Random Matrix Advances in Machine Learning
(Colloquium de Bordeaux)

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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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- If $y_1 \sim \mathcal{N}(0, C_p)$, ML estimator for C_p is the sample covariance matrix (SCM)

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  or equivalently, in spectral norm

$$\left\| \hat{C}_p - C_p \right\| \xrightarrow{\text{a.s.}} 0.$$

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- For practical p, n with $p \simeq n$, leads to dramatically wrong conclusions
- **Even for** $p = n/100$.

The Marčenko–Pastur law

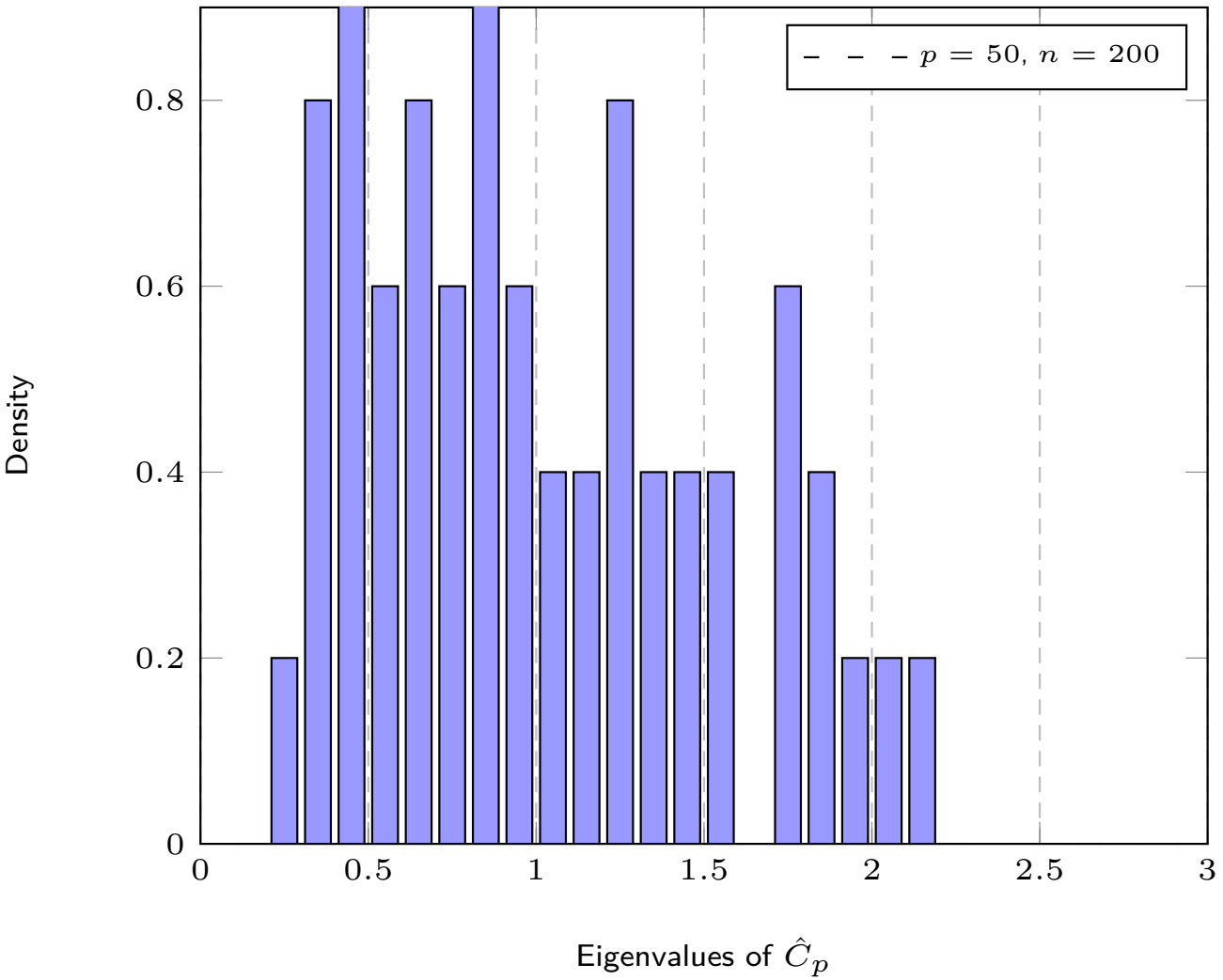

Figure: Histogram of the eigenvalues of $\hat{C}_p$ for $c = 1/4$, $C_p = I_p$.

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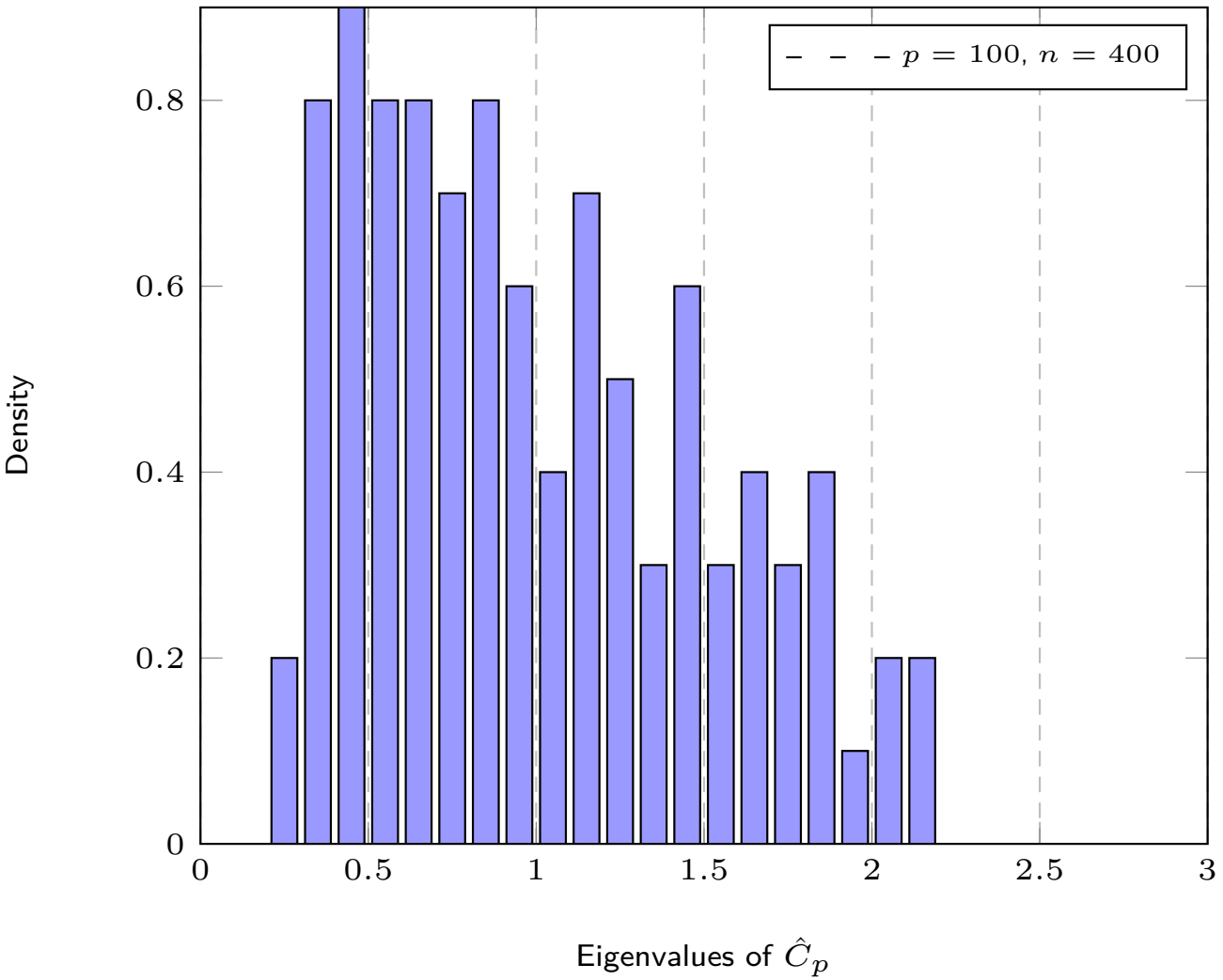

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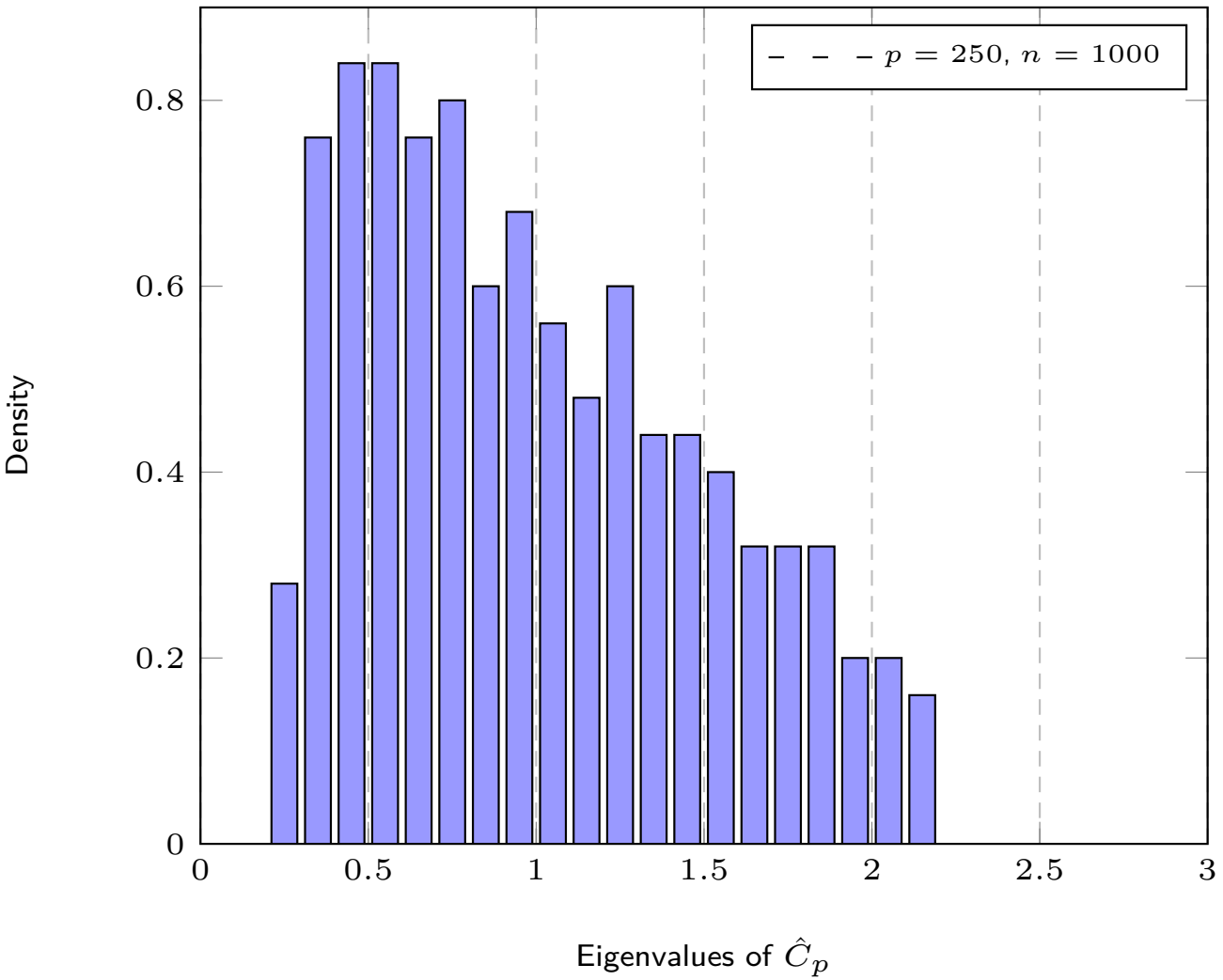

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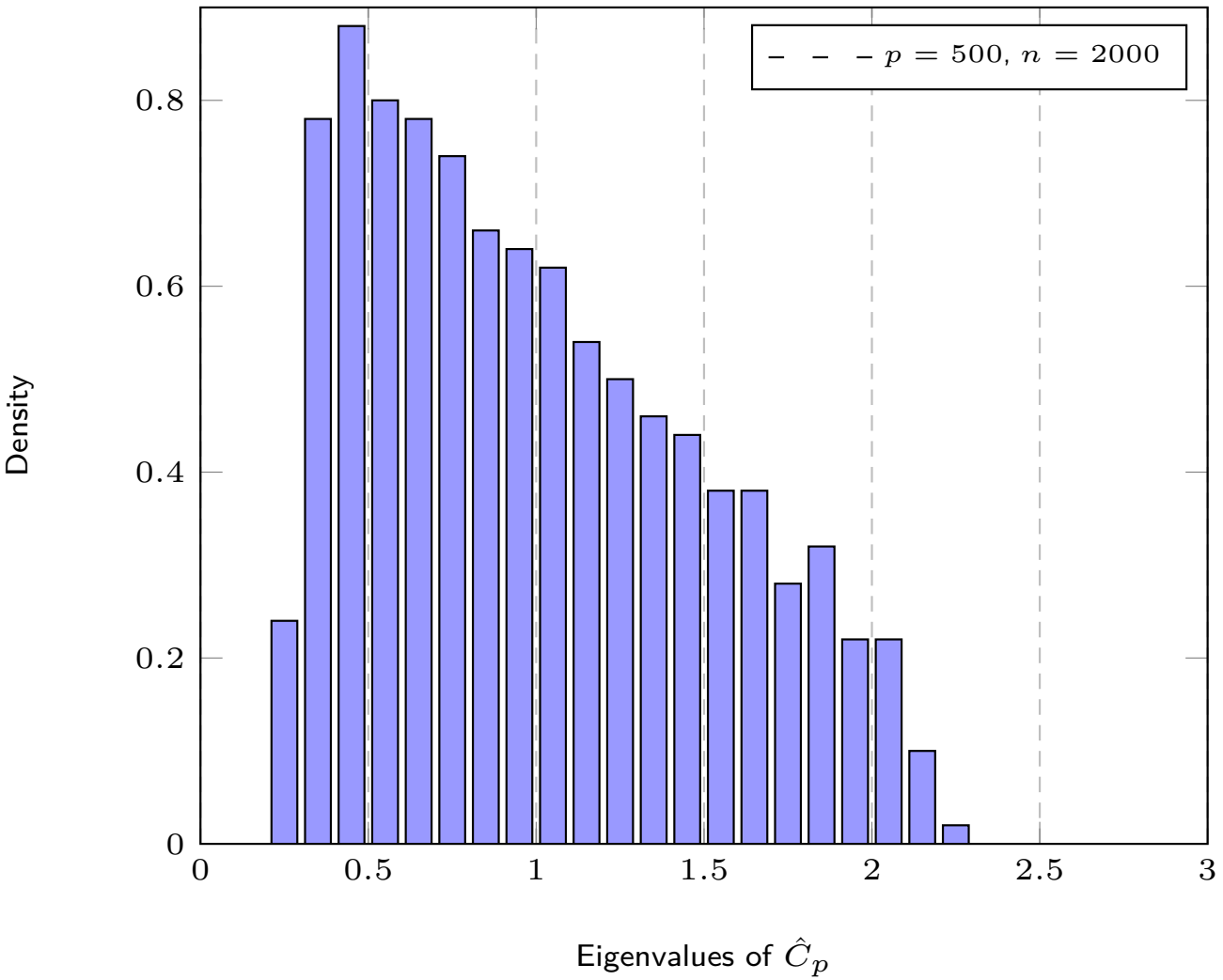

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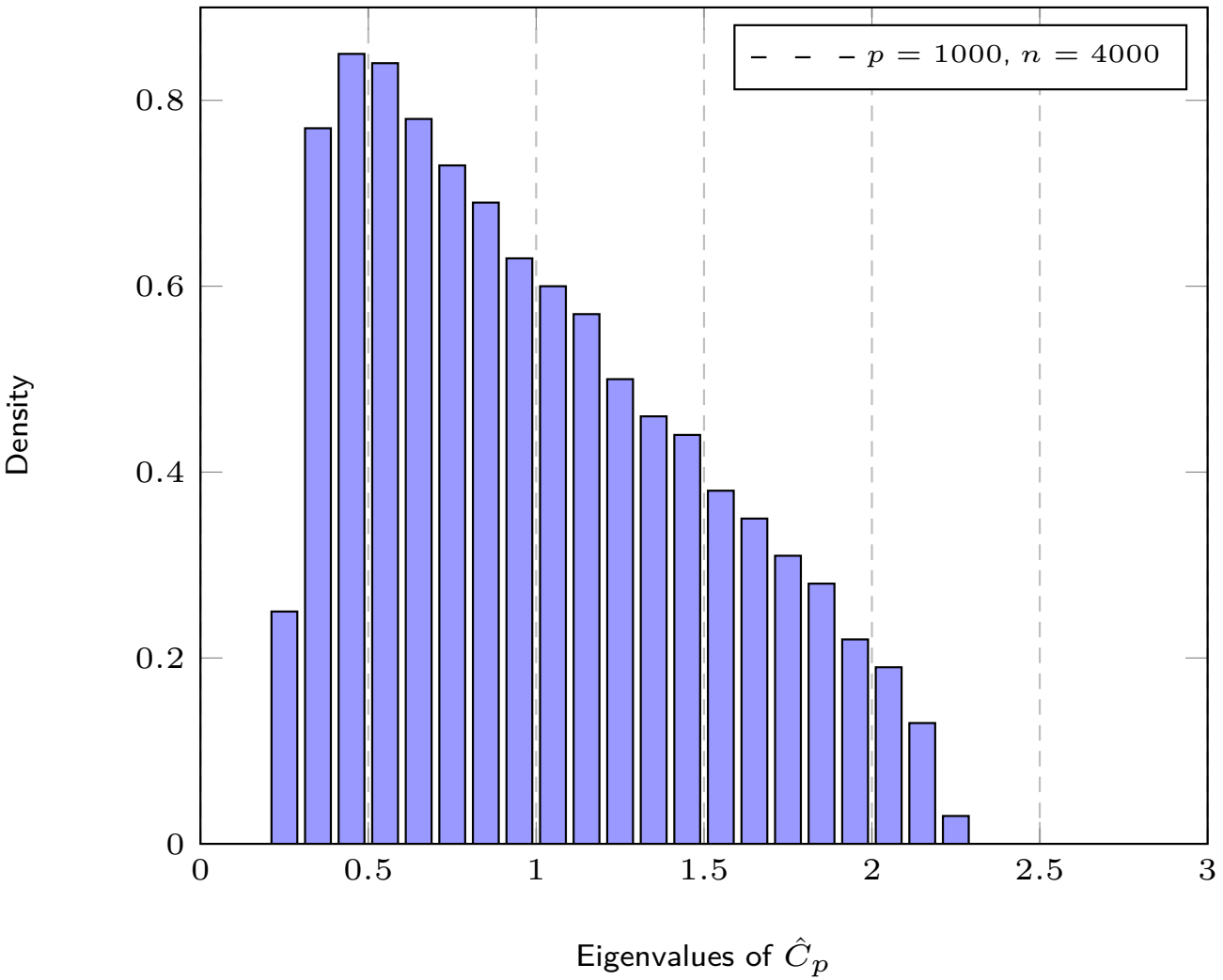

