Random Matrices: Invertibility, Structure, and Applications

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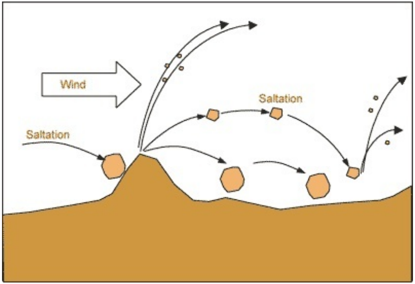
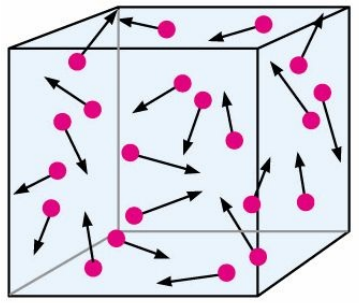
Chaos and Order

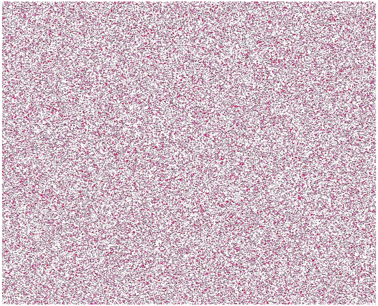
Many complex systems that occur in nature and society exhibit chaos on the **microscopic** level and order on the **macroscopic** level.



Chaos and Order

Gas molecules:





Statistical mechanics: randomness at the microscopic level averages out at the macroscopic level.

Probability Theory

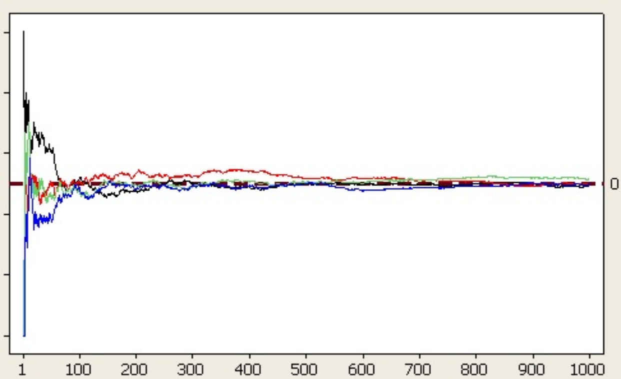
- **Microscopic:** independent random variables $X_1, X_2, \dots$
- **Macroscopic:** function $f(X_1, \dots, X_n)$ where n is large.
- Example: Bernoulli r.v's $X_i = \pm 1$ with probabilities $\frac{1}{2}$.
  At each game, gain \$1 or lose \$1 independently.
  Macroscopic quantity: average gain

$$f(X_1, \dots, X_n) = \frac{X_1 + \cdots + X_n}{n}.$$

Probability Theory

Limit theorems describe the macroscopic picture as $n \to \infty$.

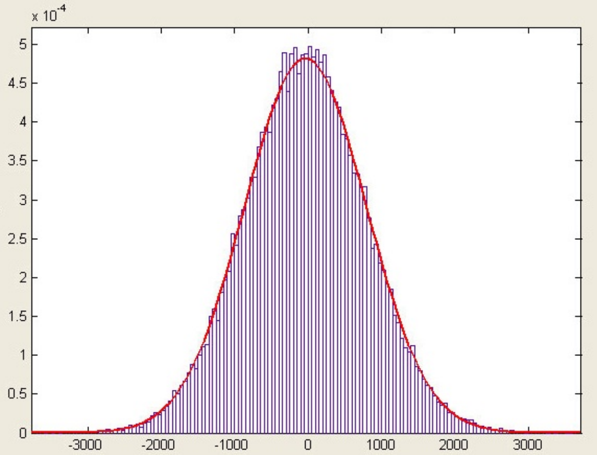
Law of Large Numbers:



$$\frac{X_1 + \cdots + X_n}{n} \to 0 \quad \text{almost surely}$$

Probability Theory

Central Limit Theorem:



$$X_1 + \cdots + X_n \approx N(0, \sqrt{n}) \quad \text{in distribution}$$

Probability Theory

- **Microscopic:** independent random variables $X_1, X_2, \ldots$
- **Macroscopic:** function $f(X_1, \ldots, X_n)$.
- Functions may be **more complex** than the sum $X_1 + \cdots + X_n$.
- Example: **random matrix theory**.

