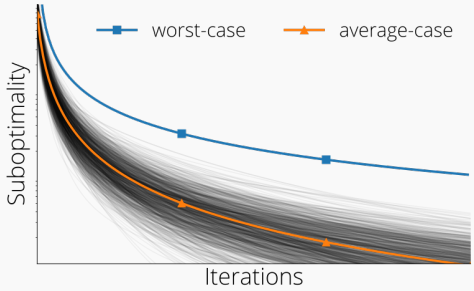


Source: [Papyan, 2020]

Random Matrices in Machine Learning: Numerical Algorithms

Analyze algorithms with **random** data.

- Simplex [Borgwardt, 1987, Smale, 1983, Spielman and Teng, 2004, Vershynin, 2009] etc.
- Conjugate Gradient [Deift and Trogdon, 2017, Paquette and Trogdon, 2020]
- Acceleration [Pedregosa and Scieur, 2020, Lacotte and Pilanci, 2020]



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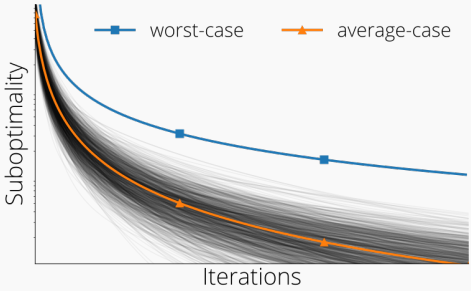
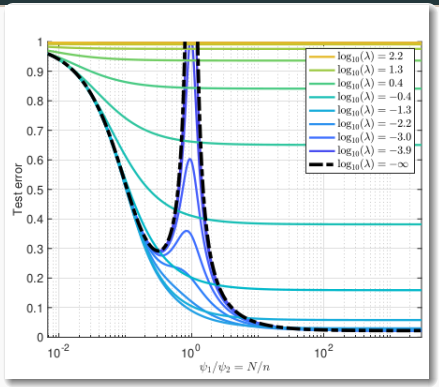


Topic of Part 3 of this tutorial

Random Matrices in Machine Learning: Generalization

As a model for generalization [Hastie et al., 2019, Mei and Montanari, 2019, Adlam and Pennington, 2020, Liao et al., 2020]



Random Matrices can be used to model the **double descent** generalization curve. Source: [Mei and Montanari, 2019] *The generalization error of random features regression: Precise asymptotics and double descent curve*

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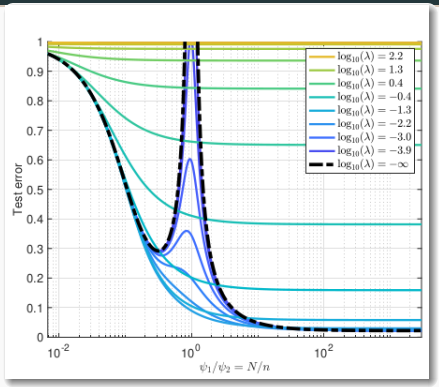

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Part 4 of this tutorial

Building Blocks

Classical Random Matrix Ensembles

Gaussian Orthogonal Ensemble (GOE)

Motivation: Model Hamiltonian heavy nuclei

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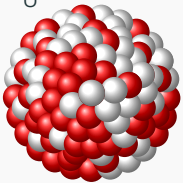

Gaussian Orthogonal Ensemble (GOE)

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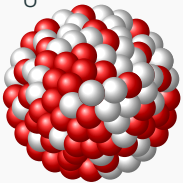

- **Rotational invariant**
  for any fixed orthogonal matrix O,

$$A \overset{\text{law}}{=} O^T A O\,.$$

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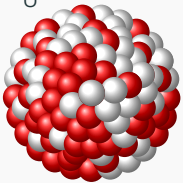

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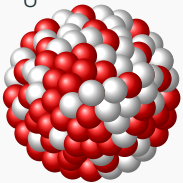

- **Rotational invariant**
  for any fixed orthogonal matrix O,

$$A \overset{\text{law}}{=} O^T A O\,.$$

- **Symmetric** matrix.

- **Independence**
  Entries A_{ij}, $i \leq j$ are independent.

Gaussian Orthogonal Ensemble (GOE)

- real $n \times n$ matrix

$$\frac{1}{\sqrt{n}} \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{13} & a_{14} & \cdots \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} & \cdots \\ a_{13} & a_{32} & a_{33} & a_{34} & a_{35} & \cdots \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}$$

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- real $n \times n$ matrix
- $\mathcal{N}(0, 1)$ above diagonal

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Gaussian Orthogonal Ensemble (GOE)

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- Symmetric
- $\mathcal{N}(0,2)$ diagonal

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Eigenvalues of GOE

Python pseudocode

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import numpy as np
import matplotlib.pyplot as plt

A = np.random.randn(n, n)
GOE = (A+A.T)/np.sqrt(2*n)

eig = np.linalg.eigvals(GOE)
plt.hist(eig)
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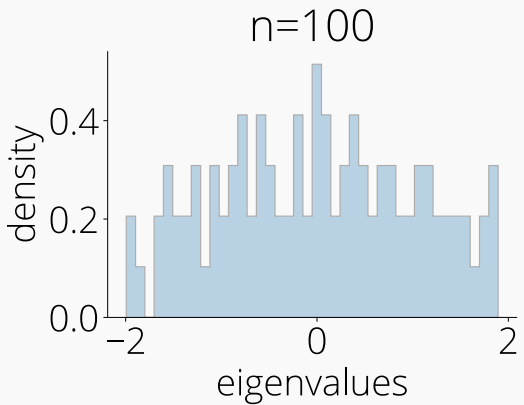

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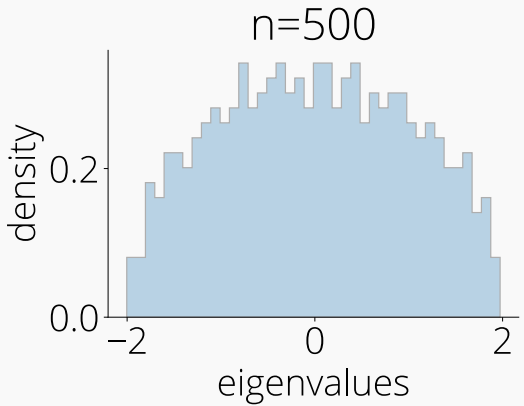

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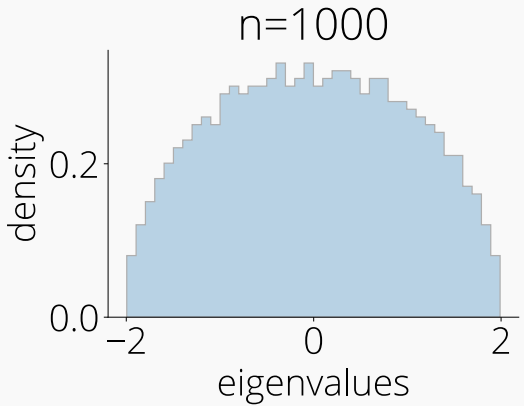

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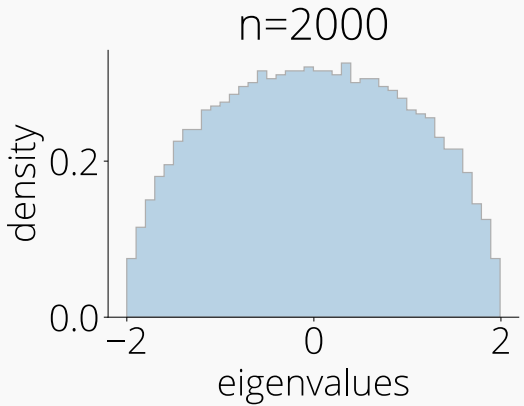

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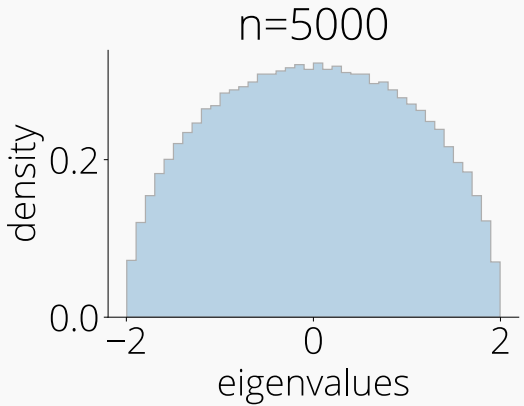

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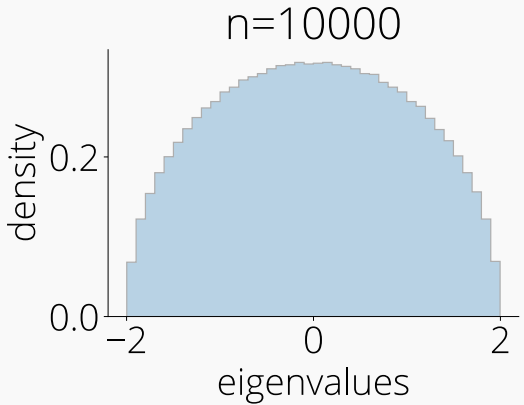
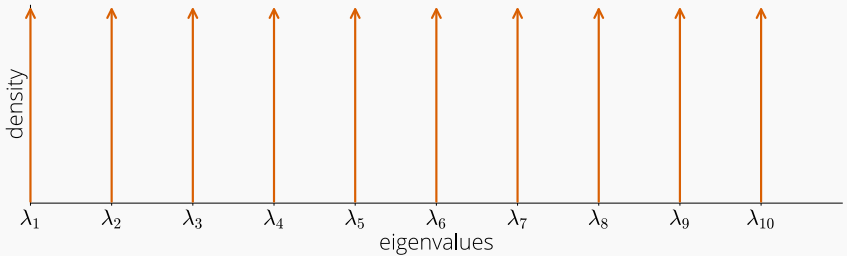


Empirical Spectral Distribution (ESD)

ESD of matrix A_n = p.d.f. of an eigenvalue chosen uniformly at random

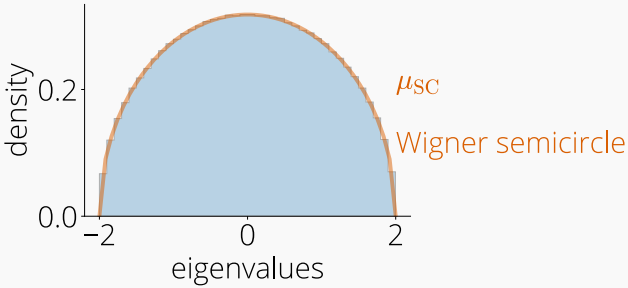
$$\mu_{\text{ESD}} = \mu_n \overset{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i(A_n)}.$$



Wigner Semicircle Law

μ_{ESD} converges as $n \to \infty$ to the semicircular distribution,

$$\mu_{\text{SC}}(x) \overset{\text{def}}{=} \frac{1}{2\pi}\sqrt{(4-x^2)_+}\,\mathrm{d}x\,.$$



To know more: [Tao, 2012, Bai and Silverstein, 2010].

Wishart ensemble

Wishart

- X = random $(d \times n)$ matrix with entries i.i.d. $\mathcal{N}(0,1)$
- Wishart $(d \times d)$ matrix, $W = \frac{XX^T}{n}$

Remarks

- W is symmetric, positive semi-definite

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- Parameter $r = \frac{d}{n}$

Wishart ensemble

Python pseudocode

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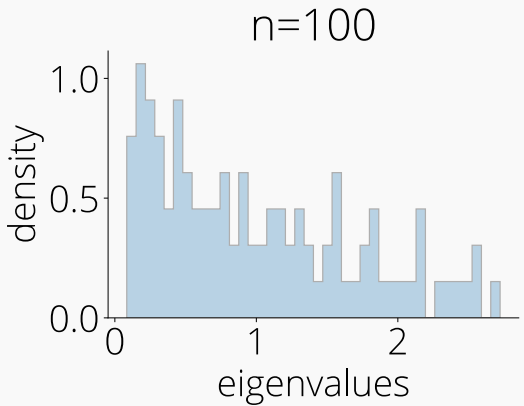
import matplotlib.pyplot as plt