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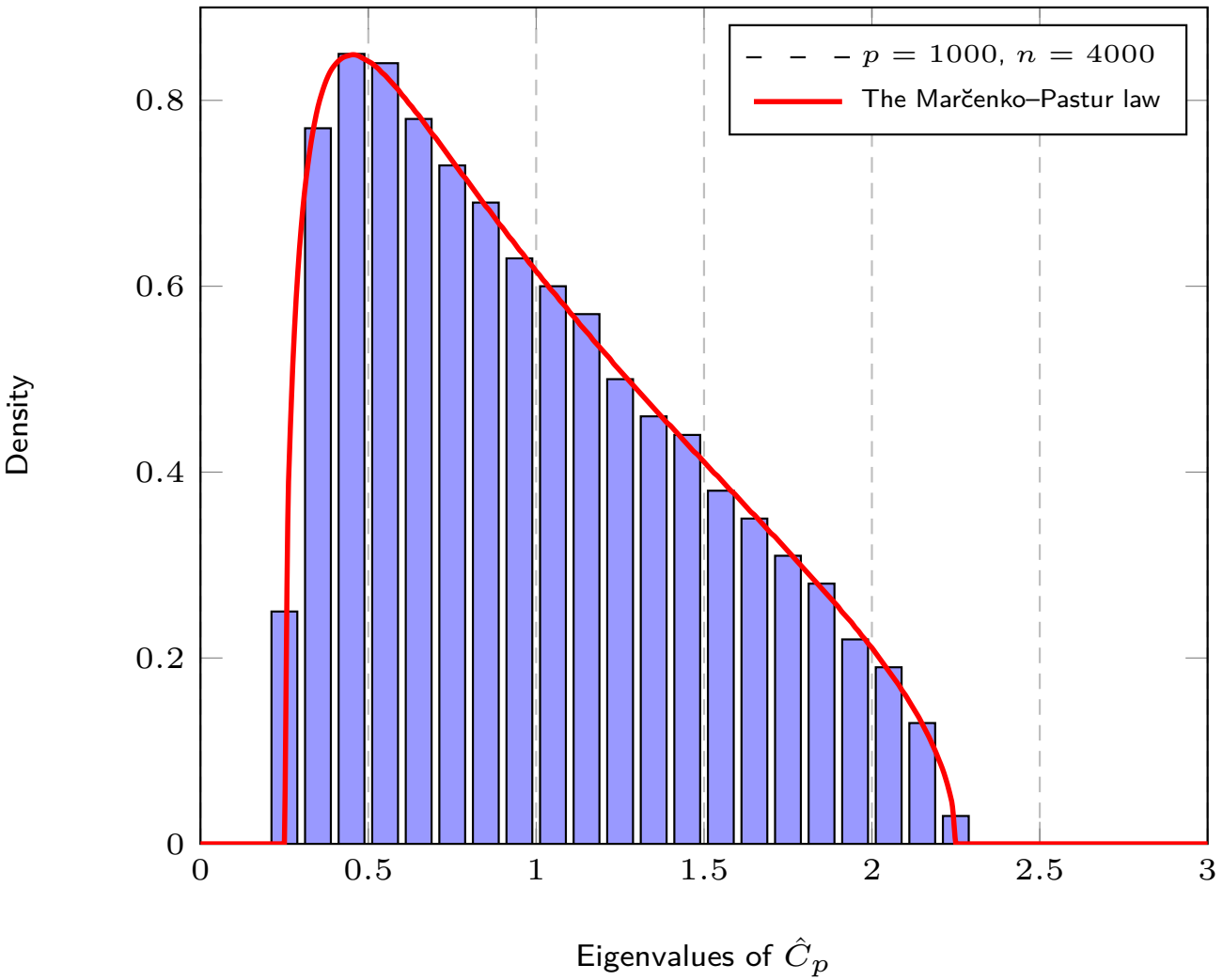

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Definition (Empirical Spectral Density)

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

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Theorem (Marčenko–Pastur Law **[Marčenko,Pastur'67]**)

$X_p \in \mathbb{C}^{p\times n}$ 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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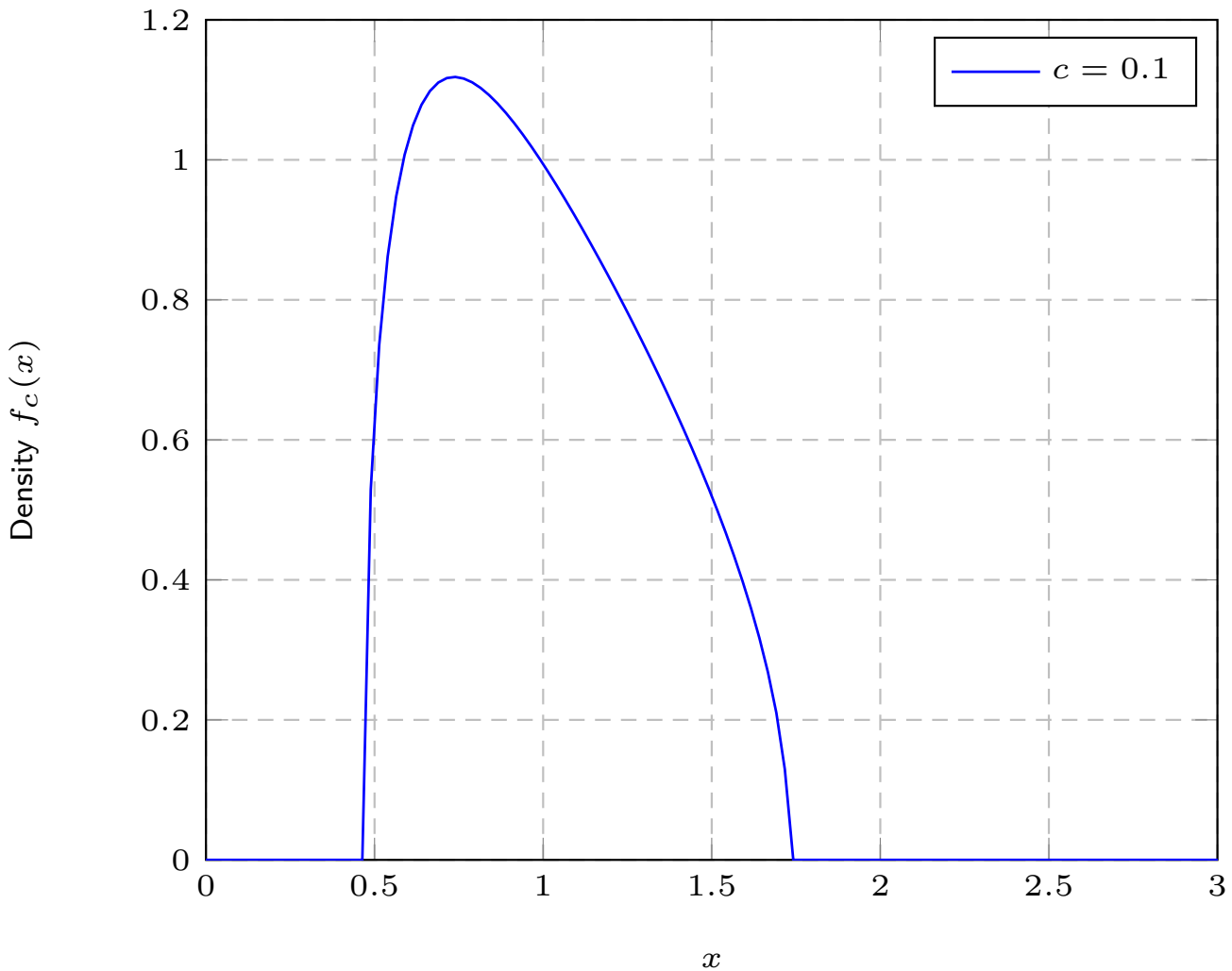

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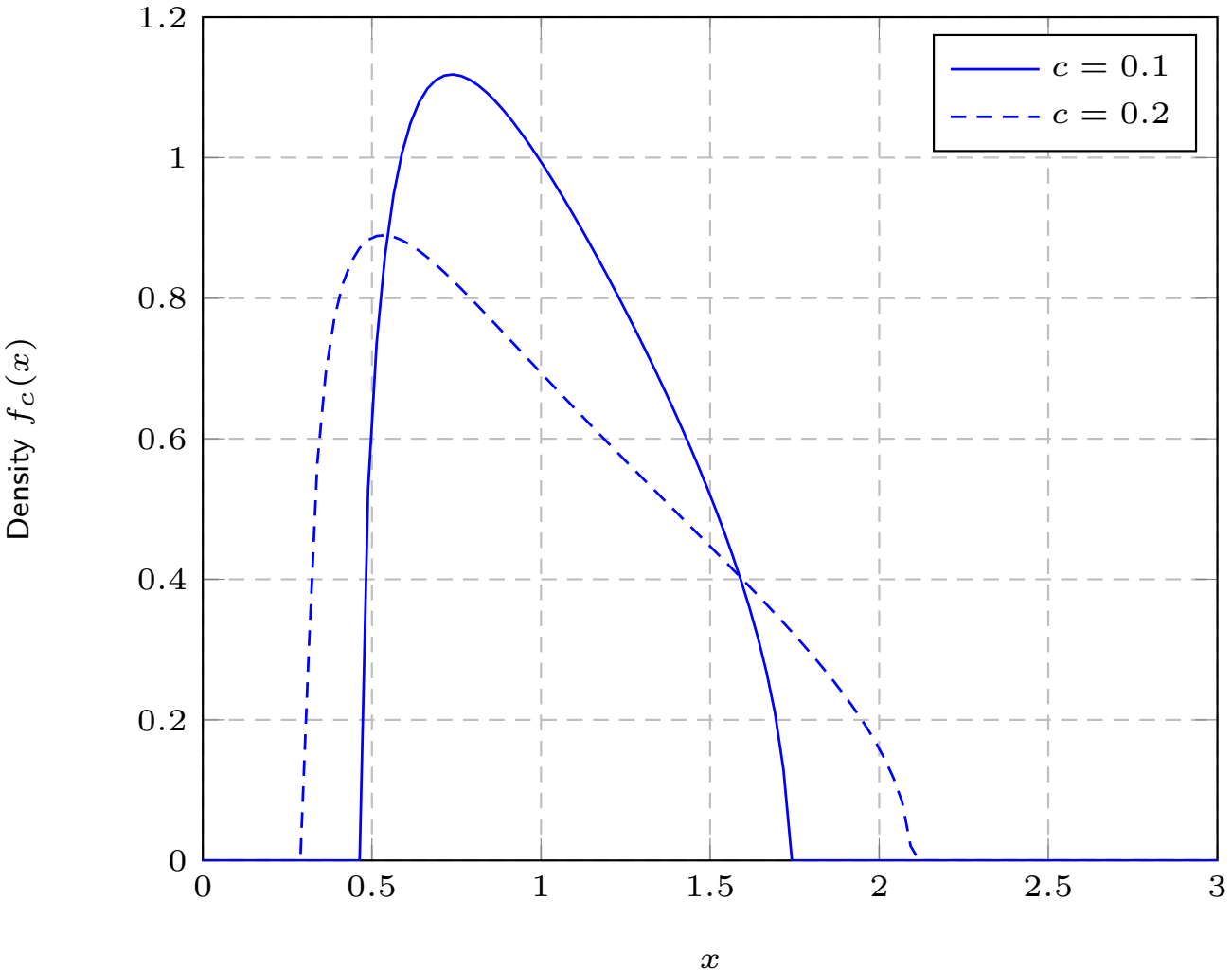

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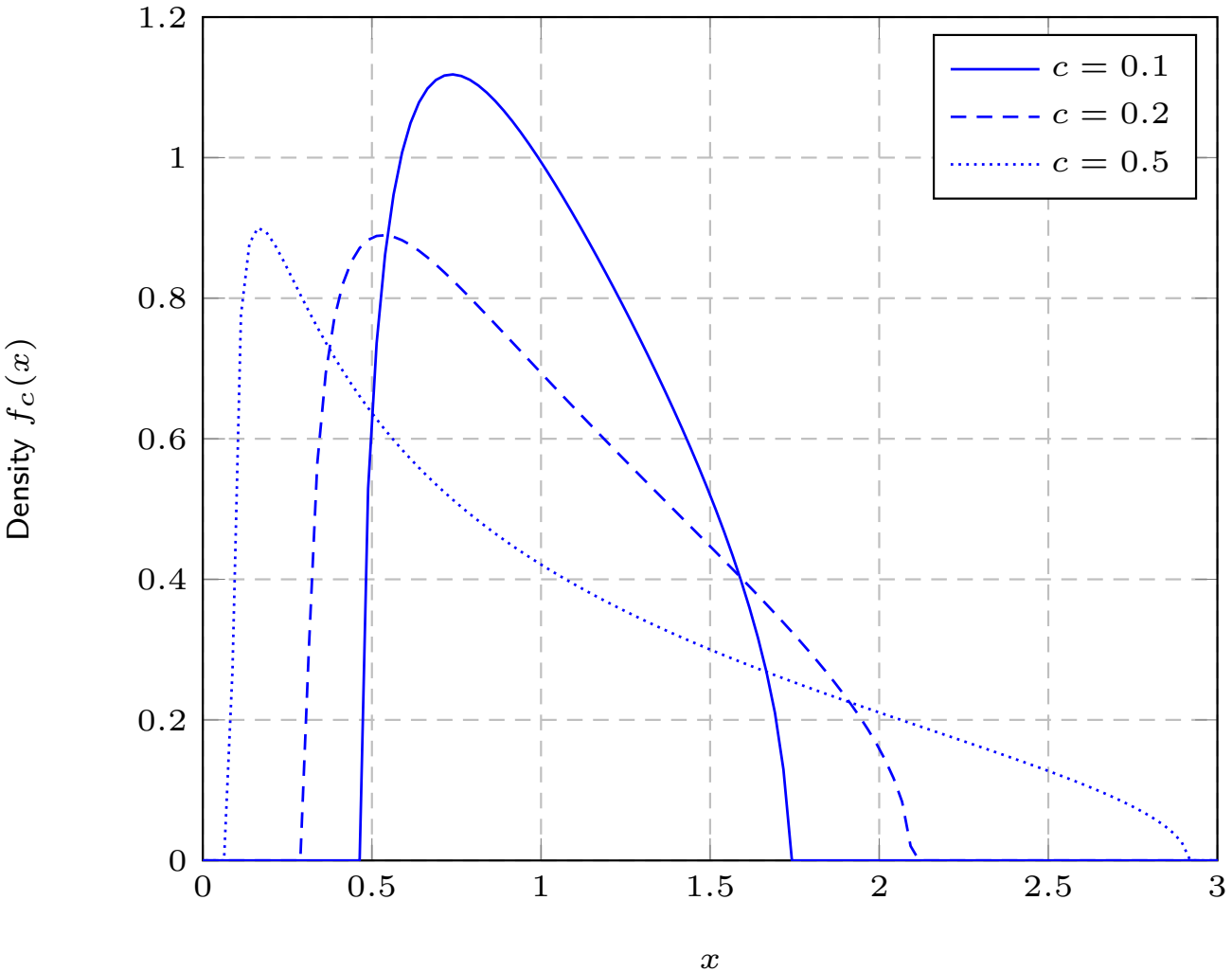

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Small rank perturbation: $C_p = I_p + P$, P of low rank.

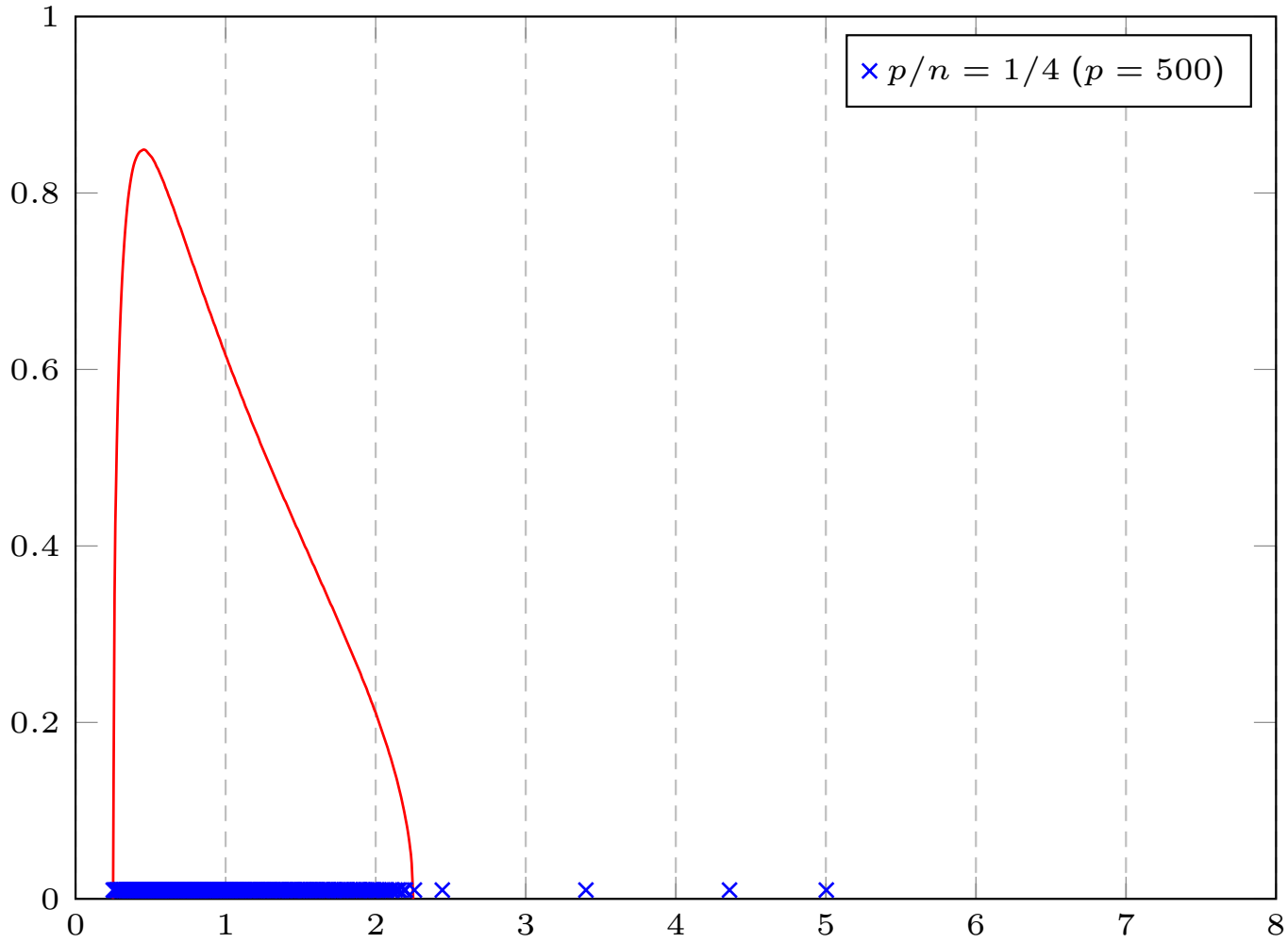

Figure: Eigenvalues of $\frac{1}{n} Y_p Y_p^{\mathsf{T}}$, $\mathrm{eig}(C_p) = \{\underbrace{1, \ldots, 1}_{p-4}, 2, 3, 4, 5\}$.