Random Matrix Theory

- **Microscopic:** independent random variables X_{ij}, arranged in a matrix

$$H = \begin{pmatrix} X_{11} & X_{12} & \cdots & X_{1n} \\ X_{21} & X_{22} & \cdots & X_{2n} \\ \multicolumn{4}{c}{\dotfill} \\ X_{n1} & X_{n2} & \cdots & X_{nn} \end{pmatrix}$$

- **Macroscopic:** the eigenvalues of H

$$\lambda_1(H), \ldots, \lambda_n(H).$$

Random Matrix Theory

One can make H **symmetric** by placing independent rv's above the diagonal and reflecting:

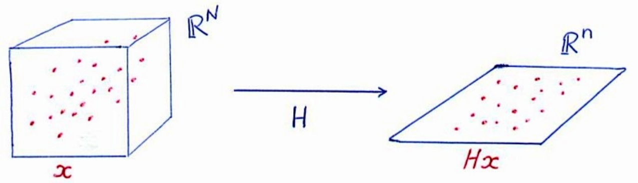
$$X_{ij} = X_{ji}$$

This is a Wigner random matrix:

$$H = \begin{pmatrix} X_{11} & X_{12} & \cdots & X_{1n} \\ X_{12} & X_{22} & \cdots & X_{2n} \\ \hdotsfor{4} \\ X_{1n} & X_{2n} & \cdots & X_{nn} \end{pmatrix}$$

Why Random Matrices?

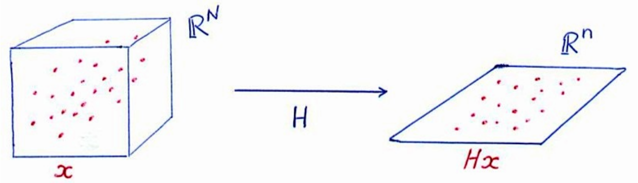
- Computer Science, Information Theory (1990's+): random matrices provide a mechanism for **dimension reduction**.
- Data points $x \in \mathbb{R}^N$ (high dimension) need to be mapped into $\mathbb{R}^n$ (low dimension) while preserving the essential information in the data.



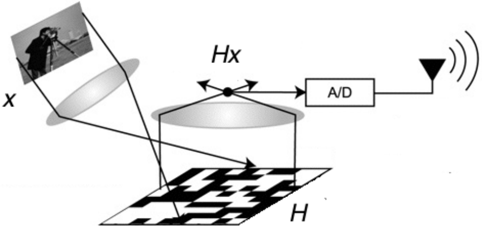
- Use a random linear transformation, given by an $n \times N$ **random matrix** H with independent entries.

Johnson-Lindenstrauss Lemma '84: *Given m data points in $\mathbb{R}^N$, one can reduce the dimension to $n \sim \log m$ while approximately preserving all pairwise distances between the points.*

Why Random Matrices?



Compressed Sensing (2004+): allows one to exactly **recover the data** $x \in \mathbb{R}^N$ from its random measurement $Hx \in \mathbb{R}^n$, provided the data x has "low information content", i.e. x is a **sparse** vector. In polynomial time.



Why Random Matrices?

- Numerical Analysis [Von Neumann et al. 40's]: analysis of algorithms for solving large **linear equations**

$$Ax = b.$$

- Use a **random matrix** A to test the quality (speed and accuracy) of a linear solver.
- Here one models a **"typical"** input A of an algorithm as a **random** input. Average analysis of algorithms.
- Many algorithms perform better when A is well conditioned, i.e. the condition number

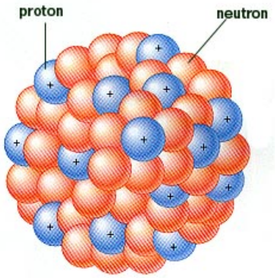
$$\kappa(A) = \|A\| \|A^{-1}\|$$

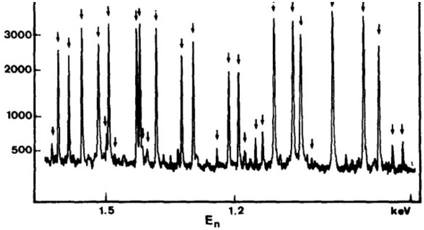
is not too large.

