Random Matrix Advances in Machine Learning

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September 27, 2019

Outline

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Context

Baseline scenario: $y_1, \ldots, y_n \in \mathbb{C}^p$ (or $\mathbb{R}^p$) i.i.d. with $E[y_1] = 0$, $E[y_1 y_1^*] = C_p$:

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- **Even for** $p = n/100$.

The Marčenko–Pastur law

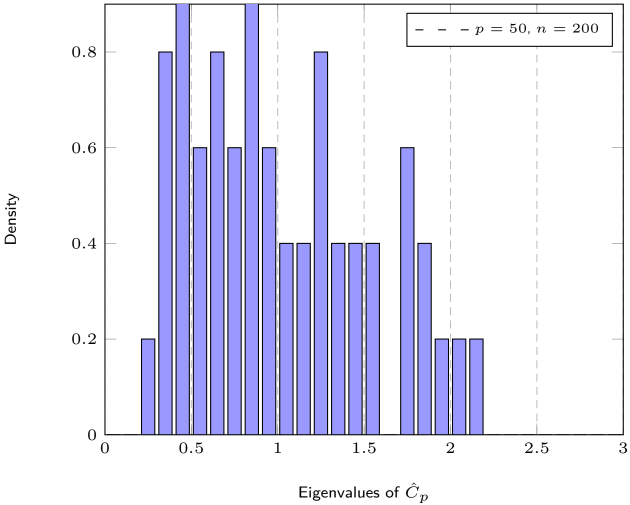

Figure: Histogram of the eigenvalues of $\hat{C}_p$ for $c = 1/4$, $C_p = I_p$.

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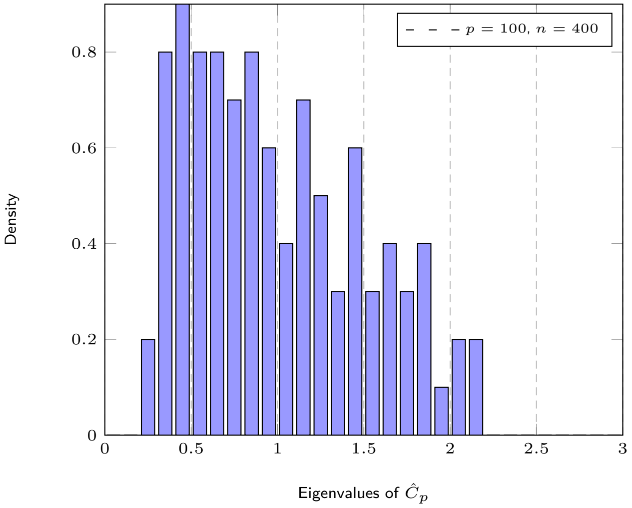

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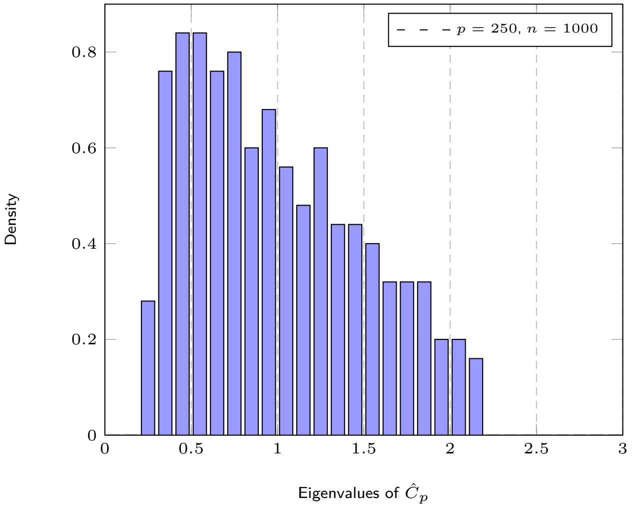

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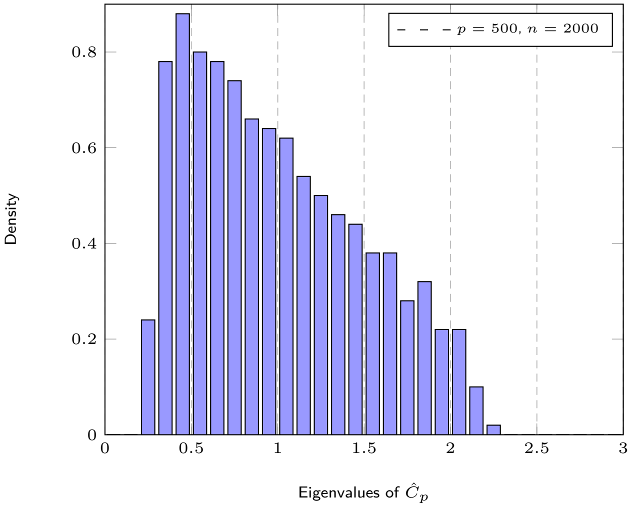

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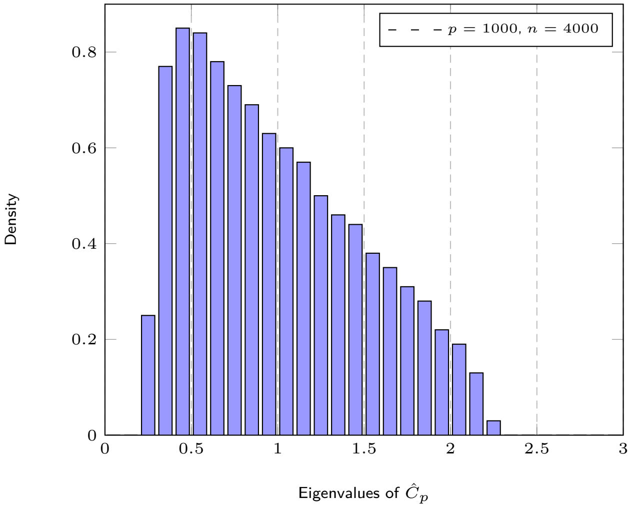

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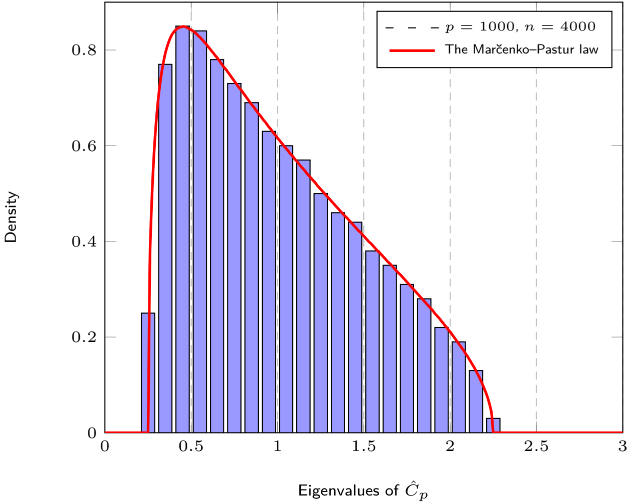

