Random Matrix Theory for Big-Data and Machine Learning

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CEA List & Centralesupélec

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Outline

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- We are given data

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- **How does it behave?**

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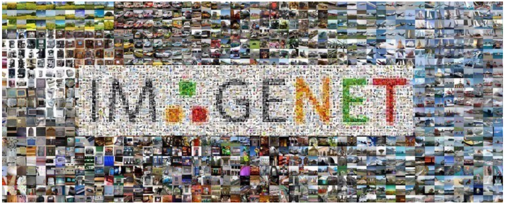

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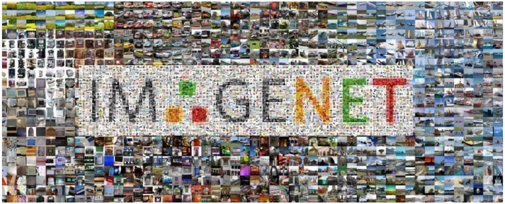

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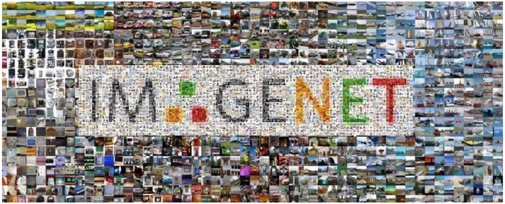

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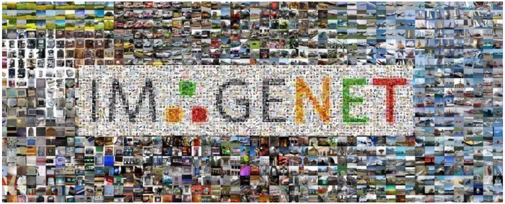

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- Which is the **Random Matrix Theory Regime**

$$\boxed{p, n \to \infty, \text{ with } p/n \to c \in (0, \infty)}$$

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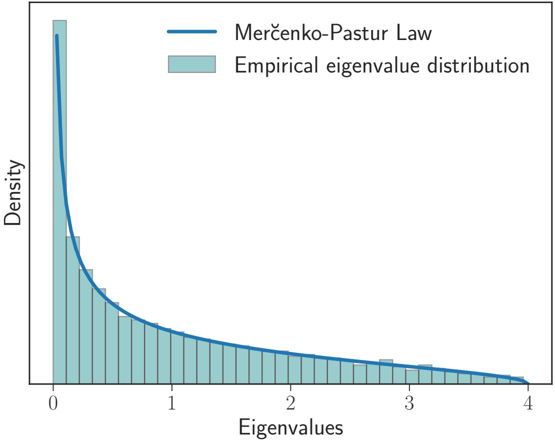

Figure 1: Histogram of the eigenvalues of $\frac{1}{p}\mathbf{X}^\intercal\mathbf{X}$ for $n = p = 1000$.

The Marčenko–Pastur law [Marčenko,Pastur'67]

Definition (Empirical Spectral Density)

Empirical Spectral Density (e.s.d.) μ_n of Hermitian matrix $\mathbf{A}_n \in \mathbb{R}^{n \times n}$ is $\mu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{\lambda_i(\mathbf{A}_n)}$.

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Theorem (Marčenko–Pastur law)

$\mathbf{X} \in \mathbb{R}^{p\times n}$ *with i.i.d. zero mean, unit variance entries.*
As $p, n \to \infty$ *with* $n/p \to c \in (0,\infty)$, *e.s.d.* μ_n *of* $\frac{1}{p}\mathbf{X}^\mathsf{T}\mathbf{X}$ *satisfies*

$$\mu_n \xrightarrow{a.s.} \mu_c$$

weakly, where μ_c *has continuous density* f_c *with compact support* $[\lambda^-, \lambda^+] = [(1-\sqrt{c})^2, (1+\sqrt{c})^2]$

