

Recent Advances in Random Matrix Theory for Modern Machine Learning

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May 2, 2019, Kraków, Poland



Outline

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- 2 Sample covariance matrix for large dimensional data
- 3 RMT for machine learning: kernel spectral clustering
- 4 RMT for machine learning: random neural networks
- 5 From theory to practice

Motivation: the pitfalls of large dimensional statistics

- The big data era: both **large dimensional** and **massive amount** of data, the number of instances n and their dimension p are both large,
 - ▶ large size high resolution images, more involved machine learning systems.
- Counterintuitive phenomenon in the large n, p regime, e.g.,
 - ▶ The “curse of dimensionality” phenomenon: **little** difference between Euclidean distance $\|\mathbf{x}_i - \mathbf{x}_j\|$ from the same or different clusters (classes), $\mathbf{x}_i, \mathbf{x}_j \in \mathbb{R}^p$ for p large.
 - ▶ Classical machine learning algos (e.g., kernel spectral clustering) still **work** for large dimensional data, although we **do not** understand why . . .
- In need of **refinement** to **understand** and **improve** modern machine learning methods for large dimensional problems, made possible with **RMT**.
- From a RMT viewpoint: with **nonlinearity** involved and of **implicit** solution (from an optimization problem)

Sample covariance matrix in the large n, p regime

- For $\mathbf{x}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$, estimate the **covariance matrix** from n data samples $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathbb{R}^{p \times n}$.
- Classical maximum likelihood sample covariance matrix:

$$\hat{\mathbf{C}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top = \frac{1}{n} \mathbf{X} \mathbf{X}^\top \in \mathbb{R}^{p \times p}$$

of rank **at most** n .

- In the regime where $n \sim p$, conventional wisdom breaks down, for $\mathbf{C} = \mathbf{I}_p$ with $n < p$, SCM will **never** be correct:

$$\|\mathbf{C} - \hat{\mathbf{C}}\| \not\rightarrow 0, n, p \rightarrow \infty$$

with at least $p - n$ **zero eigenvalues!**

- Typically what happens in deep learning: try to fit an **enormous** statistical model (60.2 M of ResNet-152) with **insufficient**, but still **numerous** data (14.2 M images of ImageNet dataset).

When is one under random matrix regime?

For $\mathbf{C} = \mathbf{I}_p$, as $n, p \rightarrow \infty$ with $p/n \rightarrow c \in (0, \infty)$: the Marčenko–Pastur law

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

where $a = (1 - \sqrt{c})^2$, $b = (1 + \sqrt{c})^2$ and $(x)^+ \equiv \max(x, 0)$.

- eigenvalues span on $[(1 - \sqrt{c})^2, (1 + \sqrt{c})^2]$.
- for $n = 100p$, spread on a range of $4\sqrt{c} = 0.4$ around the true value 1.

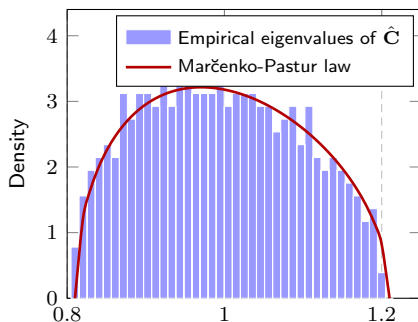
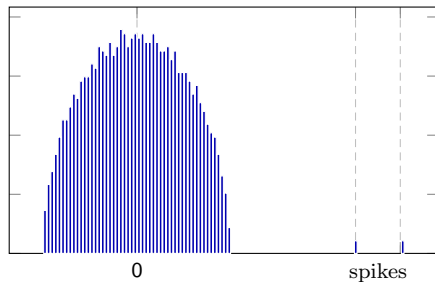


Figure: Eigenvalue distribution of $\hat{\mathbf{C}}$ versus Marčenko–Pastur law, $p = 500$, $n = 50\,000$.