r = 1/2  # for example
X = np.random.randn(n * r, n)
W = np.dot(X, X.T) / n

eig = np.linalg.eigvals(W)
plt.hist(eig)
```



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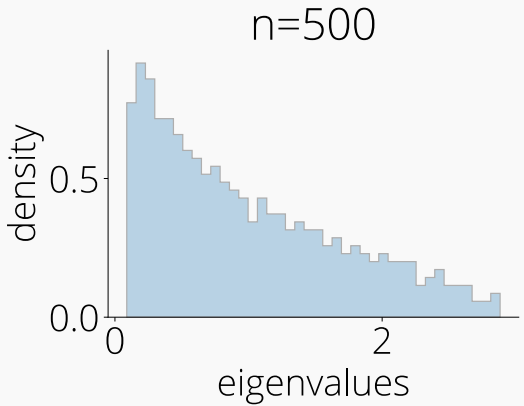

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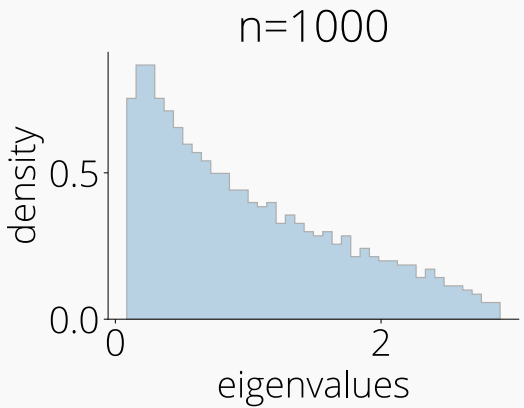

Wishart ensemble

Python pseudocode

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import numpy as np
import matplotlib.pyplot as plt

r = 1/2  # for example
X = np.random.randn(n * r, n)
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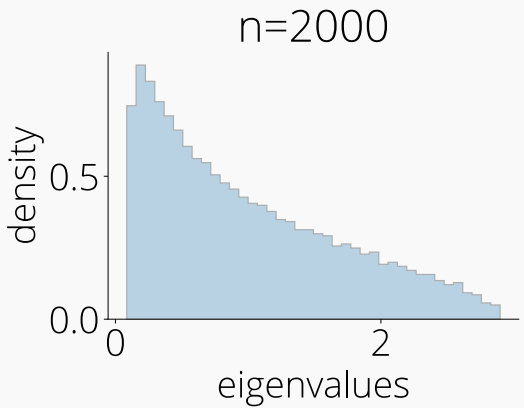

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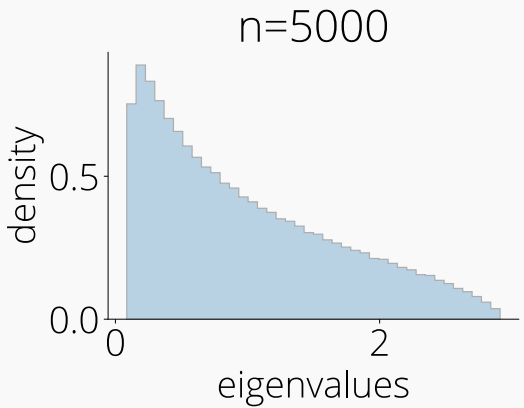

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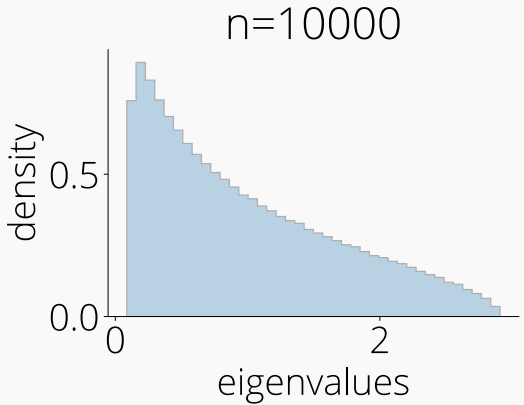


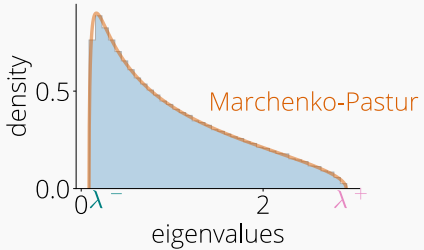
Limit of Wishart matrices

Marchenko-Pastur (MP) law [Marčenko and Pastur, 1967]

As $n, d \to \infty$, $\frac{d}{n} \to r$, μ_{ESD} converges to the Marchenko-Pastur distribution:

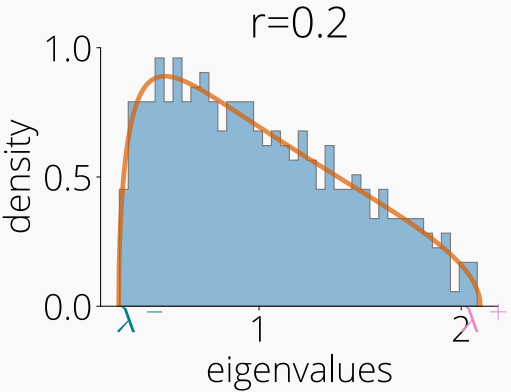
$$\mu_{\text{MP}}(x) \overset{\text{def}}{=} \underbrace{(1 - \tfrac{1}{r})_+ \delta_0(x)}_{\text{nonzero if } r > 1} + \frac{\sqrt{(\lambda^+ - x)(x - \lambda^-)}}{2\pi r x} 1_{x \in [\lambda^-, \lambda^+]} \, \mathrm{d}x \,.$$

$$\text{with } \lambda^- = (1 - \sqrt{r})^2, \lambda^+ = (1 + \sqrt{r})^2$$



The $r = \frac{d}{n}$ parameter

- $r < 1 \implies d < n \implies W$ is product of two **fat** matrices.
- $r > 1 \implies d > n \implies W$ is product of two **thin** matrices (rank-deficient).



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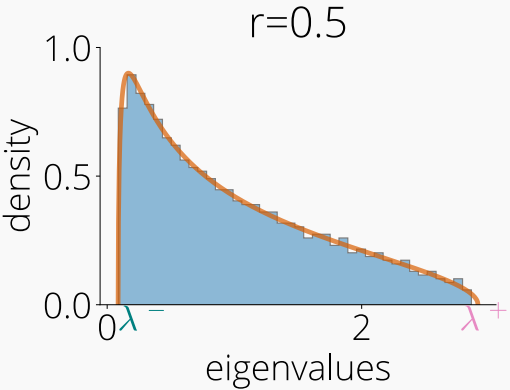

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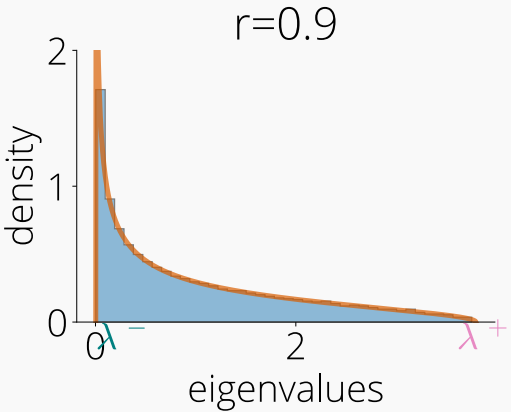

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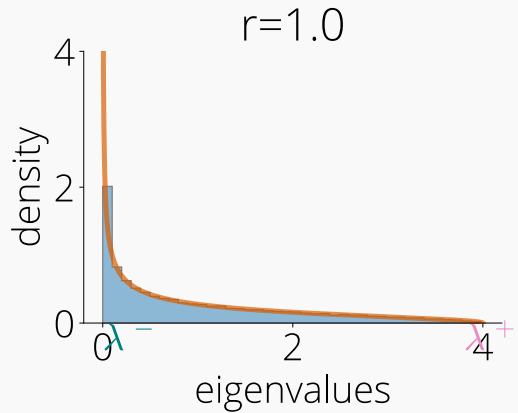

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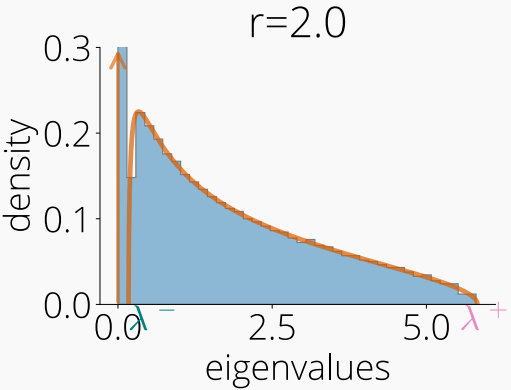

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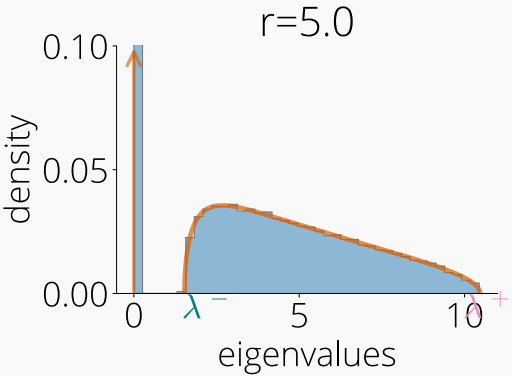

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Universality

Covariance matrices $W = \frac{1}{n} X X^\top$

What happens if we replace the $\mathcal{N}(0,1)$ with a different distribution?

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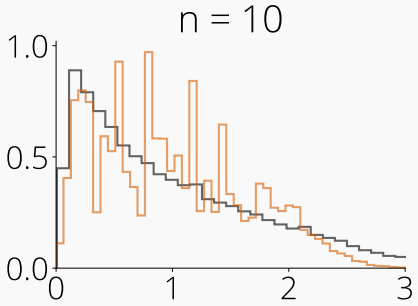

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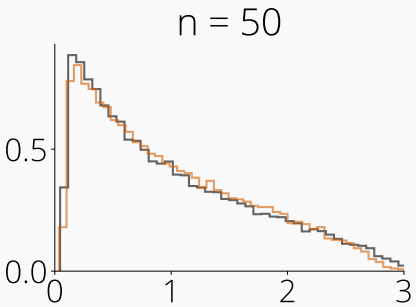

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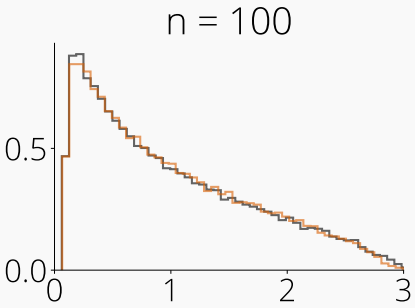

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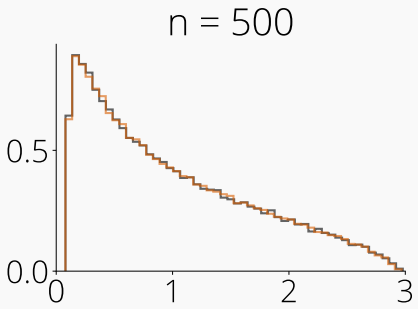

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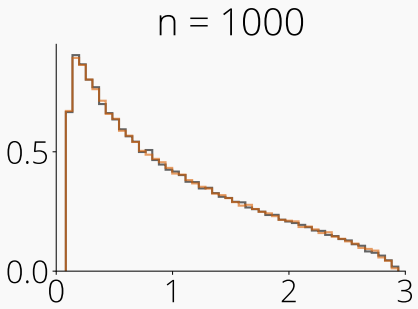

Universality

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- Statistics only mildly depend on the lower order moments of distribution of the entries

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Example: Marchenko-Pastur [Marčenko and Pastur, 1967]

Let X be a $d \times n$ random matrix with i.i.d. entries that verifies

$$\mathbb{E}[X_{ij}] = 0, \quad \mathbb{E}[X_{ij}^2] = 1, \quad \mathbb{E}[X_{ij}^4] < \infty$$

Universality: As $n, d \to \infty$ with $\frac{d}{n} \to r$, the ESD of $W = \frac{XX^T}{n}$ converges to Marchenko-Pastur(r)

May others ...

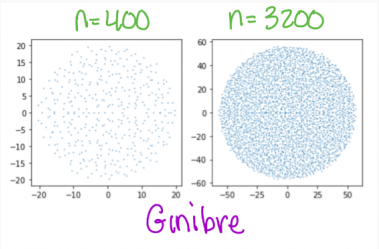
Other matrix ensembles

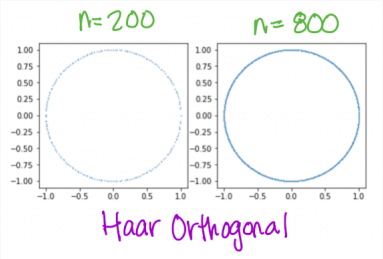
- **Ginibre.** Let G_n be $n \times n$ matrix of i.i.d. $N(0,1)$, (bilinear games [Domingo-Enrich et al., 2020])

$$\text{(Circle law)} \quad \text{ESD of } G_n/\sqrt{n} \to \text{Unif(disk)}\,.$$

- Uniform probability measure on **orthogonal matrices**. $V \sim \text{Unif}(O(n))$,

$$\text{ESD of } V \to \text{Unif}(\mathbb{S}^1)\,.$$





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Random Matrix Theory for Machine Learning

Introduction to Random Matrix Theory

Fabian Pedregosa, Courtney Paquette, Tom Trogdon, Jeffrey Pennington

https://random-matrix-learning.github.io

Table of contents

1. Stieltjes Transform

2. *R*-Transform

Stieltjes Transform

Maximum entropy principle

A disordered (real world) system will be random in all ways that are not explicitly prevented.

Conversely, a matrix is interesting only in those ways it fails to look like a random matrix.

Notes of Elliot Paquette and the thesis, *A random matrix framework for large dimensional machine learning and neural networks* by Zhenyu Liao

Example MNIST

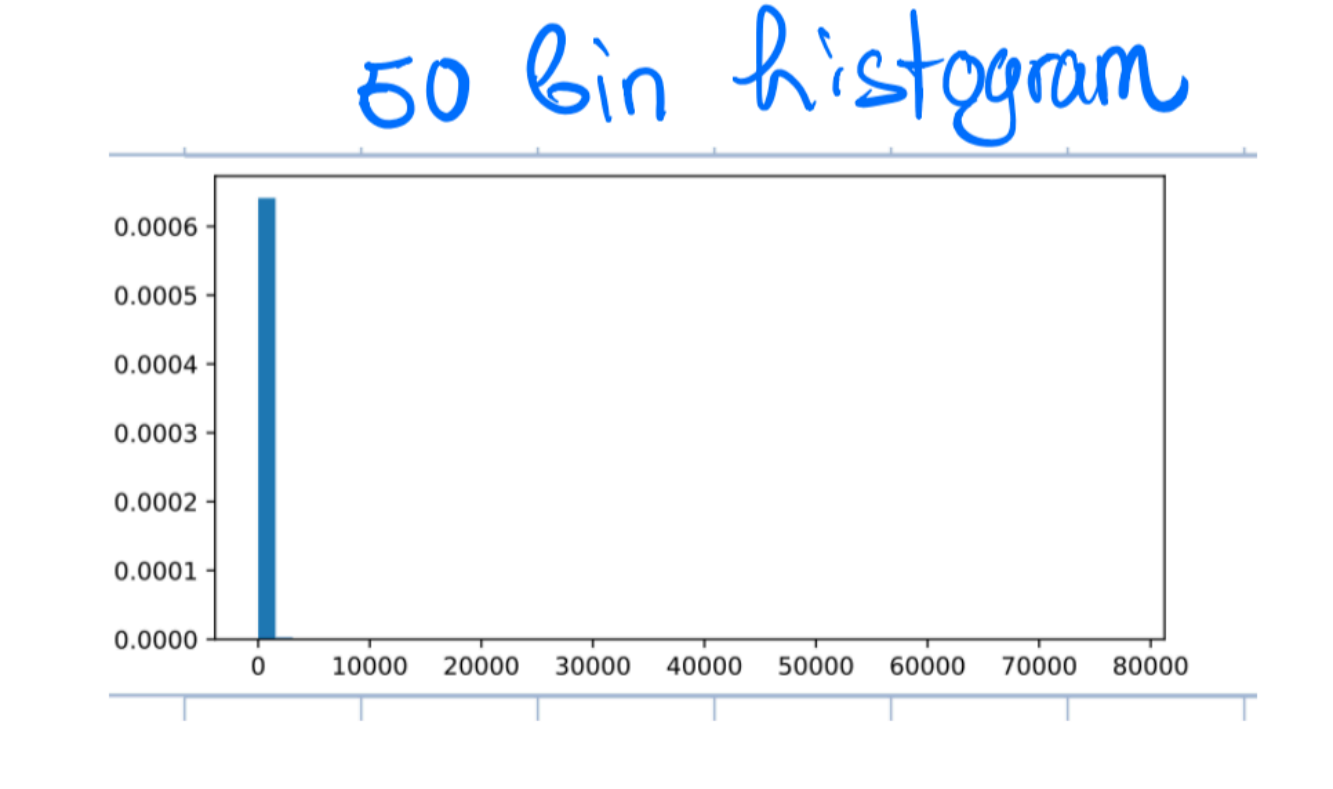
MNIST $\boldsymbol{M}$ $(60,000 \times 28 \times 28)$, form sample covariance matrix, $\boldsymbol{S} = \boldsymbol{M}\boldsymbol{M}^T$

Does $\boldsymbol{S}$ look like a random matrix?

Example MNIST

MNIST M $(60,000 \times 28 \times 28)$, form sample covariance matrix, $S = MM^T$

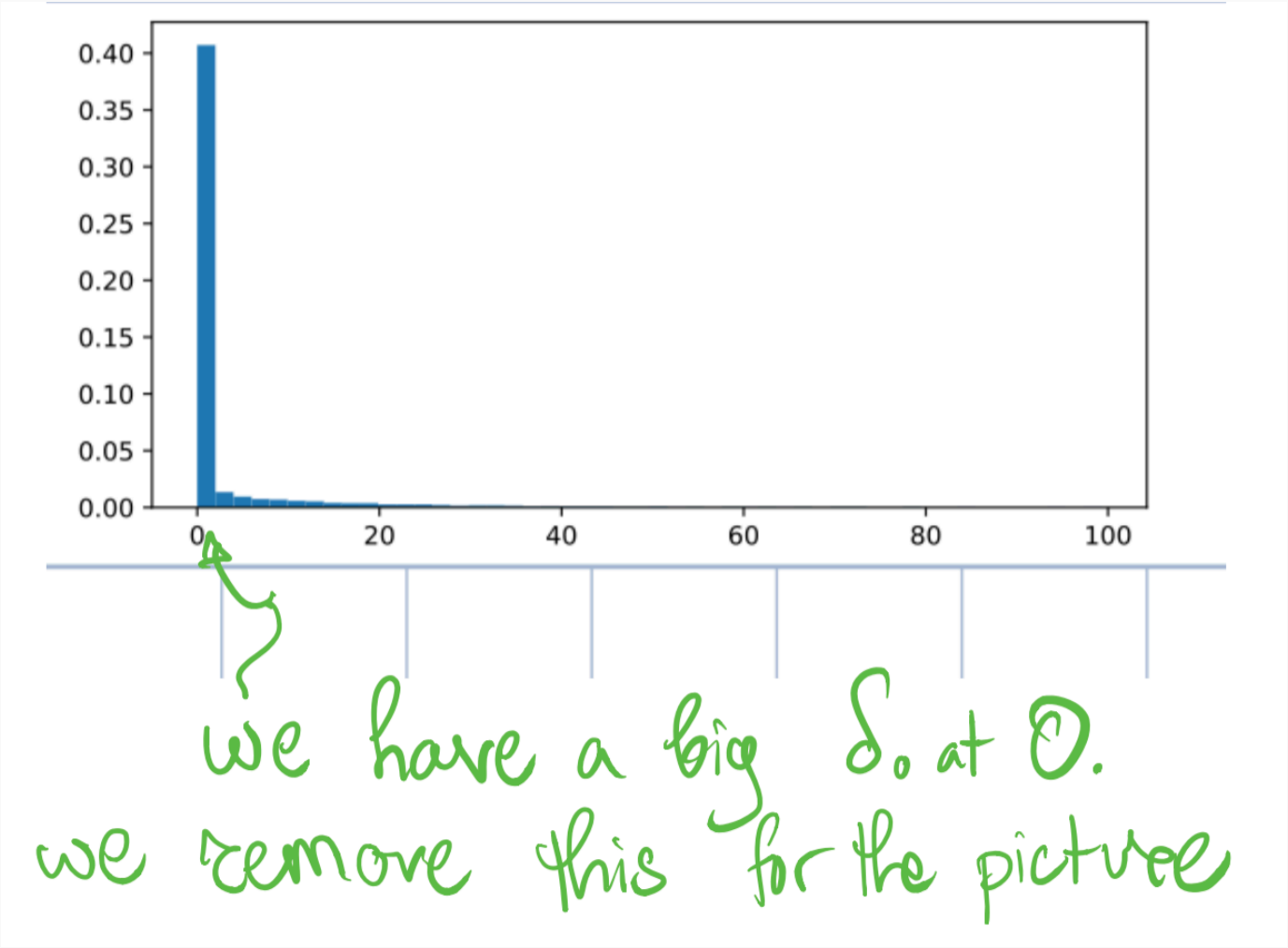
Does S look like a random matrix?



Observation 1: 1 giant eigenvalue, M has non-zero mean

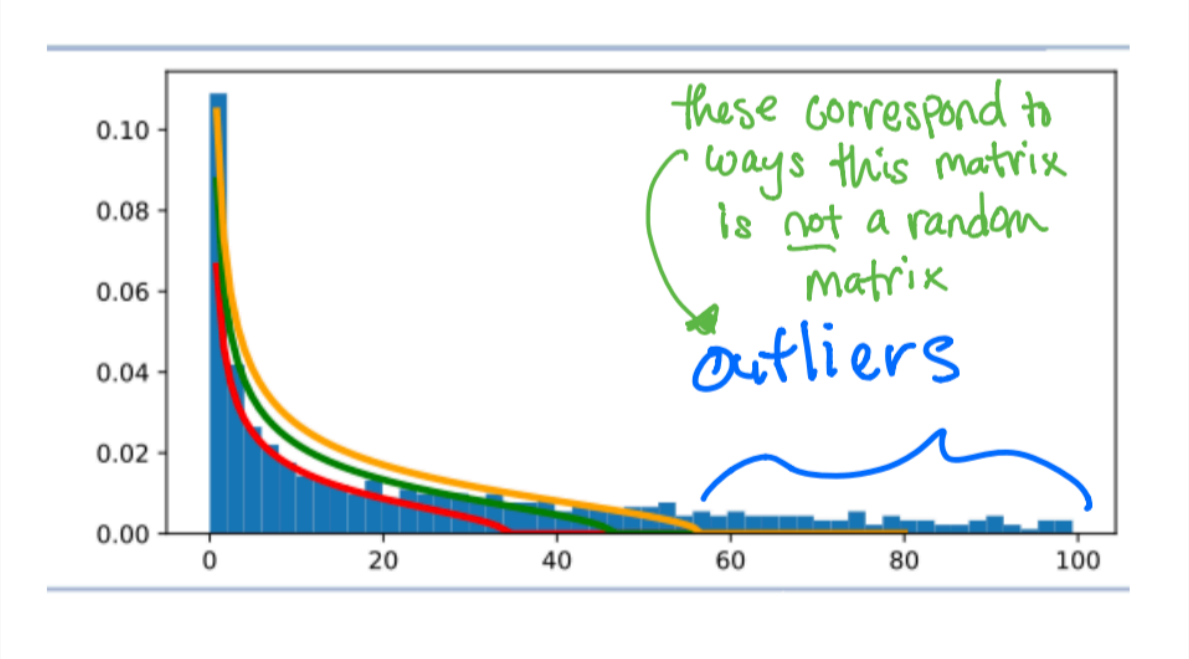
Example MNIST

Remove large eigenvalue



Example MNIST

Observation 2: There is a bulk component



- Fit bulk with Marchenko-Pastur(1) to correspond to point mass
- Large eigenvalue correspond to interesting outliers
- May be ”hidden” (weak) outliers in the bulk eigenvalues

Method 1: Stieltjes transform

Stieltjes transform

$$m_\mu(z) = \int_{\mathbb{R}} \frac{1}{t-z}\,\mu(\mathrm{d}t)$$

$$z \in \mathbb{C}, \quad \Im(z) > 0, \quad \mu \text{ is } \mathbb{P}\text{-measure on } \mathbb{R}$$

Theorem (Stieltjes inversion)

$$\lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \Im\left(m_\mu(x+i\varepsilon)\right) \xrightarrow[\varepsilon \to 0]{} \mu$$

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Example: μ is law of Unif$([-1,1])$

Stieltjes transform:

$$m_\mu(z) = \frac{1}{2}\int_{\mathbb{R}} \frac{1}{t-z} 1\left(\{|t| \le 1\}\right) \mathrm{d}t = \frac{1}{2}\int_{-1}^{1} \frac{\mathrm{d}t}{t-z} = \frac{1}{2}\log\left(\frac{1-z}{-1-z}\right)$$

Inversion

$$\lim_{\varepsilon \downarrow 0} \frac{\Im}{\pi}\left(\frac{1}{2}\log\left(\frac{1-z}{-1-z}\right)\right)\Big|_{z=x+i\varepsilon} = \begin{cases} \frac{1}{2}, & \text{if } |x| < 1 \\ 0, & \text{if } |x| > 1 \\ \star, & |x| = 1 \end{cases}$$

Empirical spectral distribution and Stieltjes

$$\text{ESD of } \boldsymbol{A}: \quad \mu_n = \frac{1}{n}\sum_{i=1}^{n} \delta_{\lambda_i(\boldsymbol{A})}$$

Stieltjes transform of ESD

$$m_{\mu_n}(z) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{\lambda_i(\boldsymbol{A}) - z} = \frac{1}{n}\mathrm{tr}\left((\boldsymbol{A} - z\boldsymbol{I}_d)^{-1}\right)$$

Theorem

If for each $z \in \mathbb{C}$, $\Im(z) > 0$, and

$$m_{\mu_n}(z) \xrightarrow[n\to\infty]{} m_{\mu}(z) \quad \Rightarrow \quad \mu_n \xrightarrow[n\to\infty]{} \mu.$$

Resolvent

Resolvent

$$Q(z) \stackrel{\text{def}}{=} \text{Resolvent of } A = (A - zI_d)^{-1}$$

Remarks

For nice random matrices (GOE, Wishart, sample covariance),

$$\text{Resolvent of } A \approx m_A(z) I_d$$

where m_A is the Stieltjes transform of A. That is, for any unit vector u independent of A,

$$u^T (A - zI_d)^{-1} u \cong m_A(z) \qquad \text{(weak sense)}$$

*This gives not only eigenvalues but also eigenvectors

Marchenko-Pastur and Stieltjes

Lemma:
Suppose $x \in \mathbb{R}^p$ has i.i.d. entries of mean zero, unit variance. Then