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Empirical spectral density (e.s.d.) μ_p of Hermitian matrix $A_p \in \mathbb{C}^{p \times p}$ is

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$X_p \in \mathbb{C}^{p\times n}$ with i.i.d. zero mean, unit variance entries.
As $p,n\to\infty$ with $p/n \to c \in (0,\infty)$, e.s.d. μ_p of $\frac{1}{n}X_pX_p^*$ satisfies

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weakly, where

- $\mu_c(\{0\}) = \max\{0, 1-c^{-1}\}$
- *on $(0,\infty)$, μ_c has continuous density f_c supported on $[(1-\sqrt{c})^2, (1+\sqrt{c})^2]$*

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

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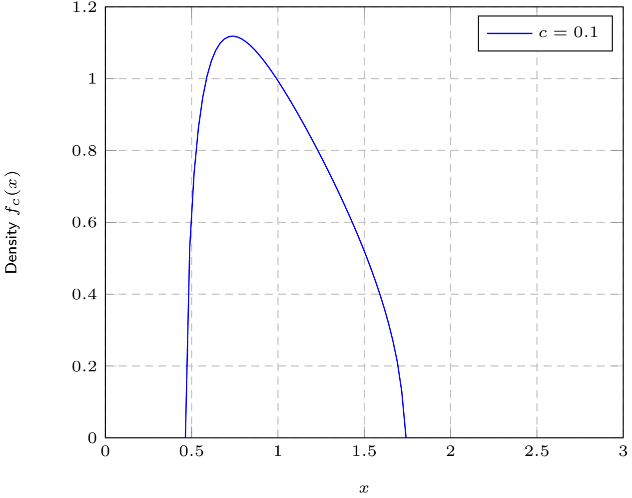
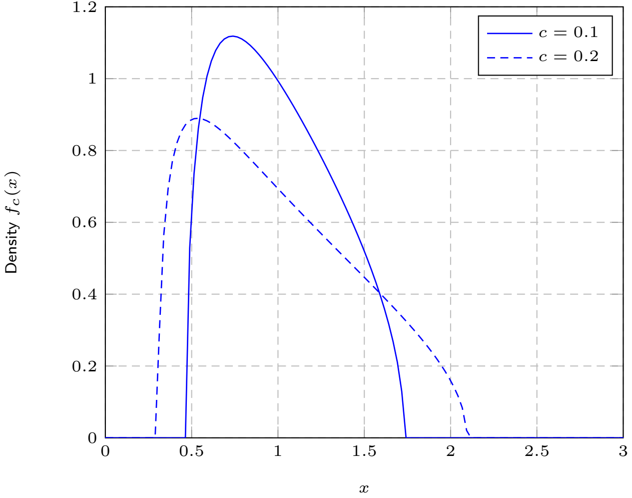


Figure: Marčenko-Pastur law for different limit ratios $c = \lim_{p \to \infty} p/n$.



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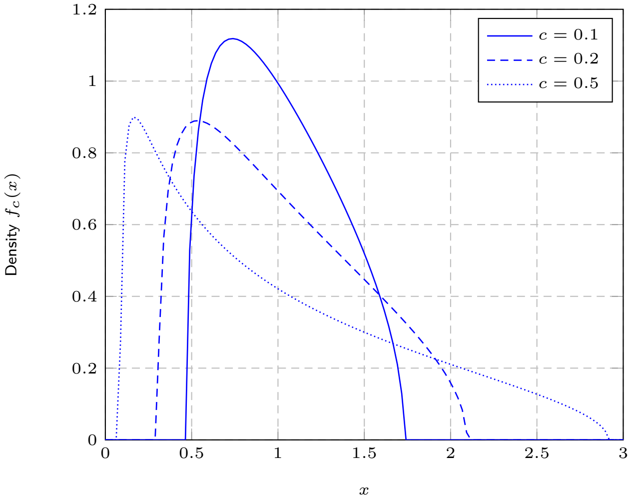

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Small rank perturbation: $C_p = I_p + P$, P of low rank.

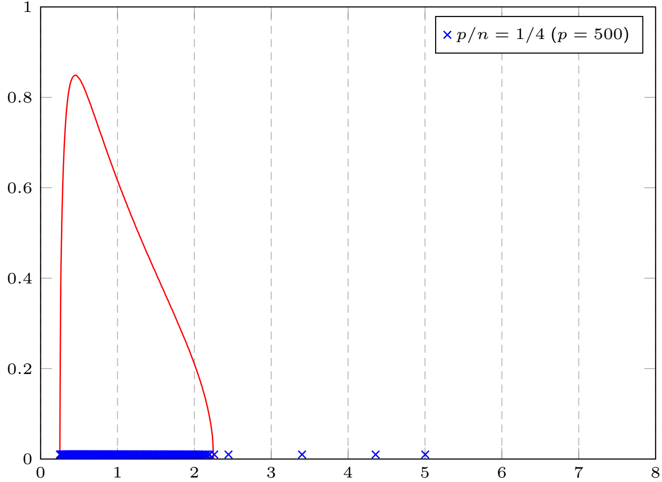

Figure: Eigenvalues of $\frac{1}{n} Y_p Y_p^\mathsf{T}$, $\mathrm{eig}(C_p) = \{\underbrace{1, \ldots, 1}_{p-4}, 2, 3, 4, 5\}$.

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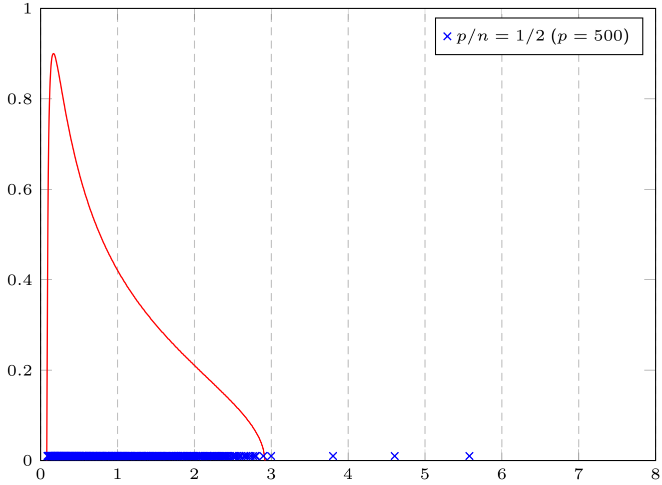

