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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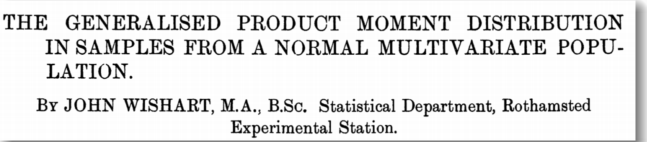
Goal of Random Matrix Theory is to understand their

- 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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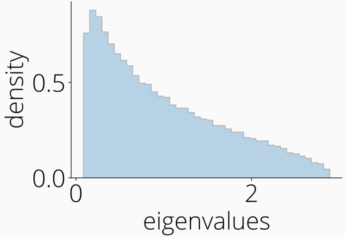

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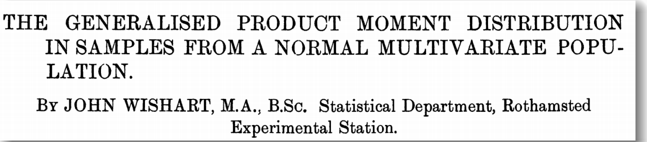

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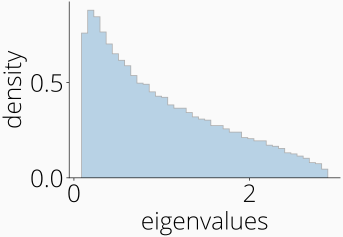
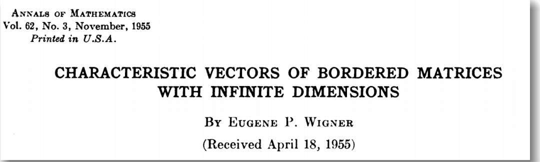


$$W = XX^\top, X_{ij} \sim \mathcal{N}(0,1)$$

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

1955: Random Symmetric Matrices



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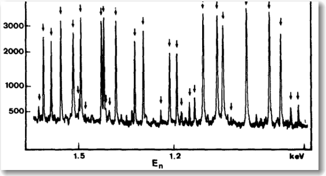
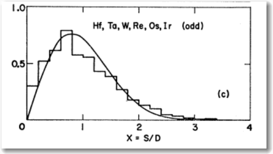
CHARACTERISTIC VECTORS OF BORDERED MATRICES WITH INFINITE DIMENSIONS

BY EUGENE P. WIGNER

(Received April 18, 1955)





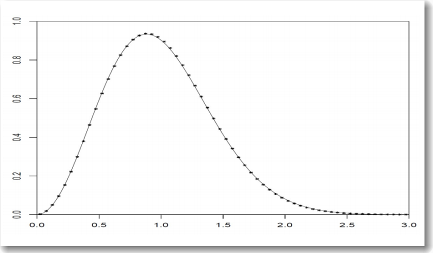
Eugene Wigner

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 ...

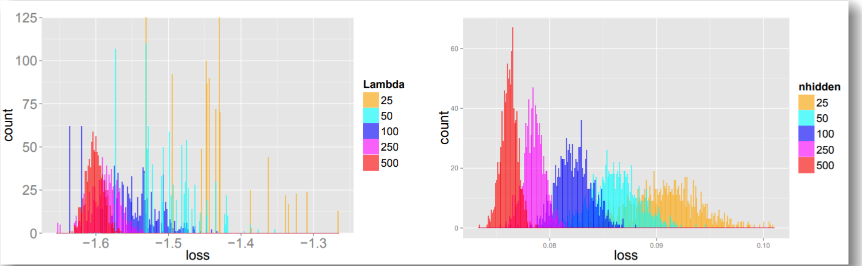


Distribution function of gaps between eigenvalues compared with histogram of gaps between ζ zeros. Source: [Odlyzko, 1987]

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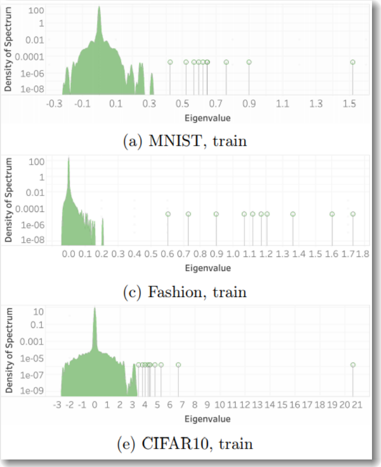
[3] *https://github.com/deep-lab/DeepnetHessian*



Source: [Papyan, 2020]

