Random Matrices and Machine Learning

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Outline

Reminders: the sample covariance matrix model

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The SCM model:

- $X_n = (X_{ij}) = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n] \in \mathbb{C}^{N \times n}$ (or $\mathbb{R}^{N \times n}$) with i.i.d. zero mean unit variance entries and

$$\Sigma_n = \frac{1}{\sqrt{n}}[\boldsymbol{s}_1, \ldots, \boldsymbol{s}_n] = \frac{1}{\sqrt{n}}[R_N^{1/2}\boldsymbol{x}_1, \cdots, R_N^{1/2}\boldsymbol{x}_n]$$

with $R_N \in \mathbb{C}^{N \times N} \succeq 0$, so that

$$n\mathbb{E}\boldsymbol{s}_1\boldsymbol{s}_1^* = R_N^{1/2}\mathbb{E}\boldsymbol{x}_1\boldsymbol{x}_1^* R_N^{1/2} = R_N.$$

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- the matrix

$$\hat{R}_N = \frac{1}{n}R_N^{1/2} X_n X_n^* R_N^{1/2} = \Sigma_n \Sigma_n^* = \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{s}_i \boldsymbol{s}_i^*$$

is the **sample covariance matrix**.

Reminders: Limiting eigenvalue distribution

Further notations:

- for $\lambda_1(A) \geq \ldots \lambda_N(A)$ the eigenvalues of Hermitian (symmetric) A:

$$L_N \equiv \frac{1}{N} \sum_{i=1}^{N} \delta_{\lambda_i(\hat{R}_N)} \quad \text{(random)}$$

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- we further denote the Stieltjes transform

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- $N/n \equiv c_n \to c > 0$
- $L_N^R \to L_\infty^R$ in distribution.

Reminders: Limiting spectral measure

Theorem (Limiting spectral distribution)

For $z \in \mathbb{C}^+ = \{w \in \mathbb{C},\ \Im[w] > 0\}$, as $n, N \to \infty$,

$$g_n(z) \xrightarrow{\text{a.s.}} t(z)$$

where $t(z)$ is the unique solution in $\mathbb{C}^+$ of

$$t(z) = \int \frac{L_\infty^R(du)}{-z(1 + uct(z)) + (1 - c)u}.$$

As a consequence,

$$L_N \xrightarrow{\text{a.s.}} \mathcal{F}$$

with $\mathcal{F}$ the unique probability measure such that $t(z) = \int (t - z)^{-1} \mathcal{F}(dt)$.

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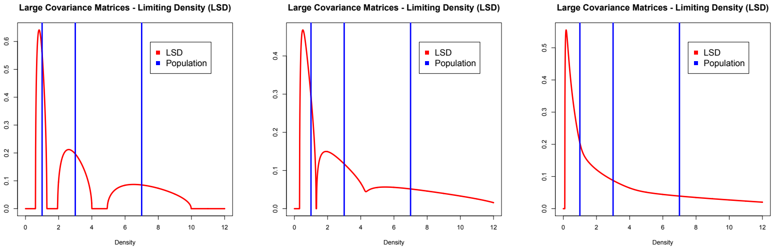

Figure: In red, limiting density for $c = .1$, $c = .3$, $c = .6$. In blue, 3 population eigenvalues of R_N, each of equal multiplicity.

Restating the theorem

The co-resolvent result: In the following it will be more convenient to work with $\Sigma_n^* \Sigma_n \in \mathbb{C}^{n \times n}$ than $\Sigma_n \Sigma_n^* \in \mathbb{C}^{N \times N}$.

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For $z \in \mathbb{C}^+$, $\tilde{t}(z) = \int (\lambda - z)^{-1} \tilde{\mathcal{F}}(d\lambda)$ is the unique solution in $\mathbb{C}^+$ of

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Remark. $t(z), \tilde{t}(z)$ are linked by $czt(z) = 1 - c + z\tilde{t}(z)$ (from $\tilde{\mathcal{F}} = (1-c)\delta_0 + c\mathcal{F}$).