Reminder on kernel spectral clustering

Two-step classification of n data points based on similarity $\mathbf{S} \in \mathbb{R}^{n \times n}$:



↓ **Top eigenvectors** ↓

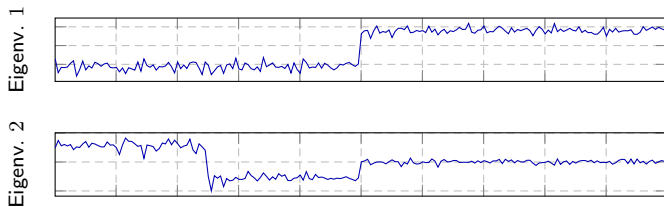
Eigenv. 1



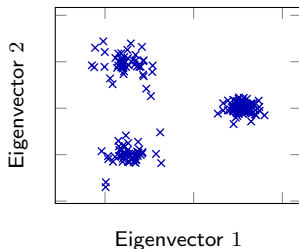
Eigenv. 2



Reminder on kernel spectral clustering



⇓ k -dimensional representation ⇓



EM or k -means clustering.

Loss of relevance of Euclidean distance

- Simplest binary Gaussian mixture classification setting

$$\mathcal{C}_1 : \mathbf{x} = \boldsymbol{\mu} + \mathbf{z}, \quad \mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{I}_p);$$

$$\mathcal{C}_2 : \mathbf{x} = -\boldsymbol{\mu} + (\mathbf{I}_p + \mathbf{E})^{\frac{1}{2}} \mathbf{z}, \quad \mathbf{x} \sim \mathcal{N}(-\boldsymbol{\mu}, \mathbf{I}_p + \mathbf{E}).$$

for $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$.

- Neyman-Pearson test tells us: classification is **non-trivial** only when

$$\|\boldsymbol{\mu}\| \geq O(1), \quad \|\mathbf{E}\| \geq O(p^{-1/2}), \quad |\text{tr } \mathbf{E}| \geq O(\sqrt{p}), \quad \|\mathbf{E}\|_F^2 \geq O(1).$$

- In this **non-trivial** setting, for $\mathbf{x}_i \in \mathcal{C}_a, \mathbf{x}_j \in \mathcal{C}_b$,

$$\frac{1}{p} \|\mathbf{x}_i - \mathbf{x}_j\|^2 = \begin{cases} \frac{1}{p} \|\mathbf{z}_i - \mathbf{z}_j\|^2 + Ap^{-1/2}, & \text{for } a = b = 2; \\ \frac{1}{p} \|\mathbf{z}_i - \mathbf{z}_j\|^2 + Bp^{-1/2}, & \text{for } a = 1, b = 2 \end{cases} \quad (2)$$

- For A, B both of order $O(1)$ and $A > B$ with high probability for p large, so

$$\max_{1 \leq i \neq j \leq n} \left\{ \frac{1}{p} \|\mathbf{x}_i - \mathbf{x}_j\|^2 - 2 \right\} \rightarrow 0 \quad (3)$$

almost surely as $n, p \rightarrow \infty$.

Kernel spectral clustering for large dimensional data

Objective: “cluster” data $\mathbf{x}_1, \dots, \mathbf{x}_n$ into K similarity classes.

Consider the RBF kernel matrix $\mathbf{K}_{ij} = \exp\left(-\frac{1}{2p}\|\mathbf{x}_i - \mathbf{x}_j\|^2\right)$.