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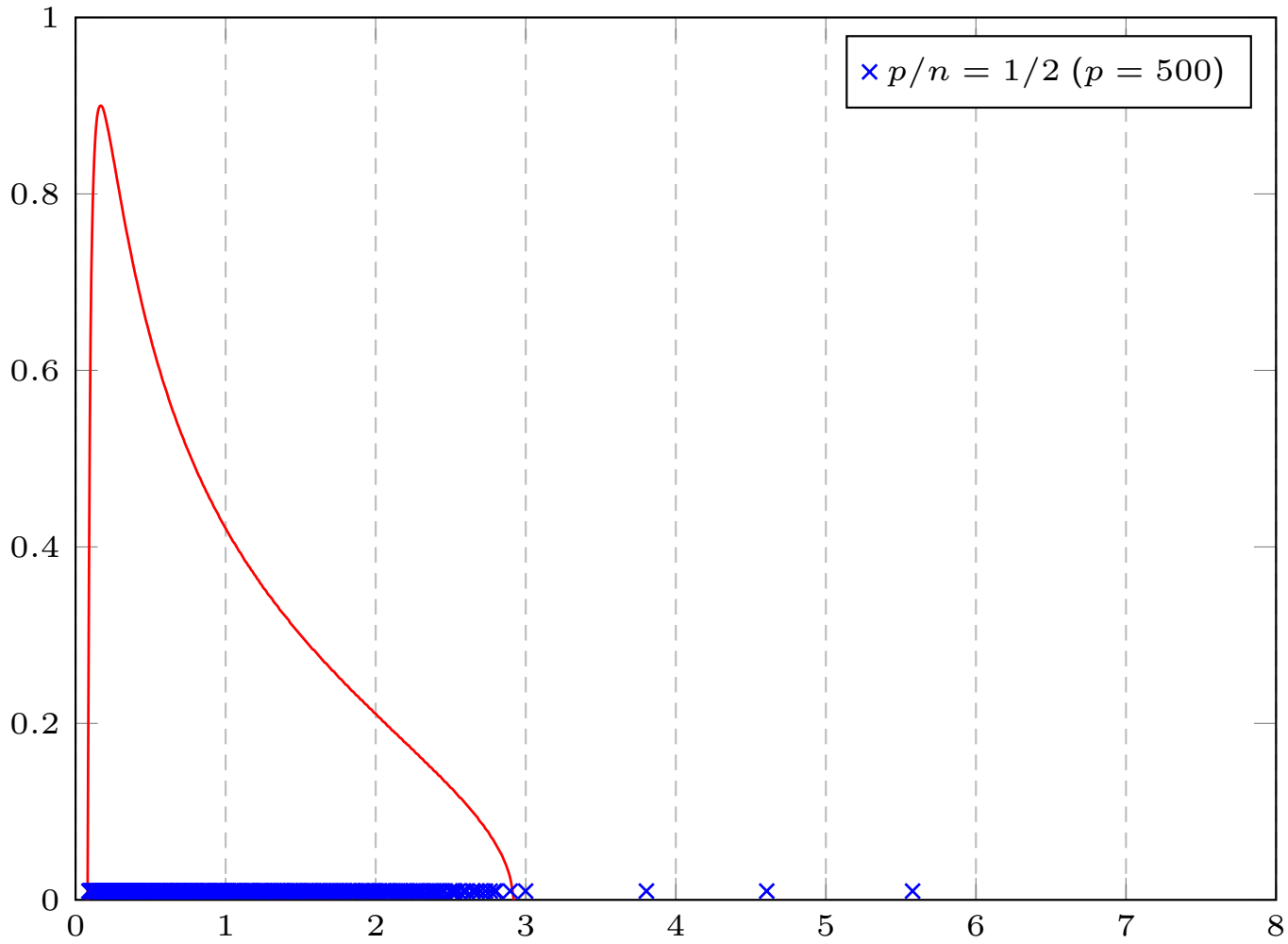

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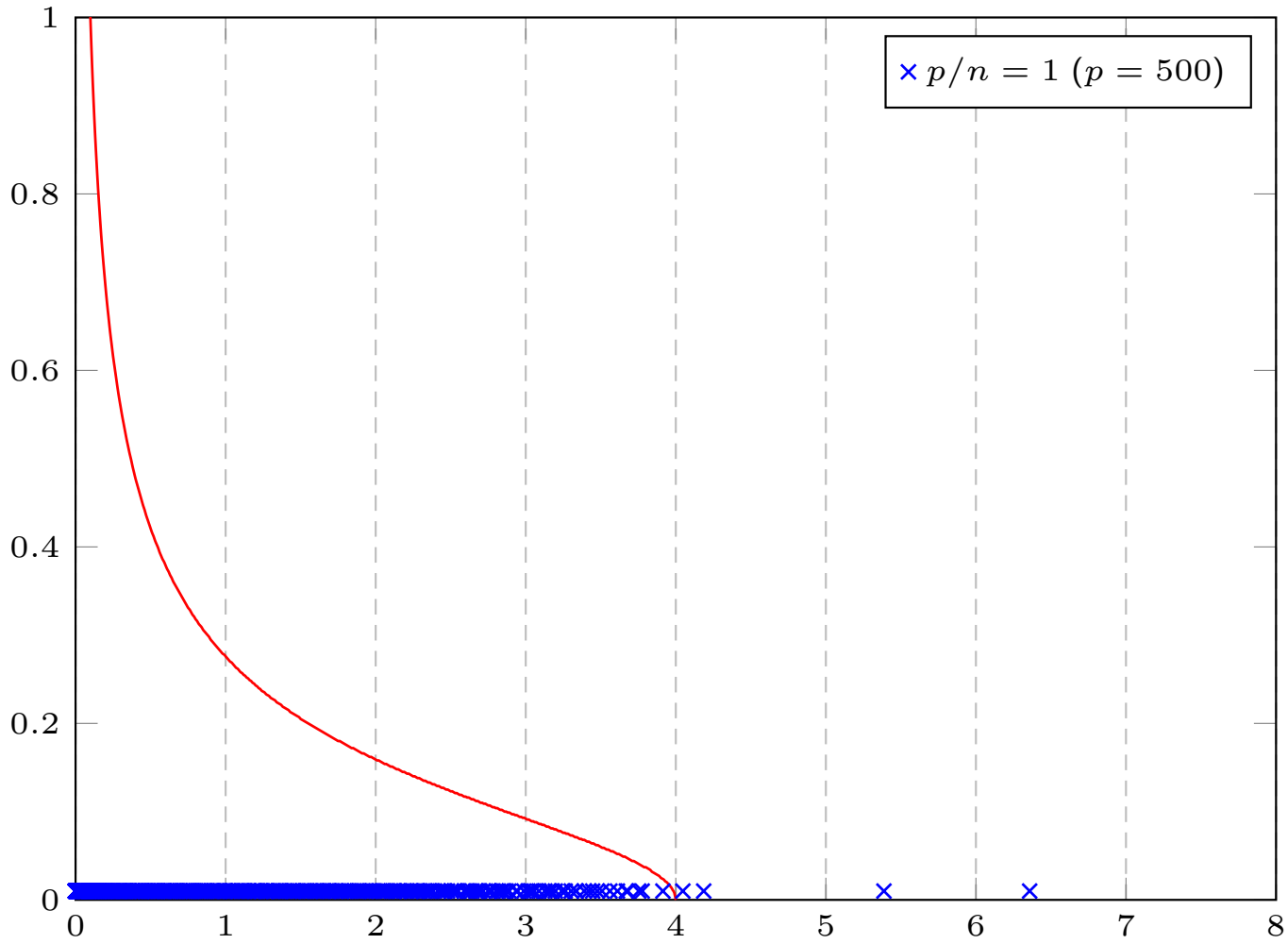

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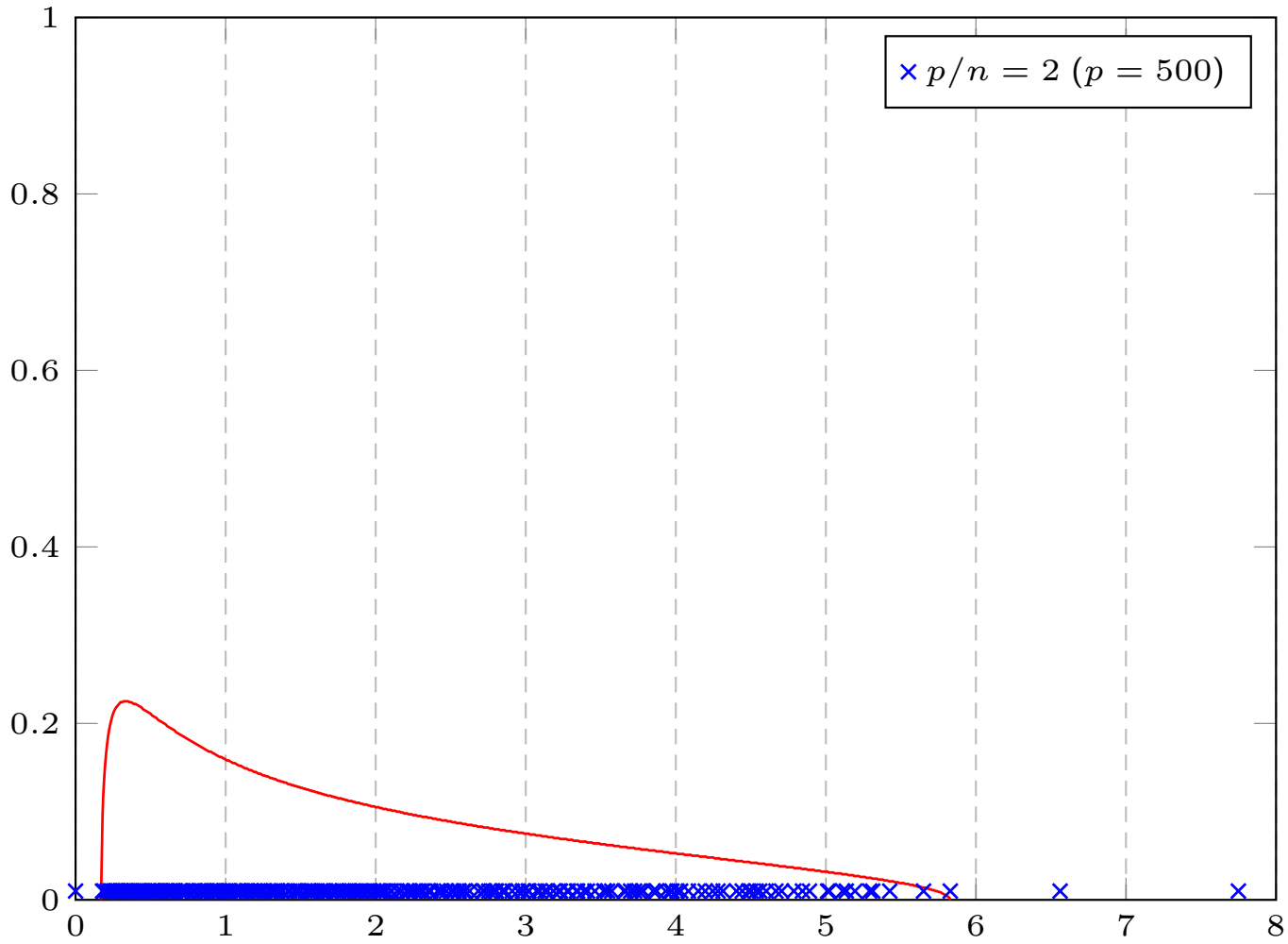

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Theorem (Eigenvalues **[Baik,Silverstein'06]**)

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,*

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

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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

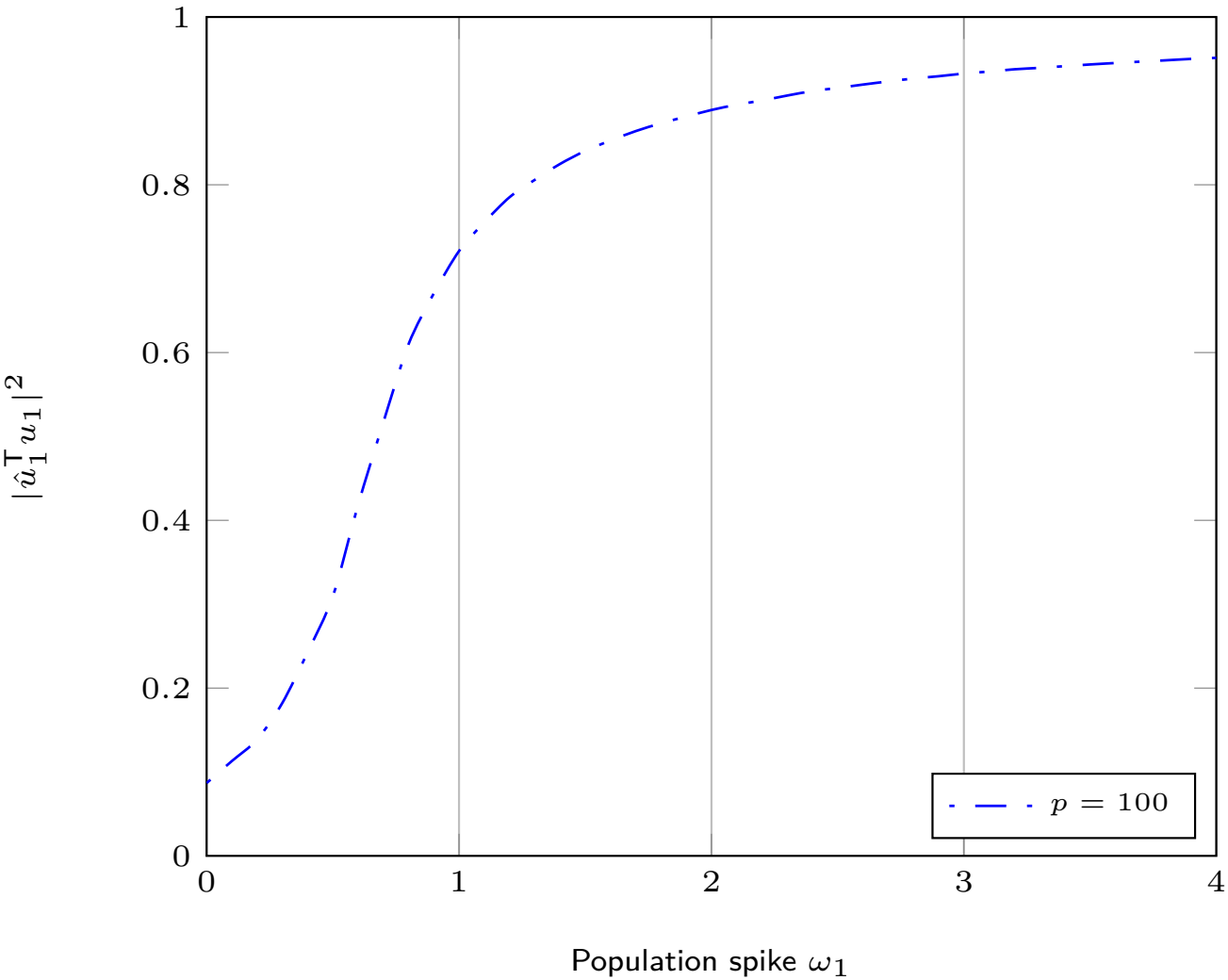

Figure: Simulated versus limiting $|\hat{u}_1^{\mathsf{T}} u_1|^2$ for $Y_p = C_p^{\frac{1}{2}} X_p$, $C_p = I_p + \omega_1 u_1 u_1^{\mathsf{T}}$, $p/n = 1/3$, varying ω_1.

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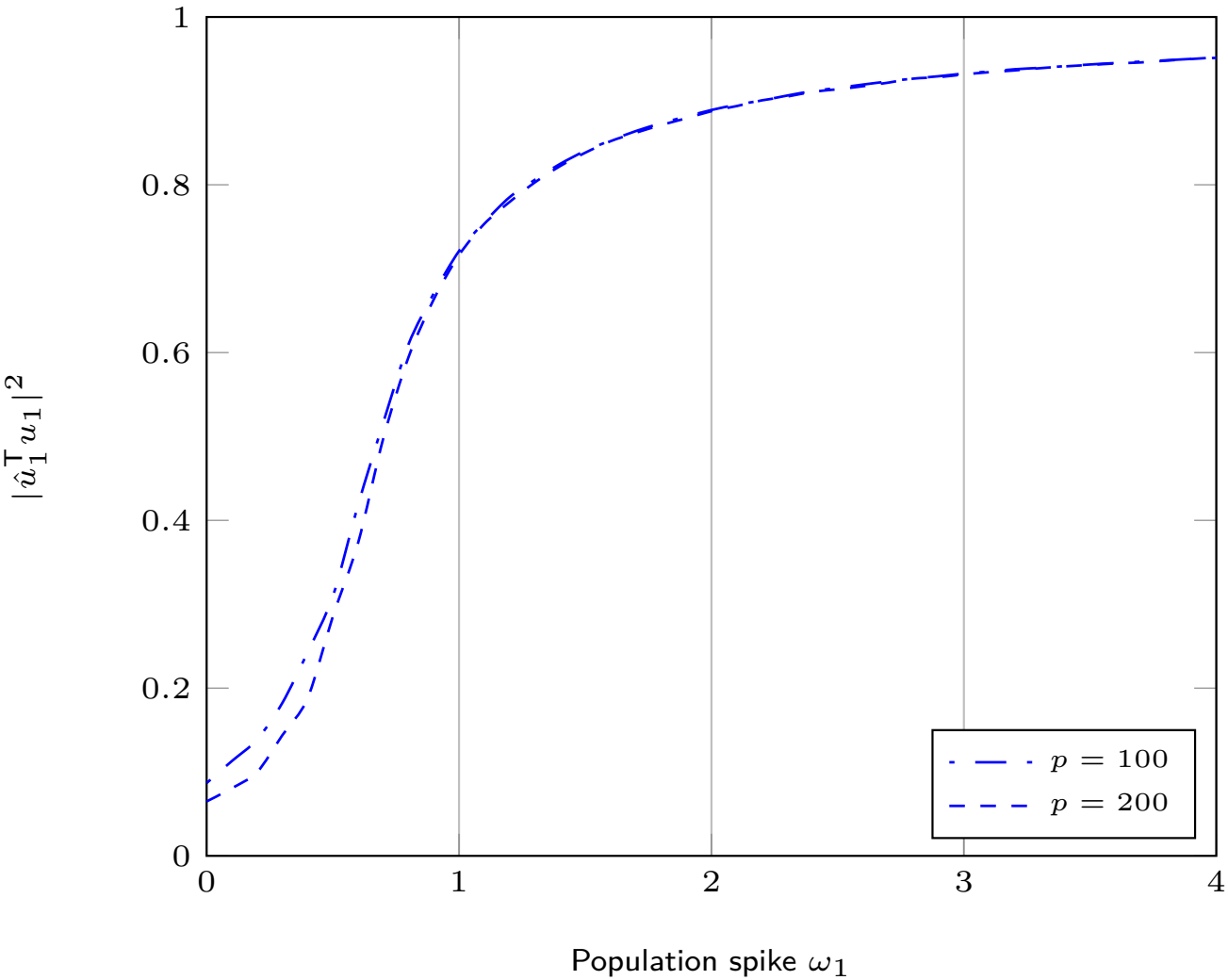