Restating the theorem

Proof. Starting from the result (inverted on both sides):

$$\frac{1}{\tilde{t}(z)} = -z + c \int \frac{u L_\infty^R(du)}{1 + u\tilde{t}(z)}$$

multiply by $\tilde{t}(z)$ ($\neq 0$) to get

$$1 = -z\tilde{t}(z) + c \left(1 - \int \frac{L_\infty^R(du)}{1 + u\tilde{t}(z)} \right)$$

so that, using $czt(z) = 1 - c + z\tilde{t}(z)$,

$$t(z) = -\frac{1}{z} \int \frac{L_\infty^R(du)}{1 + u\tilde{t}(z)} = \int \frac{L_\infty^R(du)}{-z - zu\tilde{t}(z)}$$

and finally, again with $czt(z) = 1 - c + z\tilde{t}(z)$,

$$t(z) = \int \frac{L_\infty^R(du)}{-z(1 + uct(z)) + (1-c)u}.$$

Both results are thus equivalent.

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- we only have the link

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how to go backwards?

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- from $\Sigma_n \Sigma_n^*$, estimate eigenvectors $u_1(R_N), \dots, u_N(R_N)$?

Outline

From Stieltjes transform to measure

Proposition (Condition on density measure)

For g_μ Stieltjes transform of μ with real support and finite mass. Assume

$$\frac{1}{\pi} \lim_{y \downarrow 0} \Im \left[g_\mu(x_0 + \imath y) \right] \equiv I(x_0) \text{ exists}$$

for all $x \in \mathcal{V}(x_0)$. Then μ has a density in x_0 equal to $I(x_0)$.

Proof. See course notes.

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Beyond the spectrum: Most importantly, this is a required first step to:

- create a **strong link** between R_N and $\Sigma_n\Sigma_n^*$
- provide **new statistical inference** tools on R_N (eigenvalues and eigenvectors).

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Two fundamental identities: for all $z_1, z_2 \in \mathbb{C} \setminus \mathbb{R}$,

$$(\star) \quad (\tilde{t}(z_1) - \tilde{t}(z_2)) \left(1 - c \int \frac{\tilde{t}(z_1)\tilde{t}(z_2) u^2 L_\infty^R(du)}{(1 + u\tilde{t}(z_1))(1 + u\tilde{t}(z_2))} \right) = (z_1 - z_2)\tilde{t}(z_1)\tilde{t}(z_2)$$

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Elements of proof.

- follows immediately from the "scalar resolvent identity": $a^{-1} - b^{-1} = a^{-1}b^{-1}(b - a)$ (remember the matrix form $A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}$).
- applied to the scalar inverse $\tilde{t}(z) = (-z + c\int u/(1 + u\tilde{t}(z))L_\infty^R(du))^{-1}$.

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Important corollary: taking $z_1 = z \in \mathbb{C}^+$ and $z_2 = \bar{z}$ in $(\star)$,

$$2\imath\Im[\tilde{t}(z)]\left(1 - c|\tilde{t}(z)|^2 \int \frac{u^2 L_\infty^R(du)}{|1+u\tilde{t}(z)|^2}\right) = 2\imath\Im[z]|\tilde{t}(z)|^2$$

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so that, since $\Im[z] > 0$ and $\Im[\tilde{t}(z)] > 0$ (Stieltjes transform of real supported measure),

$$\boxed{(\star\star\star) \quad \forall z \in \mathbb{C}^+, \quad 1 - c|\tilde{t}(z)|^2 \int \frac{u^2 L_\infty^R(du)}{|1+u\tilde{t}(z)|^2} > 0.}$$

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Theorem (Existence of a density)

For all $x \in \mathbb{R} \setminus \{0\}$,

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Step 2. Extract **converging subsequences** $(z_n, \tilde{t}(z_n)) \to (x, \tilde{t})$ and show that $\tilde{t}$ is unique.