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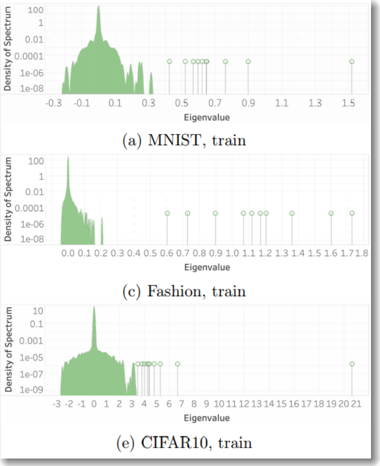
RMT model for the Hessian still an open problem [Liao and Mahoney, 2021, Baskerville et al., 2021] ...



(a) MNIST, train

(c) Fashion, train

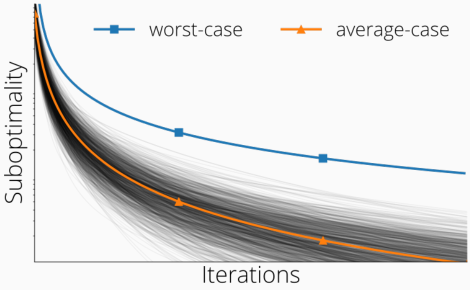
(e) CIFAR10, train

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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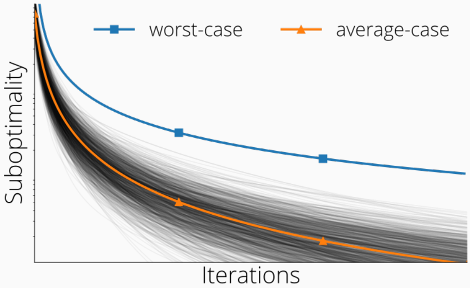
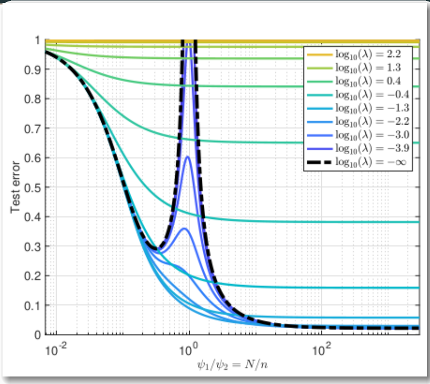


Topic of Part 3 of this tutorial

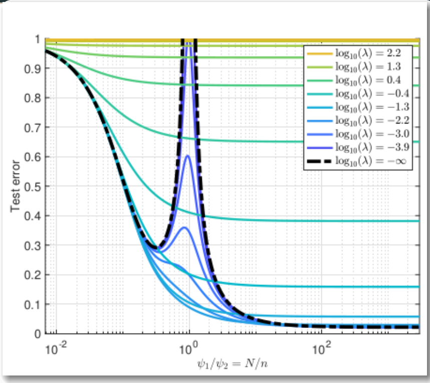
Random Matrices in Machine Learning: Generalization

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*

Random Matrices in Machine Learning: Generalization



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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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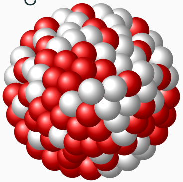

Gaussian Orthogonal Ensemble (GOE)

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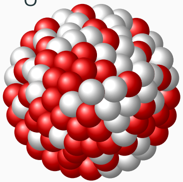

- **Rotational invariant**
  for any fixed orthogonal matrix O,

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

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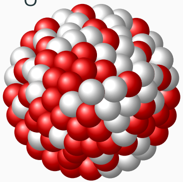

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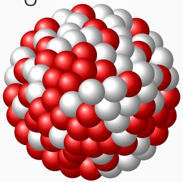