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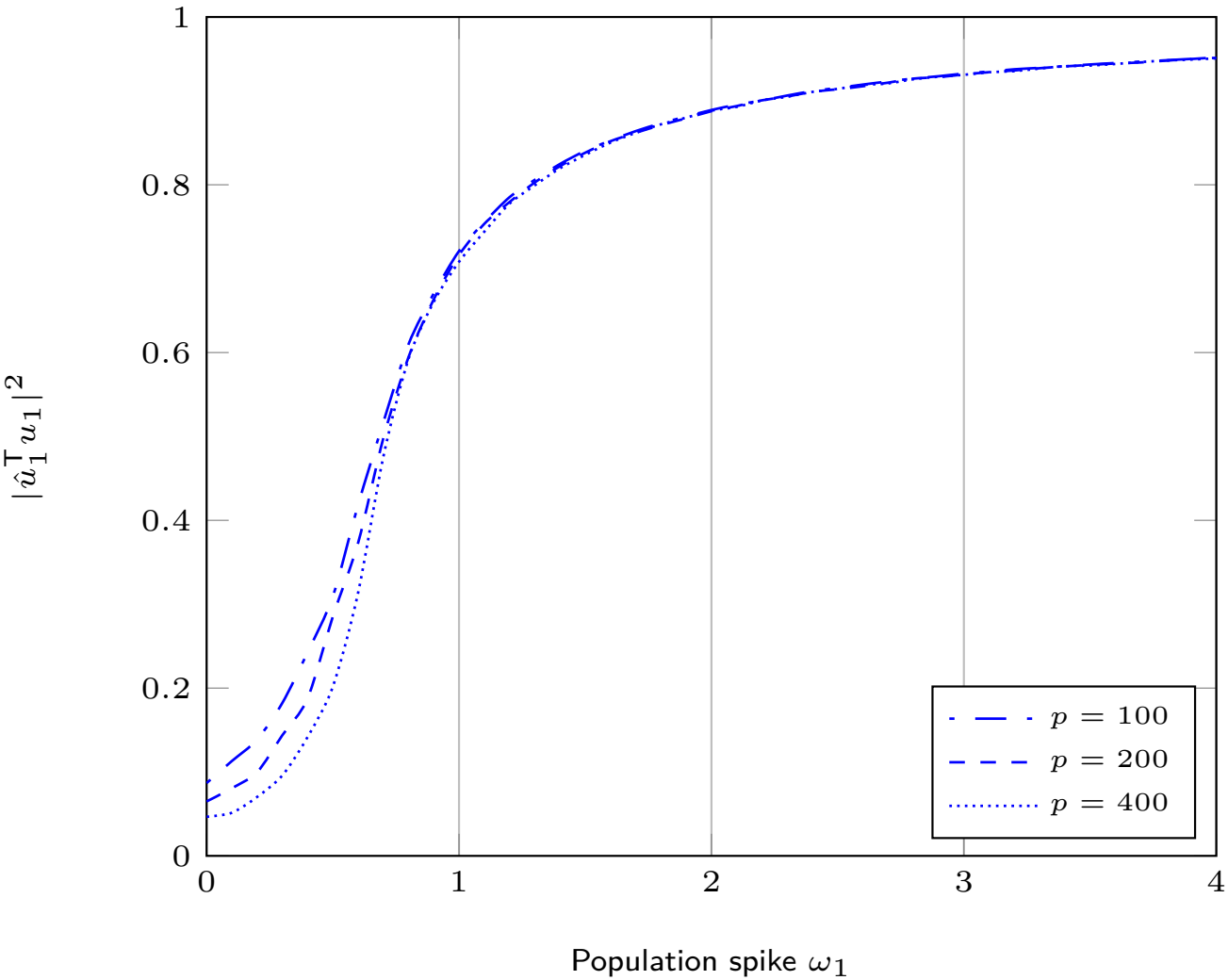

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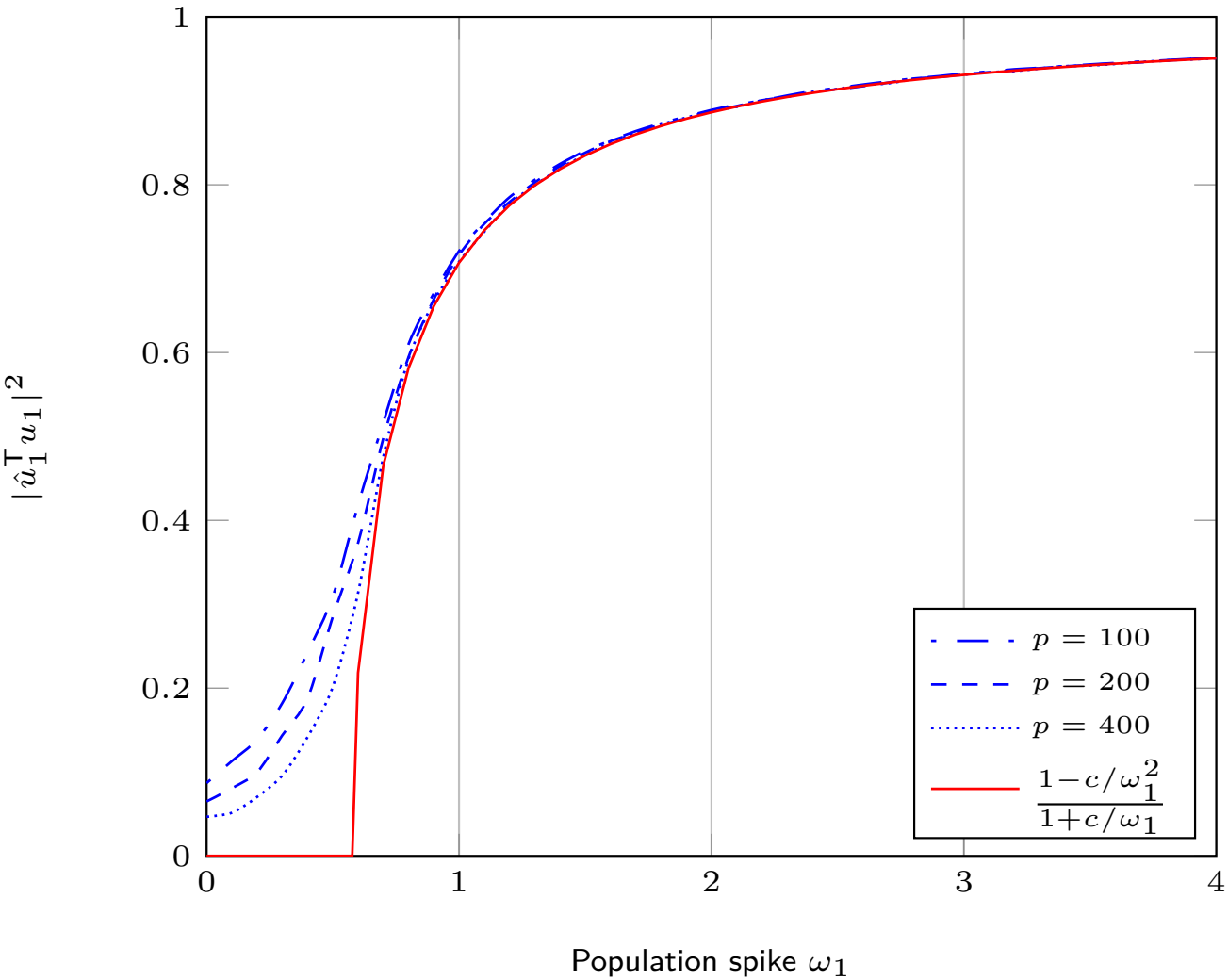

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Other Spiked Models

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 2**: In these "non-trivial" settings, **RMT explains a lot of things and can improve algorithms!**
- **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"

The curse of dimensionality and its consequences

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- GMM setting: $x_1^{(a)}, \ldots, x_{n_a}^{(a)} \sim \mathcal{N}(\mu_a, C_a)$, $a = 1, \ldots, k$
- Non-trivial task:

$$\|\mu_a - \mu_b\| = O(1), \quad \mathsf{tr}\,(C_a - C_b) = O(\sqrt{p}), \quad \mathsf{tr}\,[(C_a - C_b)^2] = O(p)$$

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- Why? **Finite-dimensional intuition**

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

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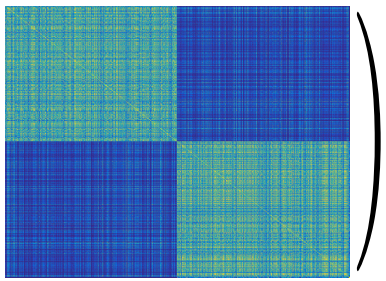
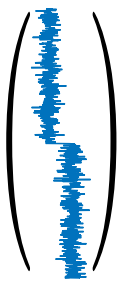
$K =$  $v_2 =$ 

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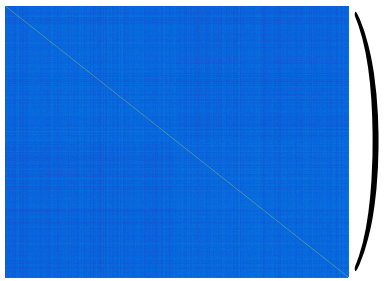
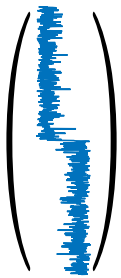
$K =$  $v_2 =$ 

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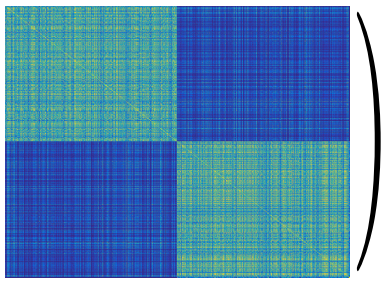
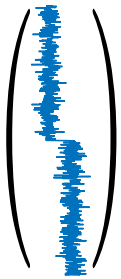
$K =$  $v_2 =$ 

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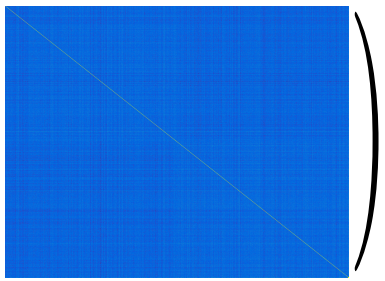
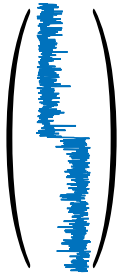
$K =$  $v_2 =$ 

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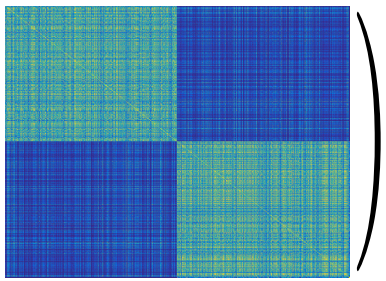
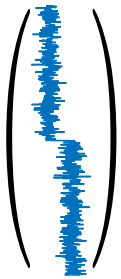
$K =$  $v_2 =$ 

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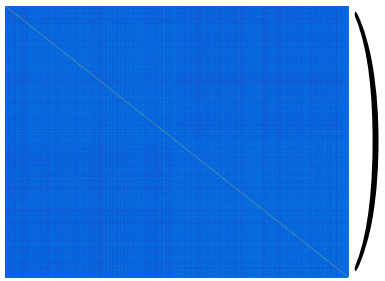
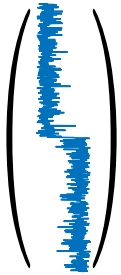
$K =$  $v_2 =$ 

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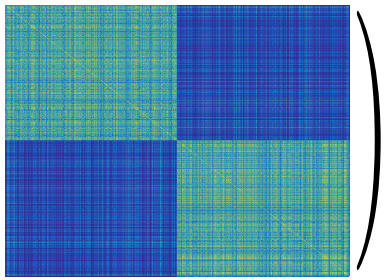
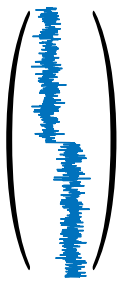
$K =$  $v_2 =$ 

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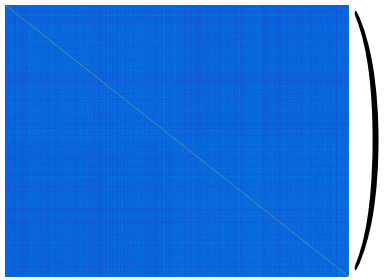
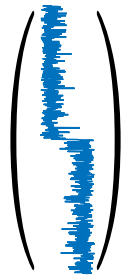
$K =$  $v_2 =$ 

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- more importantly, **in non-trivial settings, data are neither close, nor far!**

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RMT can explain tools engineers (and researchers) have used blindly for decades!

Isolated eigenvalues: Gaussian inputs

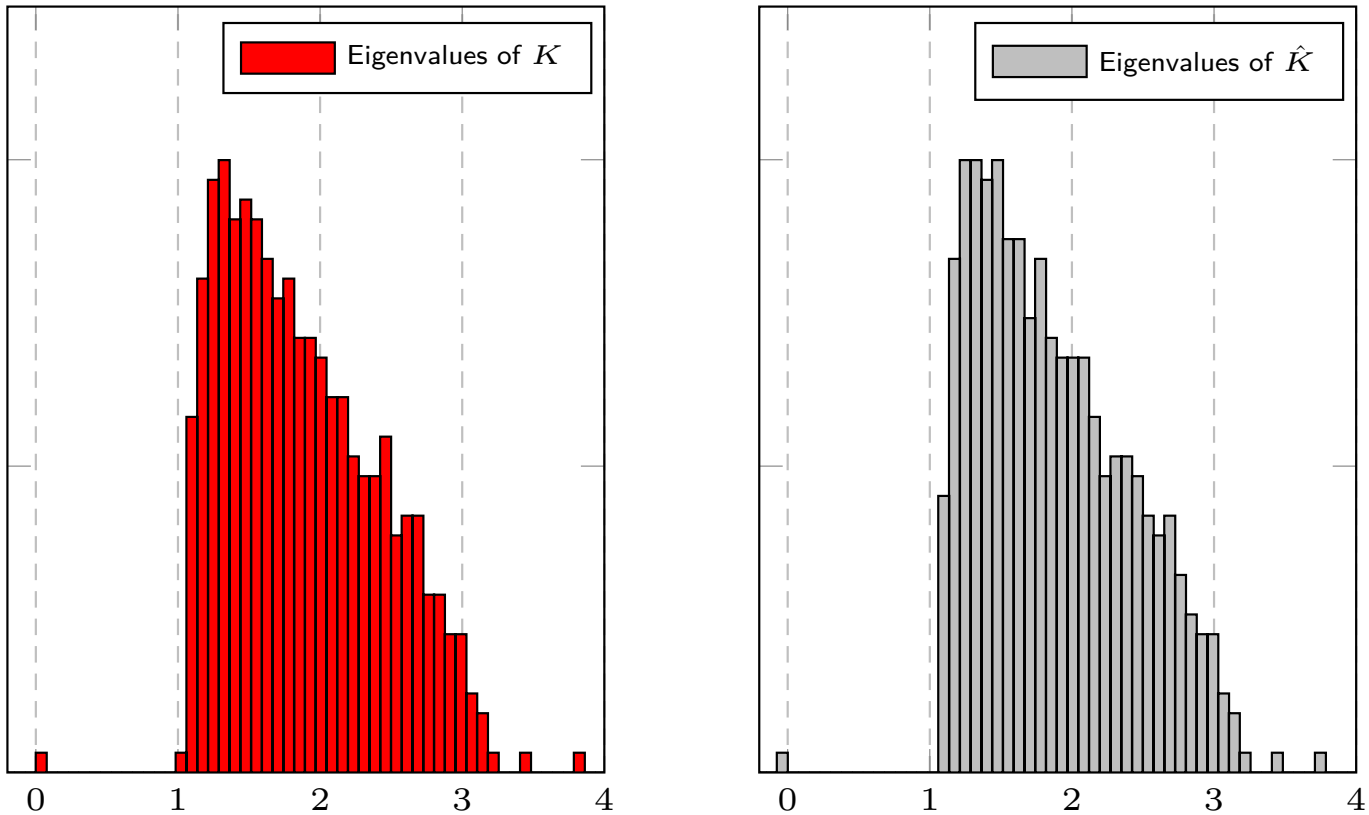

Figure: Eigenvalues of K and $\hat{K}$, $k = 3$, $p = 2048$, $n = 512$, $c_1 = c_2 = 1/4$, $c_3 = 1/2$, $[\mu_a]_j = 4\boldsymbol{\delta}_{aj}$, $C_a = (1 + 2(a-1)/\sqrt{p})I_p$, $f(x) = \exp(-x/2)$.

Theoretical Findings versus MNIST

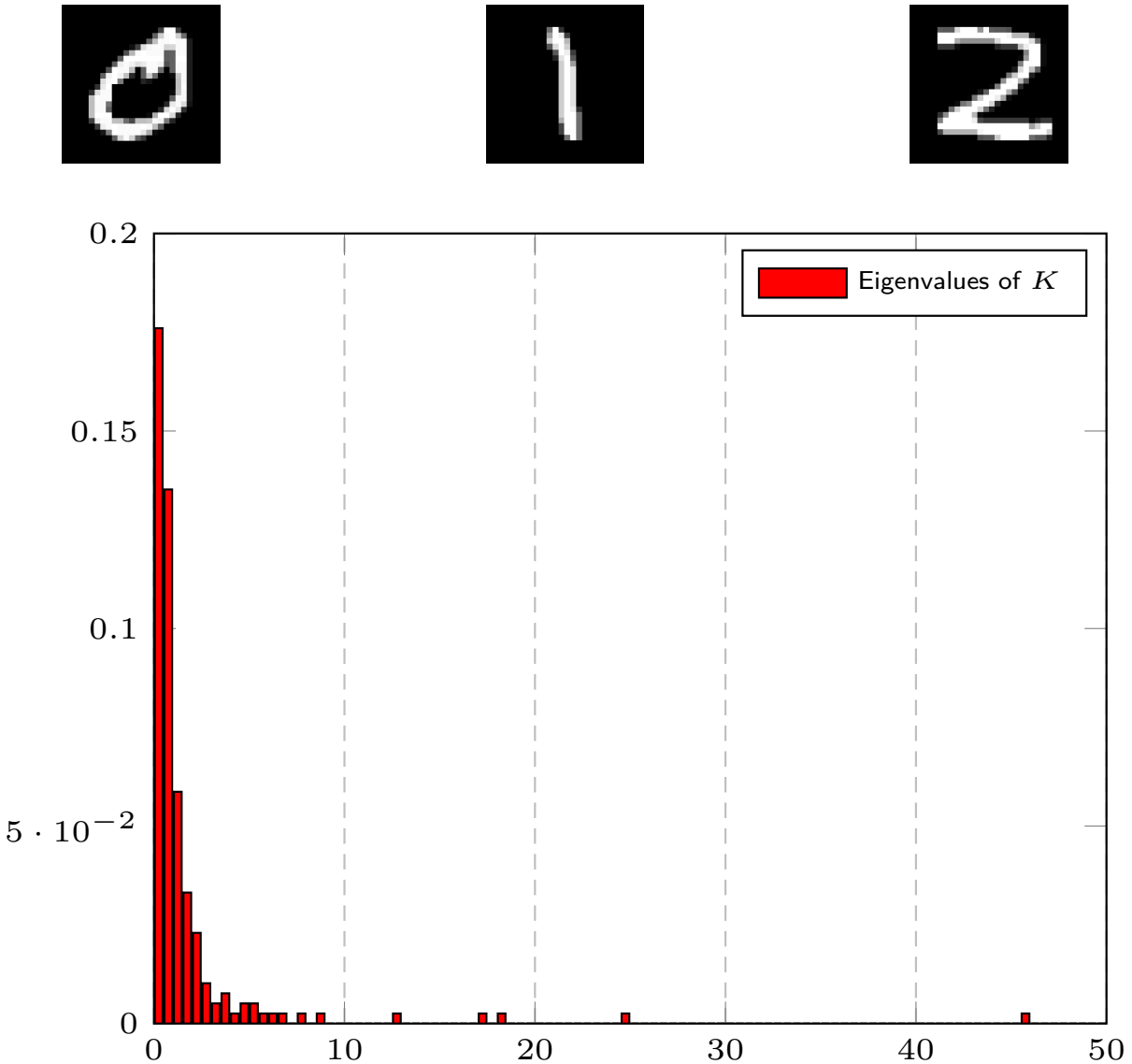

Figure: Eigenvalues of K (red) and (equivalent Gaussian model) $\hat{K}$ (white), MNIST data, $p = 784$, $n = 192$.