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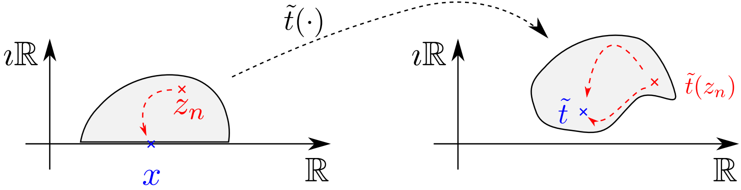
Step 2. Extract **converging subsequences** $(z_n, \tilde{t}(z_n)) \to (x, \tilde{t})$ and show that $\tilde{t}$ is unique.



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- **Careful!** left inequality is strict because $\int \frac{|\tilde{t}(z_0)|^2 u^2 L_\infty^R(du)}{|1+u\tilde{t}(z_0)|^2} < 1$ but $\lim_n \int \frac{|\tilde{t}(z_n)|^2 u^2 L_\infty^R(du)}{|1+u\tilde{t}(z_n)|^2} \le 1$ only!

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This concludes the proof. $\square$

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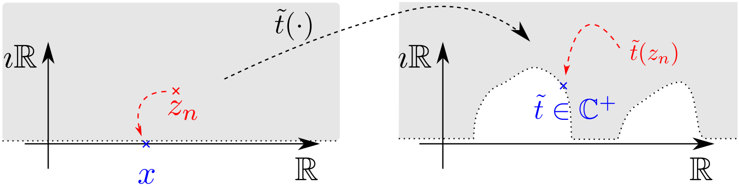

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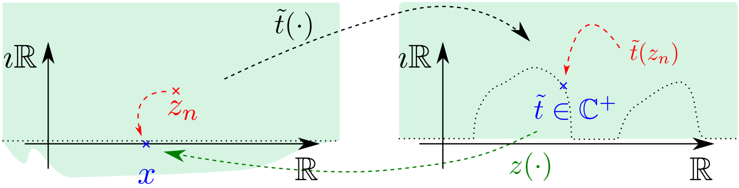

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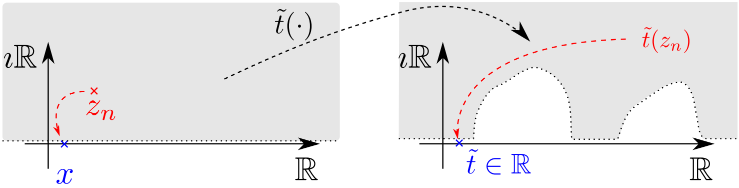

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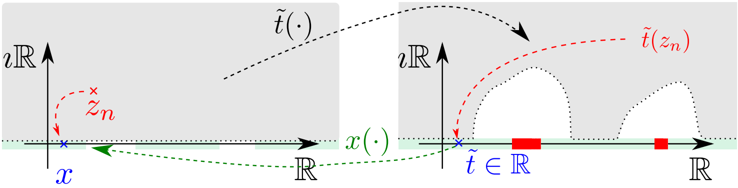

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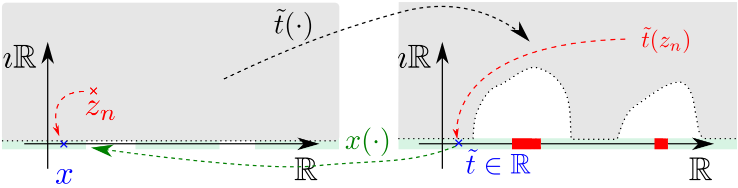

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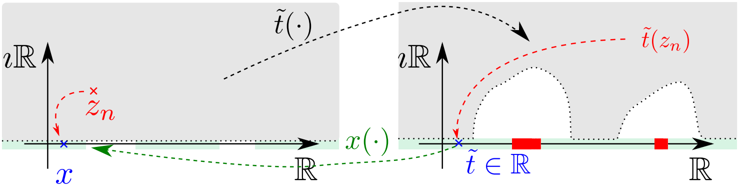
Application to the SCM model