- **Rotational invariant**
  for any fixed orthogonal matrix O,

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- **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

```python
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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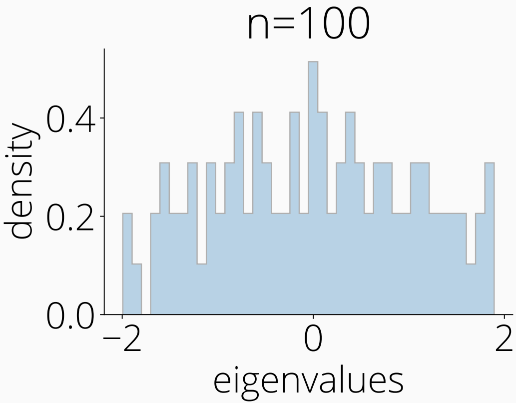

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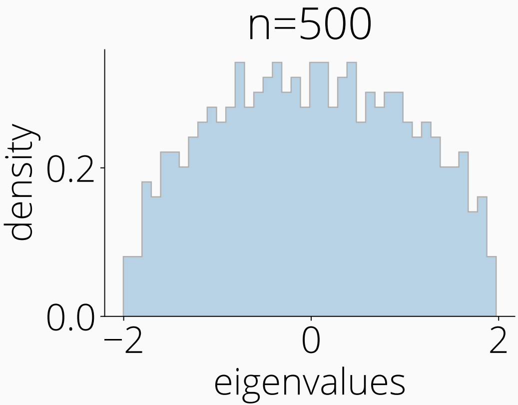

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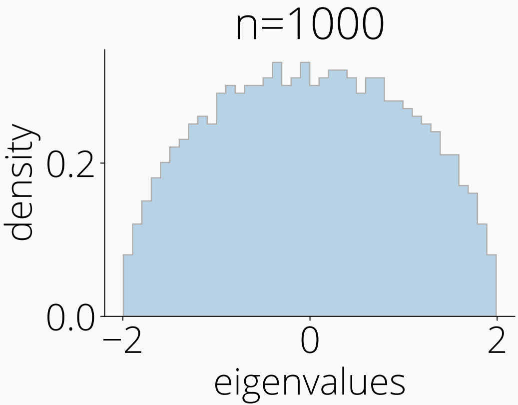

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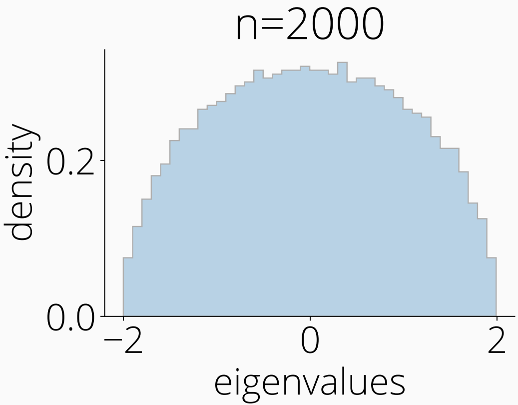

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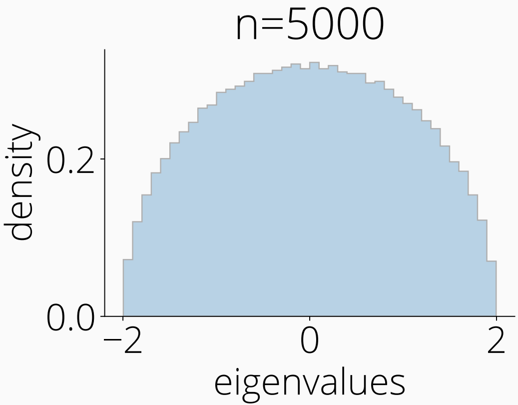

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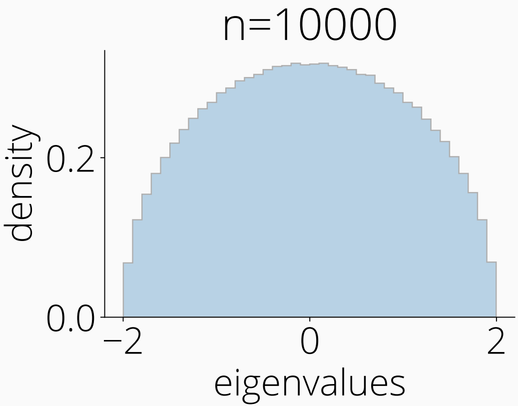
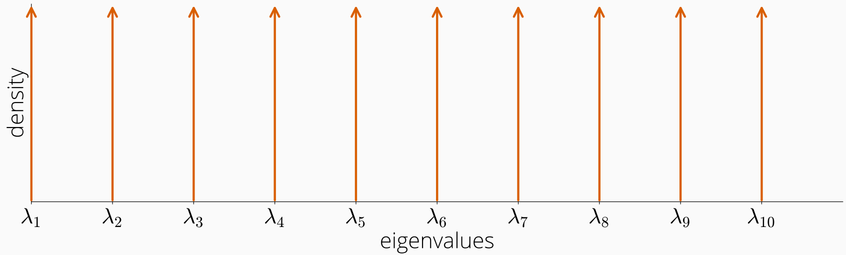


Empirical Spectral Distribution (ESD)

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

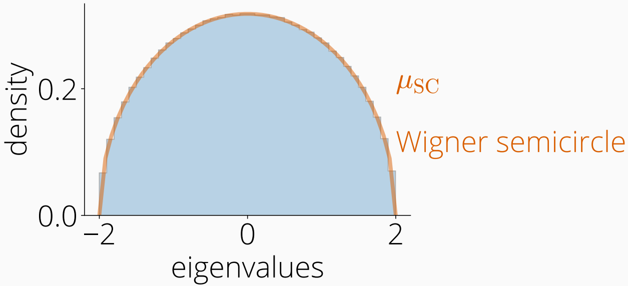