$$f_c(x) = \frac{1}{2\pi c x}\sqrt{(x-\lambda^-)(\lambda^+ - x)}$$

The Marčenko–Pastur law

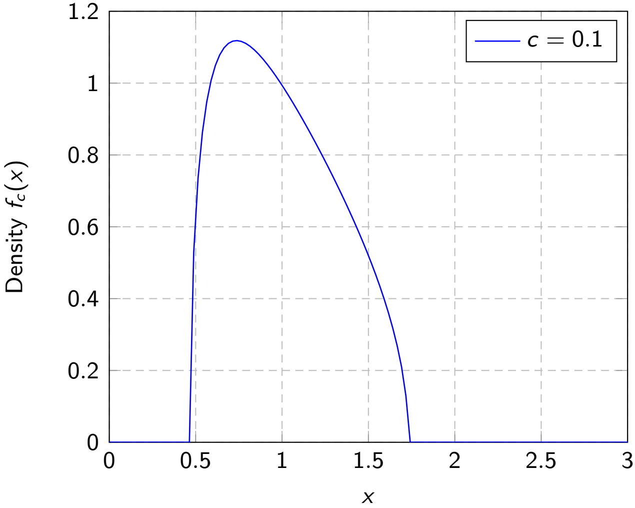

Figure 2: Marčenko-Pastur law for different limit ratios $c = \lim_{p\to\infty} p/n$.

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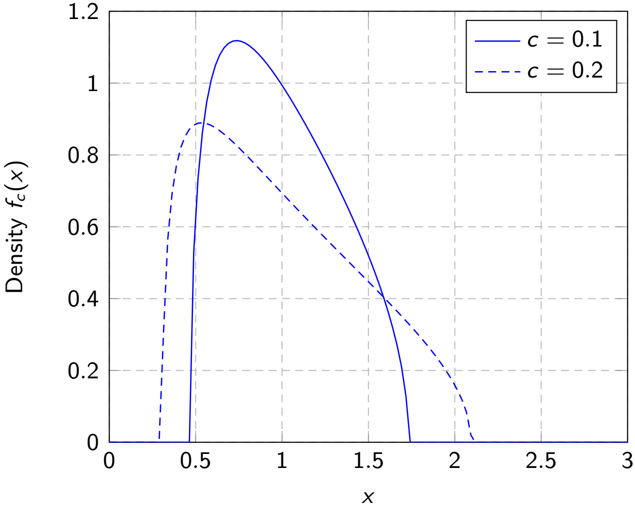

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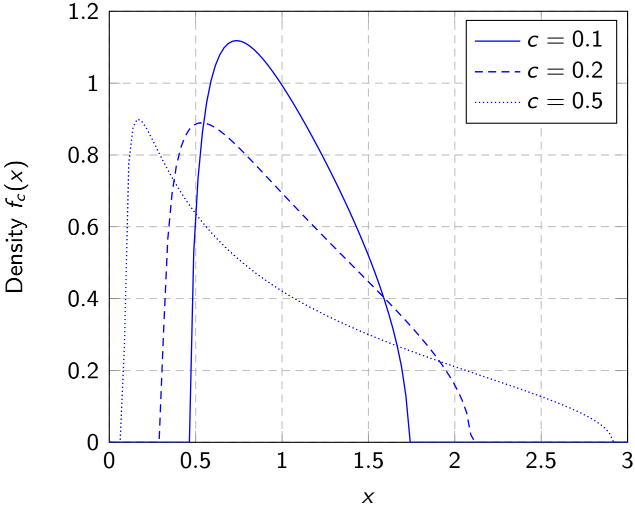

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Gaussian Mixtures (Spiked Model)

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- Which can be written as

$$\mathbf{X} = \mathbf{m}\,\mathbf{y}^\mathsf{T} + \mathbf{Z}$$

where $\mathbf{y} \in \{+1, -1\}^n$ is the vector of labels and $\mathbf{Z}$ has $\mathcal{N}(0, 1)$ entries.