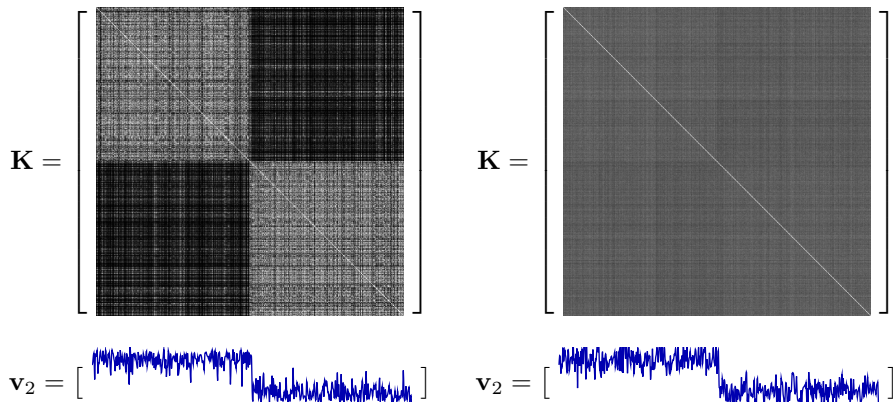


Figure: Kernel matrices \mathbf{K} and the second top eigenvectors \mathbf{v}_2 for small (left, $p=5, n=500$) and large (right, $p=250, n=500$) dimensional data.

But why kernel spectral clustering works?

The **accumulated effect** of the small “hidden” statistical information (in $\boldsymbol{\mu}, \mathbf{E}$).

$$\mathbf{K} = \exp(-1) \left(\mathbf{1}_n \mathbf{1}_n^\top + \frac{1}{p} \mathbf{Z}^\top \mathbf{Z} \right) + g(\boldsymbol{\mu}, \mathbf{E}) \frac{1}{p} \mathbf{j} \mathbf{j}^\top + * + o_{\|\cdot\|}(1) \quad (4)$$

with $\mathbf{Z} = [\mathbf{z}_1, \dots, \mathbf{z}_n] \in \mathbb{R}^{p \times n}$ and $\mathbf{j} = [\mathbf{1}_{n/2}; -\mathbf{1}_{n/2}]$, the class-information vector.

Therefore

- **entry-wise**: for $\mathbf{K}_{ij} = \exp\left(-\frac{1}{2p} \|\mathbf{x}_i - \mathbf{x}_j\|^2\right)$,

$$\mathbf{K}_{ij} = \exp(-1) \left(1 + \underbrace{\frac{1}{p} \mathbf{z}_i^\top \mathbf{z}_j}_{O(p^{-1/2})} \right) \pm \underbrace{\frac{1}{p} g(\boldsymbol{\mu}, \mathbf{E})}_{O(p^{-1})} + *$$

so that $\frac{1}{p} g(\boldsymbol{\mu}, \mathbf{E}) \ll \frac{1}{p} \mathbf{z}_i^\top \mathbf{z}_j$;

- **spectrum-wise**: $\|\frac{1}{p} \mathbf{Z}^\top \mathbf{Z}\| = O(1)$ and $\|g(\boldsymbol{\mu}, \mathbf{E}) \frac{1}{p} \mathbf{j} \mathbf{j}^\top\| = O(1)$ as well!

Neural networks and deep learning

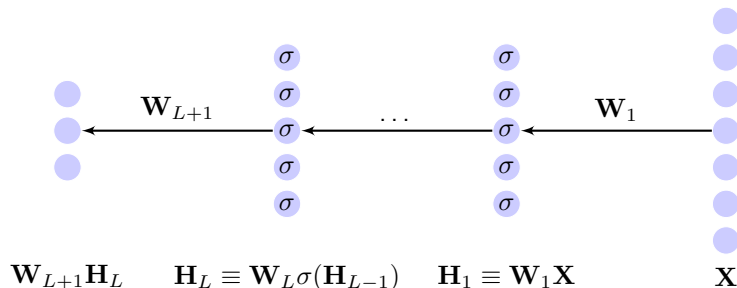
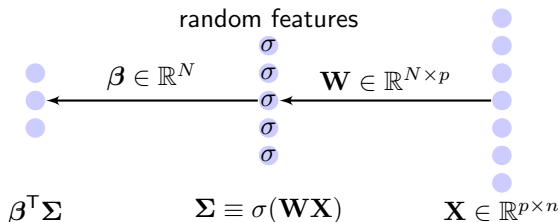


Figure: Illustration of L -hidden-layer nonlinear neural networks

with **nonlinear** activation function $\sigma(z)$: ReLU(z) = $\max(z, 0)$, Leaky ReLU $\max(z, az)$ ($a > 0$) or sigmoid $\sigma(z) = (1 + e^{-z})^{-1}$, arctan, tanh, etc.