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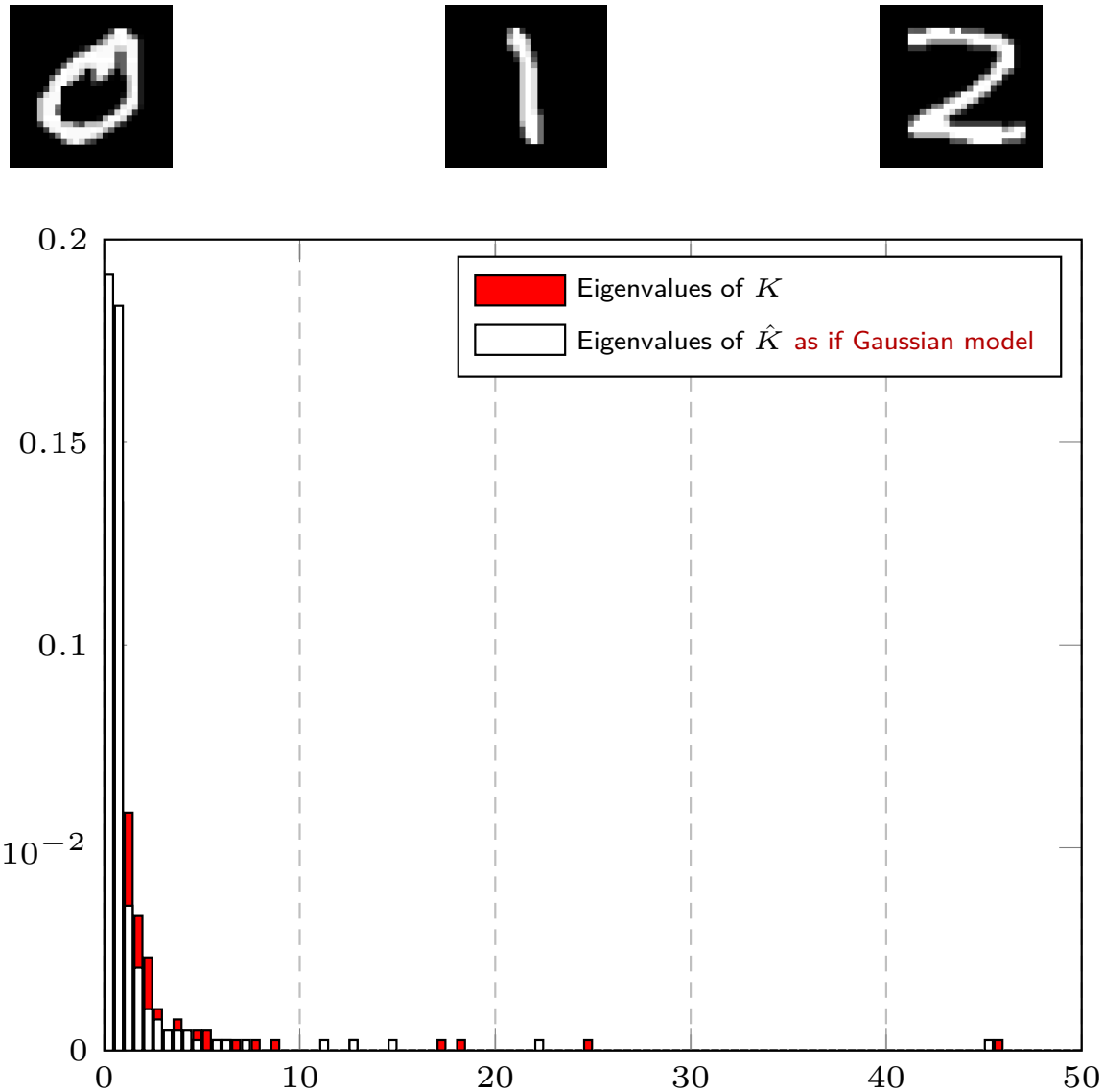

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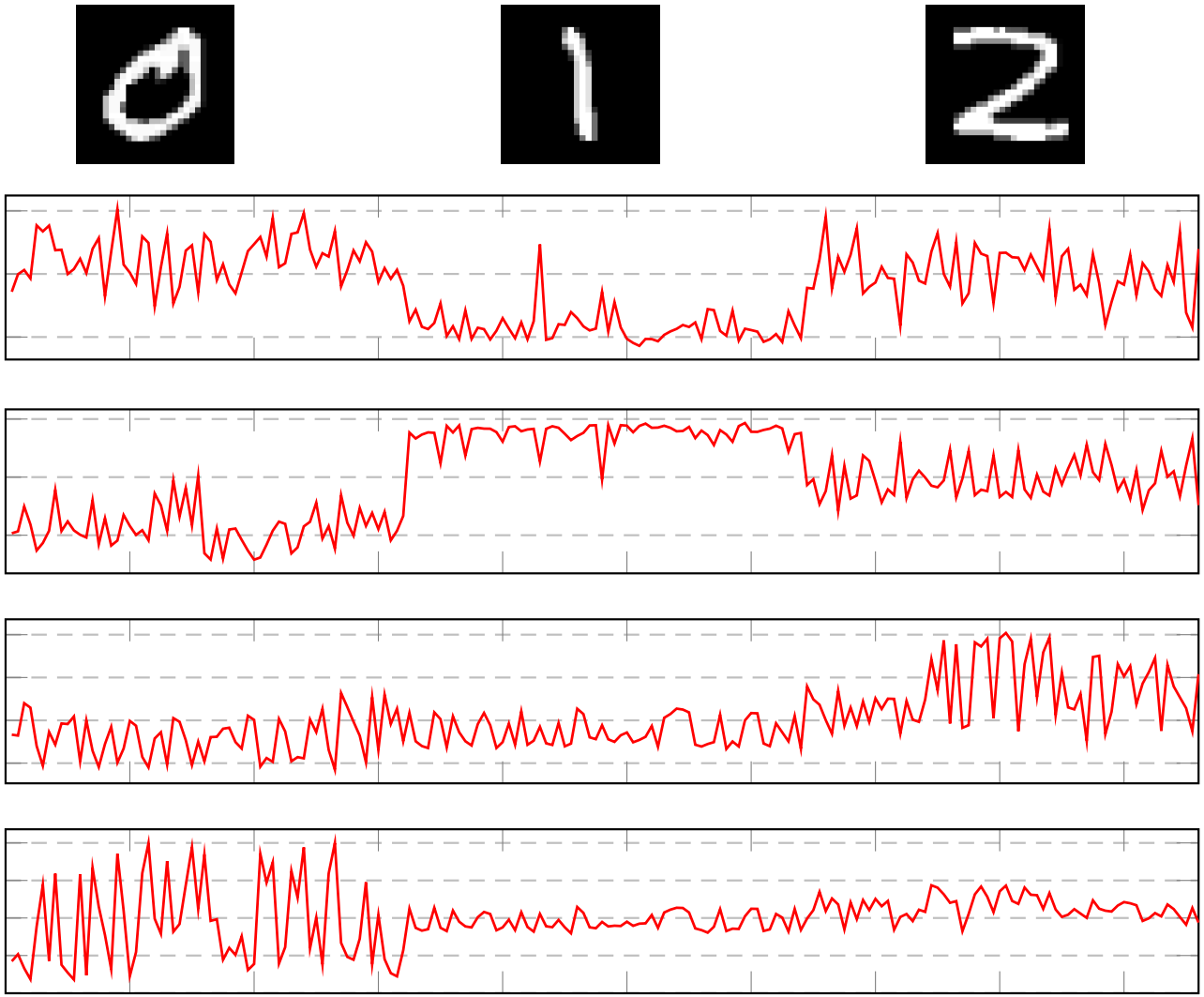

Figure: Leading four eigenvectors of K for MNIST data (**red**) and theoretical findings (**blue**).

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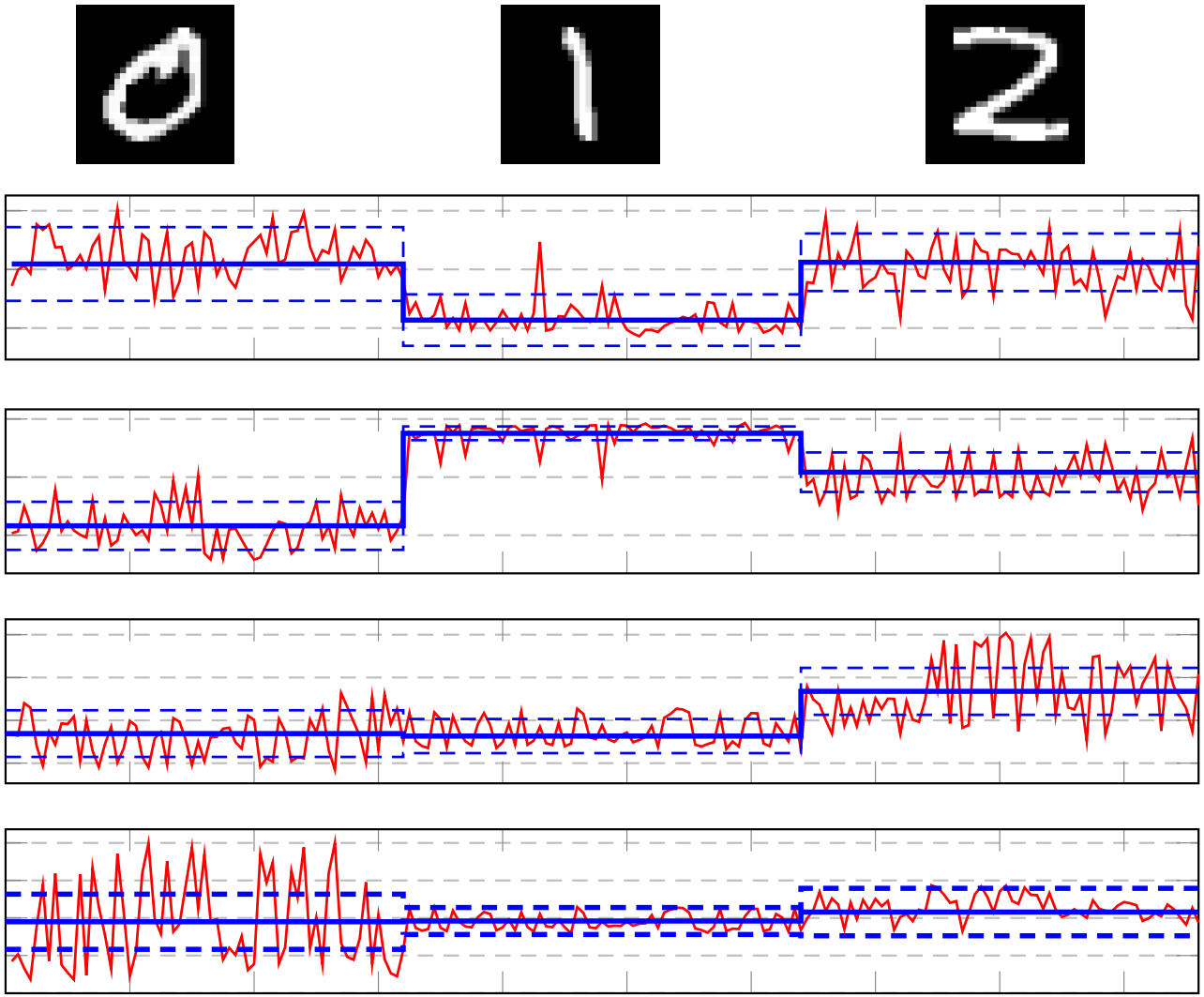

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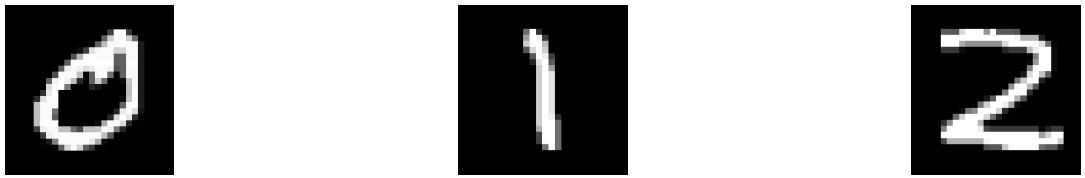
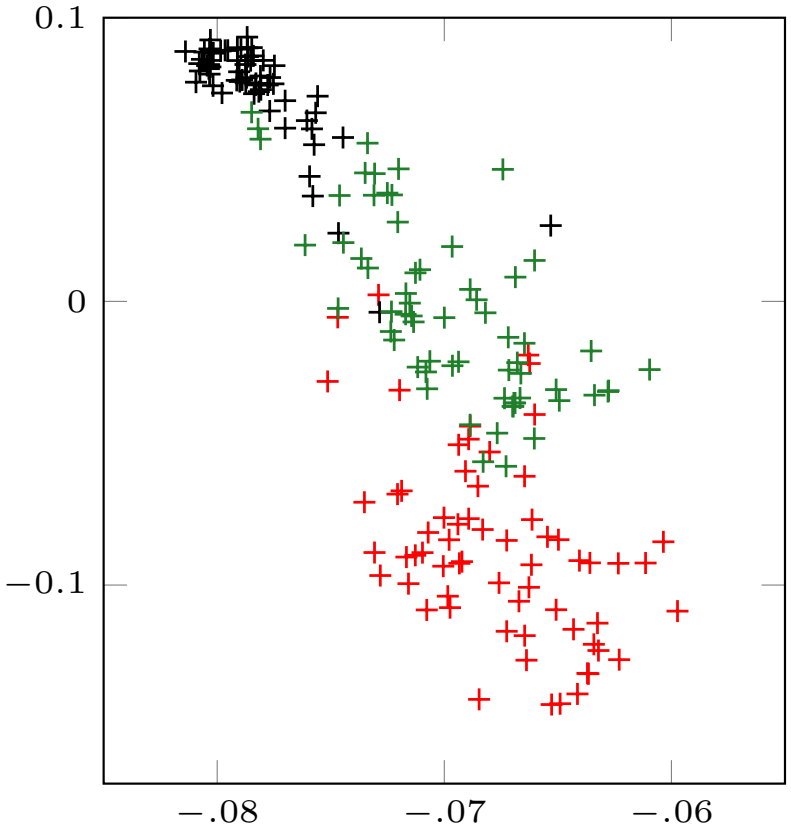
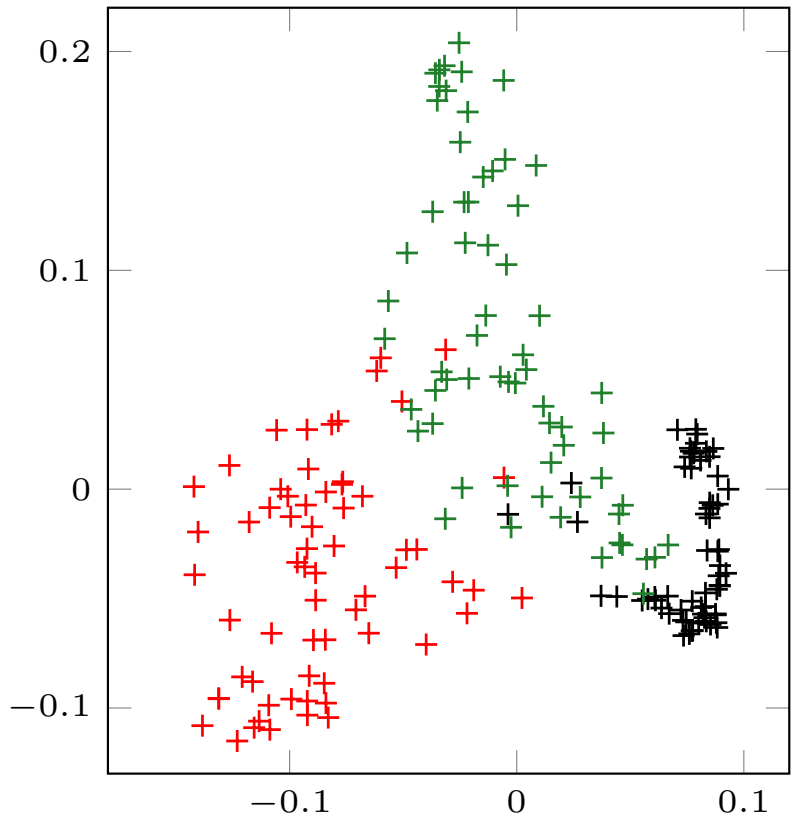


Eigenvector 2/Eigenvector 1



Eigenvector 3/Eigenvector 2



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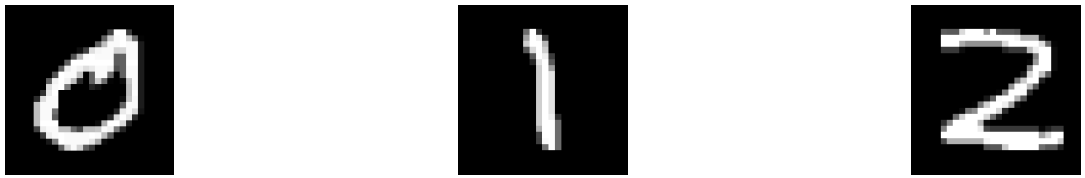