$$\mu_{\mathrm{ESD}} = \mu_n \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i(A_n)}.$$



Wigner Semicircle Law

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

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



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 $\mathbf{r} = \frac{d}{n}$

Wishart ensemble

Python pseudocode

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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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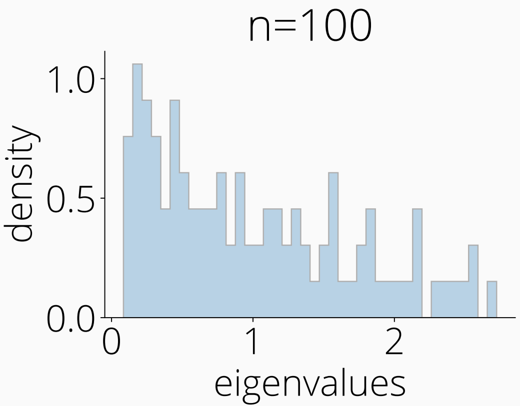

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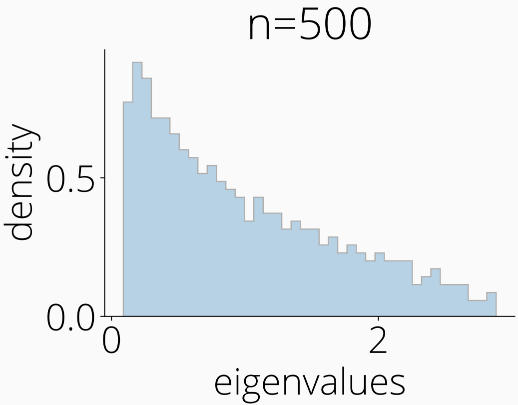

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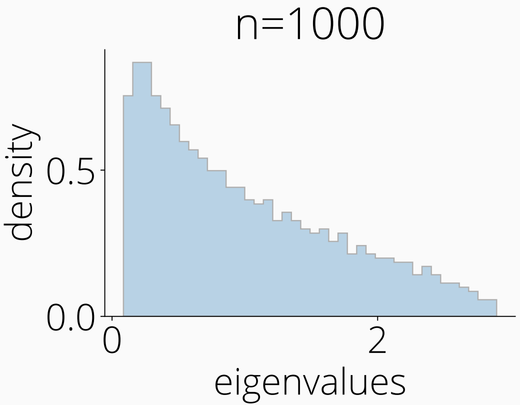

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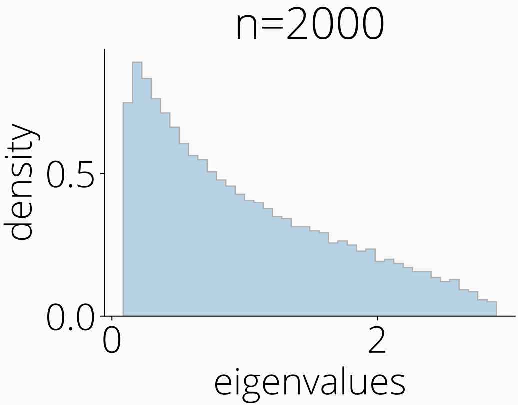

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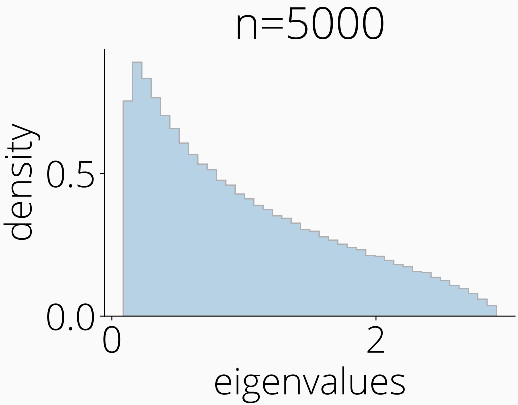


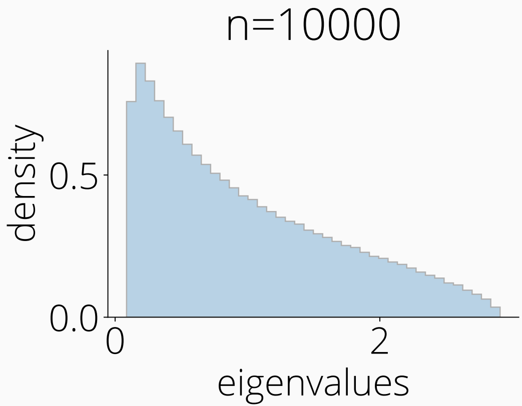
Wishart ensemble

Python pseudocode