- Question: *Are random matrices well conditioned?*

Why Random Matrices?

- Physics: Excitation spectrum of heavy nuclei, e.g. U_{238}. **Excitation spectrum** = the energy levels for which a neutron will bounce off the nucleus (scattering resonances).





- Protons and neutrons in the nucleus of U_{238} interact with each other in a complicated way. The Hamiltonian is too complex. Its spectrum is **difficult to compute** either theoretically or by simulation.

Why Random Matrices?

- Wigner 50's: One models the complicated Hamiltonian as an $n \times n$ **symmetric random matrix**

$$H = \begin{pmatrix} X_{11} & X_{12} & \cdots & X_{1n} \\ X_{12} & X_{22} & \cdots & X_{2n} \\ \multicolumn{4}{c}{\dotfill} \\ X_{1n} & X_{2n} & \cdots & X_{nn} \end{pmatrix}$$

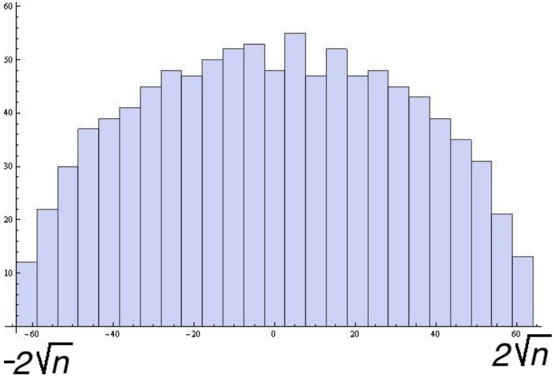
- The excitation spectrum = the eigenvalues

$$\lambda_1(H), \ldots, \lambda_n(H).$$

- The **distribution of the eigenvalues** now becomes computable. So, what is it?

Semicircle Law

The **histogram** of the eigenvalues of a 1000 × 1000 symmetric matrix with independent $N(0,1)$ entries:



Benedek Valkó's course on random matrices `http://www.math.wisc.edu/~valko/courses/833/833.html`

After rescaling...

Semicircle Law

Semicircle law [Wigner '55]: *Let H be a symmetric random matrix with $N(0,1)$ entries. Then the eigenvalue histogram of $\frac{1}{\sqrt{n}}H$ (i.e. the "empirical spectral distribution") converges to the semi-circle supported in $[-2,2]$.*

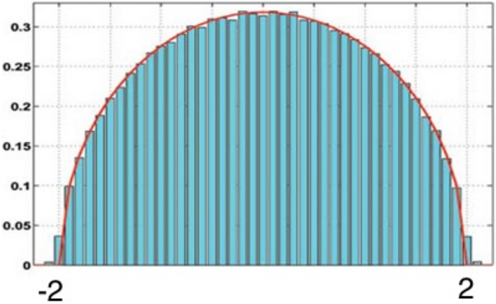
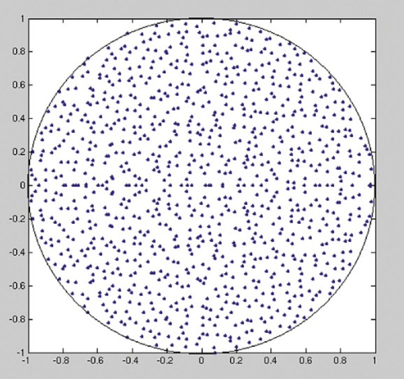


Image by Alan Edelman, MIT open courseware 18.996 / 16.399 Random Matrix Theory and Its Applications

Circular Law

Circular law [Mehta '67]: *Let H be a random matrix with all independent $N(0,1)$ entries. Then the empirical spectral distribution of $\frac{1}{\sqrt{n}}H$ converges to the uniform measure on the unit disc in $\mathbb{C}$.*



Universality

- The limit laws of random matrix theory (semicircle, circular) are **the same for different distributions** of entries X_{ij}, e.g. normal $N(0,1)$, Bernoulli ± 1 etc.
- **Microscopic** laws may be different (and even unknown), but **macroscopic** picture is the same. Importance: one can replace the unknown distribution by normal.