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- We have then

$$\frac{1}{p}\mathbf{X}^\intercal\mathbf{X} = \underbrace{\|\mathbf{m}\|^2\,\bar{\mathbf{y}}\bar{\mathbf{y}}^\intercal}_{\text{(Low-rank) Information}} + \underbrace{\frac{1}{p}\mathbf{Z}^\intercal\mathbf{Z} + *}_{\text{Noise}} \quad \text{where } \bar{\mathbf{y}} = \mathbf{y}/\sqrt{p}$$

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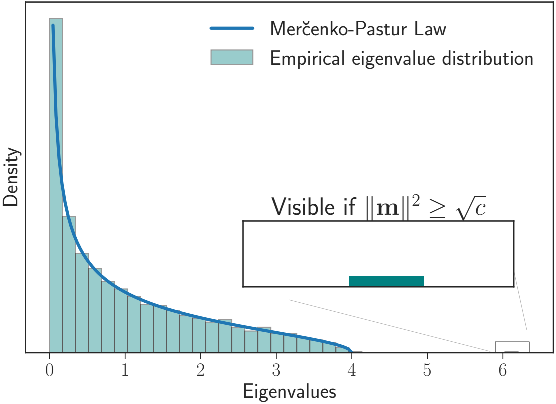

Figure 3: Histogram of the eigenvalues of $\frac{1}{p}\mathbf{X}^\intercal\mathbf{X}$ for $n = p = 1000$.

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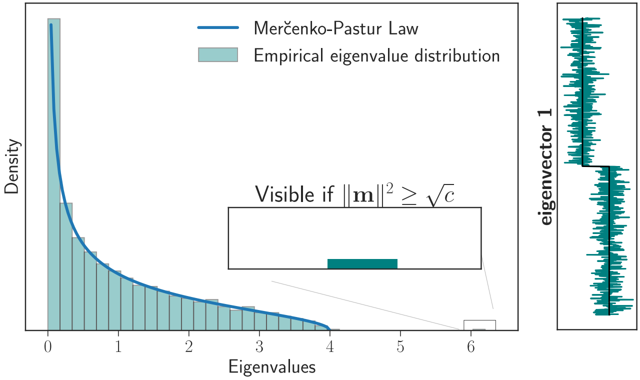

Figure 4: Histogram of the eigenvalues of $\frac{1}{p}\mathbf{X}^\intercal\mathbf{X}$ and its dominant eigenvector for $n = p = 1000$.

Spiked Models

Theorem (Eigenvalues [Baik, Silverstein'06])

Let

- $\mathbf{Z}$ *with i.i.d. zero mean, unit variance,* $\mathbb{E}|Z_{ij}|^4 < \infty$
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Then, under the RMT regime, if $\|\mathbf{m}\|^2 > \sqrt{c}$

$$\lambda_\ell \left(\frac{1}{p} \mathbf{X}^\mathsf{T} \mathbf{X} \right) \xrightarrow{a.s.} 1 + \|\mathbf{m}\|^2 + c \frac{1 + \|\mathbf{m}\|^2}{\|\mathbf{m}\|^2} > (1 + \sqrt{c})^2$$

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Then, under the RMT regime, for $\mathbf{a}, \mathbf{b} \in \mathbb{R}^p$ *deterministic and* $\hat{\mathbf{u}}$ *eigenvector corresponding to* $\lambda_{\max}\left(\frac{1}{p}\mathbf{X}^\mathsf{T}\mathbf{X}\right)$,

$$\mathbf{a}^\mathsf{T}\hat{\mathbf{u}}\hat{\mathbf{u}}^\mathsf{T}\mathbf{b} - \frac{1 - c\|\mathbf{m}\|^{-4}}{1 + c\|\mathbf{m}\|^{-2}}\mathbf{a}^\mathsf{T}\hat{\mathbf{u}}\hat{\mathbf{u}}^\mathsf{T}\mathbf{b} \cdot 1_{\|\mathbf{m}\|^2 > \sqrt{c}} \xrightarrow{a.s.} 0$$

In particular,

$$|\hat{\mathbf{u}}^\mathsf{T}\mathbf{u}|^2 \xrightarrow{a.s.} \frac{1 - c\|\mathbf{m}\|^{-4}}{1 + c\|\mathbf{m}\|^{-2}} \cdot 1_{\|\mathbf{m}\|^2 > \sqrt{c}}.$$