```
import numpy as np
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)
```



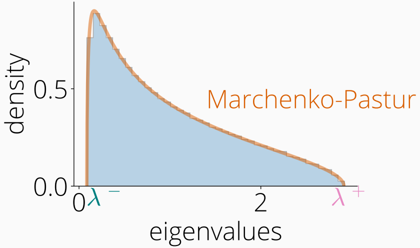
Limit of Wishart matrices

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

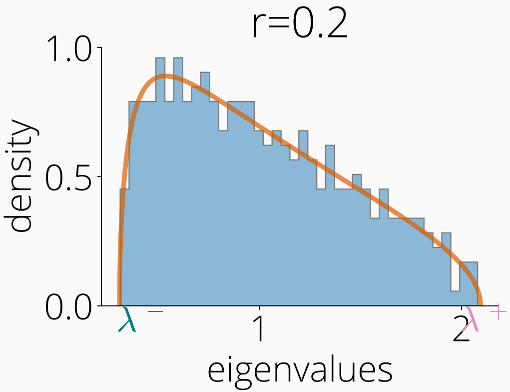
As $n, d \to \infty$, $\frac{d}{n} \to r$, μ_{ESD} converges to the Marchenko-Pastur distribution:

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

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



- $r < 1 \implies d < n \implies W$ 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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The $r = \frac{d}{n}$ parameter

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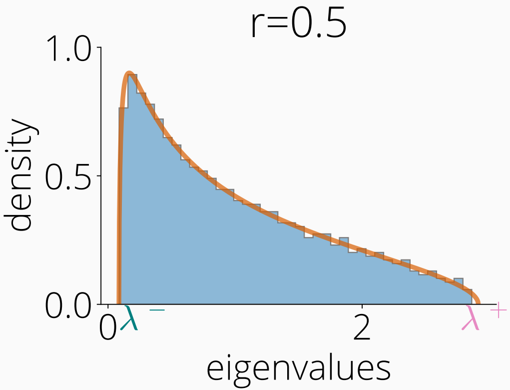

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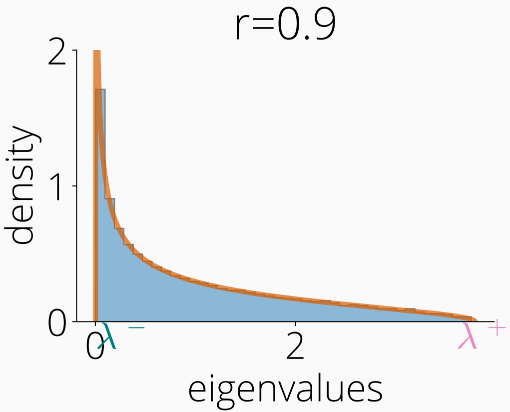

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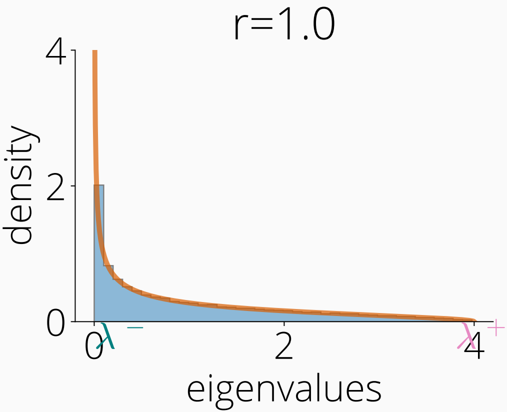

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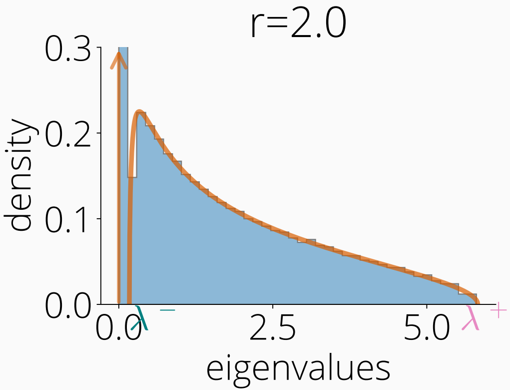

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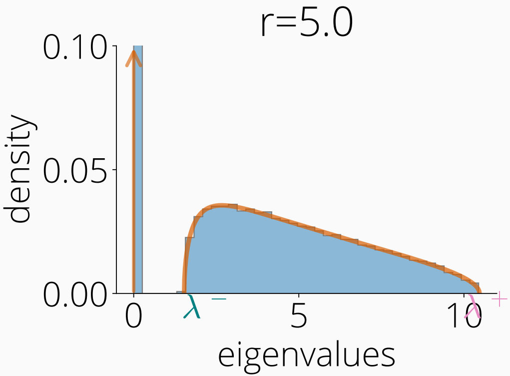

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Universality

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