$$x^T A x - \mathrm{tr} A \to 0$$

Wishart: $W = \frac{1}{n} X X^T, \quad X \in \mathbb{R}^{d \times n}, \quad d/n \to r \in (0 \infty)$

$$X = \begin{bmatrix} | & | & \cdots & | \\ x_1 & x_2 & \cdots & x_n \\ | & | & \cdots & | \end{bmatrix} \Rightarrow \text{Resolvent of } W = Q_n(z) = \left(\frac{1}{n} \sum_{i=1}^{n} x_i x_i^T - z I_d \right)^{-1}$$

Question: What is the Stieltjes transform of Wishart W?

Suppose $\exists\ Q(z) \in \mathbb{C}^{d \times d}$ s.t. $\frac{1}{d} \mathrm{tr}(Q_n(z) - Q(z)) \to 0$ (Stieltjes of MP $= \mathrm{tr}(Q(z))$)

Fact: $\left| \frac{1}{d} \mathrm{tr}\left(Q_n(z) (Q(z)^{-1} + z I_d) Q(z) \right) - \frac{1}{n} \frac{1}{d} \sum_{i=1}^{n} x_i^T Q(z) Q_n(z) x_i \right| \to 0$

Marchenko-Pastur and Stieltjes

Linear algebra to construct self-consistent equation for $\mathrm{tr}(Q_n(z))$:

Remove 1 column and 1 row:

$$Q_n = \left(\frac{1}{n}\sum_{i=1}^{n} x_i x_i^T - zI_d\right)^{-1} = \left(\frac{1}{n}x_1 x_1^T + \overbrace{\frac{1}{n}\sum_{i=2}^{n} x_i x_i^T - zI_d}^{Q_n^{(1)}}\right)^{-1}$$

$$= Q_n^{(1)} - \frac{n^{-1}Q_n^{(1)}x_1 x_1^T Q_n^{(1)}}{1 + n^{-1}x_1^T Q_n^{(1)} x_1} \quad \text{(Sherman-Morrison)}$$

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$Q_n^{(1)}, x_1$ independent $\Rightarrow x_1^TQQ_n^{(1)}x_1 = tr(QQ_n^{(1)})$ and $x_1^TQ_n^{(1)}x_1 = tr(Q_n^{(1)})$

$$d^{-1}x_1^TQQ_nx_1 \quad = \quad \frac{d^{-1}\mathrm{tr}(QQ_n^{(1)})}{1+n^{-1}\mathrm{tr}(Q_n^{(1)})} \approx \frac{d^{-1}\mathrm{tr}(QQ_n)}{1+n^{-1}\mathrm{tr}(Q_n)}$$

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$$\begin{array}{ccc} \frac{1}{nd}\sum_{i=1}^{n} x_i^TQQ_nx_i & \approx & \frac{d^{-1}\mathrm{tr}(QQ_n)}{1+n^{-1}\mathrm{tr}(Q_n)} \\ \downarrow & & \downarrow \\ d^{-1}\mathrm{tr}\big(Q_n(Q^{-1}+zI_d)Q\big) & \approx & \frac{d^{-1}\mathrm{tr}(QQ_n)}{1+n^{-1}\mathrm{tr}(Q_n)} \end{array} \Rightarrow \quad Q^{-1} + zI_d = \frac{1}{1+n^{-1}\mathrm{tr}(Q_n)}I_d$$

$$Q = \left(-z + \frac{1}{1+n^{-1}\mathrm{tr}(Q_n)}\right)^{-1} I_d$$

Marchenko-Pastur and Stieltjes

$$\text{Stieltjes of } W_n = m_{W_n}(z) = d^{-1}\mathrm{tr}(Q_n) \approx d^{-1}\mathrm{tr}(Q) = \left(-z + \frac{1}{1 + r \cdot d^{-1}\mathrm{tr}(Q_n)}\right)^{-1}$$

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Fixed point equation for trace ($r = \lim_{n\to\infty} \frac{d}{n}$):

$$m_{W_n}(z) = \frac{1}{-z + \frac{1}{1+r\cdot m_{W_n}(z)}} + \varepsilon(n,z), \qquad \varepsilon(n,z) \xrightarrow[n\to\infty]{} 0$$

Fixed point for Marchenko-Pastur, MP:

$$m_{\mathrm{MP}}(z) = \frac{1}{-z + \frac{1}{1+r\cdot m_{\mathrm{MP}}(z)}}, \qquad \text{Note: } m(z) \sim \frac{-1}{z} \text{ as } z \to \infty$$

✓ solve numerically ✓ many dist. satisfy fixed point eqn.

Marchenko-Pastur and Stieltjes

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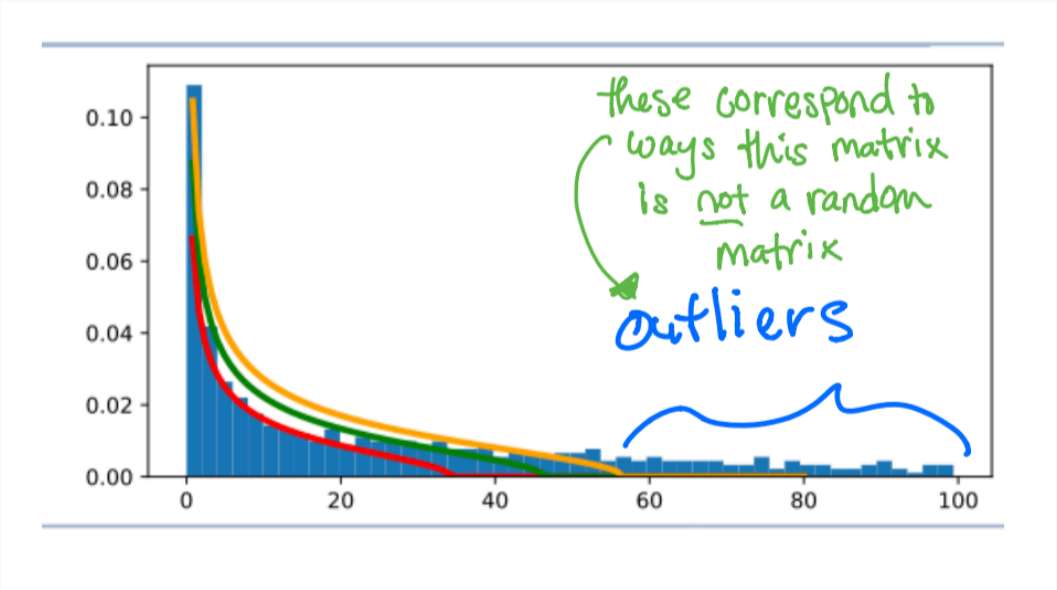
✓ solve numerically ✓ many dist. satisfy fixed point eqn.

Stieltjes transform of Marchenko-Pastur

$$m_{\mathrm{MP}}(z) = \frac{1 - r - z + \sqrt{((1+\sqrt{r})^2 - z)((1-\sqrt{r})^2 - z)}}{2rz}$$

Bulk + outliers

How do we model this?



	Bulk	+	Outliers
	↓		↓
Model:	Marchenko-Pastur	+	Spikes

Sample covariance matrices

Set-up

- Covariance matrix, C, (symmetric, positive semi-definite matrix)
- Noise matrix, $Z \in \mathbb{R}^{d \times n}$ (mean 0, variance 1, i.i.d.)
- $n^{1/\delta} \leq d \leq n^{\delta}$ for some $\delta > 0$
- $X = C^{1/2}Z$; Form $\dfrac{XX^T}{n}$
- $\|C\|_2 \leq$ constant, independent of n

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Theorem (Bai, Krishnaiah, Silverstein, Yin, '80s-'90s)

$$\text{Stieltjes of } \frac{XX^T}{n} = \operatorname{tr}\left[\left(I_d - z\frac{XX^T}{n}\right)^{-1}\right] \approx \frac{n}{d}\widetilde{m}(z) + \frac{1-\frac{d}{n}}{\frac{d}{n}z}$$

$$\text{where} \qquad \widetilde{m}(z) = \left(-z + \frac{1}{n}\operatorname{tr}[C(I_d - \widetilde{m}(z)C)^{-1}]\right)^{-1}$$

✓ $\widetilde{m}(z) \approx$ Stieltjes transform $\frac{X^TX}{n}$ ✓ implicit eqn, solved numerically

Examples of Sample Covariances

See Colab for details

R-Transform

Example Hessian of 2-layer Network Model

Setup

- $W^{(1)} \in \mathbb{R}^{n_1 \times n_0}$ and $W^{(2)} \in \mathbb{R}^{n_2 \times n_1}$ weight matrices, i.i.d. $N(0,1)$
- $x \in \mathbb{R}^{n_0 \times m}$ is input data and $y \in \mathbb{R}^{n_2 \times m}$ targets
- $g : \mathbb{R} \to \mathbb{R}$ activation function
- $n = n_0 = n_1 = n_2$ and $\phi = \frac{2n}{m}$

outputs: $\widehat{y} = W^{(2)} g(W^{(1)} x)$ residuals: $e_{ij} = \widehat{y}_{ij} - y_{ij}$

Goal: $$\min_{\theta = [W^{(1)}, W^{(2)}]} \left\{ f(\theta) = \frac{1}{2m} \| W^{(2)} g(W^{(1)} x) - y \|^2 \right\}$$

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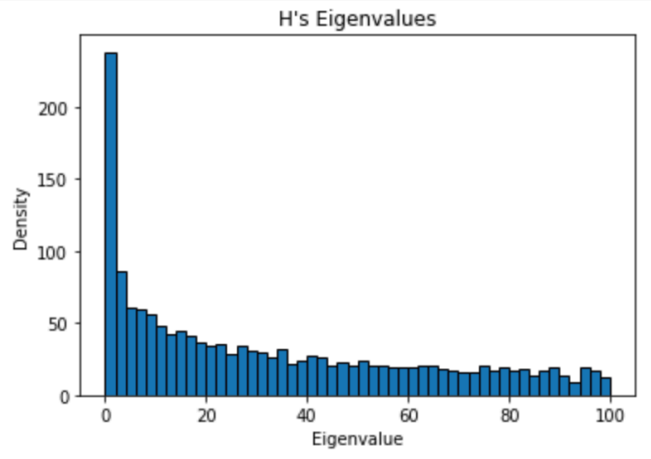
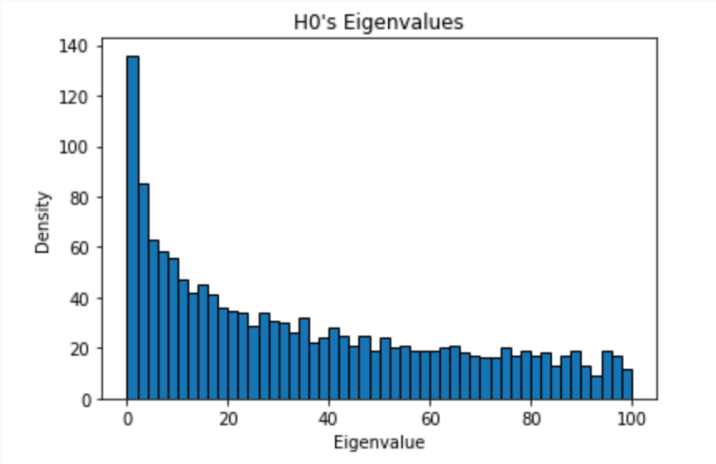
Hessian: $H = H_0 + H_1$

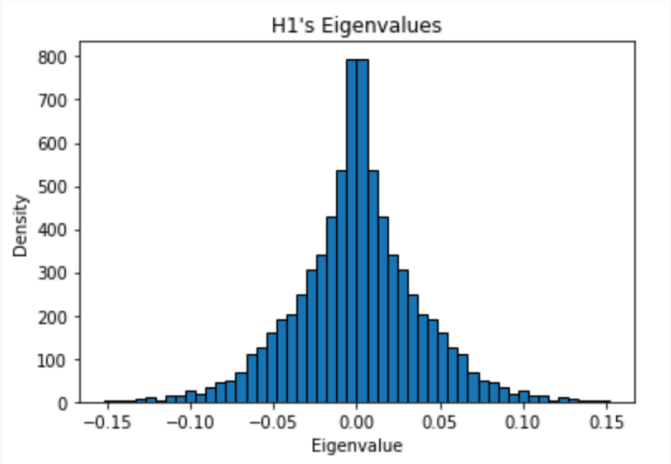
$$[H_0]_{\alpha\beta} = \frac{1}{m} \sum_{i,j=1}^{n_2,m} \frac{\partial \hat{y}_{ij}}{\partial \theta_\alpha} \frac{\partial \hat{y}_{ij}}{\partial \theta_\beta} \quad \text{and} \quad [H_1]_{\alpha\beta} = \frac{1}{m} \sum_{i,j}^{n_2,m} e_{ij} \frac{\partial^2 \hat{y}_{ij}}{\partial \theta_\alpha \partial \theta_\beta}$$

Snapshots of the Hessian during Training

Hessian: $H = H_0 + H_1$







Question: How do you model eigenvalues of H from H_0 and H_1?

Images by McGill undergraduate, Ria Stevens

R-Transform

R-Transform

Tool for writing simple formulas for densities from known densities

Definitions

Free convolution of measures, $\mu_A \boxplus \mu_B$

If A, B two random matrices with ESD, μ_A and μ_B,

$$\text{ESD of } A + B = \mu_A \boxplus \mu_B$$

provided matrix sizes large and matrices asymptotically free.

(side note: product of matrices version)

Asymptotically free matrices

Orthogonal invariance

An A random symmetric matrix is orthogonally invariance if for any fixed orthogonal matrix O

$$O^T A O \overset{\text{law}}{=} A$$

Examples

- Multiples of the Identity
- Wishart with Gaussian entries
- GOE with Gaussian entries

Asymptotically free matrices

Sufficient condition

Suppose $\{A_n\}$ and $\{B_n\}$ are $n \times n$ random matrices. If the following

- A_n and B_n are independent
- A_n is orthogonally invariant

Then A_n and B_n are asymptotically free and $\mu_{A_n} \boxplus \mu_{B_n} \cong \mu_{A_n+B_n}$

Intuition: Eigenvectors of A_n are completely unaligned from B_n

Stieltjes and R-transform

R-transform

R-transform is inverse of Stieltjes of m

$$R(-m(z)) - \frac{1}{m(z)} = z.$$

Examples

- $\beta \boldsymbol{u}\boldsymbol{u}^T$ is $R_{\beta \boldsymbol{u}\boldsymbol{u}^T} = \frac{\beta}{n(1-s\beta)}$
- $R_{\text{Marchenko-Pastur(r)}}(s) = \frac{1}{1-sr}$
- $R_{\text{semicircle}}(s) = s$

Calculus for spectral densities

Theorem

If A and B are asymptotically free,

$$R_{\mu_{A+B}} = R_{\mu_A \boxplus \mu_B} = R_{\mu_A}(s) + R_{\mu_B}(s).$$

Remark

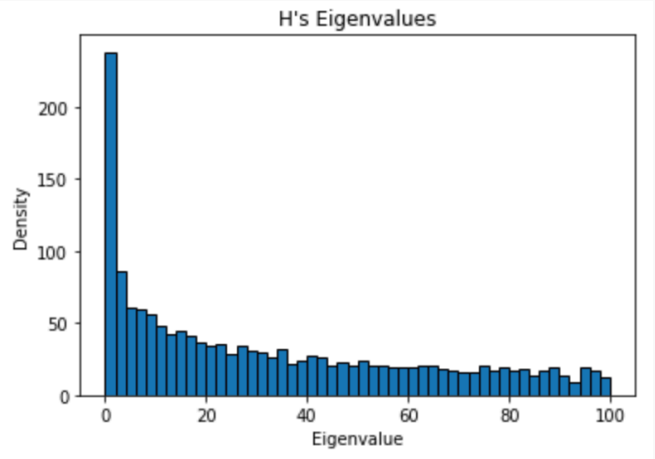
R-transform $\Leftrightarrow$ Stieltjes transform $\Leftrightarrow$ Spectral density

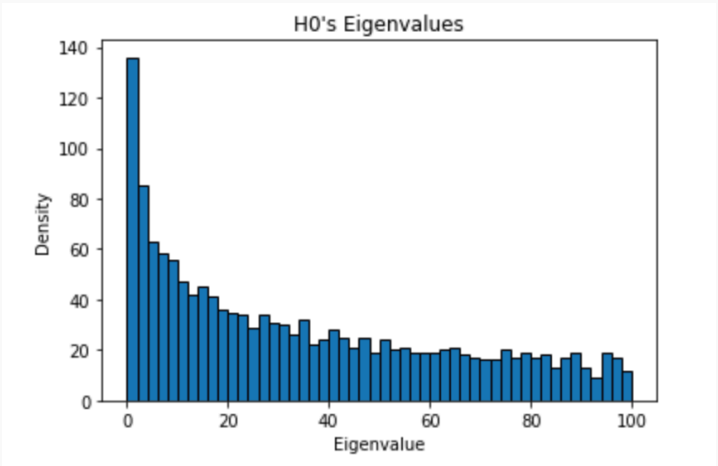
Example

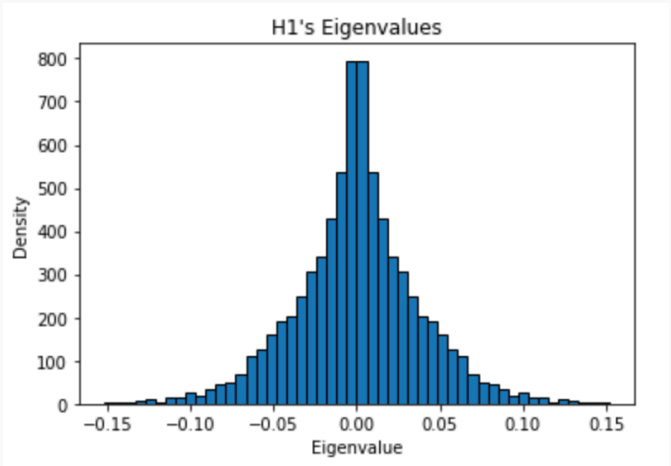
$$R_{\text{GOE + Wishart}} = R_{\text{semicircle}} + R_{\text{MP}} = \underbrace{s}_{\text{GOE}} + \underbrace{\frac{1}{1 - sr}}_{\text{Wishart}}$$