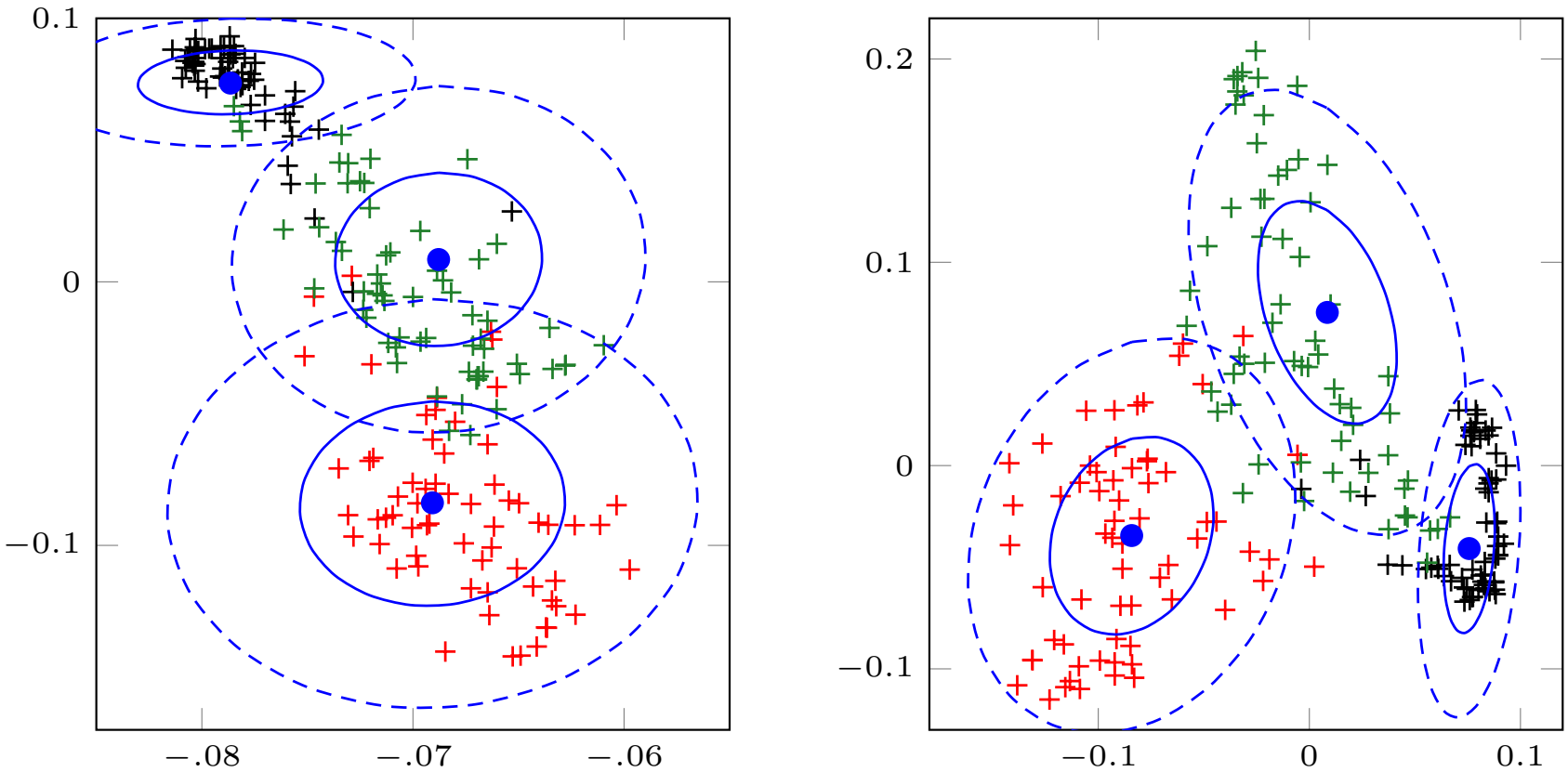

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Takeaway Message 2

"RMT Reassesses and Improves Data Processing"

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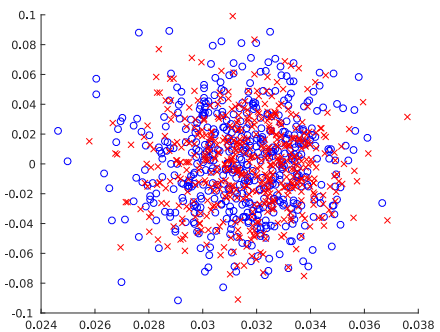
Gaussian vectors $\mathcal{N}(0, C_1)$ vs. $\mathcal{N}(0, C_2)$



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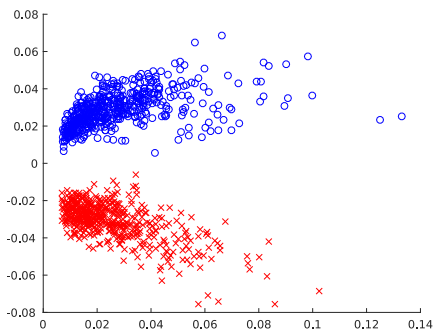

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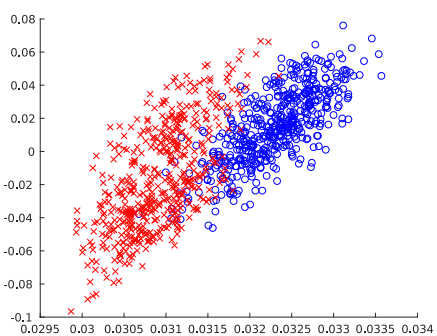
Real EEG data



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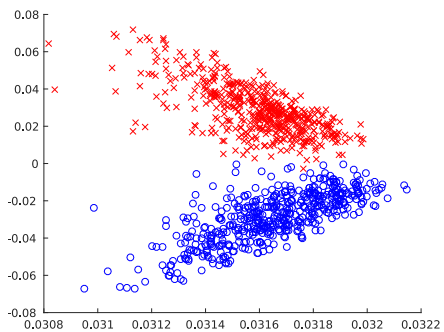

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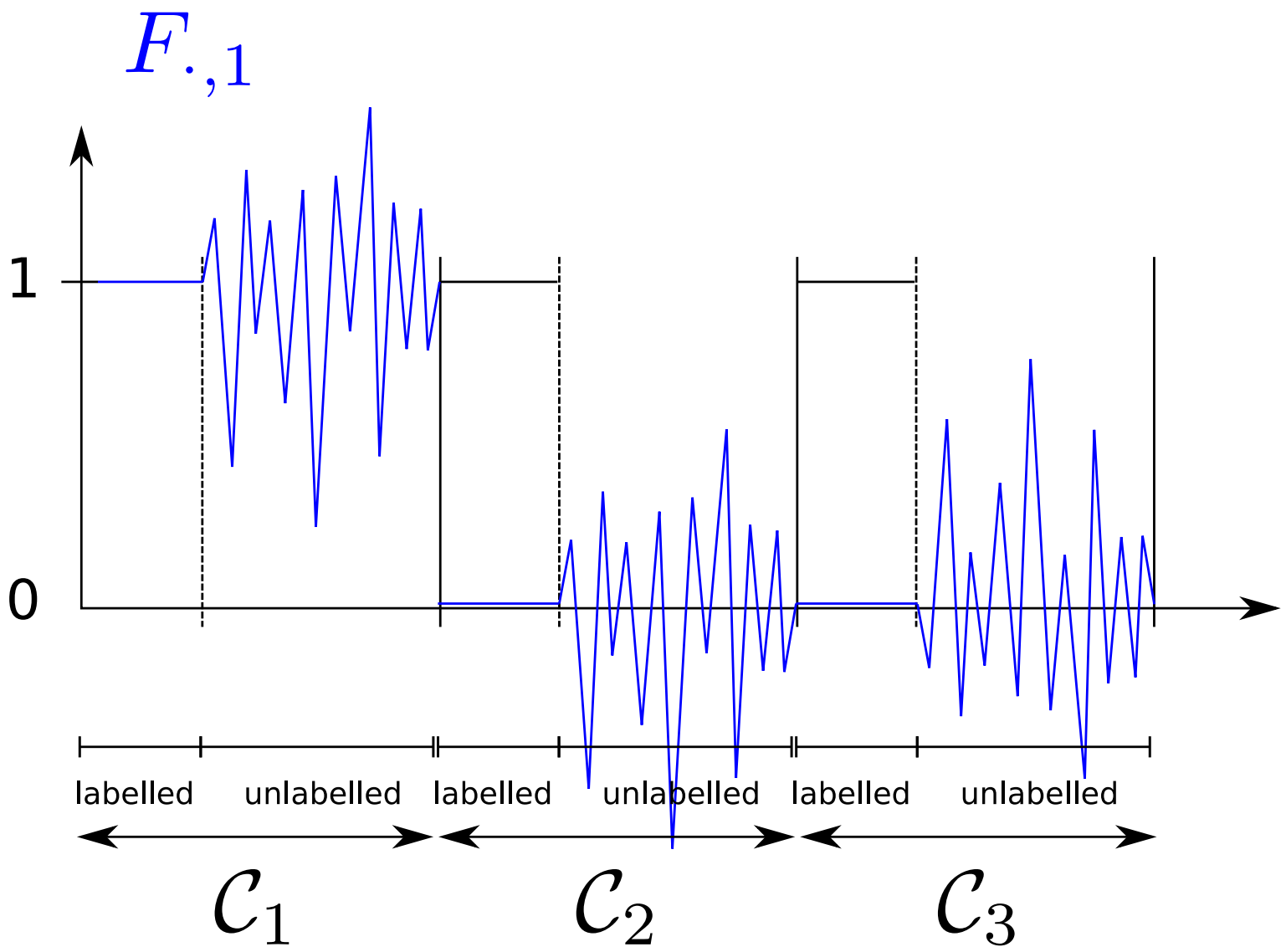
- **Explicit solution**:

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

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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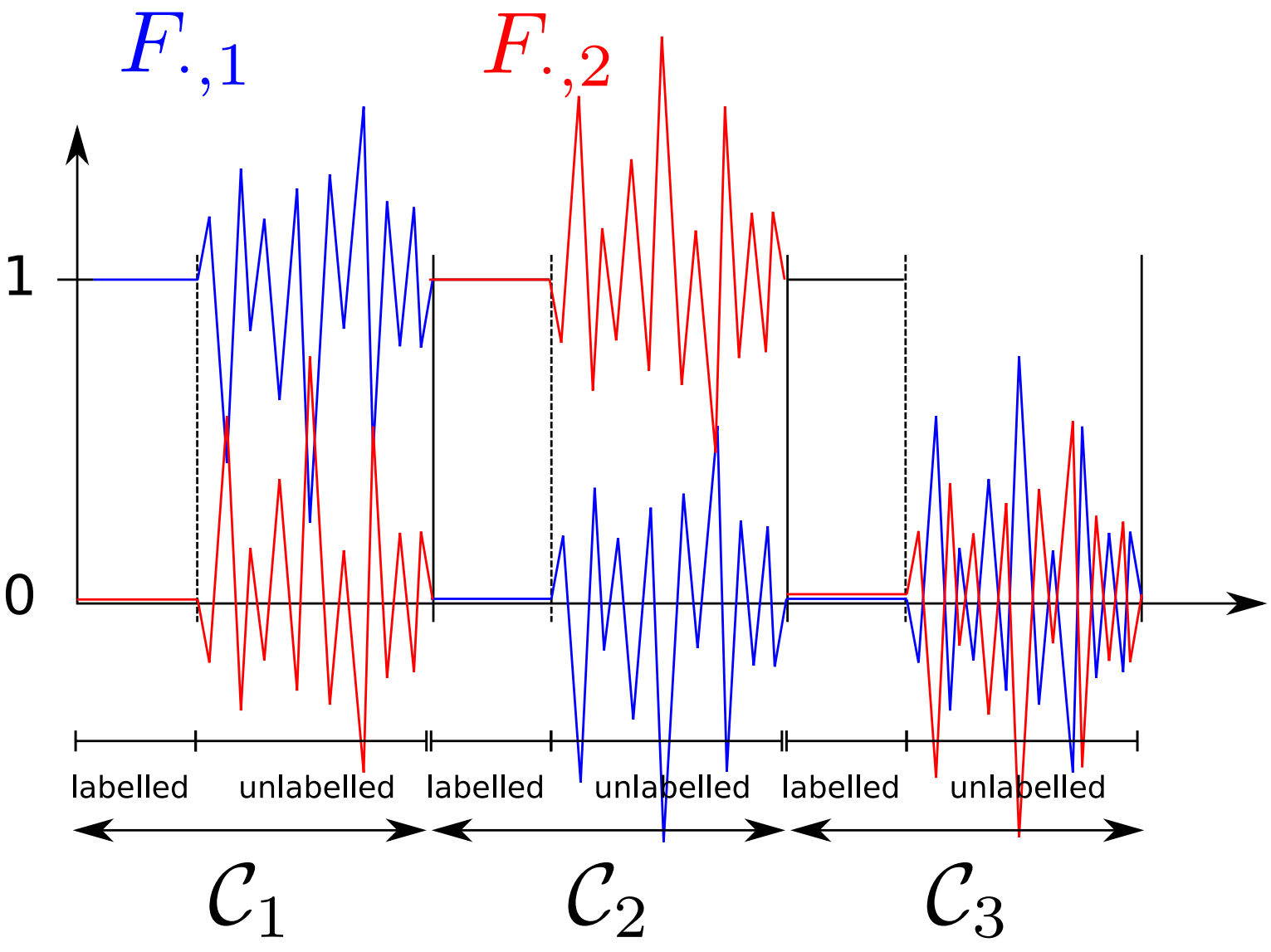

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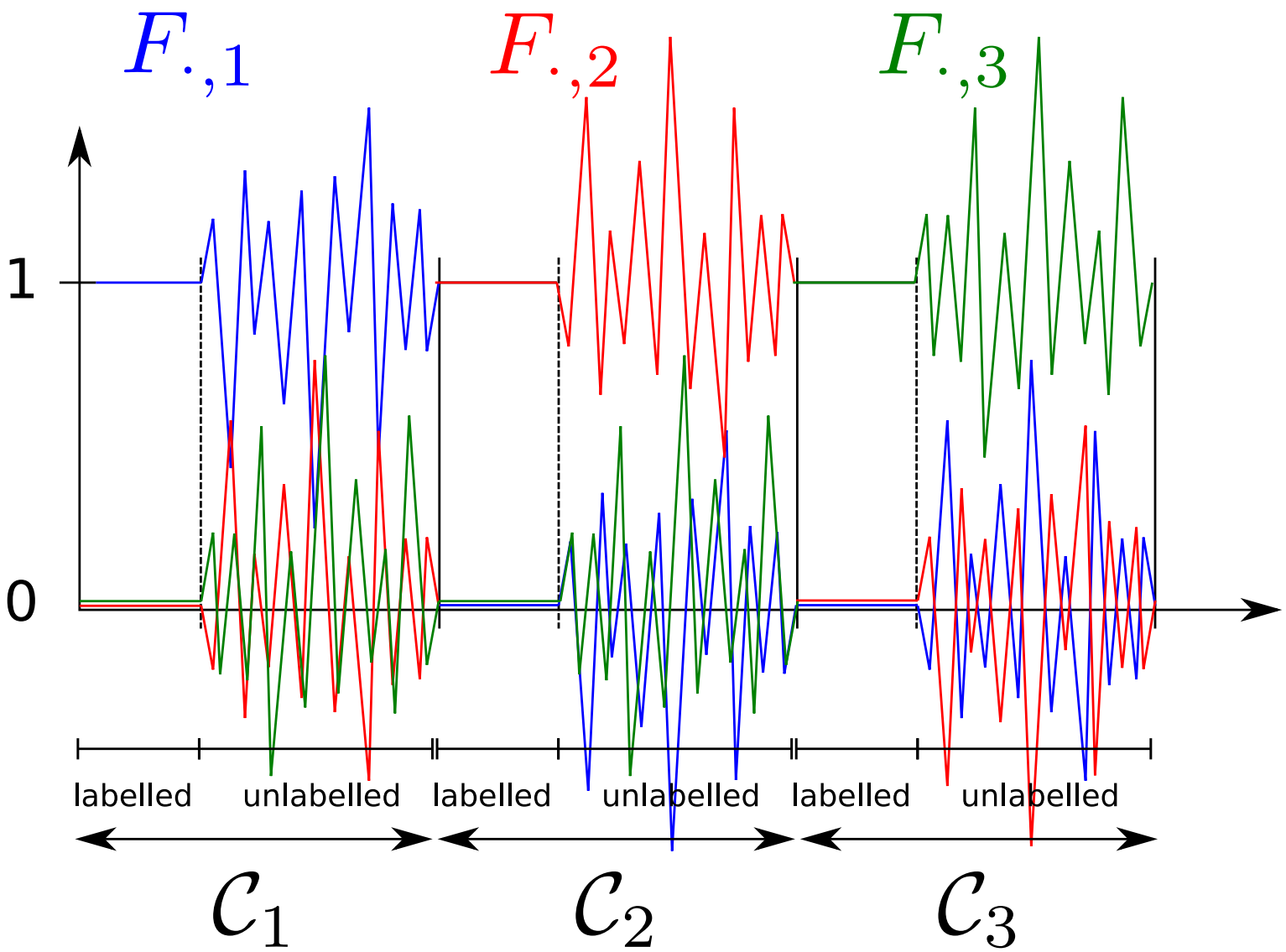
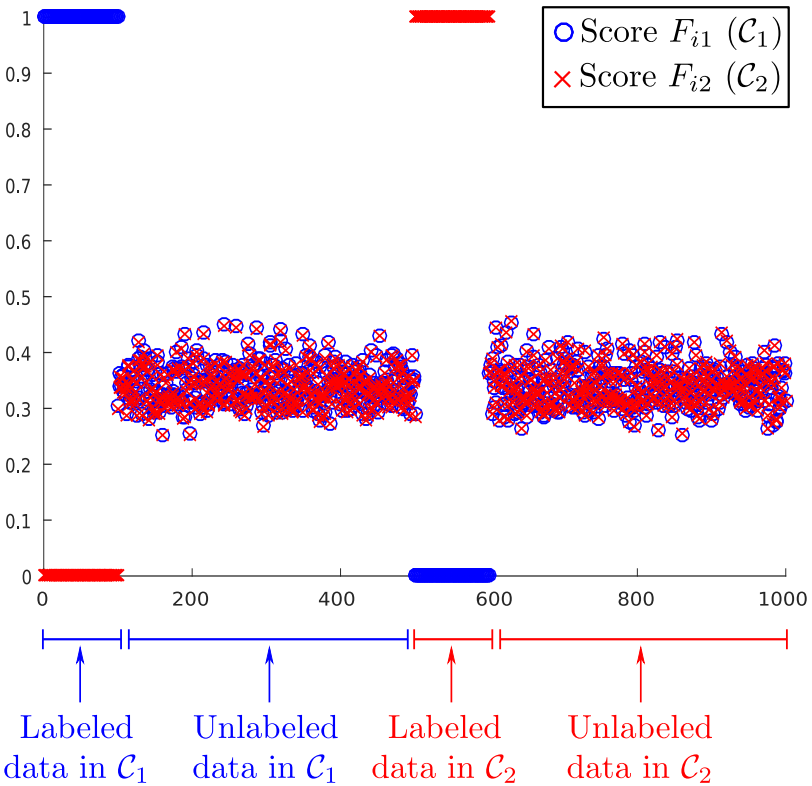
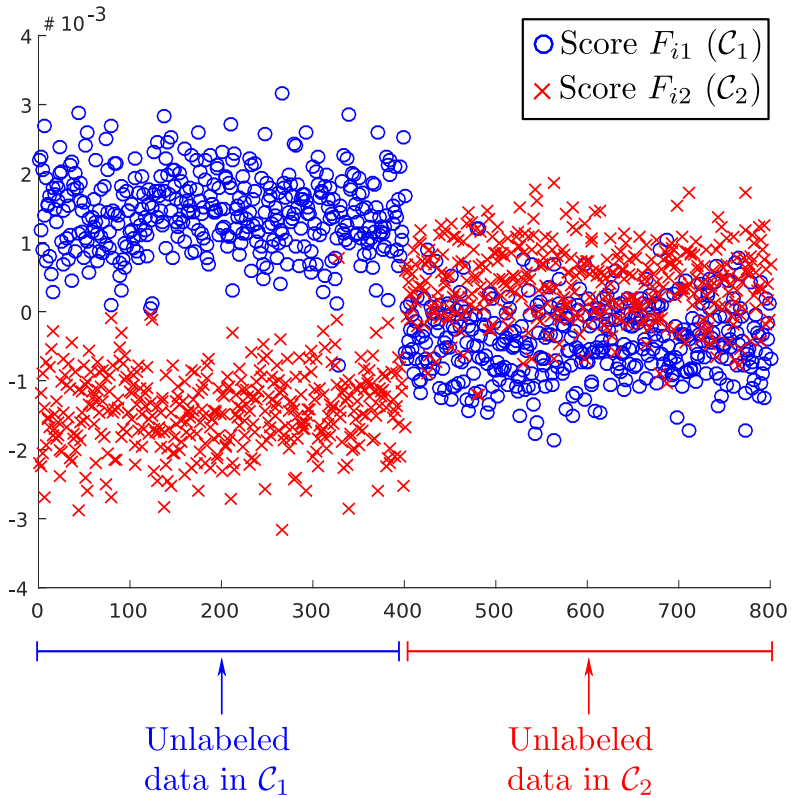


The reality: What we see!