- The same phenomenon as in the Central Limit Theorem:

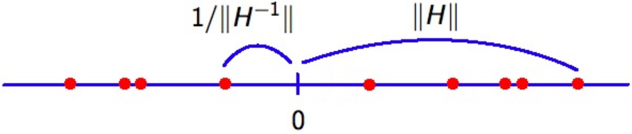
$$X_1 + \cdots + X_n \approx N(0, \sqrt{n}).$$

  The same limit **regardless of the distribution** of X_i.
- For semicircle law, universality was proved by [Pastur'73], see [Bai-Silverstein'10]. For circular law, universality was established by [Girko'84, Edelman'97, Bai'97, Götze-Tikhomirov'07, Pan-Zhou'07, Tao-Vu'07-08].

Local Regime

- The limit laws are **global**; they state something for the **bulk** of the eigenvalues (say, for 10% or 1% of eigenvalues).
- Where are **individual eigenvalues**? Local regime.

  There is extensive recent work, with many questions answered [Tao-Vu'05+, Rudelson-V'07+, V, L. Erdös-Schlein-Yau'08+].
- Why local regime? The eigenvalue **nearest** 0 determines the **invertibility** properties of H. The eigenvalue farthest from 0 determines the operator norm of H:



- If there is an eigenvalue at 0, then H is **singular**. Otherwise H has **full rank**.
- The limit laws do not preclude **one** eigenvalue to stick to 0 almost surely.

Invertibility

Invertibility Problem: *Are random matrices H likely singular or full rank?*

- Answer: likely to have full rank.
- 1. For $n \times n$ matrices with **all independent entries**.

Conjecture [P. Erdös]: *For Bernoulli matrices with ± 1 entries,*

$$\mathbb{P}\{H \text{ is singular}\} = \Big(\frac{1}{2} + o(1)\Big)^n$$

$\approx \mathbb{P}\{$*two rows or two columns of H are equal up to a sign*$\}$.

- Best known result: $\big(\frac{1}{\sqrt{2}} + o(1)\big)^n$ [Bourgain-Wood-Vu'10].
- For **general distributions** of entries, one still has [Rudelson-V'08]:

$$\mathbb{P}\{H \text{ is singular}\} \leq \exp(-cn).$$

Invertibility

- 2. For **symmetric matrices**, the invertibility conjecture is the same. For **Bernoulli** symmetric matrices with ±1 entries,

$$\mathbb{P}\{H \text{ is singular}\} = \Big(\frac{1}{2} + o(1)\Big)^n ?$$

- Best known result [V'11]:

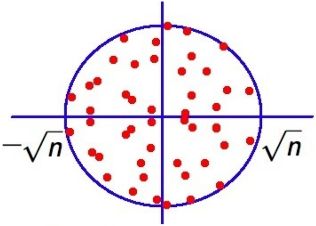
$$\mathbb{P}\{H \text{ is singular}\} \le \exp(-n^c).$$

This also holds for **general** distributions of entries.

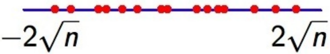
Delocalization

More general phenomenon:

The spectrum of a random matrix H is **delocalized**.



All independent entries

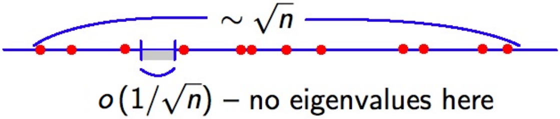


Symmetric

- 1. Eigenvalues of H **do not stick to any particular point.** The probability that the spectrum **hits** a particular point is $\exp(-cn)$ for matrices H with all independent entries [Rudelson-V'08].
- Similarly for symmetric matrices H: $\exp(-n^c)$ [V'11].

Delocalization

- 2. Moreover, the eigenvalues of H **do not stick to small intervals**.
- The specturm of a symmetric random matrix **misses** any fixed interval smaller than the **average eigenvalue gap** (which is $1/\sqrt{n}$). [Erdös-Schlein-Yau, Tao-Vu, V'11].