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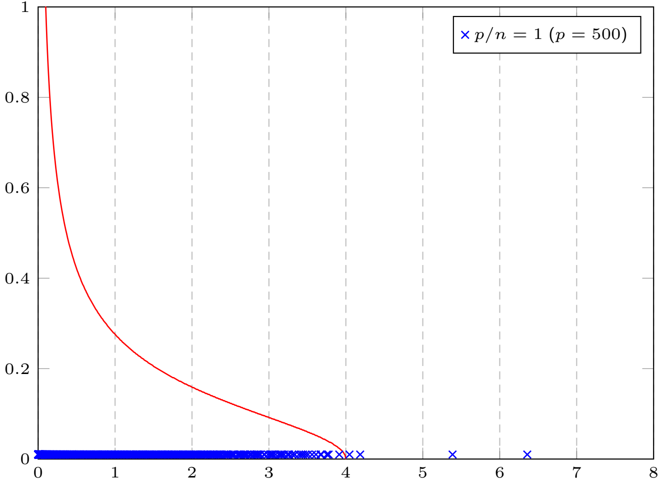

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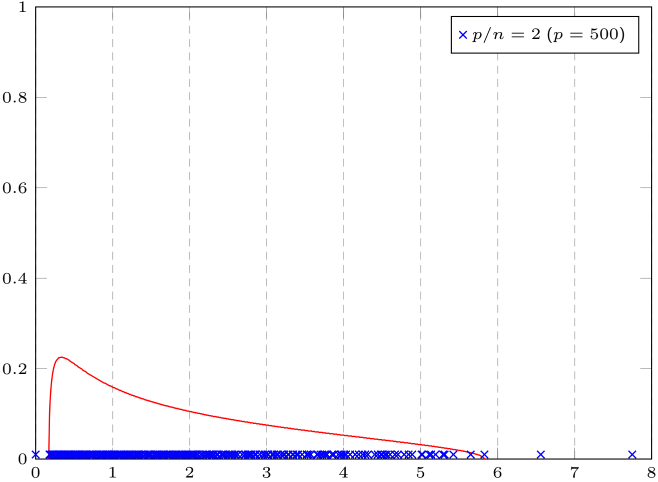

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Theorem (Eigenvalues [Baik,Silverstein'06])

Let $Y_p = C_p^{\frac{1}{2}} X_p$, *with*

- X_p *with i.i.d. zero mean, unit variance,* $E[|X_p|_{ij}^4] < \infty$.
- $C_p = I_p + P$, $P = U\Omega U^*$, *where, for* K *fixed,*

$$\Omega = \operatorname{diag}(\omega_1, \ldots, \omega_K) \in \mathbb{R}^{K \times K}, \text{ with } \omega_1 \geq \ldots \geq \omega_K > 0.$$

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Then, as $p, n \to \infty$, $p/n \to c \in (0, \infty)$, *denoting* $\lambda_m = \lambda_m(\frac{1}{n} Y_p Y_p^*)$ *(*$\lambda_m > \lambda_{m+1}$*),*

$$\lambda_m \xrightarrow{\text{a.s.}} \begin{cases} 1 + \omega_m + c\frac{1+\omega_m}{\omega_m} > (1+\sqrt{c})^2 & , \ \omega_m > \sqrt{c} \\ (1+\sqrt{c})^2 & , \ \omega_m \in (0, \sqrt{c}]. \end{cases}$$

Theorem (Eigenvectors **[Paul'07]**)

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Then, as $p, n \to \infty$*,* $p/n \to c \in (0, \infty)$*, for* $a, b \in \mathbb{C}^p$ *deterministic and* $\hat{u}_i$ *eigenvector of* $\lambda_i(\frac{1}{n} Y_p Y_p^*)$*,*

$$a^* \hat{u}_i \hat{u}_i^* b - \frac{1 - c\omega_i^{-2}}{1 + c\omega_i^{-1}} a^* u_i u_i^* b \cdot 1_{\omega_i > \sqrt{c}} \xrightarrow{\text{a.s.}} 0$$

In particular,

$$|\hat{u}_i^* u_i|^2 \xrightarrow{\text{a.s.}} \frac{1 - c\omega_i^{-2}}{1 + c\omega_i^{-1}} \cdot 1_{\omega_i > \sqrt{c}}.$$

Spiked Models

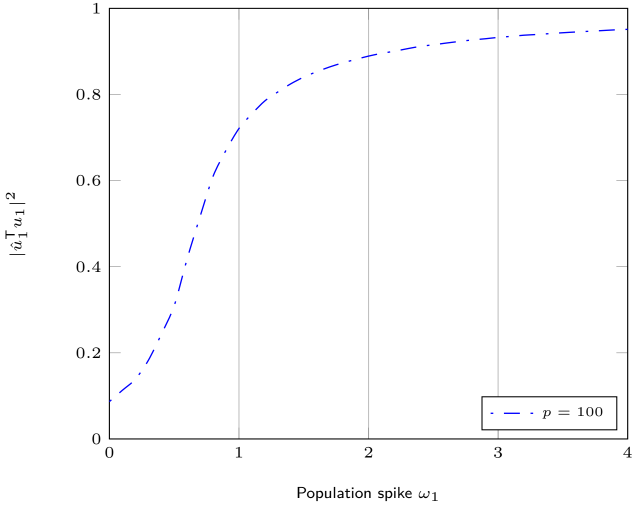
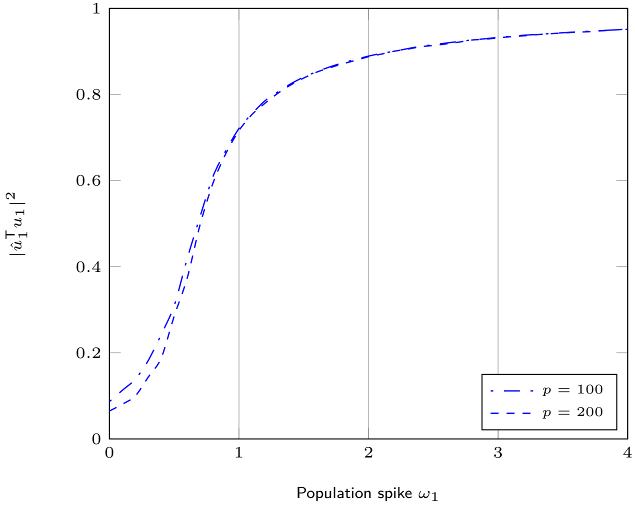


Figure: Simulated versus limiting $|\hat{u}_1^{\mathsf{T}} u_1|^2$ for $Y_p = C_p^{\frac{1}{2}} X_p$, $C_p = I_p + \omega_1 u_1 u_1^{\mathsf{T}}$, $p/n = 1/3$, varying ω_1.