Setting. $p = 400$, $n = 1000$, $x_i \sim \mathcal{N}(\pm\mu, I_p)$. Kernel $K_{ij} = \exp(-\frac{1}{2p}\|x_i - x_j\|^2)$.

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





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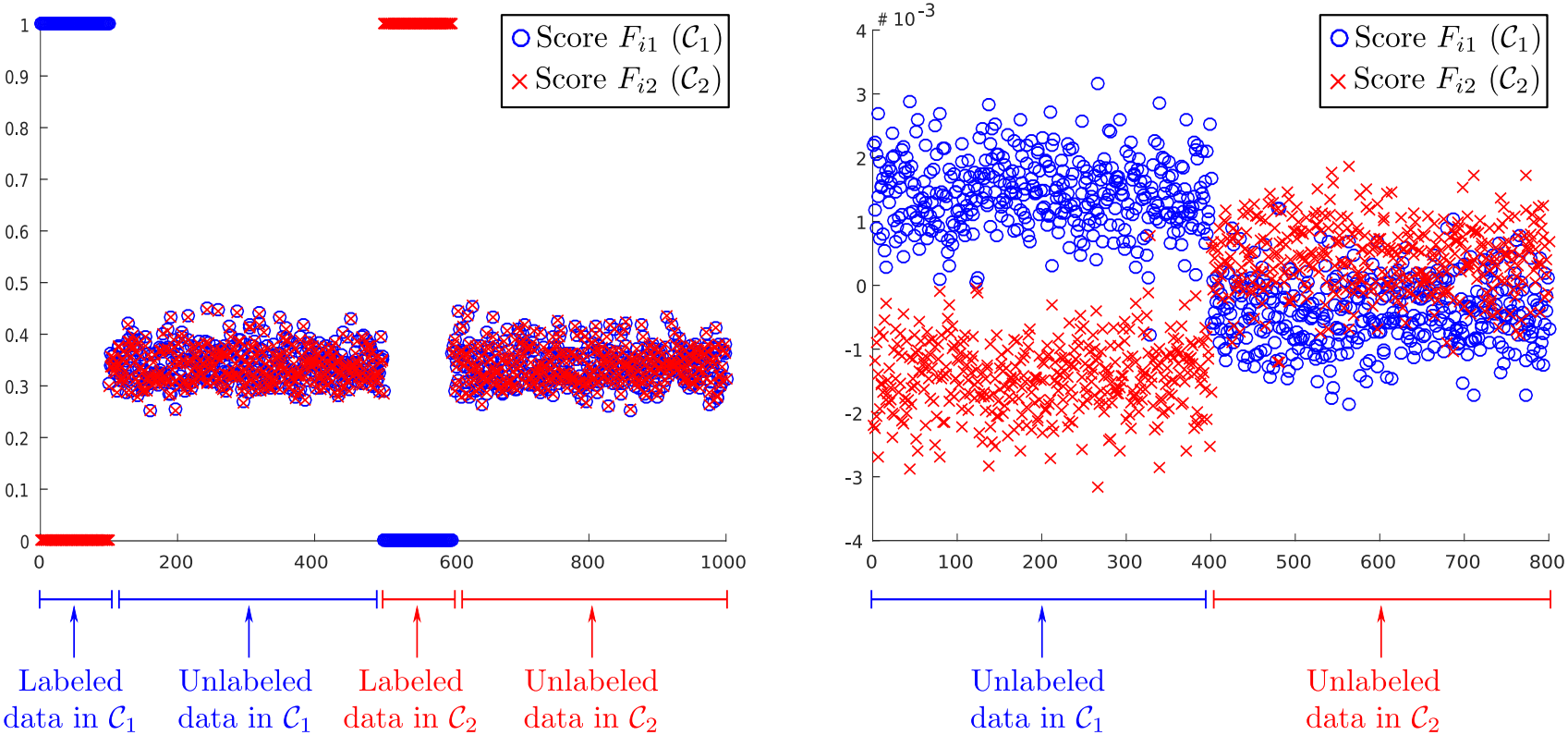

➪ **Score are almost all identical... and do not follow the labelled data!**

MNIST Data Example

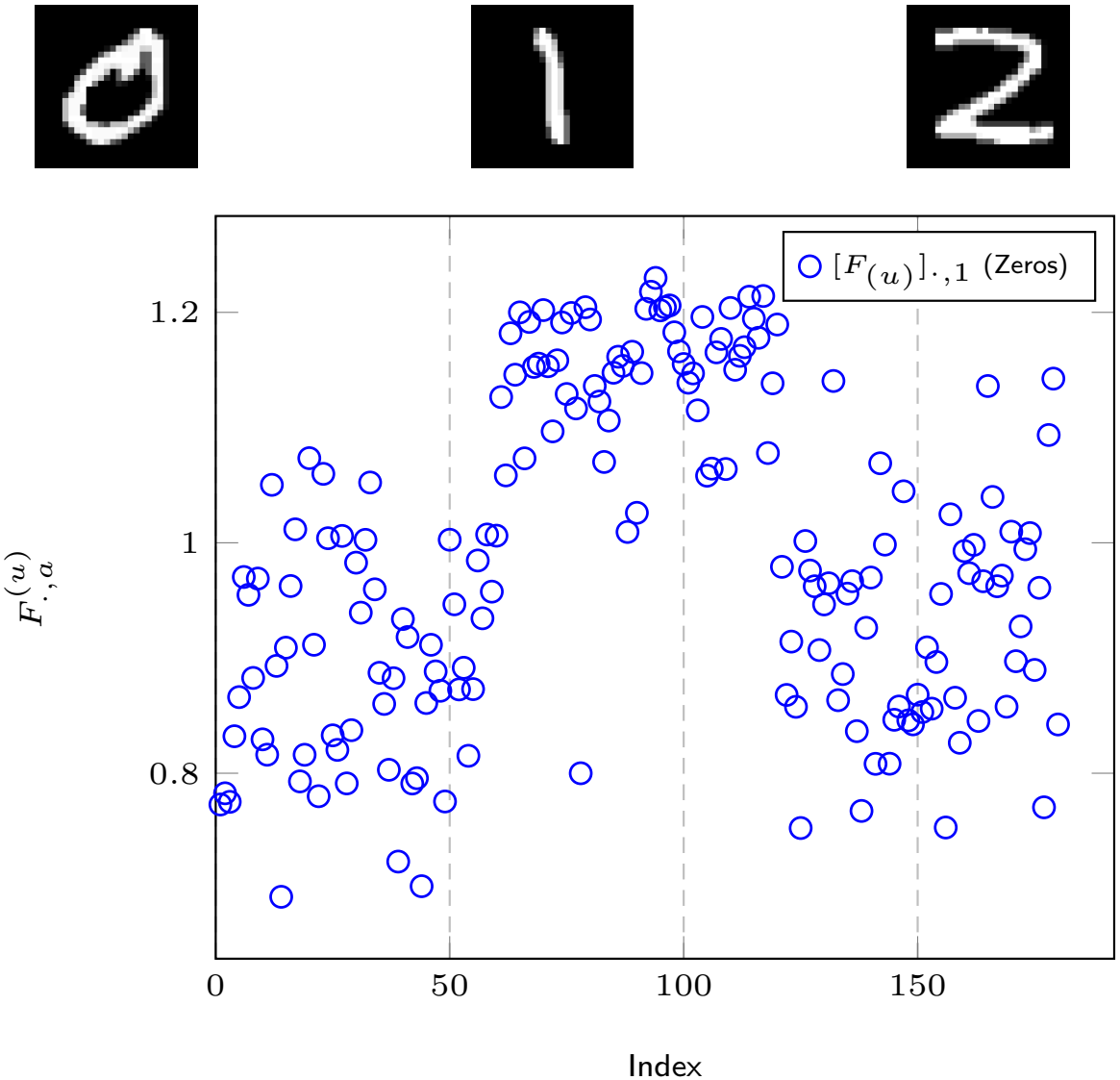

Figure: Vectors $[F^{(u)}]_{\cdot,a}$, $a = 1, 2, 3$, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

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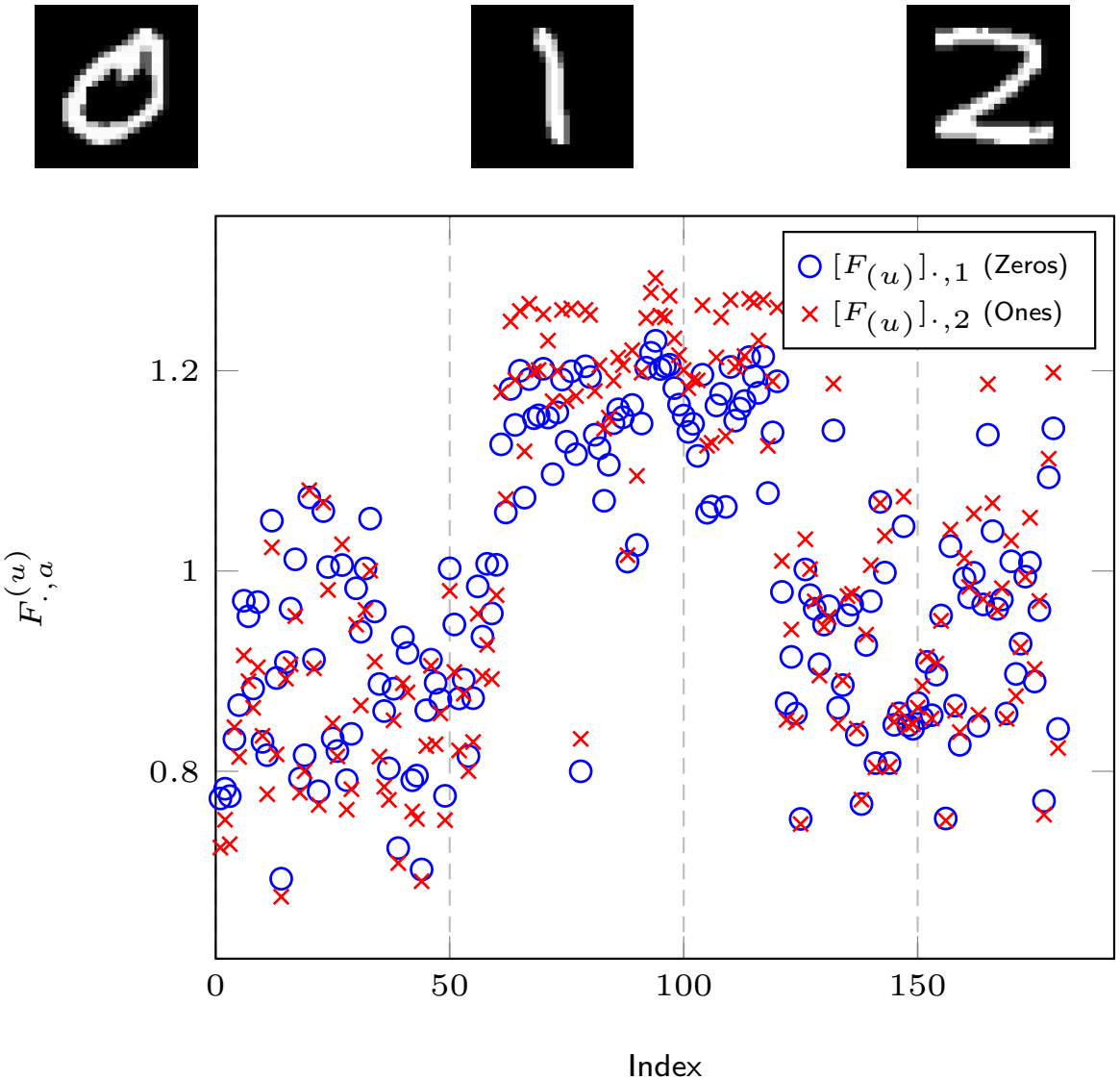

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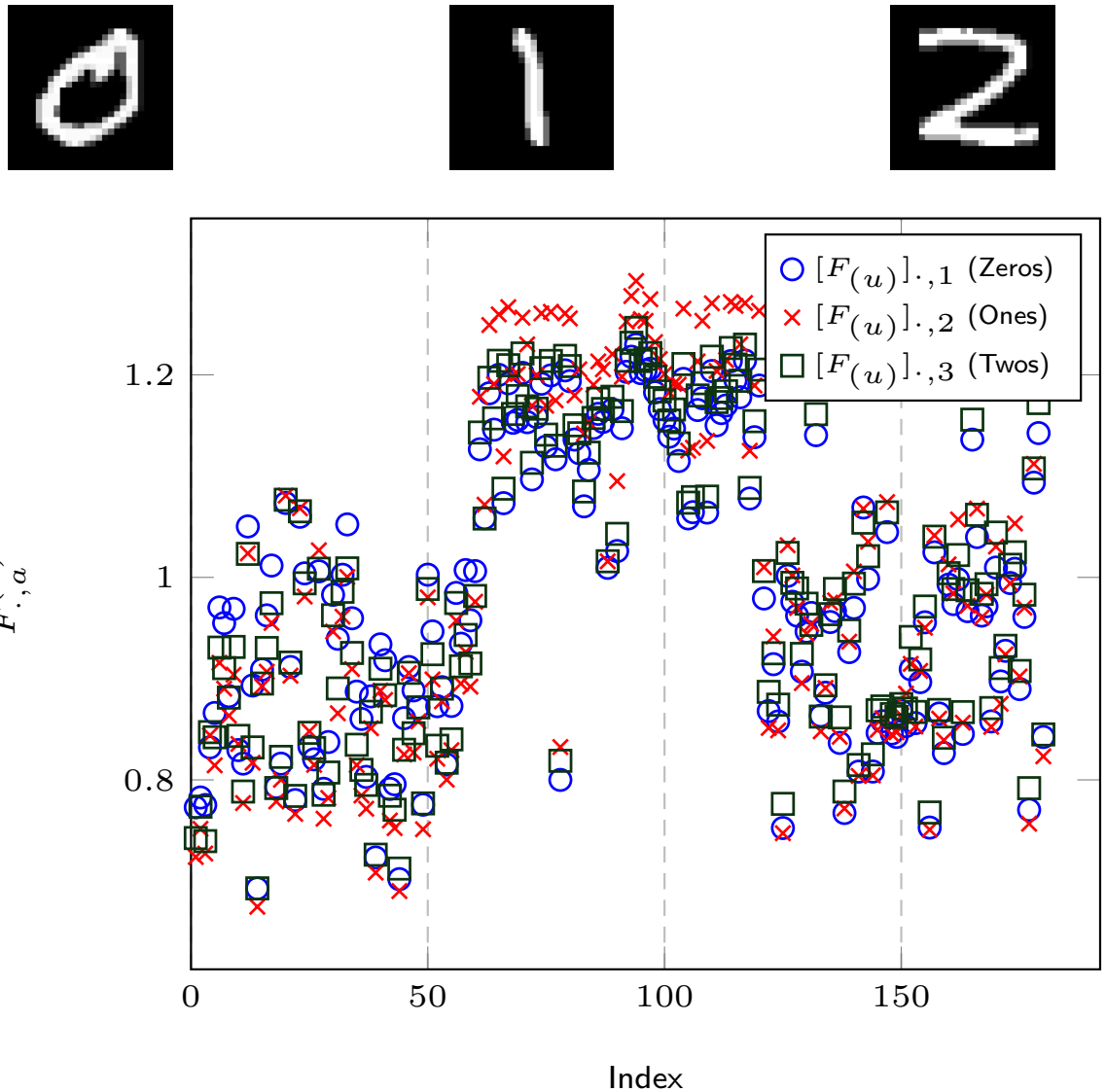

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- Update the algorithm and **provably improve unlabelled data use**.

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

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with $m_b \in \mathbb{R}^k$, $\Sigma_b \in \mathbb{R}^{k \times k}$ function of $f(\tau), f'(\tau), f''(\tau)$, $\mu_1, \ldots, \mu_k$, $C_1, \ldots, C_k$.