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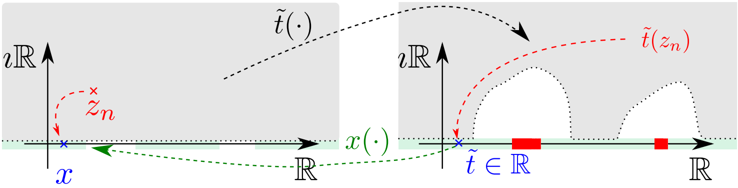

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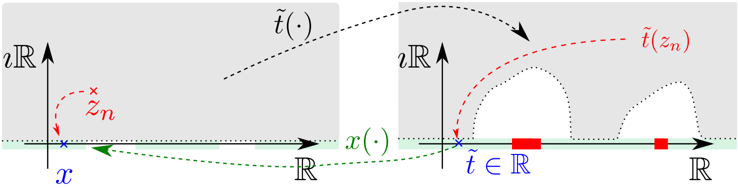

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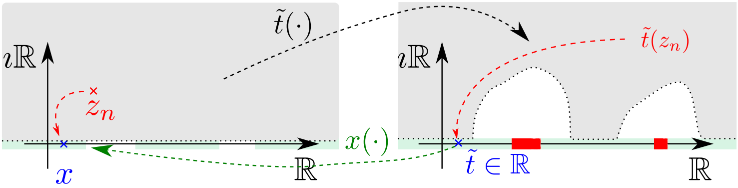

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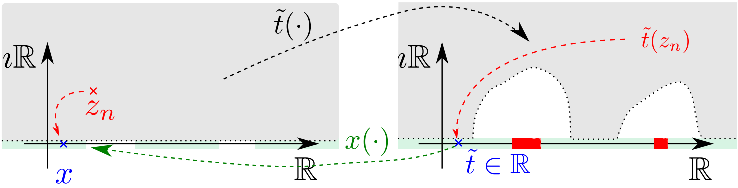

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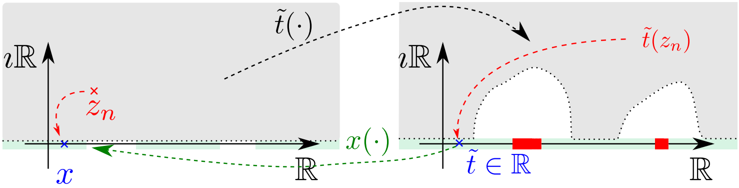

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- elsewhere, $x(\tilde{t})$ **may not** be increasing (otherwise, it would have an increasing local inverse satisfying $\tilde{t}(x)$ equation: but this is not a proof!)

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Let $z(\cdot)$ *and* $x(\cdot)$ *as above. Then,*

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   Conversely, for $\tilde{t}_0 \in \mathbb{R}^* \setminus \{\tilde{t}, -1/\tilde{t} \in \operatorname{supp}(L_\infty^R)\}$ such that $x'(\tilde{t}_0) > 0$,
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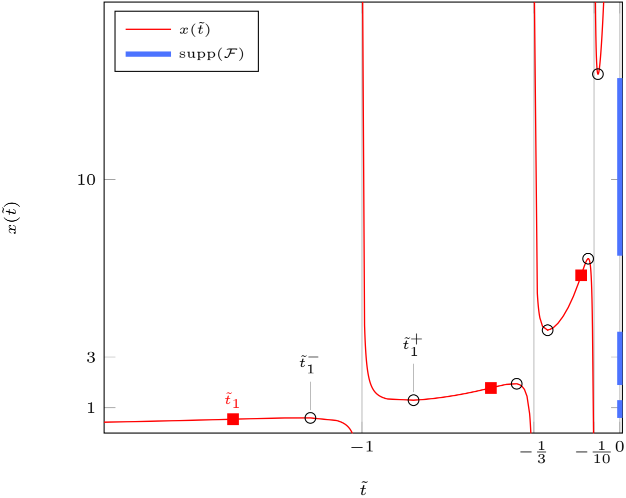

Figure: $x(\tilde{t})$ for $\tilde{t} \in \mathbb{R}$, R_N diagonal with 3 masses in 1, 3, 10, $c = 1/10$. Support $\mathrm{supp}(\mathcal{F})$ underlined on y-axis.