Snapshots of the Hessian during Training

Hessian: $H = H_0 + H_1$







Question: How do you model eigenvalues of H from H_0 and H_1?

Images by McGill undergraduate, Ria Stevens

Model for the Hessian

$$n_2\varepsilon \overset{\text{def}}{=} f(\boldsymbol{\theta}) \quad \text{Hessian:} \quad \boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{H}_1$$

Modeling Assumptions

- $\boldsymbol{H}_0$ is Marchenko-Pastur
- $\boldsymbol{H}_0$ and $\boldsymbol{H}_1$ are asymptotically free
- $n = n_0 = n_1 = n_2$ and $\phi = \frac{2n}{m}$

R-transform of $\boldsymbol{H}_1$: $$R_{\boldsymbol{H}_1}(s) = \frac{\varepsilon\phi s}{2 - \varepsilon\phi^2 s^2}$$

R-transform of $\boldsymbol{H}$

$$R_{\boldsymbol{H}}(s) = \frac{1}{1 - s\phi} + \frac{\varepsilon\phi s}{2 - \varepsilon\phi^2 s^2}$$

Questions?

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Random Matrix Theory for Machine Learning

Part 3: Analysis of numerical algorithms

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https://random-matrix-learning.github.io

Notation

In this section:

- A is typically a rectangular matrix with more rows than columns
- W is a symmetric (square) matrix
- Often $W \propto A^T A$

Motivation: Average-case versus worst-case in high dimensions

Issues with worst-case bounds in high dimensions

In some very specific cases, the high-dimensionality of a given problem provides it with enough degrees of freedom to “conspire against” a given algorithm.

Issues with worst-case bounds in high dimensions

In some very specific cases, the high-dimensionality of a given problem provides it with enough degrees of freedom to "conspire against" a given algorithm.

For, example, consider solving a $n \times n$ linear system $\boldsymbol{W}\boldsymbol{x} = \boldsymbol{b}$ using the conjugate gradient (CG) algorithm where

$$W = \begin{bmatrix} \mathfrak{r} & \sqrt{\mathfrak{r}} & & & & & \\ \sqrt{\mathfrak{r}} & 1+\mathfrak{r} & \sqrt{\mathfrak{r}} & & & & \\ & \sqrt{\mathfrak{r}} & 1+\mathfrak{r} & \sqrt{\mathfrak{r}} & & & \\ & & \sqrt{\mathfrak{r}} & \ddots & \ddots & & \\ & & & \ddots & & & \\ & & & & & \sqrt{\mathfrak{r}} & \\ & & & & \sqrt{\mathfrak{r}} & 1+\mathfrak{r} & \end{bmatrix}, \quad b = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad 0 < \mathfrak{r} < 1.$$

Issues with worst-case bounds in high dimensions

The CG algorithm is iterative and produces approximations x_k that satisfy:

$$x_k = \underset{y \in \mathbb{R}^n}{\arg\min} \left\{ (x-y)^T W (x-y)^T : y \in \operatorname{span}\{b, Wb, \ldots, W^{k-1}b\} \right\}.$$

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It can be shown that for the above choice of W, b, and $1 \leq k < n$

$$\|b - Wx_k\|^2 = \left(\frac{1}{\mathfrak{r}}\right)^k \quad \text{but} \quad \|b - Wx_n\| = 0.$$

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The residuals (or norms of the gradient) appear to diverge exponentially before the iteration finally converges!

And as n increases, this becomes worse. And a worst-case bound needs to account for this pathological example.

Instead, we may want to choose W and b to be random and consider

$$\mathbb{E}\|b - Wx_k\|^2.$$

If one chooses W to be distributed according to the Wishart distribution, as $n \to \infty$,

$$\mathbb{E}\|b - Wx_k\|^2 = \mathfrak{r}^k + o(1), \quad \mathfrak{r} = r^{-1} = \lim_{n\to\infty} \frac{n}{d}.$$

Introducing distributions

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But a valid important open problem is: To model optimization in a ML context, what distribution is relevant for W?

This is an open problem. See Liao and Mahoney [2021] for work in this direction.

Main RMT tool: Matrix moments

Main linear algebra tool

Recall Cauchy's integral formula: If f is analytic in a sufficiently large region and $\mathcal{C}$ is smooth, simple, closed curve then

$$f(z) = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} \frac{f(z')}{z' - z} \, \mathrm{d}z'.$$

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$$f(z) = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} \frac{f(z')}{z' - z} \, \mathrm{d}z'.$$

Suppose the eigenvalues of an $n \times n$ matrix W are enclosed by $\mathcal{C}$, then

$$f(W) := U f(\Lambda) U^{-1} = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} f(z) (z I_n - W)^{-1} \, \mathrm{d}z.$$

Main linear algebra tool

Recall Cauchy's integral formula: If f is analytic in a sufficiently large region and $\mathcal{C}$ is smooth, simple, closed curve then

$$f(z) = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} \frac{f(z')}{z' - z} \, \mathrm{d}z'.$$

Suppose the eigenvalues of an $n \times n$ matrix W are enclosed by $\mathcal{C}$, then

$$f(W) := U f(\Lambda) U^{-1} = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} f(z) (z I_n - W)^{-1} \, \mathrm{d}z.$$

In particular,

$$W^k = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} z^k (z I_n - W)^{-1} \, \mathrm{d}z.$$

Two consequences

$$\frac{1}{n}\operatorname{tr} W^k = \frac{1}{2\pi n \mathrm{i}} \int_{\mathcal{C}} z^k \operatorname{tr}\left(z I_n - W\right)^{-1} \mathrm{d}z$$

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$$\sum_j w_j \delta_{\lambda_j}, \quad w_j = (v_j^T u)^2$$

Analysis of matrix moments

A main RMT takeaway:

Matrix moments $\Leftrightarrow$ Classical moments of ESD $\Leftrightarrow$ Contour integrals of Stieltjes transform

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If $\mu_{\mathrm{ESD}} = \sum_{j=1}^{n} w_j \delta_{\lambda_j(\boldsymbol{W})}$, $w_j = (\boldsymbol{v}_j^T \boldsymbol{u})^2$ for eigenvectors $\boldsymbol{v}_j$ then the first $\approx$ becomes $=$.

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If μ_{ESD} is the limiting ESD then errors are typically on the order of $1/\sqrt{n}$.

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If a statistic, (which might be the error encountered in, or the runtime of, an algorithm) depends strongly on these generalized moments, it may be analyzable directly using RMT.

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Theorem (Knowles and Yin [2017])

For a large class of sample covariance matrices W there exists a deterministic measure μ_{SCM} with Stieltjes transform m_{SCM} such that

$$\Pr\left(\left|a^T(W - zI_n)^{-1}b - (a^T b)m_{\mathrm{SCM}}(z)\right| \geq \|a\|\|b\|t\right) = O(n^{-D})$$

for any $D > 0$, uniformly in a large subset of the complex plane.

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Resolvent estimates lead to moment estimates

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$$u^T P(W) u \approx \int_{\mathbb{R}} P(x) \mu_{\mathrm{SCM}}(\mathrm{d}x)$$

Algorithm halting times (runtimes)

Statistics of algorithm runtimes

Our abstract setup to analyze algorithms is as follows. Suppose first that there is a intrinsic notion of dimension n.

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- Let $\mathcal{E}$ represent a distribution from which problems P_n are drawn (e.g., a random matrix and vector for a linear system).
- The halting time is then defined as

$$T_{\mathcal{A}}(P_n, \varepsilon) = \min\{k : E_k(P_n; \mathcal{A}) < \varepsilon\}.$$

Some history