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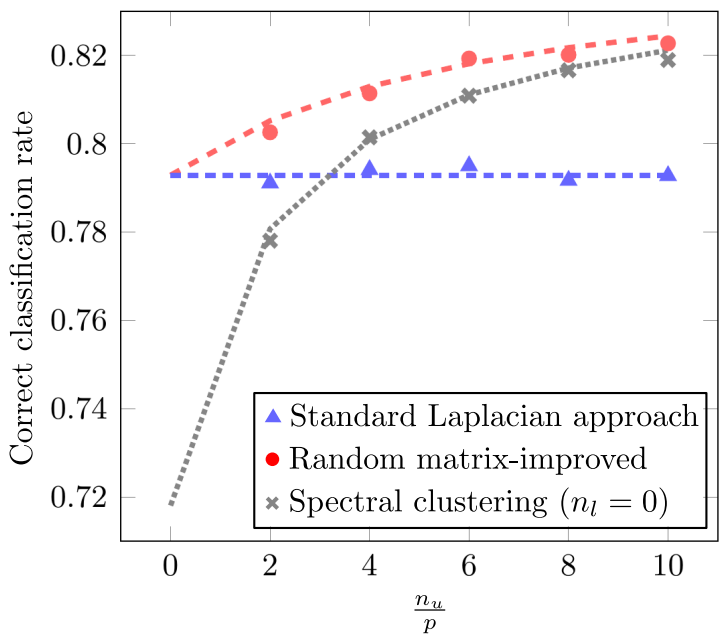
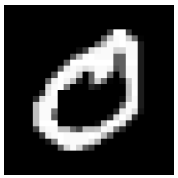
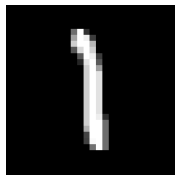


Experimental evidence: MNIST


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
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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)
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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
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Centered kernel **(RMT)**	83.6±2.4	84.6±2.4	88.7±9.4
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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"

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

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$x \in \mathbb{R}^p$ is a concentrated random vector if, for all Lipschitz $f : \mathbb{R}^p \to \mathbb{R}$, there exists $m_f \in \mathbb{R}$, wuch that

$$P\left(|f(x) - m_f| > \varepsilon\right) \leq e^{-g(\varepsilon)}, \quad g \text{ increasing function.}$$

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

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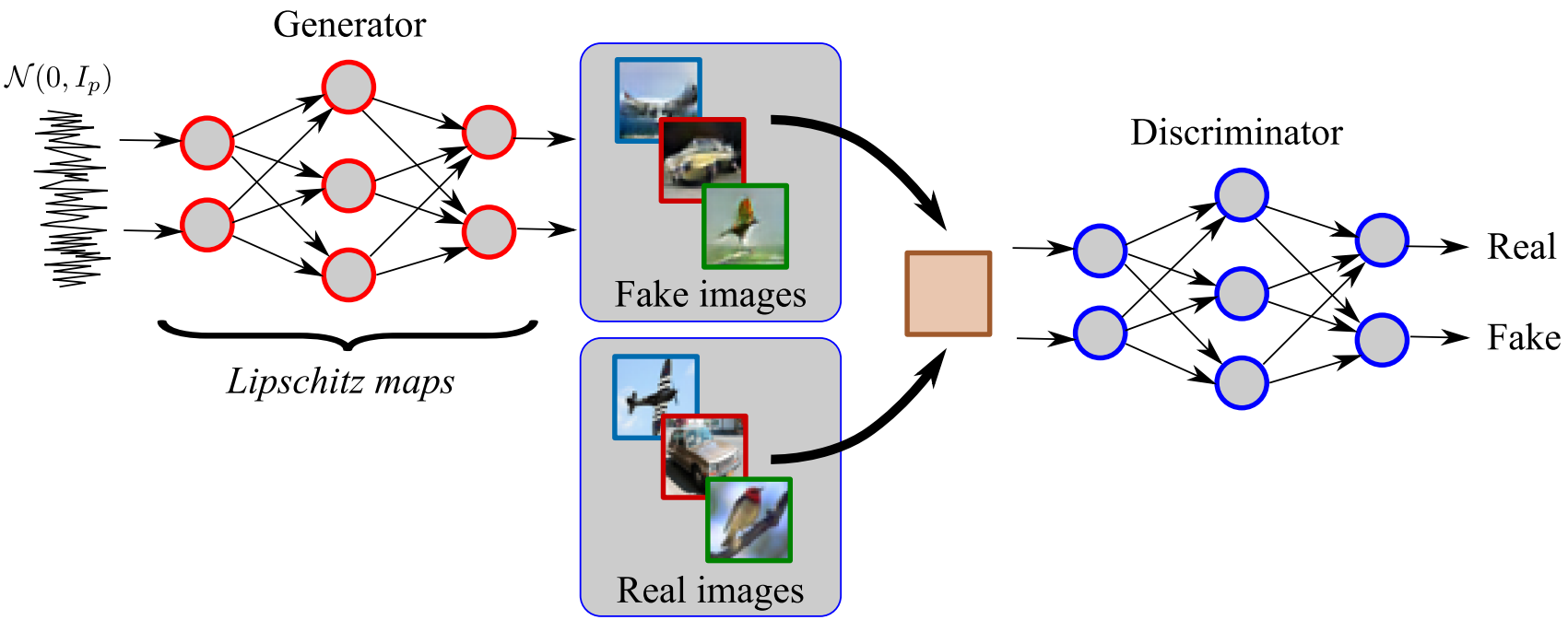
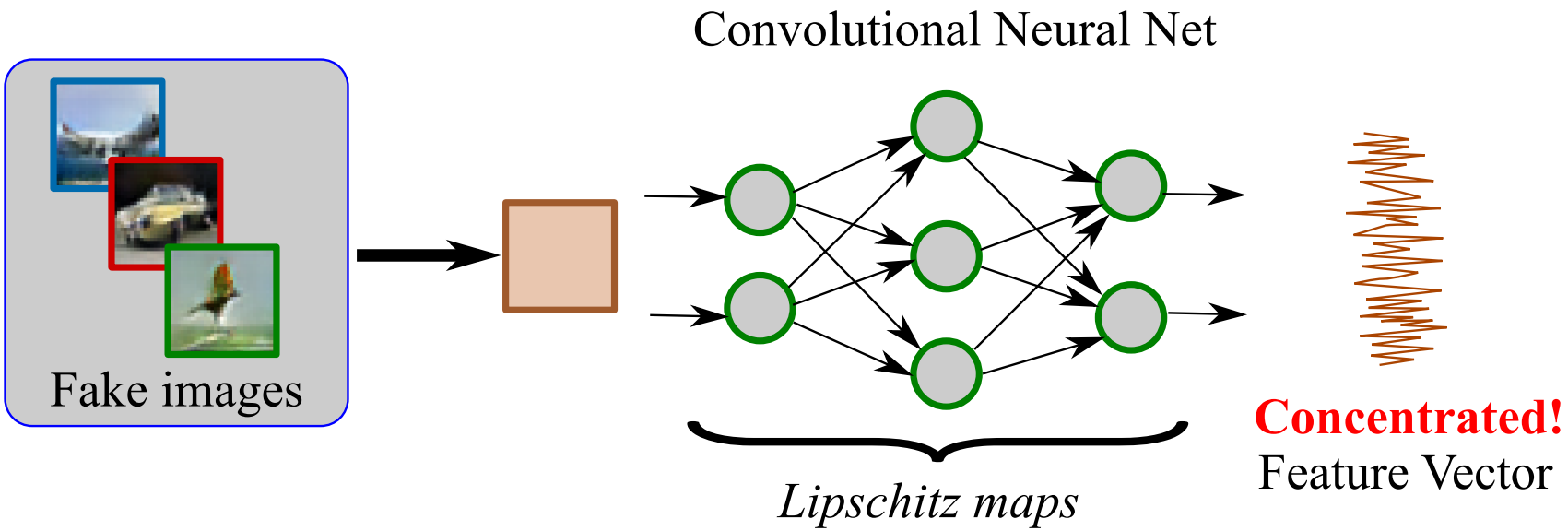
Key Finding. **Real images are "almost" concentrated random vectors!**

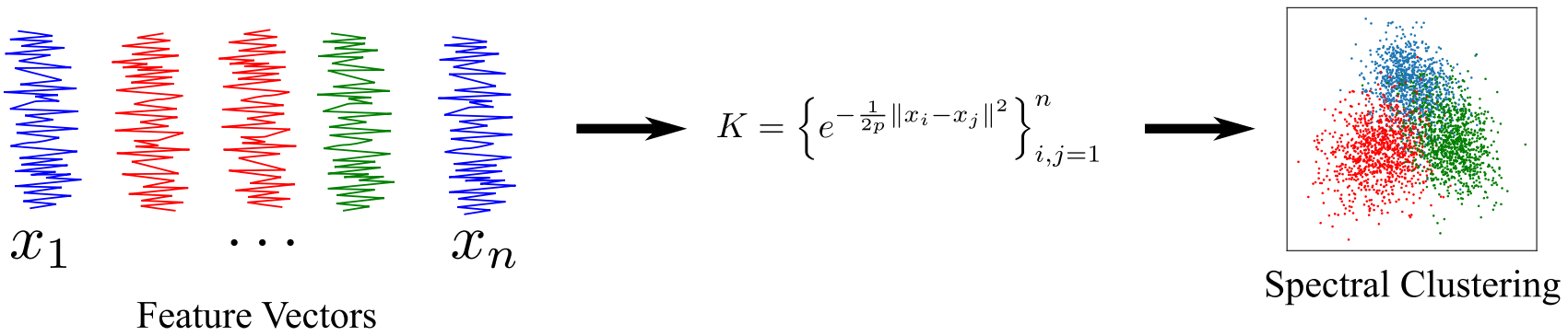
Example: GAN-generated images **are concentrated random vectors!**



Ok. . . so what?


Convolutional Neural Net
Fake images
Lipschitz maps
Concentrated!
Feature Vector

Ok. . . so what?

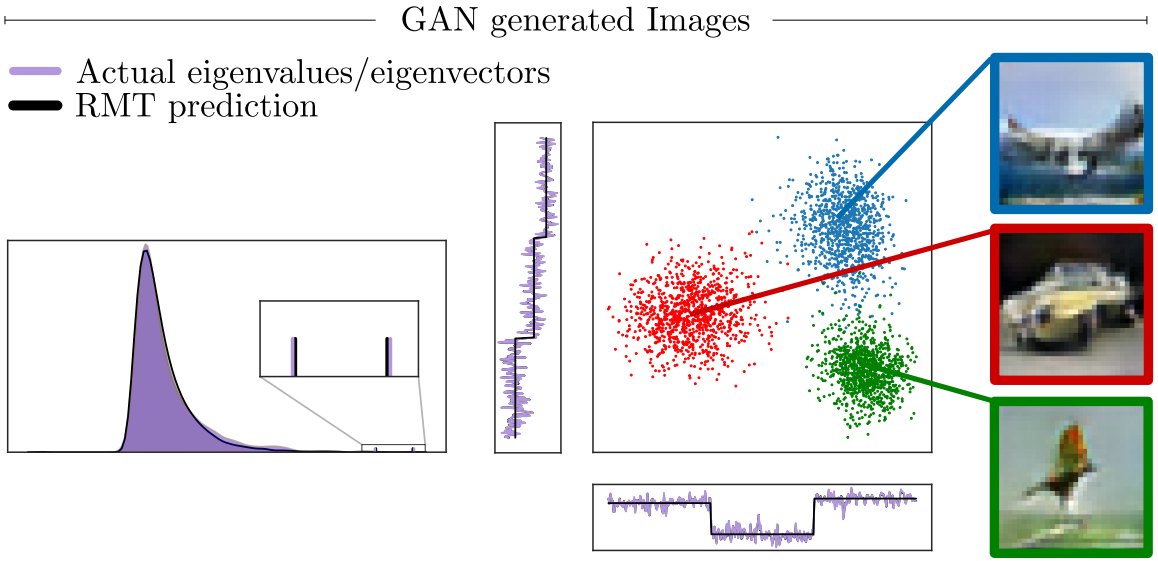


Feature Vectors

Spectral Clustering

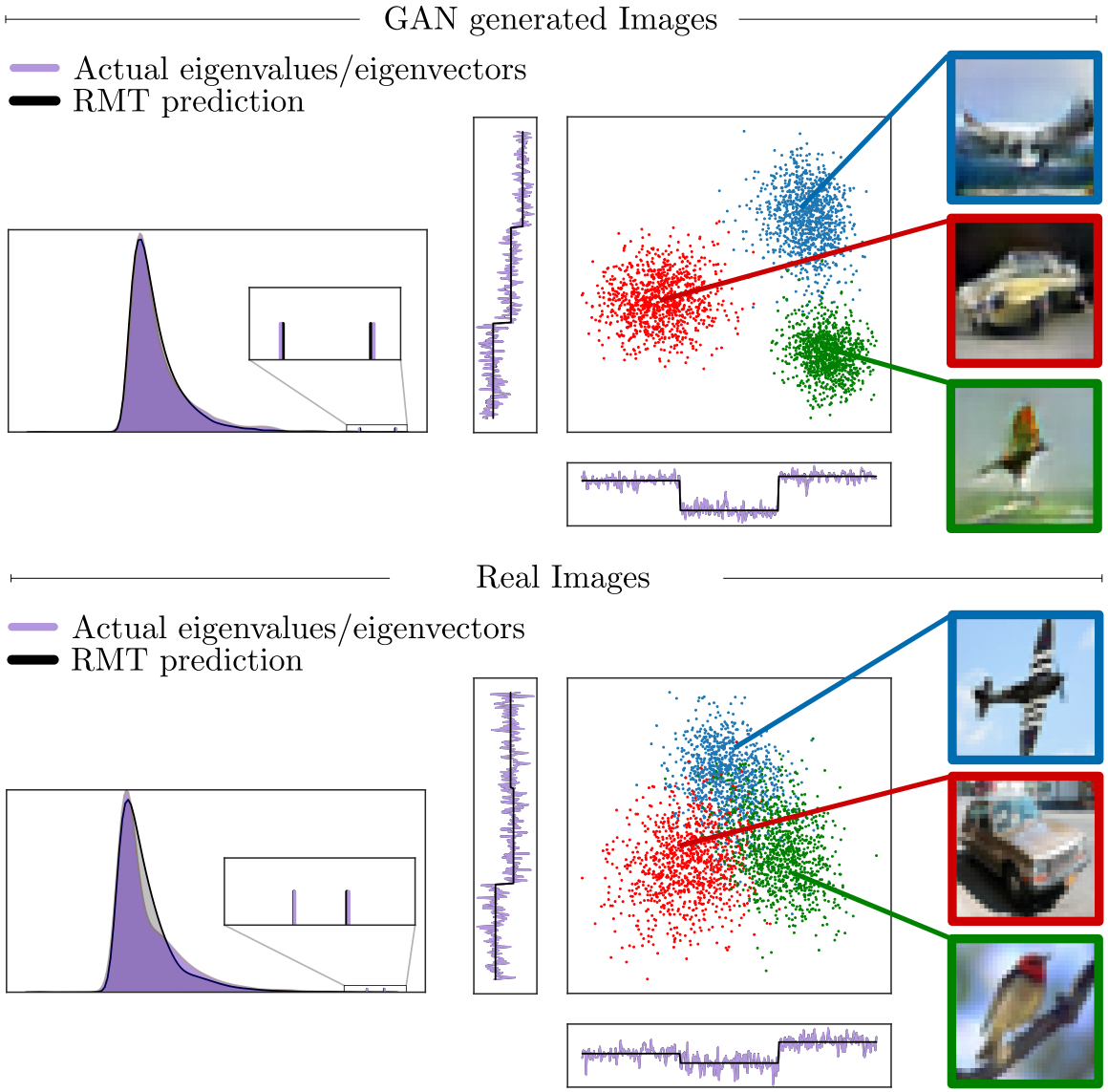
Ok. . . so what? (2)

Results. **[Seddik,C'19]**



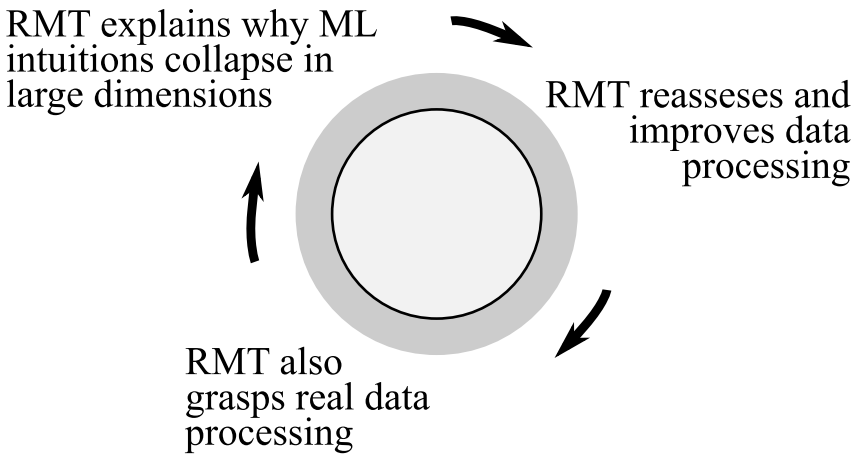
Ok. . . so what? (2)

Results. [Seddik,C'19]



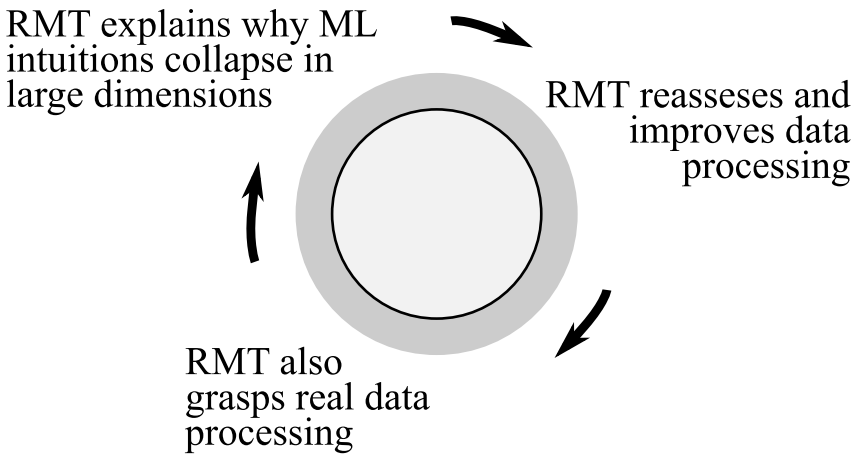
Conclusion

Reminder of Takeaway messages:



Conclusion

Reminder of Takeaway messages:

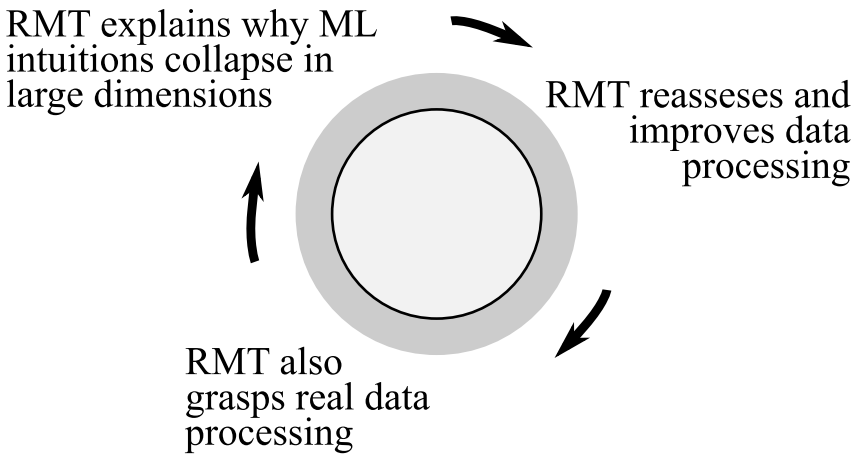


The road ahead:

- getting away from GMM models and show universality results (**concentration of measure arguments**)

Conclusion

Reminder of Takeaway messages:



The road ahead:

- getting away from GMM models and show universality results (**concentration of measure arguments**)
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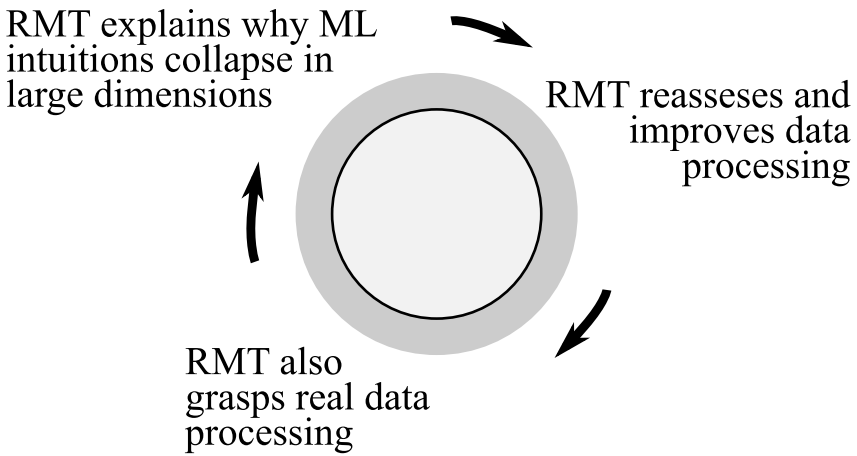
Conclusion

Reminder of Takeaway messages:



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!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