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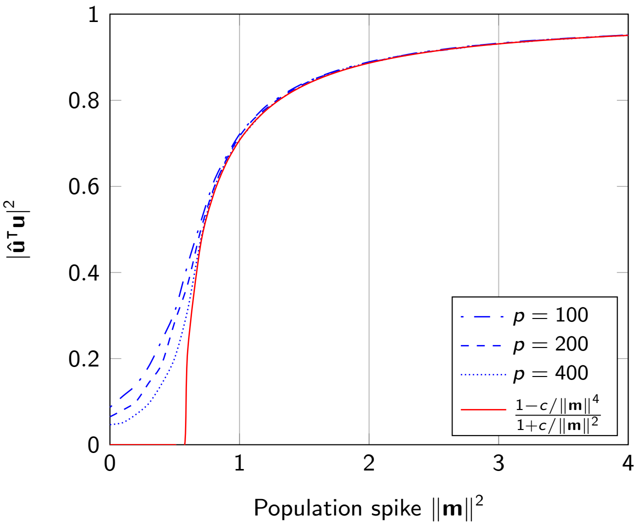

Figure 5: Simulated versus limiting $|\hat{\mathbf{u}}^\mathsf{T}\mathbf{u}|^2$, $p/n = 1/3$, varying $\|\mathbf{m}\|^2$.

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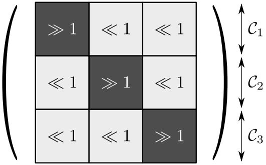

- $\mathbf{K}$ mainly low rank with class information in eigenvectors.

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3. **Covariance:** $\|\bar{\mathbf{C}}_\ell\| = \mathcal{O}(1)$, $\operatorname{tr}\bar{\mathbf{C}}_\ell = \mathcal{O}(\sqrt{p})$, $\operatorname{tr}\bar{\mathbf{C}}_a\bar{\mathbf{C}}_b = \mathcal{O}(p)$

Small Dimension vs High Dimension!

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Random Matrix Equivalent [Couillet, Benaych'15]

- **Key Observation:** *The between and within class vectors are "equidistant" in high-dimension.*

$$\boxed{\max_{1\leq i\neq j\leq n}\left\{\left|\frac{1}{p}\|\mathbf{x}_i-\mathbf{x}_j\|^2-\tau\right|\right\}\xrightarrow{a.s.}0}$$

where $\tau=\frac{2}{p}\operatorname{tr}\mathbf{C}$.

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where $\tau=\frac{2}{p}\mathrm{tr}\mathbf{C}$.

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$$\mathbf{K}\propto\underbrace{\mathbf{J}\mathbf{A}\mathbf{J}^\intercal}_{Information}+\underbrace{f'(\tau)\mathbf{Z}^\intercal\mathbf{Z}+*}_{Noise}$$

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Theory (with Gaussian assum.) versus MNIST

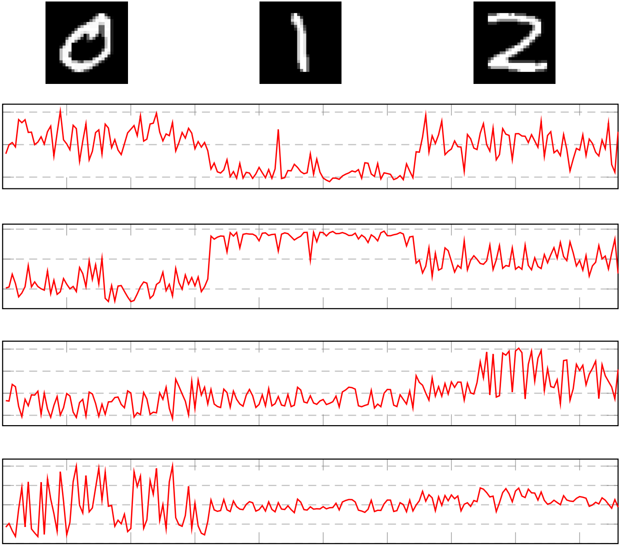

Figure 6: Leading four eigenvectors of $\mathbf{K}$ for MNIST data (**red**) and theoretical findings (**blue**).