Probably the most famous, and maybe the most influential, instance of the probabilistic analysis of an algorithm, was the analysis of the simplex algorithm developed by Dantzig [1951] for linear programming (see also Dantzig [1990]).

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Despite the existence of other algorithms for linear programming with provable polynomial runtime guarantees, the simplex method persisted as the most widely used algorithm.

Some history

Borgwardt [1987] and, independently, Smale [1983] proved that under certain probabilistic assumptions and under certain pivot rules, the expected runtime of the simplex algorithm is polynomial:

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The subsequent analysis by Spielman and Teng [2004] improved these analyses by providing estimates for randomly perturbed linear programs. This analysis has since been improved, see [Dadush and Huiberts [2020], Vershynin [2009], Deshpande and Spielman [2005]], for example.

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For any average-case analysis one hopes to continue to:

- Expand the class of distributions that can be considered.
- Increase the precision of the resulting estimates.
- Collect additional algorithms that can be analyzed with the same or similar techniques.

Some history

We also highlight two other success stories in average-case analysis. These are of a different flavor because randomization is introduced to algorithms to improve their performance. And subsequently, one has a natural distribution over which to compute averages, but the problem being solved is deterministic.

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The first algorithm is the power method with randomized starting. The power method is an algorithm to compute the dominant eigenvalue (provided it exists) of a matrix. It also also approximates the dominant eigenvector.

The power method

1. x_0 is the initial vector, $\|x_0\| = 1$ and W is given.
2. For $k = 1, 2, \ldots$
   - 2.1 Compute $v_k = Wx_{k-1}$
   - 2.2 Compute $\mu_k = v_k^T x_{k-1}$
   - 2.3 Compute $x_k = v_k / \|v_k\|$

The iterates μ_k, under mild assumptions, will converge to the dominant eigenvalue of W. It is well-known that the power method will converge at a exponential rate depending on the ratio of the largest-to-next-largest eigenvalue (a relative spectral gap).

If W is positive semi-definite and x_0 is chosen randomly ($x_0 =$ `np.random.randn(n)`, $x_0 \leftarrow x_0/\|x_0\|$), then it was shown in Kuczyński and Woźniakowski [1992] that a spectral gap is not need to get average-case error bounds of the form:

$$\mathbb{E} \underbrace{\frac{|\mu_k - \lambda_{\max}|}{|\lambda_{\max} - \lambda_{\min}|}}_{E_k(P_n;\mathrm{Power})} \leq 0.871 \frac{\log n}{k-1}.$$

The power method can also be analyzed on random matrices, see Kostlan [1988], Deift and Trogdon [2017].

Lastly, a discussion that is closer to the heart of the matter is the work of Strohmer and Vershynin [2009] on the randomized version of the original Kaczmarz algorithm [Kaczmarz [1937]] for the solution of overdetermined linear systems.

The Kaczmarz Algorithm

1. x_0 is the initial vector and A is given.
2. For $k = 1, 2, \ldots$
   2.1 Select a row a_j of A (add randomness here!)
   2.2 Compute $x_k = x_{k-1} - \frac{b_j - a_j^T x_{k-1}}{\|a_j\|^2} a_j$

For a consistent overdetermined system $Ax = b$ it was shown that the method satisfies

$$\mathbb{E} \underbrace{\|x_k - x\|^2}_{E_k(P_n;\mathrm{Kaczmarz})} \leq \left(1 - \frac{1}{\kappa(A^TA)}\right)^k \|x_0 - x\|^2$$

where $\kappa(A^TA)$ is the condition number of A^TA (to be discussed more later).

The power of random matrix theory (RMT) is that one can ask and answer more involved questions:

- If P_n is drawn randomly, then

$$T_{\mathcal{A}}(P_n, \varepsilon)$$

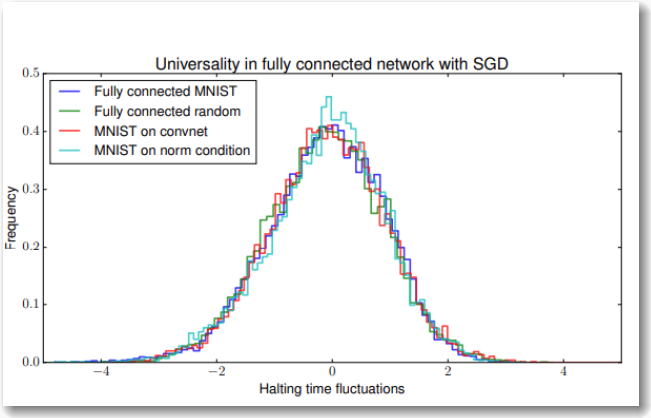
  is an integer-valued random variable. While it is important bound its expectation or moments, what about its distribution as $n \to \infty$?

- With the same considerations

$$E_k(P_n; \mathcal{A})$$

  is a random variable. Can we understand its distribution?

Universality of the halting time



Sagun et al. [2017] present experiments to demonstrate that the halting time $T_{\mathrm{SGD}}(P_n; \varepsilon)$ for a number of neural network architectures exhibits universality. That is, after proper centering and rescaling, the resulting statistics do not depend (in the limit) on the distribution on P_n.

A wide variety of numerical algorithms have been demonstrated (both empirically and rigorously) to have universal halting times (i.e., runtimes, iteration counts, etc.). The study of universality in halting time was initiated by Pfrang et al. [2014] and broaded in Deift et al. [2014].

Universality in halting time is the statement that for a given $\mathcal{A}$, and a wide class of ensembles $\mathcal{E}$, there are constants $\mu = \mu(\mathcal{E}, \varepsilon, n)$ and $\sigma = \sigma(\mathcal{E}, \varepsilon, n)$ and $\varepsilon = \varepsilon(\mathcal{E}, n)$ such that

$$\lim_{n\to\infty} \mathbb{P}_{\mathcal{E}} \left(\frac{T_{\mathcal{A}}(P_n, \varepsilon) - \mu}{\sigma} \leq t \right) = F_{\mathcal{A}}(t).$$

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$$\lim_{n\to\infty} \mathbb{P}_{\mathcal{E}} \left(\frac{T_{\mathcal{A}}(P_n, \varepsilon) - \mu}{\sigma} \leq t \right) = F_{\mathcal{A}}(t).$$

The limiting distribution is independent of the choice for $\mathcal{E}$.

A case study: Regression

A natural first step

A natural first place to combine RMT and optimization/ML with a view toward universality is in the study of linear regression:

$$\underset{x\in\mathbb{R}^n}{\arg\min}\left\{\mathcal{L}(x) := \frac{1}{2d}\|Ax-b\|^2, \quad b = Aa+\eta\right\},$$

where a is the signal, η is additive noise, and

$$\boxed{A \text{ is a } d\times n \text{ matrix}}.$$

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There are, of course, many iterative algorithms to solve this problem and we focus on two:

1. the conjugate gradient algorithm (CG) [Hestenes and Steifel [1952]], and
2. the gradient descent algorithm (GD).

The Conjugate Gradient Algorithm

1. x_0 is the initial guess.
2. Set $r_0 = A^T b - A^T A x_0$, $p_0 = r_0$.
3. For $k = 1, 2, \ldots, n$
   - 3.1 Compute $a_{k-1} = \dfrac{r_{k-1}^* r_{k-1}}{r_{k-1}^* A^T A p_{k-1}}$.
   - 3.2 Set $x_k = x_{k-1} + a_{k-1} p_{k-1}$.
   - 3.3 Set $r_k = r_{k-1} - a_{k-1} A^T A p_{k-1}$.
   - 3.4 Compute $b_{k-1} = -\dfrac{r_k^* r_k}{r_{k-1}^* r_{k-1}}$.
   - 3.5 Set $p_k = r_k - b_{k-1} p_{k-1}$.

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Why consider CG?

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CG is a highly-structured algorithm with connections to the Lanczos iteration and the theory of orthogonal polynomials. While we do not discuss many of these details, they play an important role in the analysis. CG is also a method-of-choice in the broader computational mathematics community.

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A simplification.

Instead of considering CG on the normal equations, $A^T A x = A^T b$, we first consider a slightly simpler problem:

CG applied to $A^T A x = c$.

Scaling regions

Scaling regions show up here in the relationship between n and d in a sample covariance matrix $W = \frac{A^T A}{d}$ (A is $d \times n$).