- In particular, eigenvalues are **separated from** 0 by $1/\sqrt{n}$. So

$$\|H^{-1}\| = O(\sqrt{n}), \qquad \|H\| = O(\sqrt{n}).$$

- Therefore **the condition number is linear** in n:

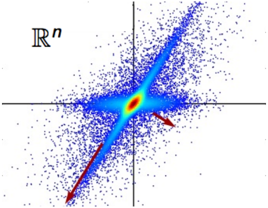
$$\kappa(H) = \|H\|\|H^{-1}\| = O(n).$$

Same if H has all independent entries [Rudelson-V'08].

- Thus: **Random matrices are well conditioned**.
  This addresses a problem of Von Neumann et al. 40's.

Random Matrices in Statistics: Covariance Estimation

- Statistics: Principal Component Analysis (PCA): determine the axes along which **most correlation occurs**. This is the **covariance structure** of the distribution.

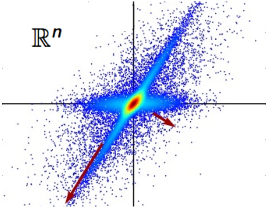


$$H = \begin{bmatrix} — X_1 — \\ — X_2 — \\ \cdots\cdots \\ — X_N — \end{bmatrix}$$

- We sample a few **data points** $X_1, \ldots, X_N \in \mathbb{R}^n$ independently from the distribution. We organize them as an $N \times n$ random matrix H with **independent rows.** Warning: not independent **entries**!
- Compute the $n \times n$ matrix $H^T H$, the Wishart random matrix. Its eigenvectors are the **principal components**.

Problem: *How many sample points $N = N(n)$ are needed to estimate the covariance structure of a distribution in $\mathbb{R}^n$?*

Random Matrices in Statistics: Covariance Estimation



$$H = \begin{bmatrix} - X_1 - \\ - X_2 - \\ \cdots\cdots \\ - X_N - \end{bmatrix}$$

- A different look at the Wishart matrix:

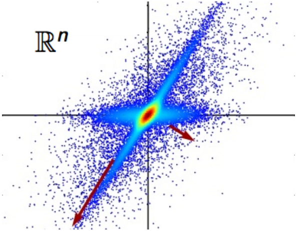
$$\Sigma_N = \frac{1}{N} H^T H = \frac{1}{N} \sum_{i=1}^{N} X_i X_i^T$$

This is the sample covariance matrix, $n \times n$ symmetric random matrix.

- Our hope: Σ_N is a good estimate for the population covariance matrix

$$\Sigma = \mathbb{E}\, X_i X_i^T.$$

Random Matrices in Statistics: Covariance Estimation



Sample and population covariance matrices:

$$\Sigma_N = \frac{1}{N}\sum_{i=1}^{N} X_i X_i^T, \qquad \Sigma = \mathbb{E}\, X_i X_i^T.$$

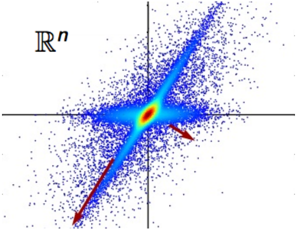
- Key: Σ_N is a **sum of independent random matrices** $X_i X_i^T$.
- Law of Large Numbers in higher dimensions implies:

$$\Sigma_N \to \Sigma \quad \text{as } N \to \infty, \quad n \text{ fixed.}$$

- But we need a **small** sample size N!
- What is the **smallest sample size** $N = N(n)$ so that $\Sigma_N \approx \Sigma$?
- $N \geq n$ is needed (for the full rank).[1]

[1] For structured data, one can have $N \ll n$, see e.g. [Levina-V'10].