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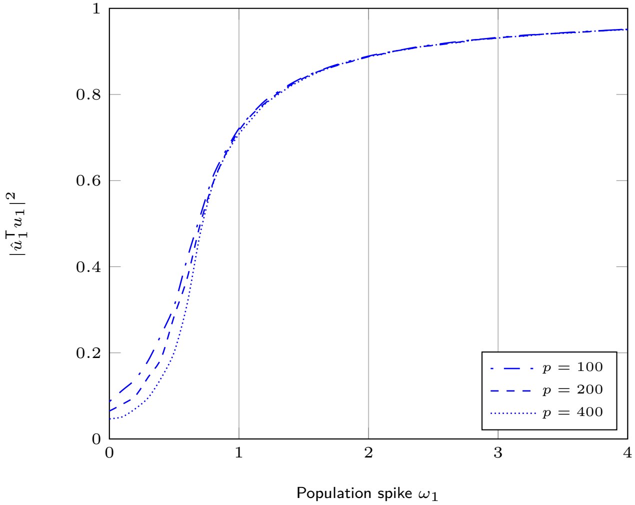

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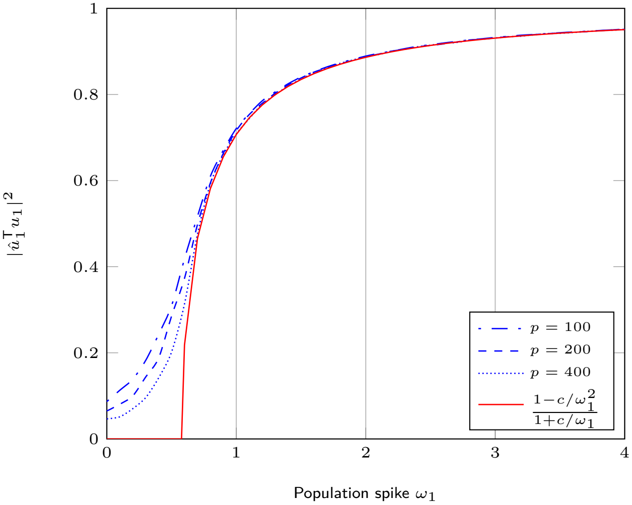

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Other Spiked Models

Similar results for multiple matrix models:

- $Y_p = \frac{1}{n}(I+P)^{\frac{1}{2}} X_p X_p^* (I+P)^{\frac{1}{2}}$
- $Y_p = \frac{1}{n} X_p X_p^* + P$
- $Y_p = \frac{1}{n} X_p^* (I+P) X$
- $Y_p = \frac{1}{n} (X_p + P)^* (X_p + P)$
- etc.

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- **Key observation 3**: Universality goes a long way...: **RMT findings are compliant with real data observations!**

Takeaway Message 1

"RMT Explains Why Machine Learning Intuitions Collapse in Large Dimensions"

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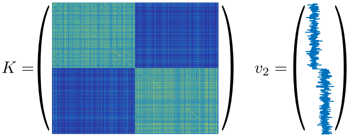
$$K = \{\kappa(x_i, x_j)\}_{i,j=1}^n, \quad \kappa(x_i, x_j) = f\left(\frac{1}{p}\|x_i - x_j\|^2\right).$$

- Why? **Finite-dimensional intuition**

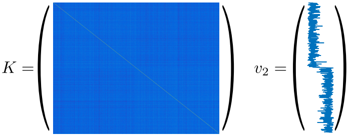
$$K = \begin{array}{cc} \begin{pmatrix} \kappa(x_i,x_j) \gg 1 & \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \ll 1 \\ \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \gg 1 & \kappa(x_i,x_j) \ll 1 \\ \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \gg 1 \end{pmatrix} & \begin{array}{c} \mathcal{C}_1 \\ \mathcal{C}_2 \\ \mathcal{C}_3 \end{array} \end{array}$$

In reality, here is what happens...

Kernel $K_{ij} = \exp(-\frac{1}{2p}\|x_i - x_j\|^2)$ and second eigenvector v_2 ($x_i \sim \mathcal{N}(\pm\mu, I_p)$, $\mu = (2, 0, \ldots, 0)^\mathsf{T} \in \mathbb{R}^p$).



$p = 4$, $n = 1000$



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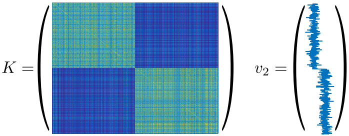

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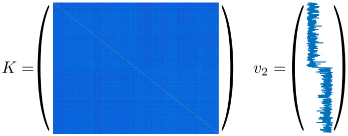

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Key observation: Under growth rate assumptions,

$$\boxed{\max_{1 \le i \ne j \le n} \left\{ \left| \frac{1}{p} \|x_i - x_j\|^2 - \tau \right| \right\} \xrightarrow{\text{a.s.}} 0}, \quad \tau = \frac{2}{p} \sum_{i=1}^{k} \operatorname{tr} \frac{n_a}{n} C_a.$$

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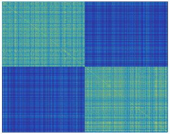
$K =$  $v_2 =$ 

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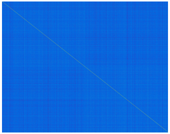
$K =$  $v_2 =$ 

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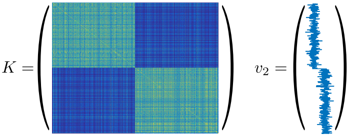

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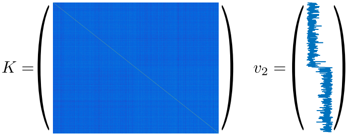

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- this suggests $K \simeq f(\tau) 1_n 1_n^\mathsf{T}$!
- more importantly, **in non-trivial settings, data are neither close, nor far!**

(Major) consequences:

The curse of dimensionality and its consequences (3)

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Under growth rate assumptions, as $p, n \to \infty$,

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- $f(\tau)$, $f'(\tau)$, $f''(\tau)$
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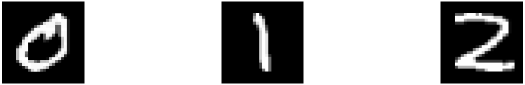
RMT can explain tools ML engineers use everyday.