Scalings of sample covariance matrices

- $d = \lfloor nr \rfloor$ for $r > 1$
- $d = n$
- $d = \lfloor n + cn^{\alpha} \rfloor$ for $0 < \alpha < 1$

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Recall that condition number of a matrix W is defined to be

$$\kappa(W) = \frac{\sigma_1(W)}{\sigma_n(W)},$$

i.e., the ratio of the largest to the smallest singular value of W.

Matrices with small condition numbers are said to be well conditioned while those with larger condition numbers are said to be ill conditioned.

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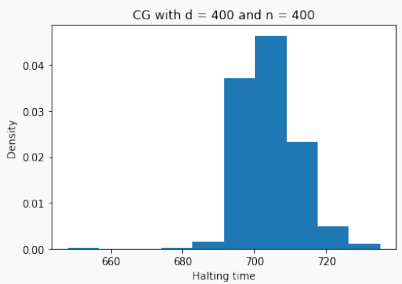
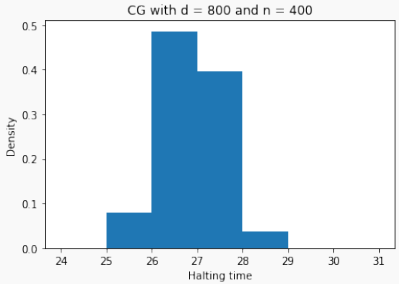
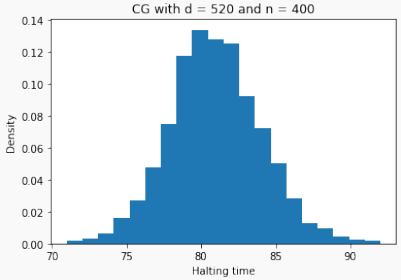
Three distinct behaviors of CG depending on scaling region







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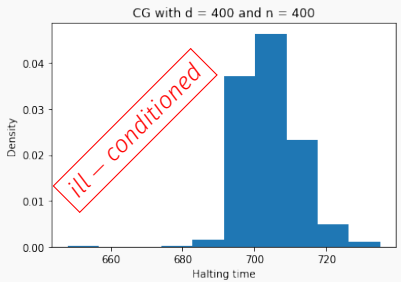

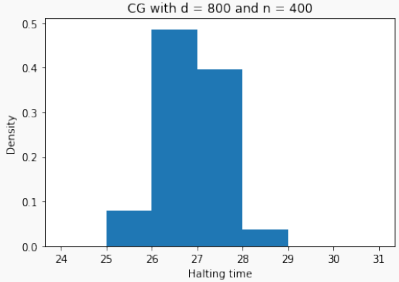

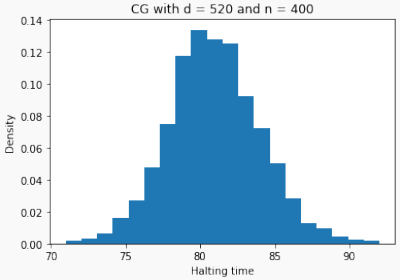

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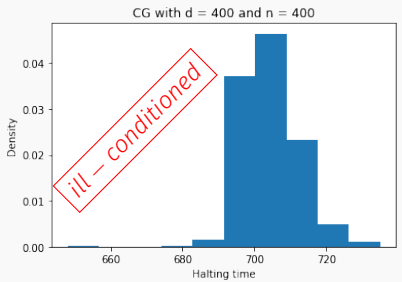

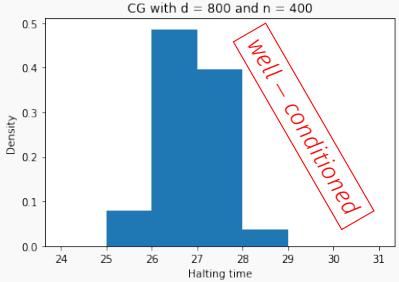

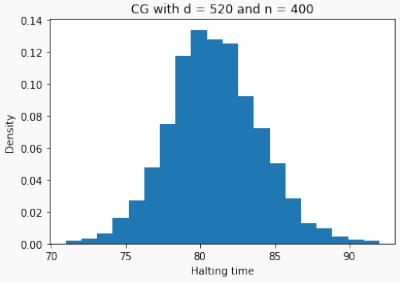

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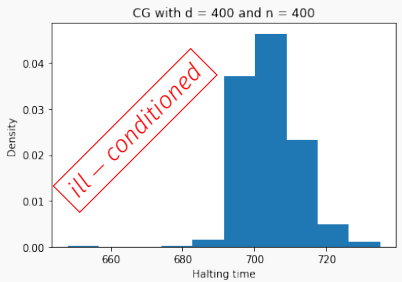
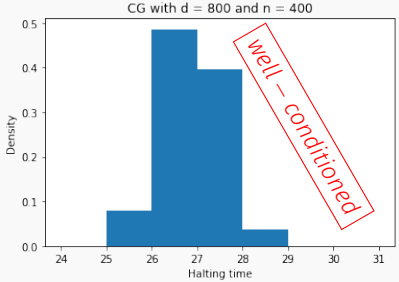
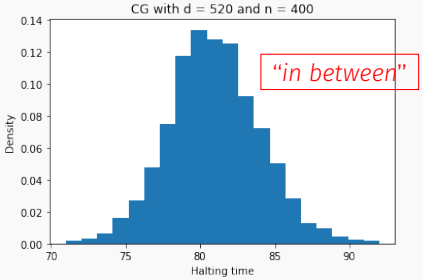
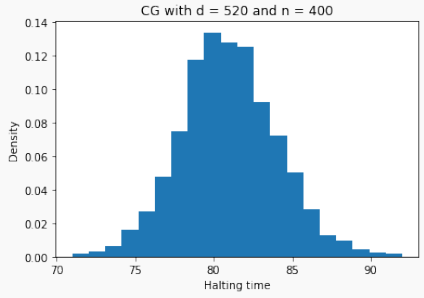
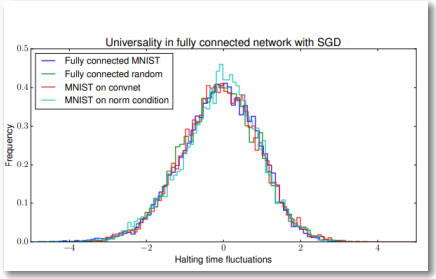






Qualitative comparison with SGD





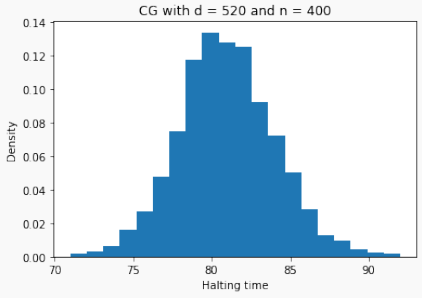
While the mechanisms behind these behaviors are surely different, we see a non-trivial histogram in each setting.

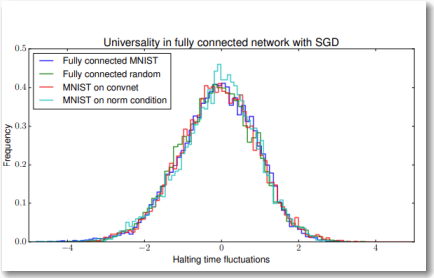
For CG on Wishart matrices, it can be shown that

$$\|r_k\| = \|c - A^T A x_k\| \overset{(\text{dist})}{=} \prod_{j=0}^{k-1} \frac{\chi_{n-j-1}}{\chi_{d-j}},$$

for independent chi-distributed random variables.

Qualitative comparison with SGD





So, if we set

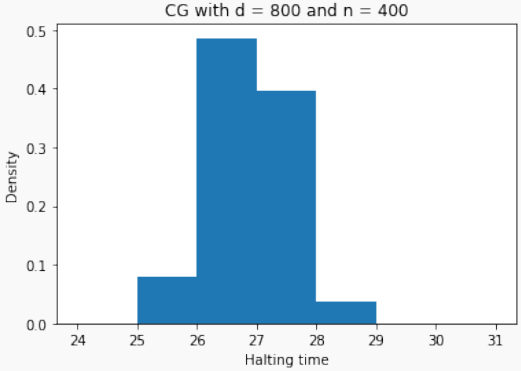
$$E_k(\mathrm{Wishart}; \mathrm{CG}) = \|r_k\|$$

we can analyze the halting time to see that

$$T_{\mathrm{CG}}(\mathrm{Wishart}, \varepsilon) \approx \frac{2}{c} n^{1-\alpha} \log \varepsilon^{-1} + O(n^{3/2-2\alpha}) \mathcal{N}(0,1),$$

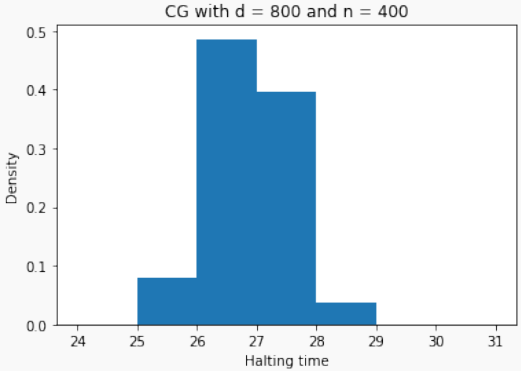
for $1/2 < \alpha < 1$.

To the well-conditioned regime!



It turns out that the errors $E_k(P_N; \mathcal{A})$ for iterative methods for a linear system involving A^TA are often analyzable in the well-conditioned, ill-conditioned and "in between" regimes. But the analysis of the halting time can be much more involved because the halting time $T_{\mathcal{A}}(P_n, \varepsilon)$ can tend to infinity with n!

To the well-conditioned regime!



So, we, for the time being, let $d = \lfloor nr \rfloor$ for $r > 1$.

The Gradient Descent Algorithm

1. x_0 is the initial vector.
2. For $k = 1, 2, \ldots$
   2.1 Select step size γ_k
   2.2 Compute $x_k = x_{k-1} - \gamma_k \nabla \mathcal{L}(x_{k-1})$

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A direction calculation reveals that

$$x_k = Q_k(W)c,$$

for a polynomial Q_k of degree $k-1$ with coefficients that depend on γ_j, $j = 1, 2, \ldots, k$.

For simplicity, suppose that W is full rank. Then if x is the true minimizer, a crucial calculation is that

$$x - x_k = W^{-1}c - Q_k(W)c = W^{-1}\underbrace{\left(I_n - WQ_k(W)\right)}_{R_k(W)}c.$$

Note that R_k is a polynomial of degree k satisfying $R_k(0) = 1$.

Then

$$\nabla \mathcal{L}(x_k) = Wx_k - Wx = R_k(W)c,$$
$$\|R_k(W)c\|^2 = c^T R_k(W)^2 c.$$

Example: GD

For GD follows that the difference $\boldsymbol{x}_k - \boldsymbol{x}$ satisfies

$$\boldsymbol{x}_k - \boldsymbol{x} = \boldsymbol{x}_{k-1} - \boldsymbol{x} - \gamma_k(W\boldsymbol{x}_{k-1} - W\boldsymbol{x}) = (\boldsymbol{I}_n - \gamma_k W)(\boldsymbol{x}_{k-1} - \boldsymbol{x}).$$

And so,

$$R_k(x) = \prod_{j=1}^{k}(1 - \gamma_j x).$$

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For CG the polynomial R_k is best characterized using the theory of orthogonal polynomials.

$$\|R_k(W)\boldsymbol{c}\|^2 = \boldsymbol{c}^T R_k(W)^2 \boldsymbol{c}$$

The error analysis of GD (and, as it turns out, CG) is reduced to:

1. The determination/characterization of the polynomial R_k.
2. The estimation of $\boldsymbol{c}^T R_k(W)^2 \boldsymbol{c}$.

For many methods of interest (CG and GD included), the coefficients of R_k depend continuously on the eigenvalues and eigenvectors of $\boldsymbol{W}$ in a sufficiently strong sense that

$$R_k(x) \xrightarrow[n\to\infty]{\Pr} \mathcal{R}_k(x) \longleftarrow \text{deterministic}.$$

Then, one can conclude

$$\boldsymbol{c}^T R_k(\boldsymbol{W})^2 \boldsymbol{c} \xrightarrow[n\to\infty]{\Pr} \int_{\mathbb{R}} \mathcal{R}_k(x)^2 \mu_{\mathrm{SCM}}(\mathrm{d}x).$$

This provides a deterministic limit for the (random) errors that are encountered throughout the algorithm.

Note: This is true only if $\boldsymbol{c}$ is independent of $\boldsymbol{W}$ and in the regression problem it is not.

Building back to true regression

For the regression problem, we have

$$c = \frac{1}{n}\left[A^T A a + A^T \eta\right].$$

Then

$$\|\mathcal{L}(x_k)\|^2 = a^T W^2 R_k(W)^2 a^T + \frac{1}{n^2}\eta^T A R_k(W)^2 A^T \eta + \underbrace{\frac{2}{n} a^T W R_k(W)^2 A^T \eta}$$

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$$\xrightarrow[n\to\infty]{\Pr} \underbrace{R\int_{\mathbb{R}} x^2 \mathcal{R}_k(x)^2 \mu_{\mathrm{SCM}}(\mathrm{d}x) + \tilde{R}\int_{\mathbb{R}} x \mathcal{R}_k(x)^2 \mu_{\mathrm{SCM}}(\mathrm{d}x)}_{\epsilon_k^2}.$$

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Important features:

- This demonstrates that the entire spectrum of W contributes via μ_{SCM}
- Nearly all probabilistic analyses of algorithms give inequalities whereas this gives true leading-order behavior.

$$\|\mathcal{L}(x_k)\|^2 \xrightarrow[n\to\infty]{\Pr} R \int_{\mathbb{R}} x^2 \mathcal{R}_k(x)^2 \mu_{\mathrm{SCM}}(\mathrm{d}x) + \tilde{R} \int_{\mathbb{R}} x \mathcal{R}_k(x)^2 \mu_{\mathrm{SCM}}(\mathrm{d}x)$$

If one has a good guess as to what the limiting distribution μ_{SCM} is then the γ_k's in GD can be chosen based on this limit — to minimize this expression, see Pedregosa and Scieur [2020].

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Furthermore, by preconditioning one can make such a guess valid, see Lacotte and Pilanci [2020].

Provided that $\mathfrak{e}_k \xrightarrow{k\to\infty} 0$, one finds that

$$\lim_{n\to\infty} \mathbb{P}\left(T_{\mathcal{A}}(P_n;\varepsilon) = \min\{k : \mathfrak{e}_k < \varepsilon\}\right) = 1,$$

for most choices of ε.

This turns out to be true for all $d \geq n$, $n \to \infty$, for the regression problem with CG or GD.

Deterministic halting for CG with $r = 2$, $\varepsilon = 10^{-4}$

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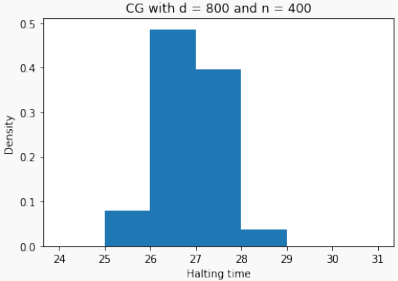

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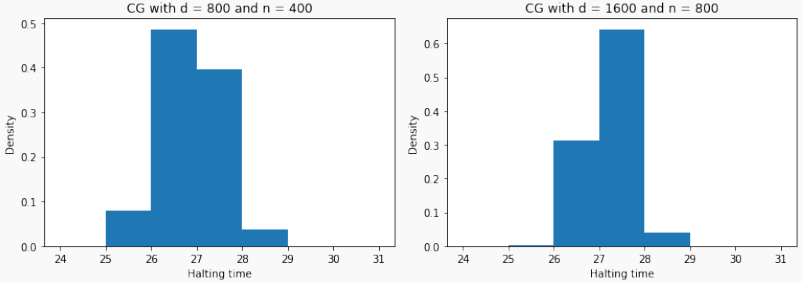

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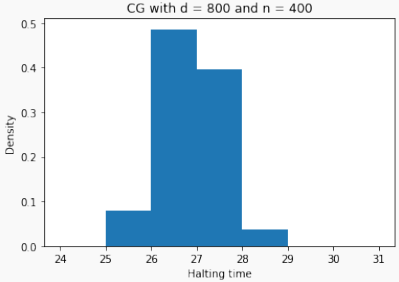

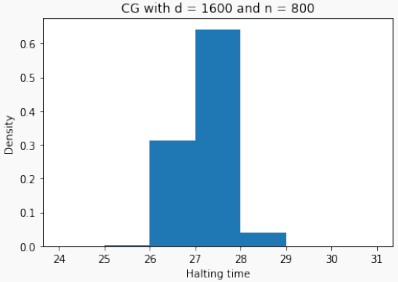

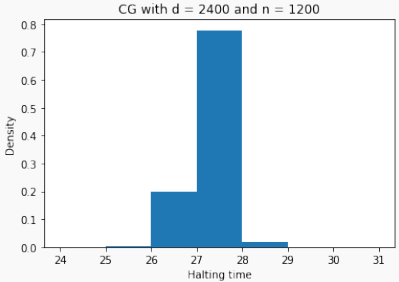

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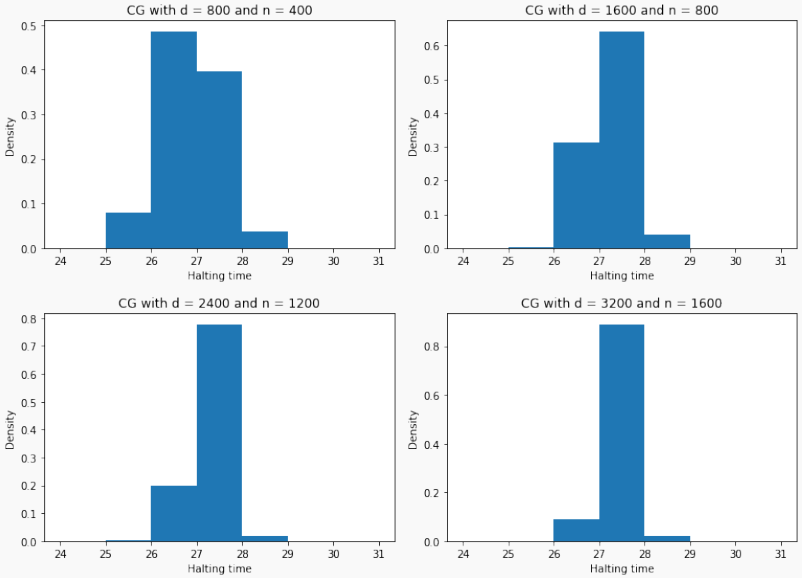

Outlook