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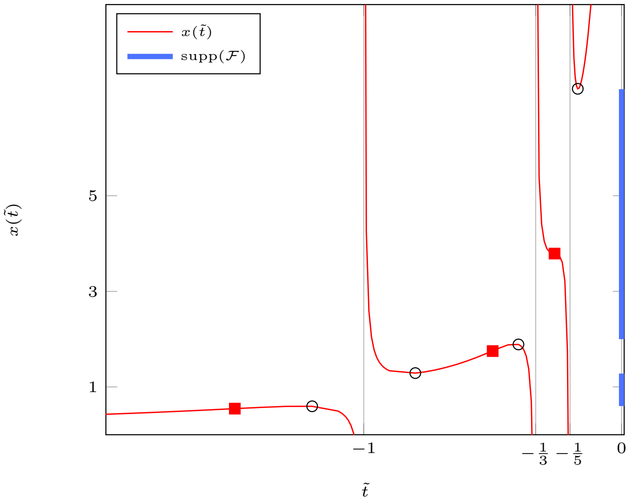

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$$x_0 = -\frac{1}{\tilde{t}^\circ(x_0)} + c \int \frac{u L_\infty^R(du)}{1 + u\tilde{t}(x_0)}$$

proving **existence**.

Application to the SCM model

[1. Uniqueness] Let

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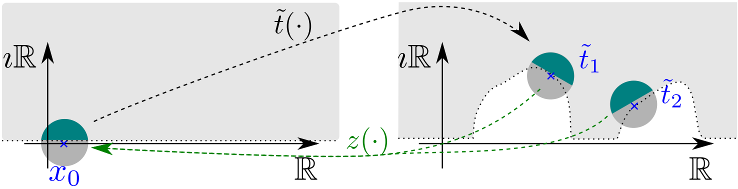

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This is a contradiction, and thus:

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Hence $x(\tilde{t}_0) \notin \operatorname{supp}(\mathcal{F})$. □

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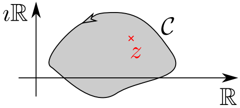

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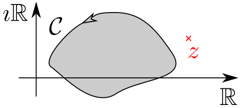

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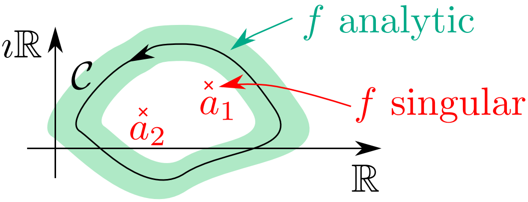

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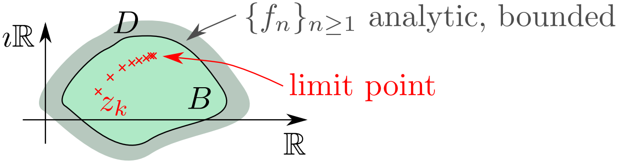

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- $f(t) = \log(1 + st)$ gives $\det(I_N + sR_N)$ (up to taking $\exp(N\cdot)$)

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- then, variable change!!!