Theoretical Findings versus MNIST



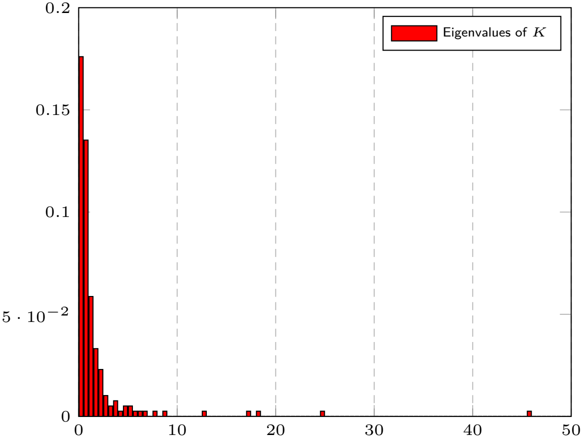
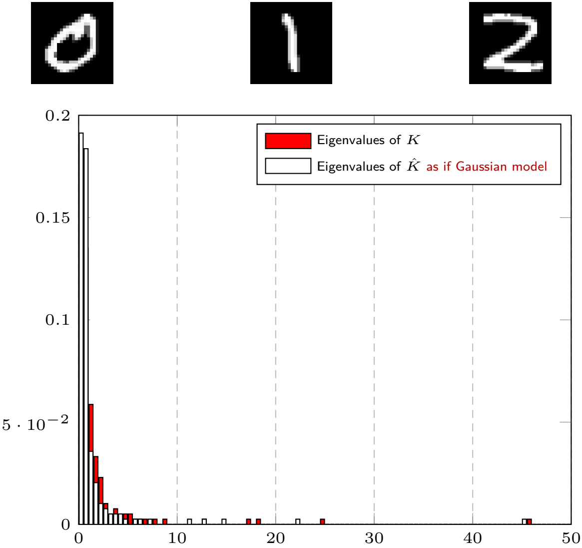


Figure: Eigenvalues of K (red) and (equivalent Gaussian model) $\hat{K}$ (white), MNIST data, $p = 784$, $n = 192$.

Theoretical Findings versus MNIST



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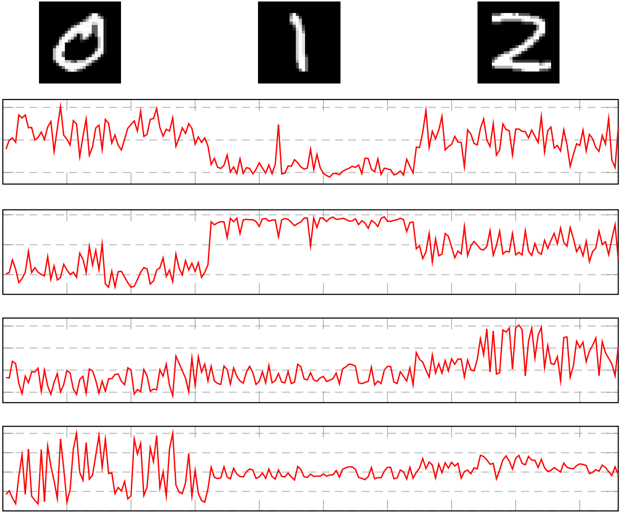

Figure: Leading four eigenvectors of K for MNIST data (**red**) and theoretical findings (**blue**).

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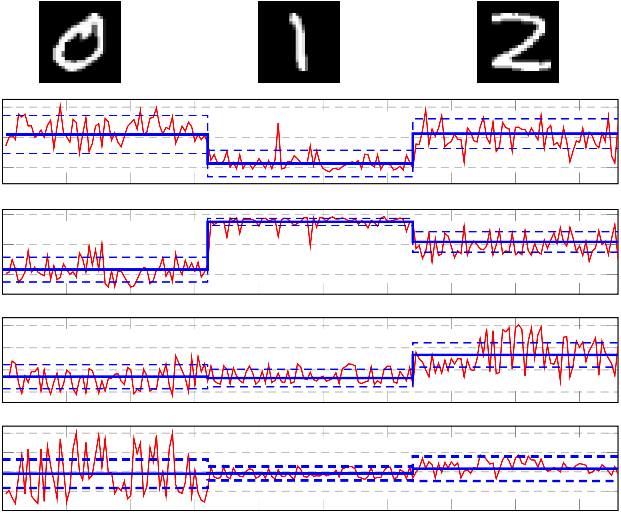

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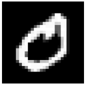
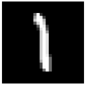
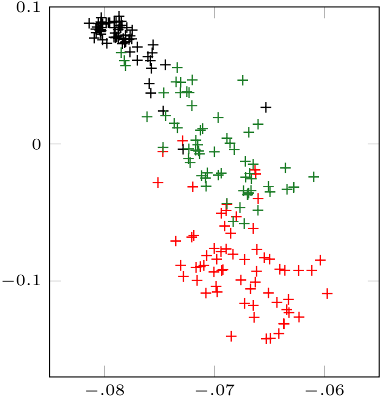
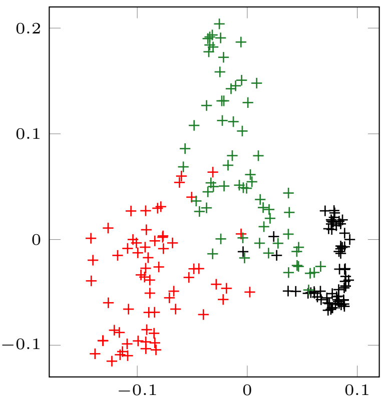
  

Eigenvector 2/Eigenvector 1



Eigenvector 3/Eigenvector 2



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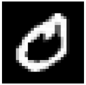
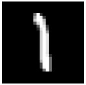


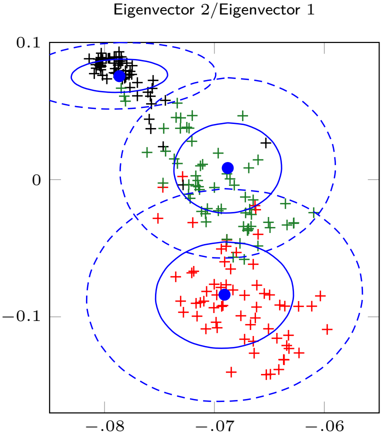

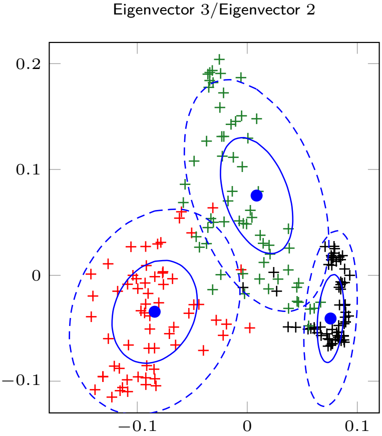

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Takeaway Message 2

"RMT Reassesses and Improves Data Processing"

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Improving Kernel Spectral Clustering