Random neural network with single hidden layer



- For random \mathbf{W} and n, p, N large, $\frac{1}{N} \Sigma^T \Sigma$ is closely related to

$$\mathbf{K} \equiv \frac{1}{N} \mathbb{E}_{\mathbf{W}}[\sigma(\mathbf{W}\mathbf{X})^T \sigma(\mathbf{W}\mathbf{X})]$$

- For Gaussian $\mathbf{W}_{ij} \sim \mathcal{N}(0, 1)$, \mathbf{K} is explicit for some $\sigma(\cdot)$ via an integral trick

$$\begin{aligned} \mathbf{K}_{ij} &= \mathbb{E}_{\mathbf{w}}[\sigma(\mathbf{w}^T \mathbf{x}_i) \sigma(\mathbf{w}^T \mathbf{x}_j)] = (2\pi)^{-\frac{p}{2}} \int_{\mathbb{R}^p} \sigma(\mathbf{w}^T \mathbf{x}_i) \sigma(\mathbf{w}^T \mathbf{x}_j) e^{-\frac{\|\mathbf{w}\|^2}{2}} d\mathbf{w} \\ &= \frac{1}{2\pi} \int_{\mathbb{R}^2} \sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}_i) \sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}_j) e^{-\frac{\|\tilde{\mathbf{w}}\|^2}{2}} d\tilde{\mathbf{w}} \end{aligned}$$

with $\tilde{\mathbf{x}}_i = [\|\mathbf{x}_i\|; 0]$ and $\tilde{\mathbf{x}}_j = \left[\frac{\mathbf{x}_i^T \mathbf{x}_j}{\|\mathbf{x}_i\|}; \sqrt{\|\mathbf{x}_j\|^2 - \frac{(\mathbf{x}_i^T \mathbf{x}_j)^2}{\|\mathbf{x}_i\|^2}} \right]$.

Nonlinearity in simple random neural networks

Table: $\mathbf{K}_{i,j}$ for commonly used $\sigma(\cdot)$, $\angle \equiv \frac{\mathbf{x}_i^\top \mathbf{x}_j}{\|\mathbf{x}_i\| \|\mathbf{x}_j\|}$.