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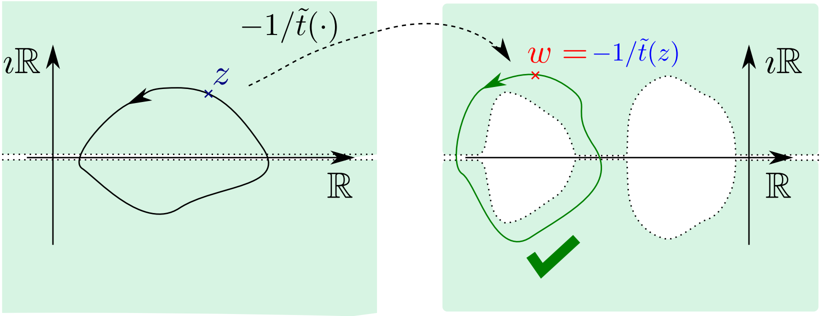

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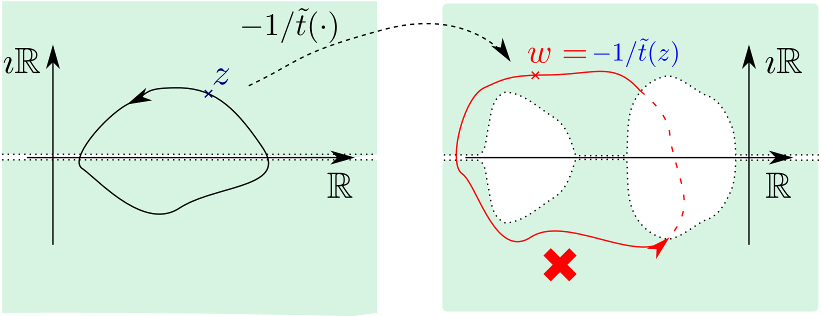

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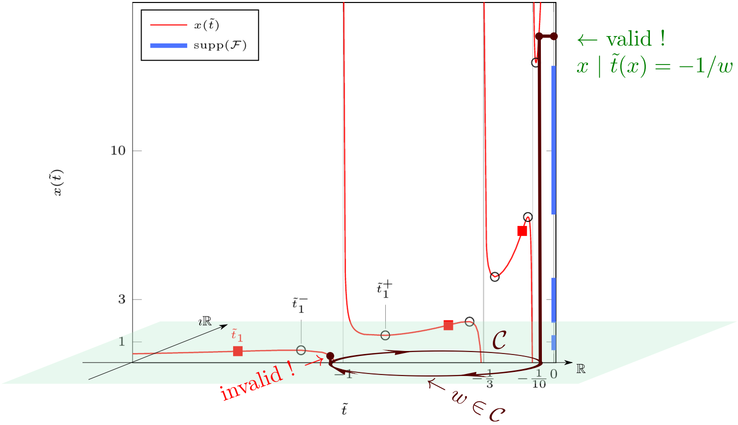
Back to $x(\tilde{t})$!: Recall $L_\infty^R = \frac{1}{3}\delta_1 + \frac{1}{3}\delta_3 + \frac{1}{3}\delta_{10}$



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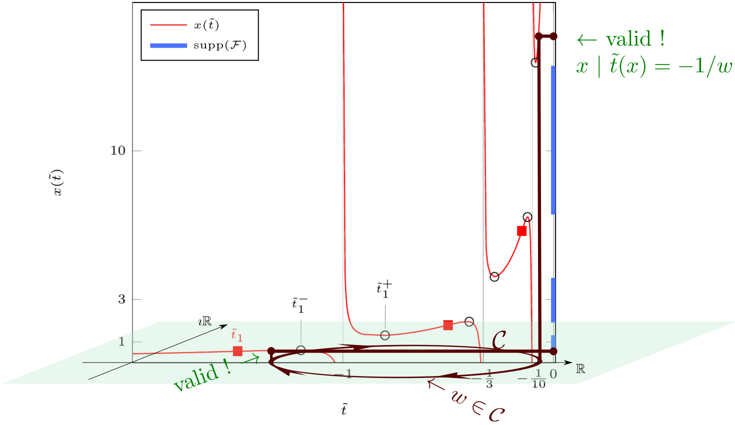