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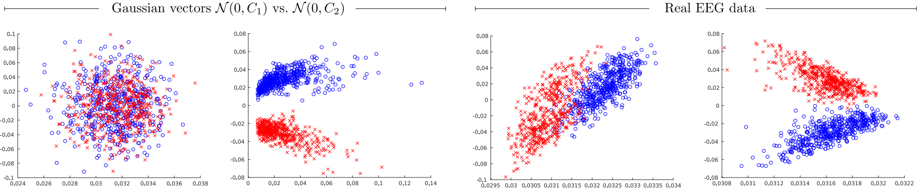

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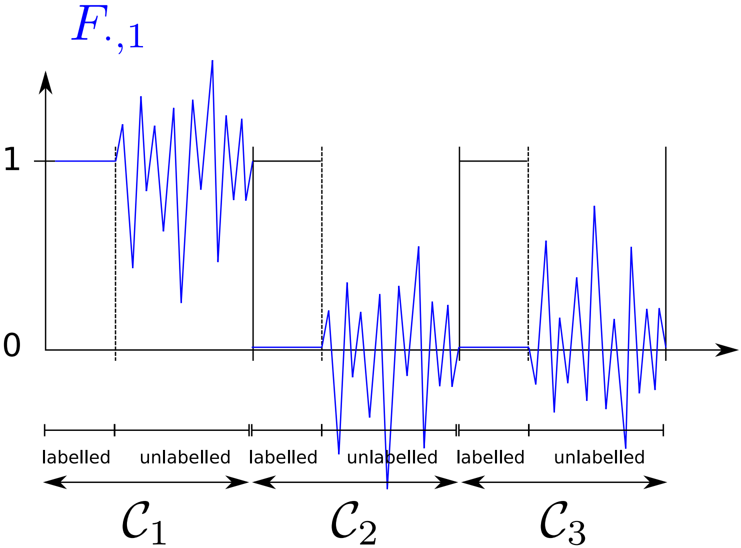
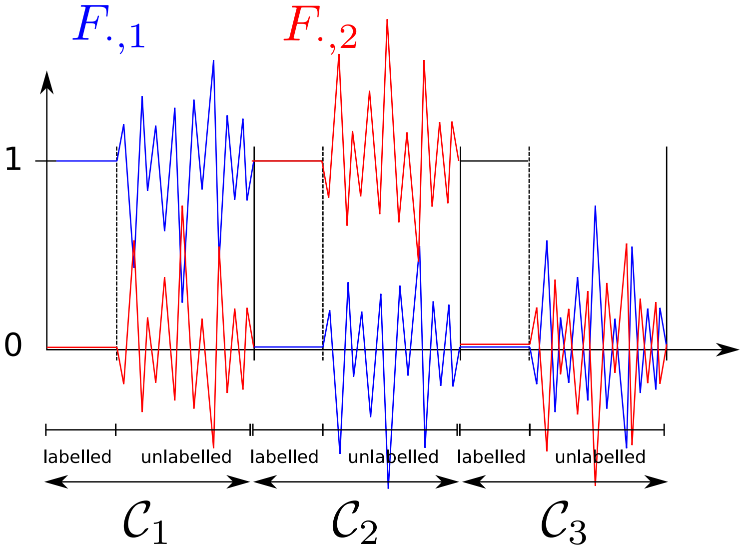
- **Explicit solution**:

$$F^{[u]} = \left(I_{n_{[u]}} - D_{[u]}^{-1} K_{[uu]} \right)^{-1} D_{[u]}^{-1} K_{[ul]} F^{[l]}$$

where $D = \operatorname{diag}(K 1_n)$ (degree matrix) and $[ul]$, $[uu]$, … blocks of **l**abeled/**u**nlabeled data.

The finite-dimensional intuition: What we expect

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$F_{\cdot,2}$
1
0
labelled
unlabelled
labelled
unlabelled
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$\mathcal{C}_1$
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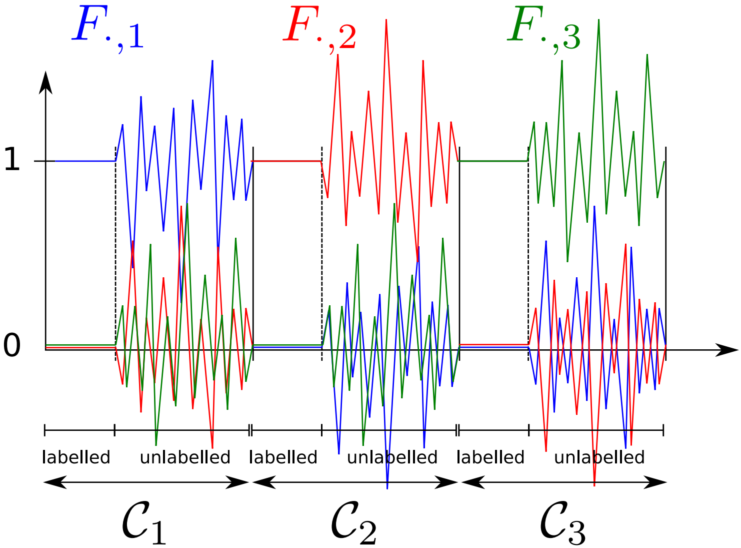

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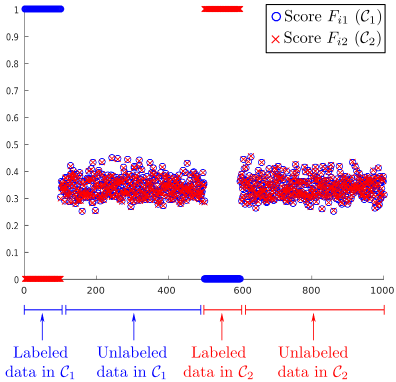
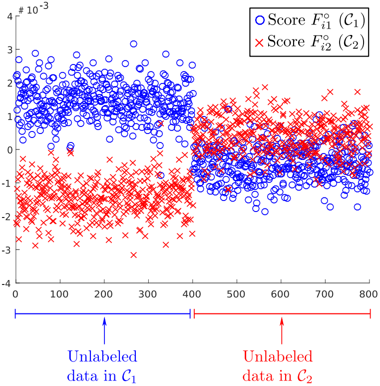
Display. Scores F_{ik} (left) and $F^\circ_{ik} = F_{ik} - \frac{1}{2}(F_{i1} + F_{i2})$ (right).





The reality: What we see!