$\sigma(t)$	$\mathbf{K}_{i,j}$
t	$\mathbf{x}_i^\top \mathbf{x}_j$
$\max(t, 0)$	$\frac{1}{2\pi} \ \mathbf{x}_i\ \ \mathbf{x}_j\ (\angle \arccos(-\angle) + \sqrt{1 - \angle^2})$
$ t $	$\frac{2}{\pi} \ \mathbf{x}_i\ \ \mathbf{x}_j\ (\angle \arcsin(\angle) + \sqrt{1 - \angle^2})$
$\varsigma_+ \max(t, 0) + \varsigma_- \max(-t, 0)$	$\frac{1}{2} (\varsigma_+^2 + \varsigma_-^2) \mathbf{x}_i^\top \mathbf{x}_j + \frac{\ \mathbf{x}_i\ \ \mathbf{x}_j\ }{2\pi} (\varsigma_+ + \varsigma_-)^2 (\sqrt{1 - \angle^2} - \angle \cdot \arccos(\angle))$
$1_{t>0}$	$\frac{1}{2} - \frac{1}{2\pi} \arccos(\angle)$
$\text{sign}(t)$	$\frac{2}{\pi} \arcsin(\angle)$
$\varsigma_2 t^2 + \varsigma_1 t + \varsigma_0$	$\varsigma_2^2 (2 (\mathbf{x}_i^\top \mathbf{x}_j)^2 + \ \mathbf{x}_i\ ^2 \ \mathbf{x}_j\ ^2) + \varsigma_1^2 \mathbf{x}_i^\top \mathbf{x}_j + \varsigma_2 \varsigma_0 (\ \mathbf{x}_i\ ^2 + \ \mathbf{x}_j\ ^2) + \varsigma_0^2$
$\cos(t)$	$\exp(-\frac{1}{2} (\ \mathbf{x}_i\ ^2 + \ \mathbf{x}_j\ ^2)) \cosh(\mathbf{x}_i^\top \mathbf{x}_j)$
$\sin(t)$	$\exp(-\frac{1}{2} (\ \mathbf{x}_i\ ^2 + \ \mathbf{x}_j\ ^2)) \sinh(\mathbf{x}_i^\top \mathbf{x}_j)$
$\text{erf}(t)$	$\frac{2}{\pi} \arcsin\left(\frac{2\mathbf{x}_i^\top \mathbf{x}_j}{\sqrt{(1+2\ \mathbf{x}_i\ ^2)(1+2\ \mathbf{x}_j\ ^2)}}\right)$
$\exp(-\frac{t^2}{2})$	$\frac{1}{\sqrt{(1+\ \mathbf{x}_i\ ^2)(1+\ \mathbf{x}_j\ ^2) - (\mathbf{x}_i^\top \mathbf{x}_j)^2}}$

\Rightarrow (still) highly **nonlinear** functions of the data \mathbf{x} !

Dig Deeper into \mathbf{K}

Data: K -class Gaussian mixture model

$$\mathbf{x}_i \in \mathcal{C}_a \Leftrightarrow \mathbf{x}_i = \boldsymbol{\mu}_a / \sqrt{p} + \mathbf{z}_i$$

with $\mathbf{z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C}_a/p)$, $a = 1, \dots, K$ of statistical **mean** $\boldsymbol{\mu}_a$ and **covariance** \mathbf{C}_a .

Non-trivial classification (again)

For p large, $\|\boldsymbol{\mu}_a - \boldsymbol{\mu}_b\| = O(1)$, $\|\mathbf{C}_a\| = O(1)$ and $\text{tr}(\mathbf{C}_a - \mathbf{C}_b) = O(\sqrt{p})$.

As a consequence,

$$\begin{aligned} \|\mathbf{x}_i\|^2 &= \underbrace{\|\mathbf{z}_i\|^2}_{O(1)} + \underbrace{\|\boldsymbol{\mu}_a\|^2/p + 2\boldsymbol{\mu}_a^\top \mathbf{z}_i / \sqrt{p}}_{O(p^{-1})} \\ &= \underbrace{\text{tr} \mathbf{C}_a/p}_{O(1)} + \underbrace{\|\mathbf{z}_i\|^2 - \text{tr} \mathbf{C}_a/p}_{O(p^{-1/2})} + \underbrace{\|\boldsymbol{\mu}_a\|^2/p + 2\boldsymbol{\mu}_a^\top \mathbf{z}_i / \sqrt{p}}_{O(p^{-1})} \end{aligned}$$

Then for $\mathbf{C}^\circ = \sum_{a=1}^K \frac{n_a}{n} \mathbf{C}_a$ and $\mathbf{C}_a = \mathbf{C}_a^\circ + \mathbf{C}^\circ$ for $a = 1, \dots, K$,

$$\Rightarrow \|\mathbf{x}_i\|^2 = \tau + O(p^{-1/2}) \text{ with } \tau \equiv \text{tr}(\mathbf{C}^\circ)/p, \quad \|\mathbf{x}_i - \mathbf{x}_j\|^2 \approx 2\tau!$$