Random Matrices in Statistics: Covariance Estimation



Sample and population covariance matrices:

$$\Sigma_N = \frac{1}{N} \sum_{i=1}^{N} X_i X_i^T, \qquad \Sigma = \mathbb{E}\, X_i X_i^T.$$

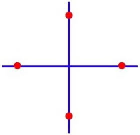
- Use **quantitative form of Law of Large Numbers** – classical deviation inequalities for sums of independent random variables (Khinchine, Bernstein, Chernoff, . . .)
- For matrices, one uses **non-commutative** versions of deviation inequalities. One obtains (for general distributions!) that

$$N = O(n \log n)$$

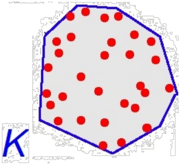
suffices for $\Sigma_N \approx \Sigma$ in the operator norm. [Rudelson'99]

Random Matrices in Statistics: Covariance Estimation

- $N = O(n \log n)$ sample points always suffice.
- In general, $\log n$ oversampling is needed (for very discrete distributions).



Problem [Kannan-Lovasz-Simonovits'97]:
$N = O(n)$ sample points should suffice for covariance estimation of the uniform distribution in an arbitrary **convex set** *K in $\mathbb{R}^n$.*



Important for **volume estimation** of K.

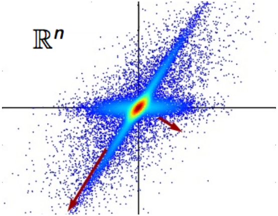
Theorem [Adamczak-Litvak-Pajor-Tomczak'09]: (UofA)
The KLS Conjecture is true.

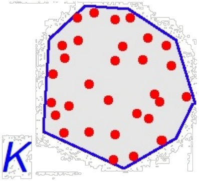
Conjecture [V'10]: $N = O(n)$ suffices for **most** distributions.

Random Matrices in Statistics: Covariance Estimation

Theorem [Srivastava-V'11]: $N = O(n)$ sample points suffice for covariance estimation for all distributions satisfying mild **regularity** assumptions.

In particular, this holds for **convex sets**, yielding an alternative approach to KLS problem.

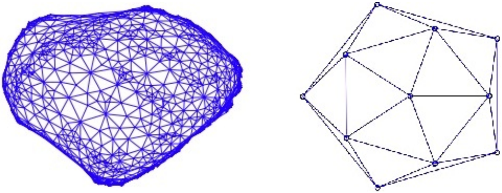




Regularity assumption: $2 + \varepsilon$ moments of k-dimensional marginals outside the ball of radius $O(\sqrt{k})$.

Covariance Estimation and the Spectral Sparsifier

- The new method: randomizing the spectral sparsifier of [Batson-Spielman-Srivastava'08].
- Spectral sparsification is a deterministic method that allows one to approximate a given **dense graph** by a **sparse graph:**



Daniel Spielman FOCS'07 tutorial on spectral graph theory

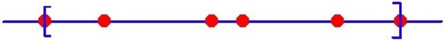
- Randomization makes the spectral sparsifier appear as a natural **method in Random Matrix Theory**.

Covariance Estimation and the Spectral Sparsifier

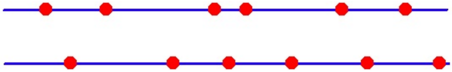
- Goal: Control the whole **spectrum** of the Wishart matrix

$$W = \sum_{i=1}^{N} X_i X_i^T,$$

i.e. the left and right **spectral edges**:



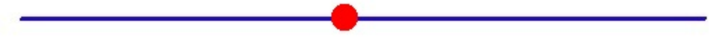
- Method: Add $X_i X_i^T$ **one at a time**, and keep track how the spectrum of W evolves.
- Eigenvalues interlace (**Cauchy interlacing theorem**):



Covariance Estimation and the Spectral Sparsifier

Evolution of the spectrum of the Wishart matrix in $\mathbb{R}^n$:

$$W = \sum_{i=1}^{N} X_i X_i^T \qquad N = 1, 2, \ldots$$



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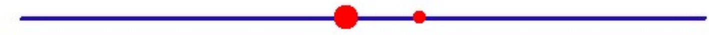

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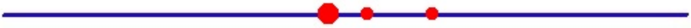

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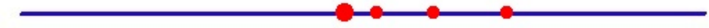

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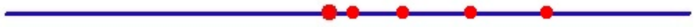

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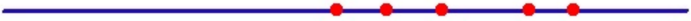

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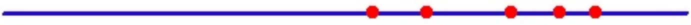

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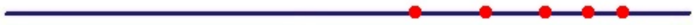