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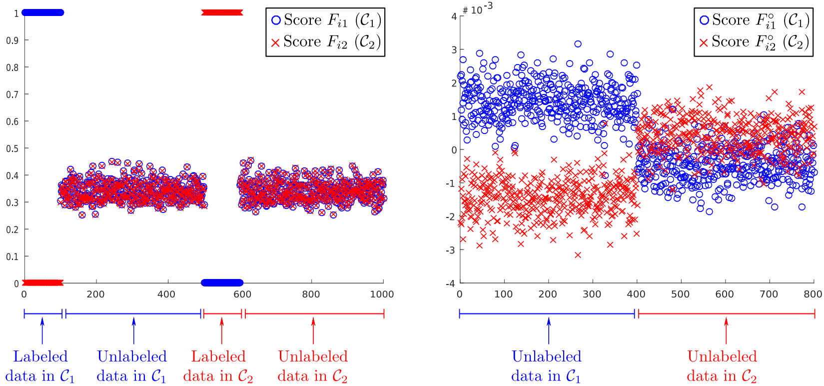
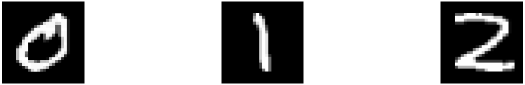


➩ **Score are almost all identical... and do not follow the labelled data!**

MNIST Data Example



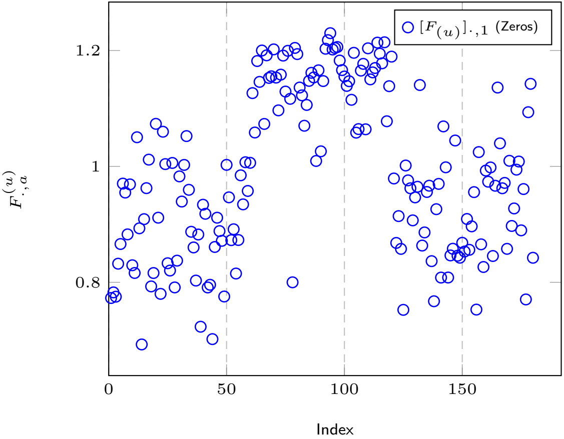


Figure: Vectors $[F^{(u)}]_{\cdot,a}$, $a = 1, 2, 3$, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

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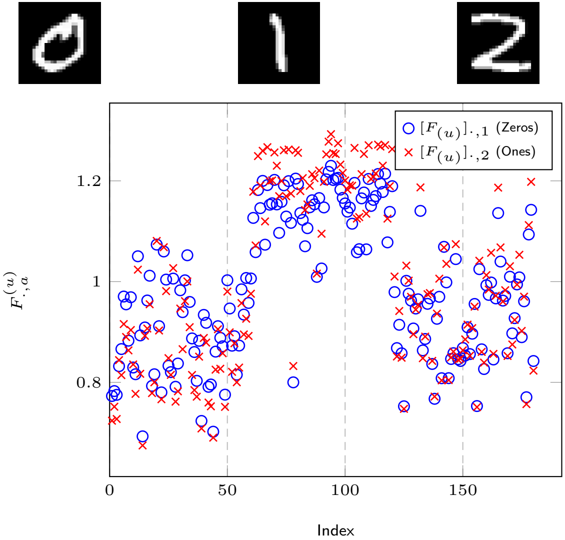

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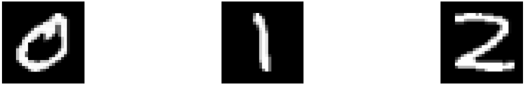

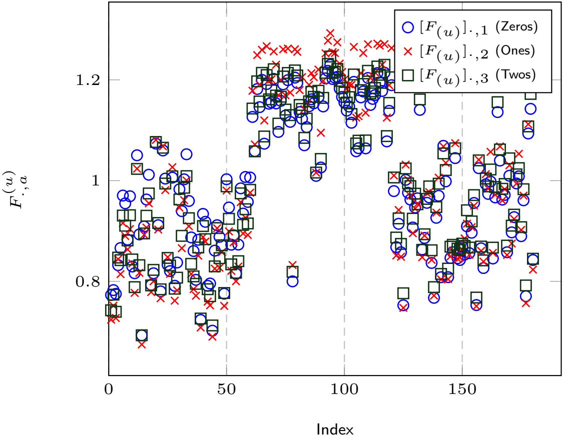

Figure: Vectors $[F^{(u)}]_{\cdot,a}$, $a = 1, 2, 3$, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

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Exploiting RMT to resurrect SSL

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- Asymptotic performance analysis: **clear understanding of what we see!**
- Update the algorithm and **provably improve unlabelled data use**.

Theorem ([Mai,C'18] Asymptotic Performance of SSL)

For $x_i \in \mathcal{C}_b$ unlabelled, score vector $F_{i,\cdot} \in \mathbb{R}^k$ satisfies:

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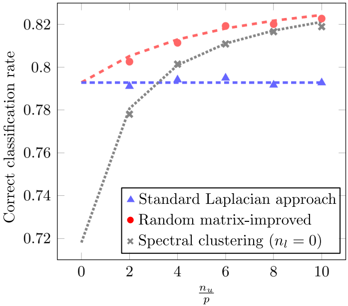
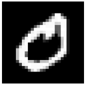
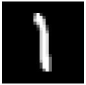


Experimental evidence: MNIST

Digits	(0,8)	(2,7)	(6,9)
$n_u = 100$			
Centered kernel **(RMT)**	**89.5±3.6**	**89.5±3.4**	**85.3±5.9**
Iterated centered kernel **(RMT)**	**89.5±3.6**	**89.5±3.4**	**85.3±5.9**
Laplacian	75.5±5.6	74.2±5.8	70.0±5.5
Iterated Laplacian	87.2±4.7	86.0±5.2	81.4±6.8
Manifold	88.0±4.7	88.4±3.9	82.8±6.5
$n_u = 1000$			
Centered kernel **(RMT)**	92.2±0.9	92.5±0.8	92.6±1.6
Iterated centered kernel **(RMT)**	**92.3±0.9**	**92.5± 0.8**	**92.9±1.4**
Laplacian	65.6±4.1	74.4±4.0	69.5±3.7
Iterated Laplacian	**92.2±0.9**	92.4±0.9	92.0±1.6
Manifold	91.1±1.7	91.4±1.9	91.4±2.0

Table: Comparison of classification accuracy (%) on MNIST datasets with $n_l = 10$. Computed over 1000 random iterations for $n_u = 100$ and 100 for $n_u = 1000$.