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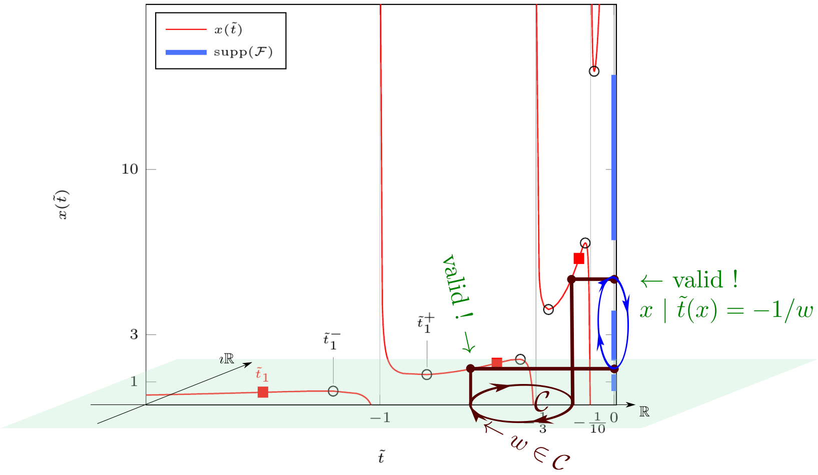
Remark: In fact, not always! e.g., estimate $\frac{1}{N}\mathrm{tr}(R_N^{-1})$ from $\hat{R}_N$ when $n < N$?

Going further...

What if we want to estimate $f(1)$, $f(3)$? : in $L_\infty^R = \frac{1}{3}\delta_1 + \frac{1}{3}\delta_3 + \frac{1}{3}\delta_5$



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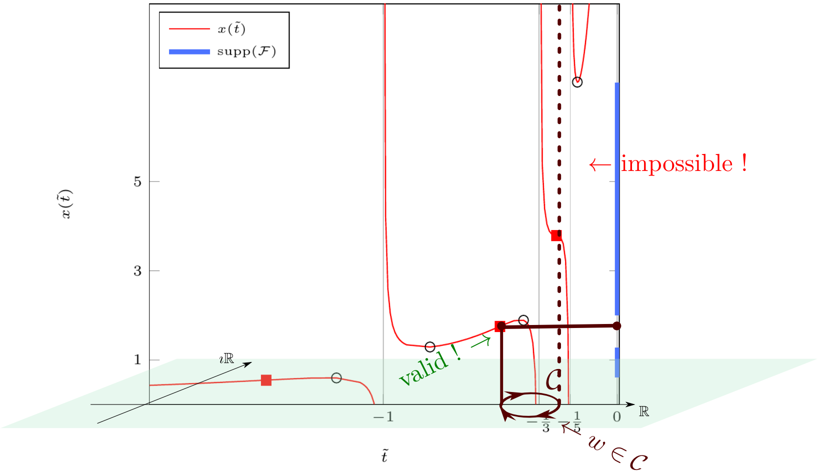

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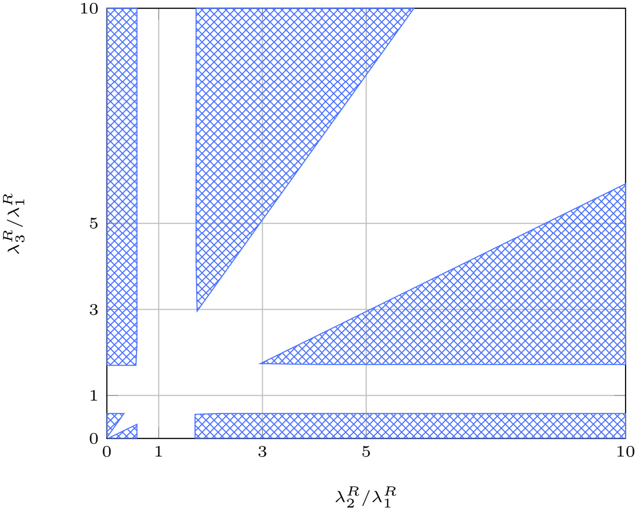

Figure: Subsets of $\lambda_1^R \leq \lambda_2^R \leq \lambda_3^R$ (hatched region) for which detectability condition over $L_\infty^R = \frac{1}{3}(\delta_{\lambda_1^R} + \delta_{\lambda_2^R} + \delta_{\lambda_3^R})$ is satisfied, $c = 1/10$.