RMT provides non-trivial tractable models to analyze the statistics of optimization algorithms.

Other algorithms are analyzable:

- MINRES algorithm
- Polyak algorithm
- Nesterov accelerated algorithm
- SGD for regression
- ...

See the preprints: Paquette and Trogdon [2020], Paquette et al. [2021], Ding and Trogdon [2021], Paquette et al. [2020]

Outlook

Other ensembles are analyzable using the following results from RMT:

- Spiked random matrices (see Baik et al. [2005], Bloemendal and Virág [2013], Ding and Yang [2019], and many more)
- Nonlinear models (see Part 4)
- Random graphs (see Erdős et al. [2013], for example)
- Invariant ensembles (see Bourgade et al. [2014], Deift [2000] and many more)

Open questions

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- To what extent can one move these ideas beyond regression? To a two-layer network? Rank-one matrix completion problem?
- What is a good probability distribution to study? Wishart is clearly the place to start but what is relevant in practice?

A CG demo

See Colab for a CG demo

https://colab.research.google.com/drive/1UZRSK665b8sqq0NQFwMCwrVabPlB-7nK?usp=sharing

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Random Matrix Theory for Machine Learning

The Mystery of Generalization: Why Does Deep Learning Work?

Fabian Pedregosa, Courtney Paquette, Tom Trogdon, Jeffrey Pennington

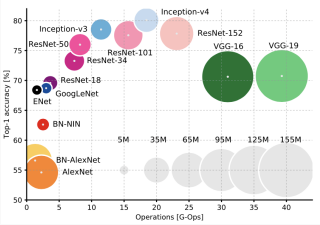
https://random-matrix-learning.github.io

Why does deep learning work?

Deep neural networks define a flexible and expressive class of functions.

State-of-the-art models have millions or billions of parameters

- Meena: 2.6 billion
- Turing NLG: 17 billion
- GPT-3: 175 billion



Source: [Canziani et al., 2016]

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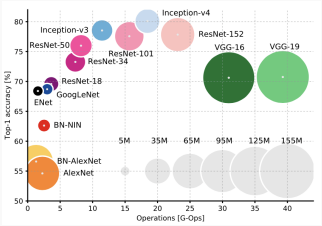
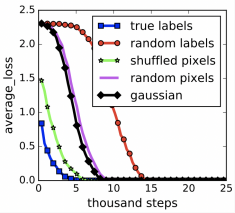


Source: [Canziani et al., 2016]

Models that perform well on real data can easily memorize noise

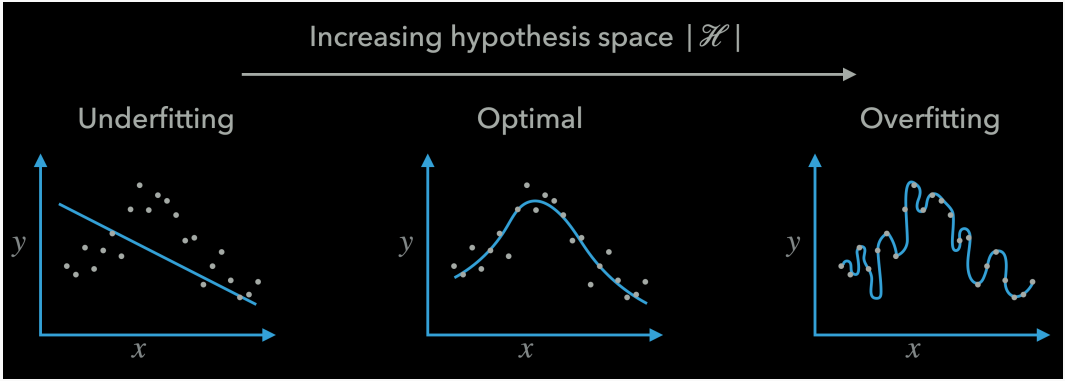


Source: [Zhang et al., 2021]

Why does deep learning work?

Deep neural networks define a flexible and expressive class of functions.

$\Rightarrow$ Standard wisdom suggests they should overfit



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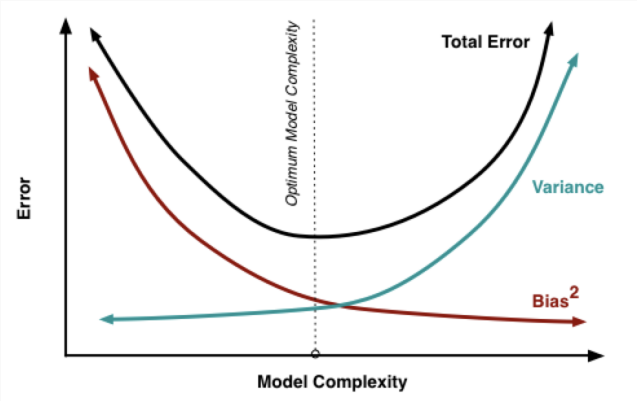
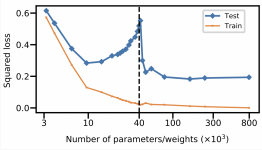
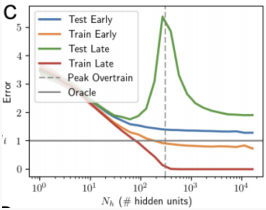


Double descent

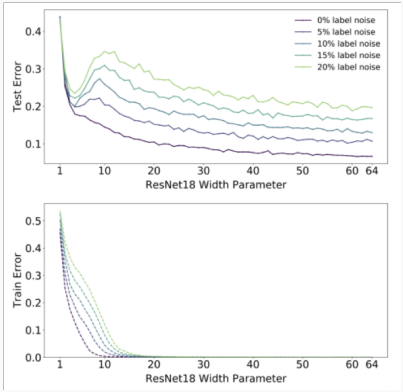
However, large neural networks do not obey the classical theory:



Source: [Belkin et al., 2019]



Source: [Advani et al., 2020]



Source: [Nakkiran et al., 2019]

The emerging paradigm of *double descent* seeks to explain this phenomenon.

Models of Double Descent

History of double descent: Kernel interpolation

1) Interpolating kernels (trained to zero error) generalize well [Belkin et al., 2018]

$\Rightarrow$ Double descent is not unique to deep neural networks

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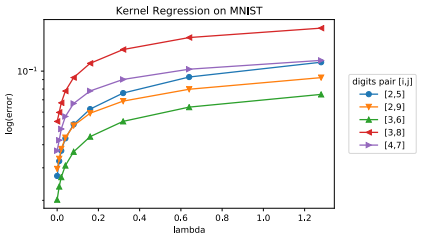

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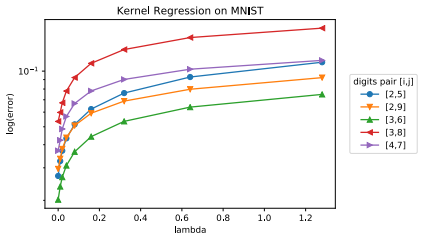


Source: [Liang and Rakhlin, 2020]

3) Consistency is a high-dimensional phenomenon [Rakhlin and Zhai, 2019]:

The estimation error of the minimum-norm kernel interpolant

$$\arg\min_{f \in \mathcal{H}} \|f\|_{\mathcal{H}} \quad \text{s.t.} \quad f(x_i) = y_i\,, \quad i = 1 \dots n$$

does not converge to zero as n grows, unless d is proportional to n.

Models of double descent: High-dimensional linear regression

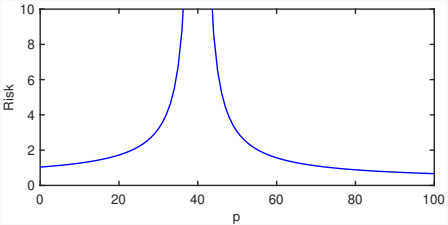
What is the simplest theoretically tractable model that exhibits double descent?

Models of double descent: High-dimensional linear regression

What is the simplest theoretically tractable model that exhibits double descent?

Linear regression suffices, but requires a mechanism to vary the effective number of parameters or samples:

- The size of randomly selected subsets of features [Belkin et al., 2020]
- The dimensionality of the low-variance subspace [Bartlett et al., 2020]
- The sparsity of the generative model [Mitra, 2019]



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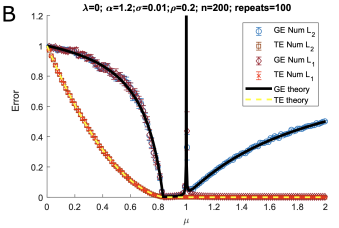


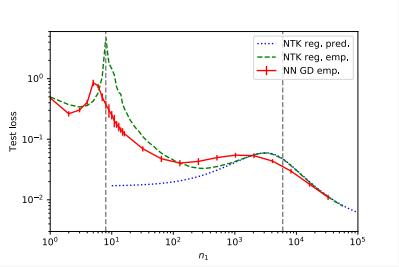
Source: [Mitra, 2019]

Models of double descent: Random feature models

In random feature regression, the number of random features controls the model capacity, and can be tuned independently from the data.

Exact asymptotic results in high dimensions exist in many settings, including:

- Unstructured random features [Mei and Montanari, 2019]
- NTK-structured random features [Adlam and Pennington, 2020]
- Random Fourier features [Liao et al., 2020]



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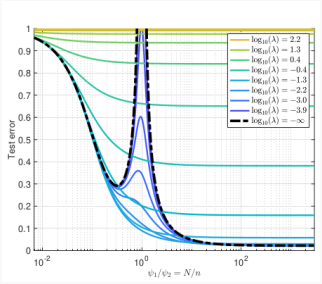

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Random feature models

Random feature regression: definition

Random feature regression is just linear regression on a transformed feature matrix, $F = f(\frac{1}{\sqrt{d}} WX) \in \mathbb{R}^{m \times n}$, where $W \in \mathbb{R}^{m \times d}$, $W_{ij} \sim \mathcal{N}(0, 1)$.

- Model given by $\beta^\top F$ (instead of $\beta^\top X$) — variable capacity (m vs d parameters)
- $f(\cdot)$ is a nonlinear activation function, acting elementwise
- F is equivalent to first post-activation layer of a NN at init

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For targets $Y \in \mathbb{R}^{1 \times n}$, the ridge-regularized loss is,

$$L(\beta; X) = \|Y - \tfrac{1}{\sqrt{m}} \beta^\top F\|_2^2 + \lambda \|\beta\|_2^2 \,,$$

and the optimal regression coefficients $\hat{\beta}$ are given by,

$$\hat{\beta} = \tfrac{1}{\sqrt{m}} Y (K + \lambda I_n)^{-1} F^\top \,, \quad K = \tfrac{1}{m} F^\top F \,.$$

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Note that $Q \equiv (K + \lambda I_n)^{-1}$ is the *resolvent* of the kernel matrix K.

Random feature regression: training error

Training error is determined by the resolvent matrix $Q \equiv (K + \lambda I_n)^{-1}$:

$$\begin{aligned} E_{\text{train}}(\lambda) &= \tfrac{1}{n} \|Y - \tfrac{1}{\sqrt{m}} \hat{\boldsymbol{\beta}}^\top F\|_2^2 \\ &= \tfrac{1}{n} \|Y - \tfrac{1}{m} YQF^\top F\|_2^2 \\ &= \tfrac{1}{n} \|Y - YQK\|_2^2 \\ &= \tfrac{1}{n} \|Y(I_n - QK)\|_2^2 \\ &= \lambda^2 \tfrac{1}{n} \|YQ\|_2^2 \,, \end{aligned}$$

where we used that $I_n - QK = I_n - Q(Q^{-1} - \lambda I_n) = I_n - (I_n - \lambda Q) = \lambda Q$.

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So we see that the training error measures the alignment between the resolvent and the label vector.

What about the test error?

Aside: Generalized cross validation (GCV)

A model's performance on the training set, or subsets thereof, can be useful for estimating its performance on the test set.

- Leave-one-out cross validation (LOOCV)

$$E_{LOOCV}(\lambda) = \frac{1}{n}\|\boldsymbol{YQ} \cdot \mathrm{diag}(\boldsymbol{Q})^{-1}\|_2^2$$

- Generalized cross validation (GCV)

$$E_{GCV}(\lambda) = \frac{1}{n}\|\boldsymbol{YQ}\|_2^2 / (\frac{1}{n}\mathrm{tr}(\boldsymbol{Q}))^2$$

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In certain high-dimensional limits, $E_{GCV}(\lambda) = E_{LOOCV}(\lambda) = E_{\text{test}}(\lambda)$:

- Ridge regression [Hastie et al., 2019]