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

- $X_{ij} \sim \mathcal{N}(0,1)$
- $X_{ij} \sim$ Rademacher $\Pr(X_{ij} = -1) = \Pr(X_{ij} = 1) = \frac{1}{2}$

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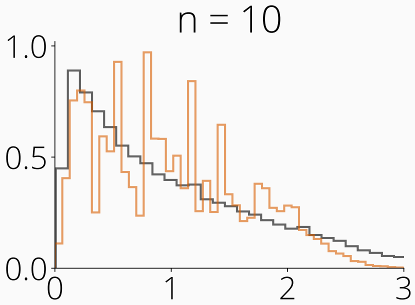

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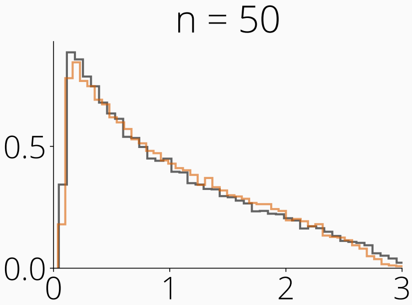

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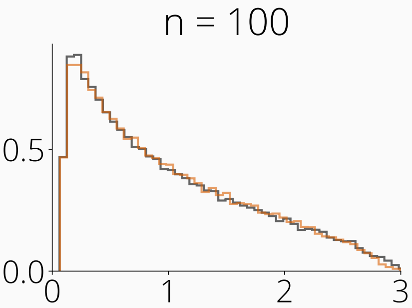

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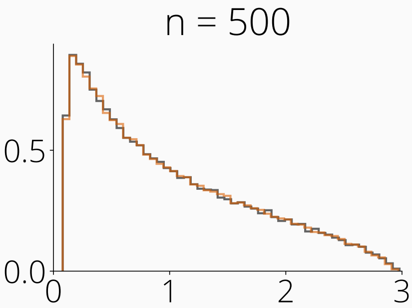

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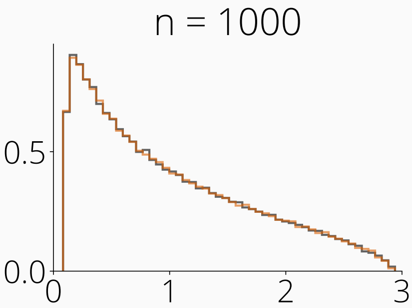

Universality

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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 ...

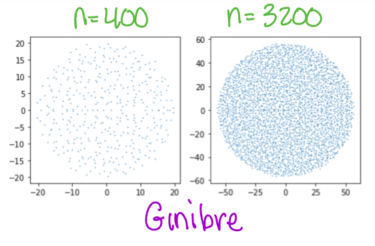
Other matrix ensembles

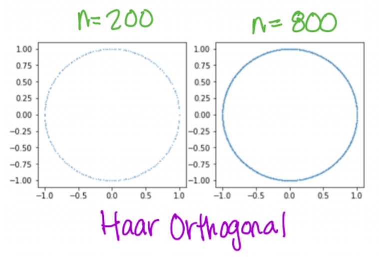
- **Ginibre.** Let G_n be $n \times n$ matrix of i.i.d. $N(0,1)$, (bilinear games [Domingo-Enrich et al., 2020])

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

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

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





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