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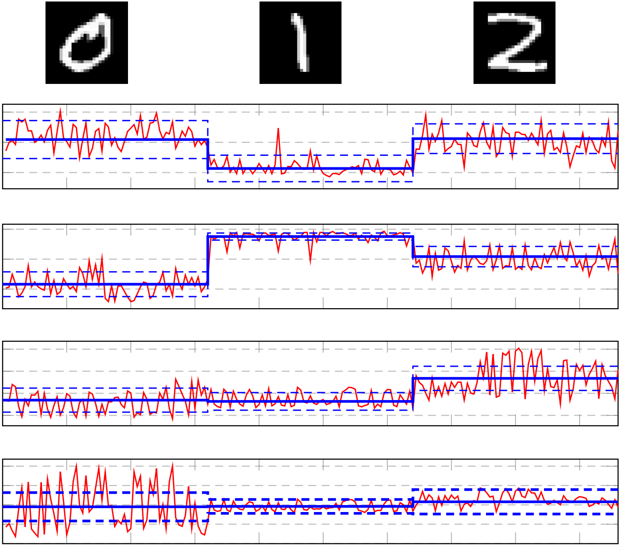

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Outline

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$\Rightarrow$ Consider data as **concentrated** vectors.

Outline

Concentrated Mixture Model

Consider data distributed in k classes as

$$\mathbf{X} = [\underbrace{\mathbf{x}_1, \ldots, \mathbf{x}_{n_1}}_{\in \mathcal{O}(e^{-\cdot^{q_1}})}, \underbrace{\mathbf{x}_{n_1+1}, \ldots, \mathbf{x}_{n_2}}_{\in \mathcal{O}(e^{-\cdot^{q_2}})}, \ldots, \underbrace{\mathbf{x}_{n-n_k+1}, \ldots, \mathbf{x}_n}_{\in \mathcal{O}(e^{-\cdot^{q_k}})}]$$

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Recall

$$\mathbf{m} = \sum_{\ell=1}^{k} \frac{n_\ell}{n} \mathbf{m}_\ell, \; \bar{\mathbf{m}}_\ell = \mathbf{m}_\ell - \mathbf{m}, \;\; \mathbf{C} = \sum_{\ell=1}^{k} \frac{n_\ell}{n} \mathbf{C}_\ell, \; \bar{\mathbf{C}}_\ell = \mathbf{C}_\ell - \mathbf{C}$$

Assumption (Growth rate)

As $n \to \infty$,

1. **Data:** $\frac{p}{n} \to c_0 \in (0, \infty)$, $\frac{n_\ell}{n} \to c_\ell \in (0, 1)$
2. **Mean:** $\|\bar{\mathbf{m}}_\ell\| = \mathcal{O}(1)$, $\mathbb{E}\|\mathbf{x}_i\| = \mathcal{O}(\sqrt{p})$
3. **Covariance:** $\|\bar{\mathbf{C}}_\ell\| = \mathcal{O}(1)$, $\operatorname{tr}\bar{\mathbf{C}}_\ell = \mathcal{O}(\sqrt{p})$, $\operatorname{tr}\bar{\mathbf{C}}_a\bar{\mathbf{C}}_b = \mathcal{O}(p)$

MP Law Still Valid for Concentrated Vectors!

Theorem (Spectrum of $\frac{1}{p}\mathbf{Z}^\intercal \mathbf{Z}$ [Louart'18])

Let $z \in \mathbb{C}^+$ and define the resolvent matrix

$$\mathbf{Q}_\delta(z) \equiv \left(\sum_{\ell=1}^{k} c_\ell \frac{\mathbf{C}_\ell}{1+\delta_\ell(z)} - z\mathbf{I}_p \right)^{-1}$$

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Then the e.s.d. $\nu_n = \frac{1}{n}\sum_{i=1}^{n}\delta_{\lambda_i}$ a.s. converges to a probability measure ν defined on a compact support $\mathcal{S}$ and having density

$$f(x) = \lim_{\epsilon\to 0,\, p\to\infty} \frac{1}{p} \mathcal{I}m\, Tr \mathbf{Q}_\delta(x+i\epsilon)$$