- Kernel ridge regression [Jacot et al., 2020]
- Random feature regression [Adlam and Pennington, 2020]

Random feature regression: high-dimensional asymptotics

To develop an analytical model of double descent, we study the high-dimensional asymptotics:

$$m, d, n \to \infty \quad \text{such that} \quad \phi \equiv \frac{d}{n}, \psi \equiv \frac{d}{m} \quad \text{are constant.}$$

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For simplicity, we focus on the specific setting in which,

$$X_{ij} \sim \mathcal{N}(0,1) \quad \text{and} \quad \boldsymbol{\beta}^* \sim \mathcal{N}(0, I_d)\,.$$

Random feature regression: test error

In the high-dimensional asymptotic setup from above, the random feature test error can be written as,

$$\begin{aligned} E_{\text{test}}(\lambda) &= E_{\text{GCV}}(\lambda) \\ &= \lim_{n\to\infty} \tfrac{1}{n}\|YQ\|_2^2/(\tfrac{1}{n}\text{tr}(Q))^2 \\ &= \lim_{n\to\infty} \tfrac{1}{n}\|(\tfrac{1}{\sqrt{d}}\beta^{*\top}X+\varepsilon)Q\|_2^2/(\tfrac{1}{n}\text{tr}(Q))^2 \\ &= \lim_{n\to\infty} \tfrac{1}{n}\text{tr}[(\sigma_\varepsilon^2 I_n + \tfrac{1}{d}X^\top X)Q^2]/(\tfrac{1}{n}\text{tr}(Q))^2 \\ &\equiv -\frac{\sigma_\varepsilon^2\tau_1'(\lambda)+\tau_2'(\lambda)}{\tau_1(\lambda)^2}\,, \end{aligned}$$

where we used that $\frac{\partial}{\partial\lambda}Q = -Q^2$, and we defined

$$\tau_1 = \lim_{n\to\infty}\tfrac{1}{n}\text{tr}(Q) \quad \text{and} \quad \tau_2 = \lim_{n\to\infty}\tfrac{1}{n}\text{tr}(\tfrac{1}{d}X^\top XQ)\,.$$

Computing the asymptotic test error

To compute the test error, we need:

$$\tau_1 = \lim_{n\to\infty} \tfrac{1}{n}\mathrm{tr}(K + \lambda I_n)^{-1} \quad \text{and} \quad \tau_2 = \lim_{n\to\infty} \tfrac{1}{n}\mathrm{tr}(\tfrac{1}{d}X^\top X(K + \lambda I_n)^{-1}) \,.$$

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Recalling the definition of K,

$$K = \tfrac{1}{m}F^\top F \,, \quad F = f(\tfrac{1}{\sqrt{d}}WX) \,,$$

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These technical challenges can be overcome with two tricks:

1. Constructing an equivalent Gaussian linearized model
2. Analyzing a suitably augmented resolvent

Computing the asymptotic test error: Gaussian equivalents

The nonlinear dependencies in $F = f(\frac{1}{\sqrt{d}}WX)$ complicate the analysis.

Can we identify a simpler matrix in the same universality class?

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There exist constants c_1 and c_2 such that

$$F \cong F_{\text{lin}} \equiv c_1 \tfrac{1}{\sqrt{d}} WX + c_2 \Theta\,, \quad \Theta_{ij} \sim \mathcal{N}(0,1)\,,$$

where $F \cong F_{\text{lin}}$ indicates the two matrices share all statistics relevant for computing the test error:

$$\tau_1 = \lim_{n\to\infty} \tfrac{1}{n}\text{tr}(\tfrac{1}{m}F^\top F + \lambda I_n)^{-1} = \lim_{n\to\infty} \tfrac{1}{n}\text{tr}(\tfrac{1}{m}F_{\text{lin}}^\top F_{\text{lin}} + \lambda I_n)^{-1}$$

$$\tau_2 = \lim_{n\to\infty} \tfrac{1}{n}\text{tr}(\tfrac{1}{d}X^\top X(\tfrac{1}{m}F^\top F + \lambda I_n)^{-1}) = \lim_{n\to\infty} \tfrac{1}{n}\text{tr}(\tfrac{1}{d}X^\top X(\tfrac{1}{m}F_{\text{lin}}^\top F_{\text{lin}} + \lambda I_n)^{-1})$$

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How can we compute these traces? Need to augment the resolvent.

Computing the asymptotic test error: resolvent method

Recall from Part 2 that the resolvent method identifies consistency relations between suitably chosen submatrices of the resolvent.

Here we can undertake a similar analysis as in Part 2, but now on an augmented matrix,

$$H = \begin{bmatrix} \lambda I_n & \frac{1}{\sqrt{m}} F_{\text{lin}}^\top \\ \frac{1}{\sqrt{m}} F_{\text{lin}} & -I_m \end{bmatrix},$$

which encodes the resolvent through $Q = (K + \lambda I_n)^{-1} = [H^{-1}]_{1:n,1:n}$.

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To derive consistency relations, we consider two submatrices: $H^{(1)}$ (leaving out row/column 1), and $H^{(n+1)}$ (leaving out row/column $n+1$).

As before, we use the Sherman-Morrison formula to compute $[H^{(1)}]^{-1}$ and $[H^{(n+1)}]^{-1}$, and relate them to Q and rows/columns of F_{lin}.

Straightforward concentration arguments eventually lead to coupled self-consistent equations for τ_1 and τ_2 [Adlam et al., 2019].

Computing the asymptotic test error: free probability

An alternative augmentation of the resolvent completely linearizes the dependence on the random matrices:

$$M = \begin{bmatrix} \lambda I_n & \frac{c_2}{m}\Theta^\top & \frac{c_1}{\sqrt{d}m}X^\top & 0 \\ c_2\Theta & -I_m & 0 & \frac{c_1}{\sqrt{d}}W \\ 0 & W^\top & -I_d & 0 \\ X & 0 & 0 & -I_d \end{bmatrix},$$

where the Schur complement formula now gives,

$$\tau_1 = \lim_{n\to\infty} \tfrac{1}{n}\mathrm{tr}([M^{-1}]_{1,1}), \quad \text{and} \quad \tau_2 = \lim_{n\to\infty} \tfrac{1}{n}\mathrm{tr}([M^{-1}]_{4,3}).$$

The asymptotic blockwise traces $\mathrm{tr}([M^{-1}]_{a,b})$ can themselves be computed using free probability [Adlam and Pennington, 2020].

Computing the asymptotic test error: free probability

M is linear in the random matrices X, W, and Θ:

$$M = \begin{bmatrix} \lambda I_n & 0 & 0 & 0 \\ 0 & -I_m & 0 & 0 \\ 0 & 0 & -I_d & 0 \\ 0 & 0 & 0 & -I_d \end{bmatrix} + \begin{bmatrix} 0 & 0 & \frac{c_1}{\sqrt{dm}} X^\top & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ X & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{c_1}{\sqrt{d}} W \\ 0 & W^\top & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & \frac{c_2}{m} \Theta^\top & 0 & 0 \\ c_2 \Theta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Can we compute the blockwise traces with free probability via the R-transform?

Computing the asymptotic test error: free probability

M is linear in the random matrices X, W, and Θ:

$$M = \begin{bmatrix} \lambda I_n & 0 & 0 & 0 \\ 0 & -I_m & 0 & 0 \\ 0 & 0 & -I_d & 0 \\ 0 & 0 & 0 & -I_d \end{bmatrix} + \begin{bmatrix} 0 & 0 & \frac{c_1}{\sqrt{dm}} X^\top & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ X & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{c_1}{\sqrt{d}} W \\ 0 & W^\top & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & \frac{c_2}{m} \Theta^\top & 0 & 0 \\ c_2 \Theta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Can we compute the blockwise traces with free probability via the R-transform?

Not naively: the additive terms are independent, but not free over $\mathbb{C}$.

However, they are free over $M_4(\mathbb{C})$, and there exists a suitable *operator-valued* generalization of the R-transform that enables the necessary computations [Mingo and Speicher, 2017].

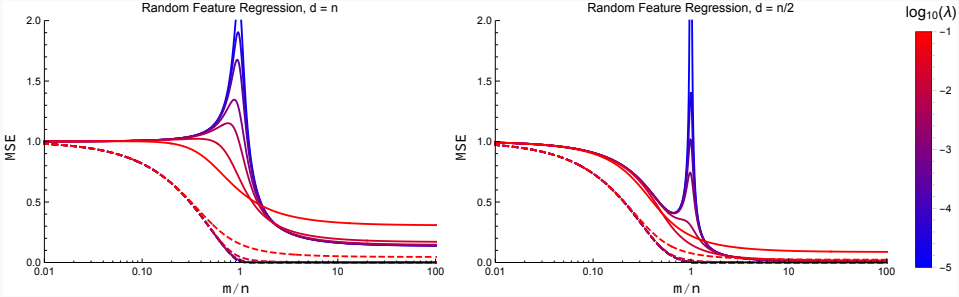
Asymptotic test error

Theorem

Let $\eta = \mathbb{E}[f(g)^2]$ and $\zeta = (\mathbb{E}[gf(g)])^2$ for $g \sim \mathcal{N}(0,1)$. Then, the asymptotic traces $\tau_1(\lambda)$ and $\tau_2(\lambda)$ are given by solutions to the polynomial system,

$$\zeta\tau_1\tau_2\left(1-\lambda\tau_1\right) = \phi/\psi\left(\zeta\tau_1\tau_2 + \phi(\tau_2-\tau_1)\right) = (\tau_1-\tau_2)\,\phi\left((\eta-\zeta)\tau_1 + \zeta\tau_2\right),$$

and, $E_{\text{train}} = -\lambda^2(\sigma_\varepsilon^2\tau_1' + \tau_2')$ and $E_{\text{test}} = -(\sigma_\varepsilon^2\tau_1' + \tau_2')/\tau_1^2$.



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