Covariance Estimation and the Spectral Sparsifier

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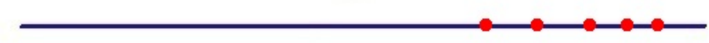

Covariance Estimation and the Spectral Sparsifier

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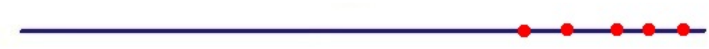

Covariance Estimation and the Spectral Sparsifier

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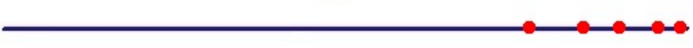
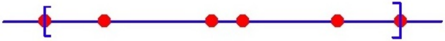


Covariance Estimation and the Spectral Sparsifier



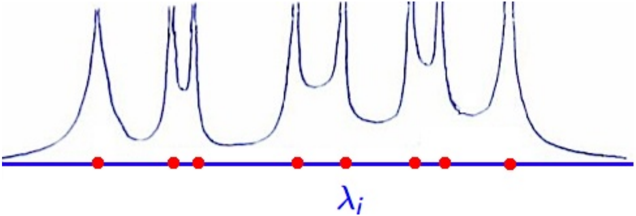
- Difficulty: The **spectral edges** (the extreme eigenvalues) are not controlled by interlacing, they are **free** on one side. They are difficult to compute.
- Solution: **Soften** the spectral edges:

Covariance Estimation via Stieltjes Transform

- **Stieltjes Transform** of the spectrum of W is the function

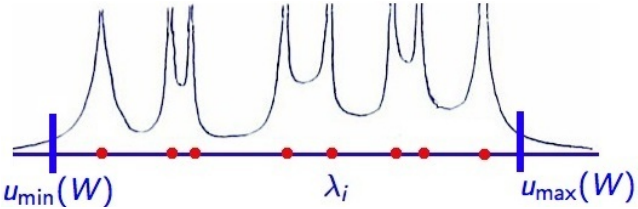
$$m_W(u) = \mathrm{trace}(uI - W)^{-1} = \sum_{i=1}^{N} \frac{1}{u - \lambda_i} \qquad u \in \mathbb{R}.$$

- Ignoring the sign, $m_W(u)$ looks like this:



- Physical interpretation: Put unit **electric charges** at points λ_i. The **electric potential** measured at u equals $m_W(u)$.

Covariance Estimation via Stieltjes Transform

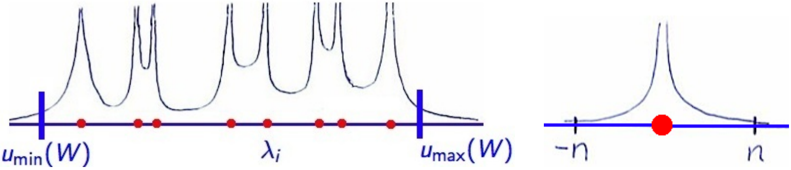


- Find the leftmost/rightmost locations $u_{\min}(W)$, $u_{\max}(W)$ where the electric **potential** is some fixed **constant**:

$$m_W(u) = \phi \qquad \text{(say, } \phi = 1000\text{).}$$

- These locations are **soft** proxies of the **spectral edges**. They "harden" as $\phi \to \infty$.

Covariance Estimation via Stieltjes Transform



- Key: As opposed to the usual spectral edges, the soft edges $u_{\min}(W), u_{\max}(W)$ **are computable**.
- Why? They are determined by the Stieltjes transform of $W = \sum_{i=1}^N X_i X_i^T$, which can be **recomputed** by adding one term at a time. (Sherman-Morrison formula).[2]
- One shows that the proxies **increase by** $1 \pm o(1)$ **at every step**.
- After N steps, they are $\approx N \pm n$. QED.

[2] For $W = V + XX^T$, one has $m_W(u) = m_V(u) + \frac{X^T(uI-V)^{-2}X}{1-X^T(uI-V)^{-1}X}$

References

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- Invertibility of Symmetric Matrices: R. Vershynin, *Invertibility of symmetric random matrices*, 2011.
- Covariance Estimation: N. Srivastava, R. Vershynin, *Covariance estimation for distributions with* $2+\varepsilon$ *moments*, 2011 (TBA).