Random Matrix Equivalent

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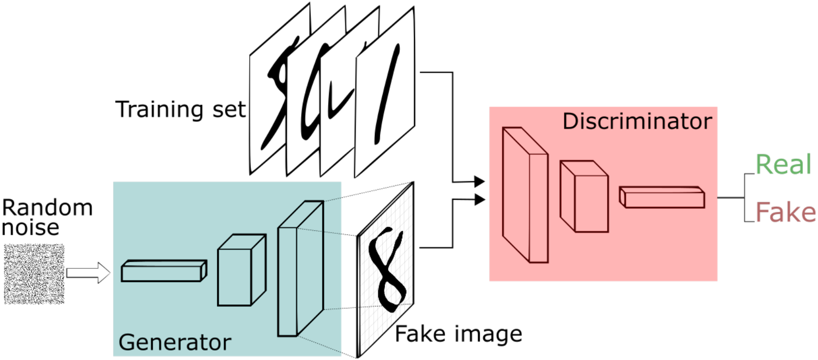
Application to GAN-generated Images



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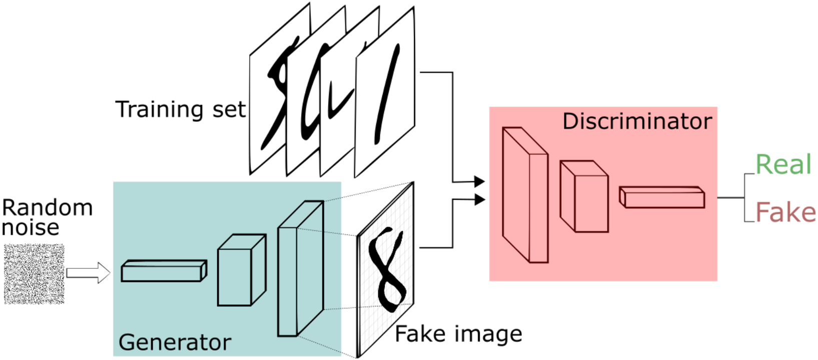

$$\min_{\mathcal{G}} \max_{\mathcal{D}} \mathbb{E}_{x \sim p(x)}[\log \mathcal{D}(x)] + \mathbb{E}_{z \sim p(z)}[\log(1 - \mathcal{D}(\mathcal{G}(z)))]$$

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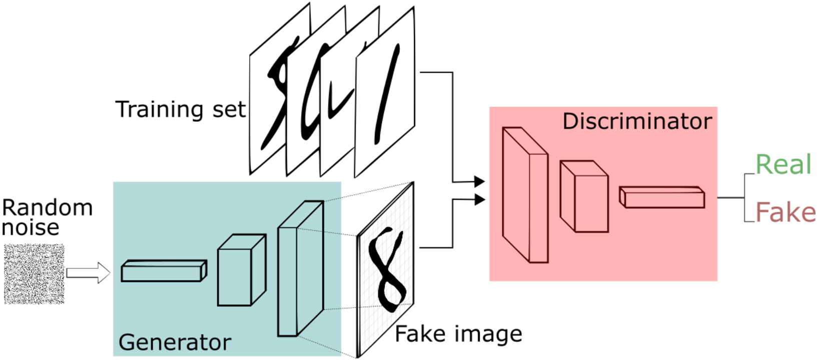

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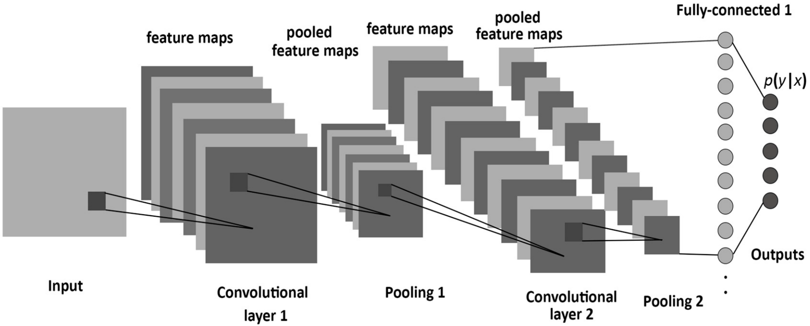
We generate data as

$$\boxed{\text{Generated images} = \mathcal{G}(\text{Gaussian})}$$

Application to GAN-generated Images

Figure 7: Images generated by a GAN model **[Brock et al.'18]**.