Understand nonlinearity in random neural networks

Asymptotic Equivalent of \mathbf{K}

For all $\sigma(\cdot)$ listed in the table above, we have, as $n \sim p \rightarrow \infty$,

$$\|\mathbf{K} - \tilde{\mathbf{K}}\| \rightarrow 0$$

almost surely, with

$$\tilde{\mathbf{K}} \equiv d_1 \left(\mathbf{Z} + \mathbf{M} \frac{\mathbf{J}^\top}{\sqrt{p}} \right)^\top \left(\mathbf{Z} + \mathbf{M} \frac{\mathbf{J}^\top}{\sqrt{p}} \right) + d_2 \mathbf{U} \mathbf{B} \mathbf{U}^\top + d_0 \mathbf{I}_n$$

and

$$\mathbf{U} \equiv \left[\frac{\mathbf{J}}{\sqrt{p}}, \phi \right], \quad \mathbf{B} \equiv \begin{bmatrix} \mathbf{t} \mathbf{t}^\top + 2\mathbf{S} & \mathbf{t} \\ \mathbf{t}^\top & 1 \end{bmatrix}.$$

$\mathbf{J} \equiv [\mathbf{j}_1, \dots, \mathbf{j}_K]$, \mathbf{j}_a canonical vector of \mathcal{C}_a , weighted by \mathbf{z} , ϕ random fluctuations of data and $\mathbf{M} \equiv [\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K]$, $\mathbf{t} \equiv \{ \text{tr} \mathbf{C}_a^\circ / \sqrt{p} \}_{a=1}^K$, $\mathbf{S} \equiv \{ \text{tr}(\mathbf{C}_a \mathbf{C}_b) / p \}_{a,b=1}^K$ the statistical information.

Table: Coefficients d_i in $\tilde{\mathbf{K}}$ for different $\sigma(\cdot)$.

$\sigma(t)$	d_1	d_2
t	1	0
$\max(t, 0)$	$\frac{1}{4}$	$\frac{1}{8\pi\tau}$
$ t $	0	$\frac{1}{2\pi\tau}$
$1_{t>0}$	$\frac{1}{2\pi\tau}$	0
$\text{sign}(t)$	$\frac{2}{\pi\tau}$	0
$s_2 t^2 + s_1 t + s_0$	s_1^2	s_2^2
$\cos(t)$	0	$\frac{e^{-\tau}}{4}$
$\sin(t)$	$e^{-\tau}$	0
$\text{erf}(t)$	$\frac{4}{\pi} \frac{1}{2\tau+1}$	0
$\exp(-\frac{t^2}{2})$	0	$\frac{1}{4(\tau+1)^3}$

Consequence

Table: Coefficients d_i in $\tilde{\mathbf{K}}$ for different $\sigma(\cdot)$.

$\sigma(t)$	d_1	d_2
t	1	0
$\max(t, 0)$	$\frac{1}{4}$	$\frac{1}{8\pi\tau}$
$ t $	0	$\frac{1}{2\pi\tau}$
$1_{t>0}$	$\frac{1}{2\pi\tau}$	0
$\text{sign}(t)$	$\frac{2}{\pi\tau}$	0
$\varsigma_2 t^2 + \varsigma_1 t + \varsigma_0$	ς_1^2	ς_2^2
$\cos(t)$	0	$\frac{e^{-\tau}}{4}$
$\sin(t)$	$e^{-\tau}$	0
$\text{erf}(t)$	$\frac{4}{\pi} \frac{1}{2\tau+1}$	0
$\exp(-\frac{t^2}{2})$	0	$\frac{1}{4(\tau+1)^3}$

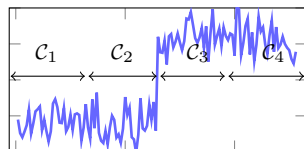
A natural classification of $\sigma(\cdot)$:

- *mean-oriented*, $d_1 \neq 0, d_2 = 0$:
 $t, 1_{t>0}, \text{sign}(t), \sin(t)$ and $\text{erf}(t)$
 \Rightarrow separate with difference in \mathbf{M} ;
- *cov-oriented*, $d_1 = 0, d_2 \neq 0$:
 $|t|, \cos(t)$ and $\exp(-t^2/2)$
 \Rightarrow track differences in cov \mathbf{t}, \mathbf{S} ;
- *"balanced"*, both $d_1, d_2 \neq 0$:
 - ▶ ReLU function $\max(t, 0)$,
 - ▶ quadratic function $\varsigma_2 t^2 + \varsigma_1 t + \varsigma_0$. \Rightarrow make use of **both** statistics!

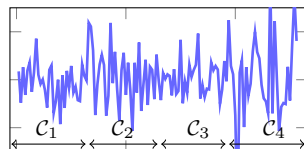
Numerical Validations: Gaussian Data

Example: Gaussian mixture data of four classes: $\mathcal{N}(\mu_1, \mathbf{C}_1)$, $\mathcal{N}(\mu_1, \mathbf{C}_2)$, $\mathcal{N}(\mu_2, \mathbf{C}_1)$ and $\mathcal{N}(\mu_2, \mathbf{C}_2)$ with different $\sigma(\cdot)$ functions.

Case 1: linear map $\sigma(t) = t$.

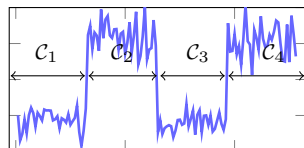


Eigenvector 1

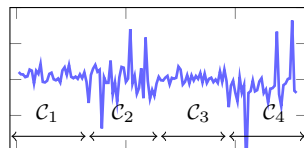


Eigenvector 2

Case 2: $\sigma(t) = |t|$.



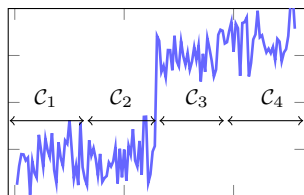
Eigenvector 1



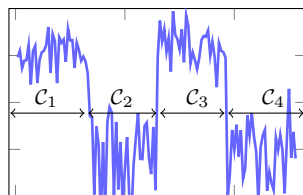
Eigenvector 2

Numerical Validations: Gaussian Data

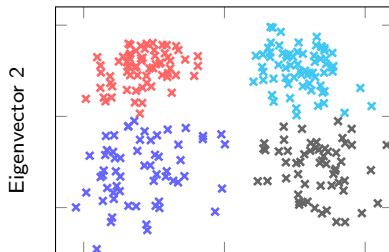
Case 3: the ReLU function $\sigma(t) = \max(t, 0)$.



Eigenvector 1



Eigenvector 2



Eigenvector 1

Numerical Validations: Real Datasets

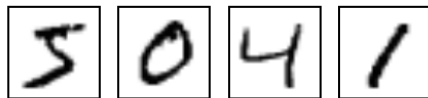


Figure: The MNIST image database.

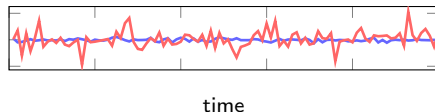


Figure: The epileptic EEG datasets.¹

Codes available at <https://github.com/Zhenyu-LIAO/RMT4RFM>.

¹<http://www.meb.unibonn.de/epileptologie/science/physik/eegdata.html>.

Numerical Validations: Real Datasets

Table: Empirical estimation of statistical information of the MNIST and EEG datasets.

	$\ \mathbf{M}^T\mathbf{M}\ $	$\ \mathbf{t}\mathbf{t}^T + 2\mathbf{S}\ $
MNIST data	172.4	86.0
EEG data	1.2	182.7

Table: Clustering accuracies on MNIST.

Table: Clustering accuracies on EEG.