Experimental evidence: Traffic signs (HOG features)

Class ID	(2,7)	(9,10)	(11,18)
$n_u = 100$			
Centered kernel **(RMT)**	79.0±10.4	77.5±9.2	78.5±7.1
Iterated centered kernel **(RMT)**	**85.3±5.9**	**89.2±5.6**	**90.1±6.7**
Laplacian	73.8±9.8	77.3±9.5	78.6±7.2
Iterated Laplacian	83.7±7.2	88.0±6.8	87.1±8.8
Manifold	77.6±8.9	81.4±10.4	82.3±10.8
$n_u = 1000$			
Centered kernel **(RMT)**	83.6±2.4	84.6±2.4	88.7±9.4
Iterated centered kernel **(RMT)**	**84.8±3.8**	**88.0±5.5**	**96.4±3.0**
Laplacian	72.7±4.2	88.9±5.7	95.8±3.2
Iterated Laplacian	83.0±5.5	88.2±6.0	92.7±6.1
Manifold	77.7±5.8	85.0±9.0	90.6±8.1

Table: Comparison of classification accuracy (%) on German Traffic Sign datasets with $n_l = 10$. Computed over 1000 random iterations for $n_u = 100$ and 100 for $n_u = 1000$.

Takeaway Message 3

"RMT Also Grasps 'Real Data' Processing"

Current Problem. Data models based on **vectors of i.i.d. entries** (or even only Gaussian).

From i.i.d. to concentrated random vectors

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Theorem (**[Louart,C'18] [Seddik,C'19]** Kernel Universality)

For $x_i \sim \mathcal{L}(\mu_a, C_a)$ concentrated random vector, under the conditions of [C-Benaych'16],

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⇨ **Same result as [C-Benaych'16]... Universality of first two moments!**

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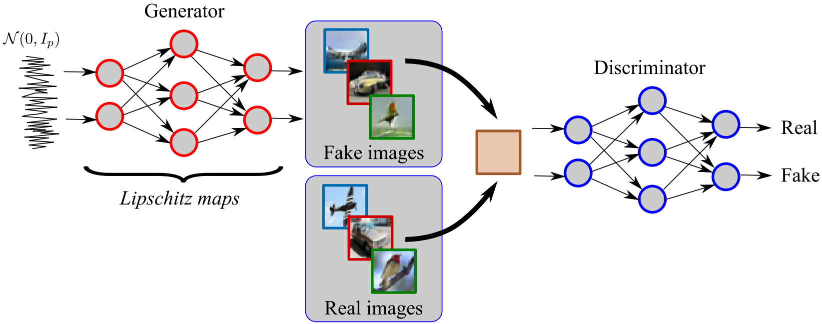

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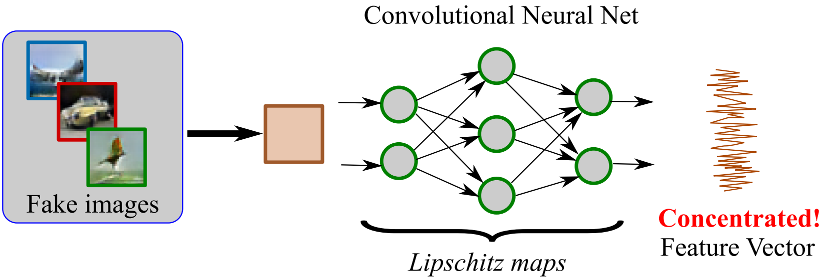
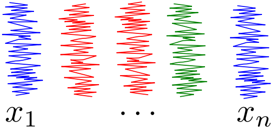


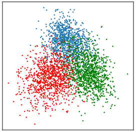
Convolutional Neural Net
Fake images
Lipschitz maps
Concentrated!
Feature Vector

Ok. . . so what?



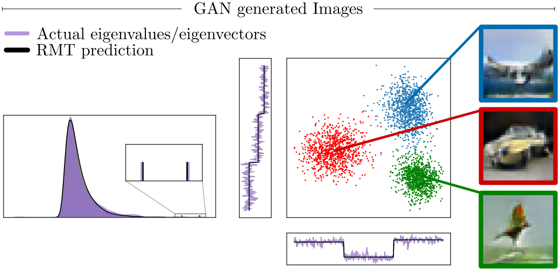
Feature Vectors

$$K = \left\{ e^{-\frac{1}{2p}\|x_i - x_j\|^2} \right\}_{i,j=1}^{n}$$



Spectral Clustering

Results. [Seddik,C'19]



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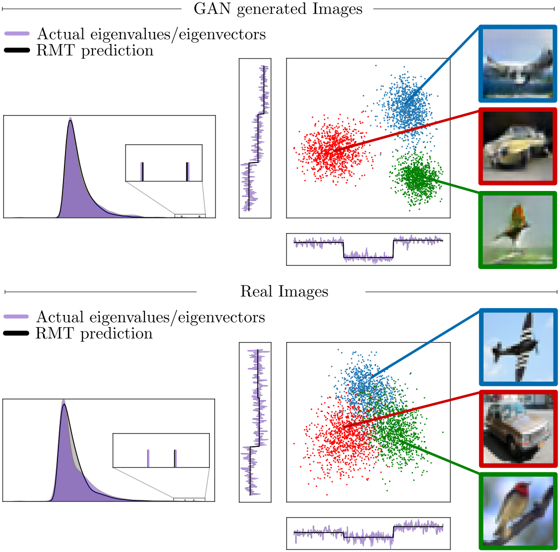
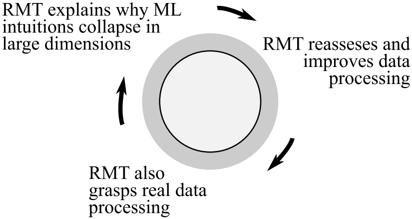


Reminder of Takeaway messages:



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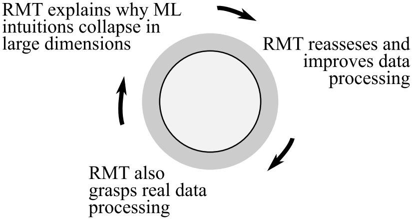

The road ahead:

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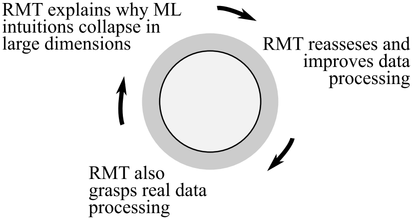

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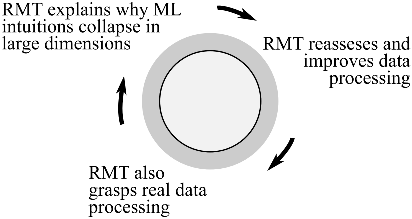

The road ahead:

- getting away from GMM models and show universality results (**concentration of measure arguments**)
- generalize the approach to problems having non-explicit solutions (such as convex optim problems)
- deep learning, recurrent neural nets... are a very different story!

Thank you!

- **[C-Benaych'16]** R. Couillet, Benaych-Georges, "Kernel Spectral Clustering of Large Dimensional Data", Electronic Journal of Statistics, vol. 10, no. 1, pp. 1393-1454, 2016. [article]
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