CNN Representations



We consider data as (commonly used in Computer Vision)

$$\mathbf{x}_i = \underbrace{\mathcal{R} \circ \mathcal{G}}_{\text{Lipschitz}}(\text{Gaussian})$$

Application to GAN-generated Images

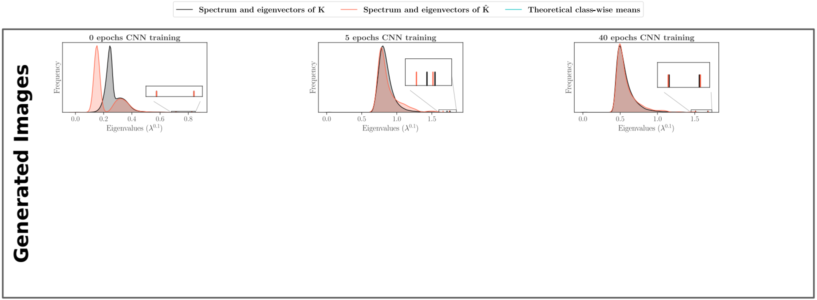


Figure 8: Spectral clustering on GAN-generated images.
$f(t) = \exp(-t)$, $k = 3$, $n = 3000$ and $p = 1024$.

Application to GAN-generated Images

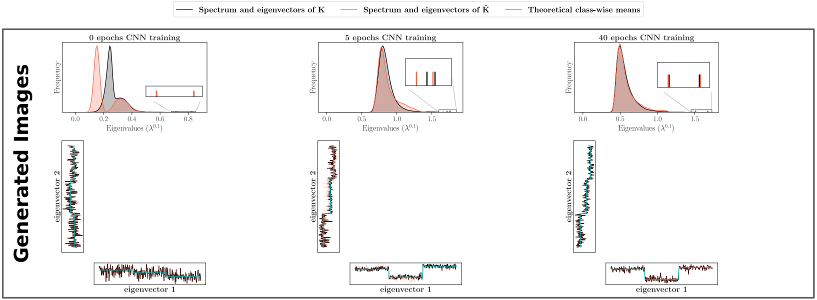


Figure 9: Spectral clustering on GAN-generated images.
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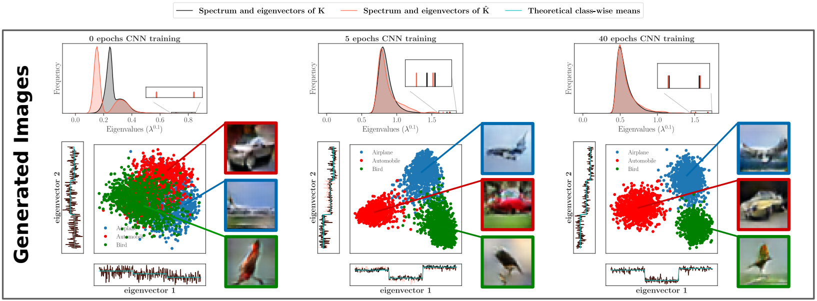

Figure 10: Spectral clustering on GAN-generated images.
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Application to Real Images

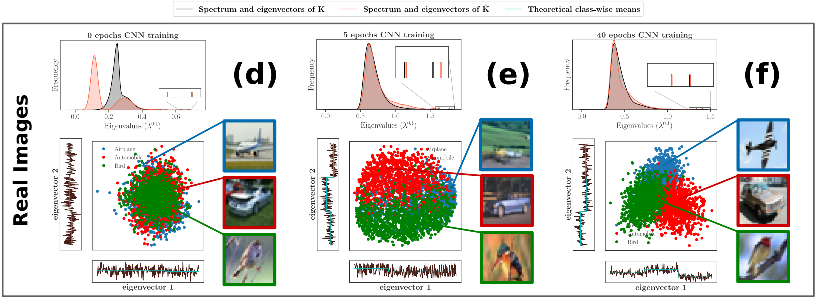

Figure 11: Spectral clustering on real images. $f(t) = \exp(-t)$, $k = 3$, $n = 3000$ and $p = 1024$.

Summary & Perspectives

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- Real data behave similar to concentrated vectors.

$\Rightarrow$ RMT is relevant for ML!

- Generalize to other ML tasks (Classification, Regression etc.).
- Use the concentration framework to understand the dynamics of neural networks and GANs.

Thanks for your attention!