	$\sigma(t)$	$n = 64$	$n = 128$		$\sigma(t)$	$n = 64$	$n = 128$
mean-oriented	t	88.94%	87.30%	mean-oriented	t	70.31%	69.58%
	$1_{t>0}$	82.94%	85.56%		$1_{t>0}$	65.87%	63.47%
	$\text{sign}(t)$	83.34%	85.22%		$\text{sign}(t)$	64.63%	63.03%
	$\sin(t)$	87.81%	87.50%		$\sin(t)$	70.34%	68.22%
cov-oriented	$ t $	60.41%	57.81%	cov-oriented	$ t $	99.69%	99.50%
	$\cos(t)$	59.56%	57.72%		$\cos(t)$	99.38%	99.36%
	$\exp(-t^2/2)$	60.44%	58.67%		$\exp(-t^2/2)$	99.81%	99.77%
balanced	$\text{ReLU}(t)$	85.72%	82.27%	balanced	$\text{ReLU}(t)$	87.91%	90.97%

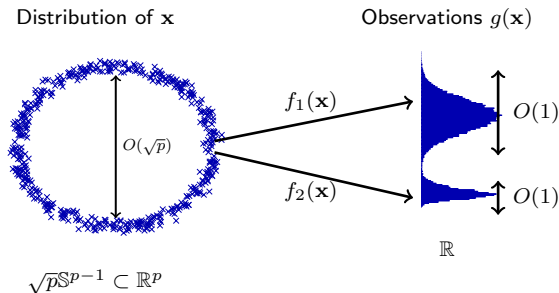
From theory to practice: concentrated random vectors

RMT often assumes \mathbf{x}_i are affine maps $\mathbf{A}\mathbf{z}_i + \mathbf{b}$ of $\mathbf{z}_i \in \mathbb{R}^p$ with i.i.d. entries.

Concentrated random vectors

For a certain family of functions $f : \mathbb{R}^p \mapsto \mathbb{R}$, there exists deterministic $m_f \in \mathbb{R}$

$$P(|f(\mathbf{x}) - m_f| > \epsilon) \leq e^{-g(\epsilon)}, \quad \text{for some strictly increasing function } g. \quad (5)$$



The theory **remains valid** for concentrated random vectors! But ... so what?

From concentrated random vectors to GANs

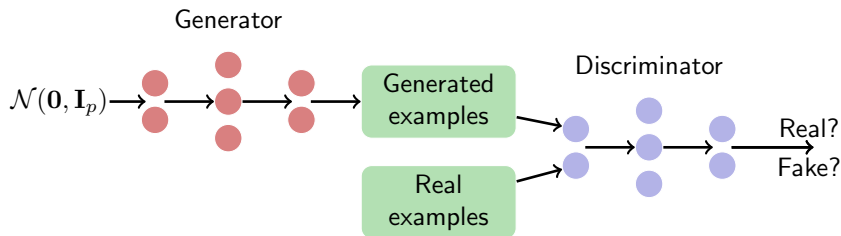


Figure: Illustration of a generative adversarial network (GAN).



Figure: Images samples generated by BigGAN (Brock *et al.*, 2018).

Take-away message and perspectives

Take-away messages:

- loss of relevance of Euclidean distance for large dimensional data
- Taylor expansion helps understand kernel spectral clustering and simple random neural nets behavior
- go beyond Gaussian or i.i.d. random vectors with concentrated random vector

Even more question:







- what can we do if Taylor expansion is not possible?
- universality? influence of higher order moments?
- more involved systems, e.g., deep neural nets?

And much more to be done!

- neural nets: loss landscape, gradient descent dynamics
- problems from convex optimization (often of *implicit solution*)
- more difficult: *non-convex* optimization problems
- transfer learning, active learning, generative networks (GANs)
- robust statistics in machine learning
- ...







Summary of Results and Perspectives

Kernel Methods: References

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Summary of Results and Perspectives

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Thank you!

Thank you!

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