Outline

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Back to the original problem:

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and we are fully in the domain of **limiting** observables!

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Assume that $\mathbb{E}[|X_{ij}|^4] < \infty$ *and*

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By integration by parts, this is, with probability 1:

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Example ($f(x) = x^2$ (continued))

Expand $\tilde{g}_n(z)$ as a rational function: the poles inside $\mathcal{C}_{\mathcal{F}}$ are such that $\tilde{g}_n(z) = 0$.

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Useful lemma:

Lemma

Let $\Lambda \in \mathbb{R}^{n\times n}$ diagonal and $a \in \mathbb{R}^n$. Then, the eigenvalues of $\Lambda - aa^*$ are either eigenvalues of Λ or the roots of $1 = a^*(\Lambda - xI_n)^{-1}a$.

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And we conclude, with probability 1,

$$G(f) = \sum_{i \in S} \frac{n}{N} \frac{1}{\tilde{g}_n'(x_i)} + o(1)$$

with $S = \{i \mid \lambda_i \text{ inside } \mathcal{C}_{\mathcal{F}}\}$.

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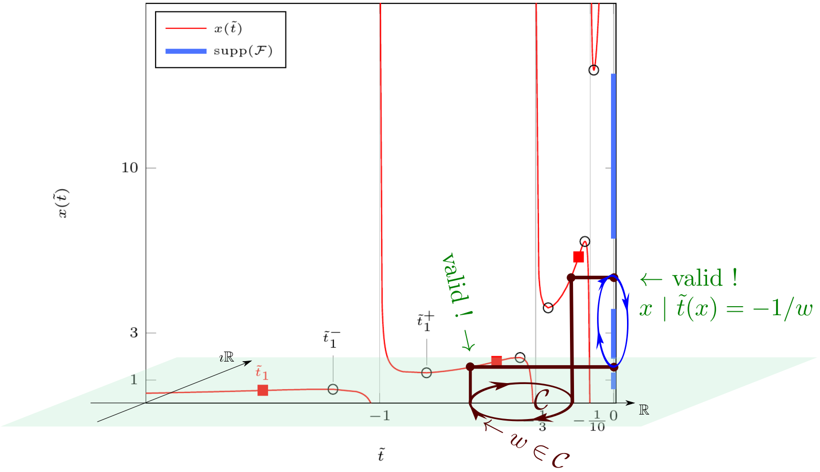

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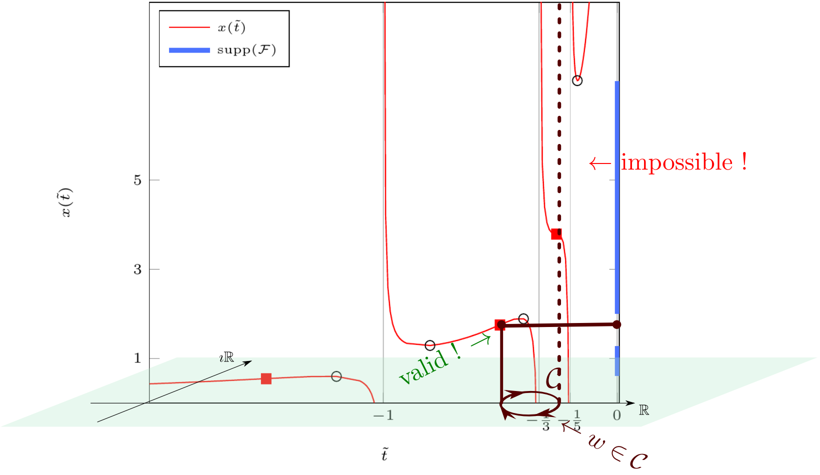

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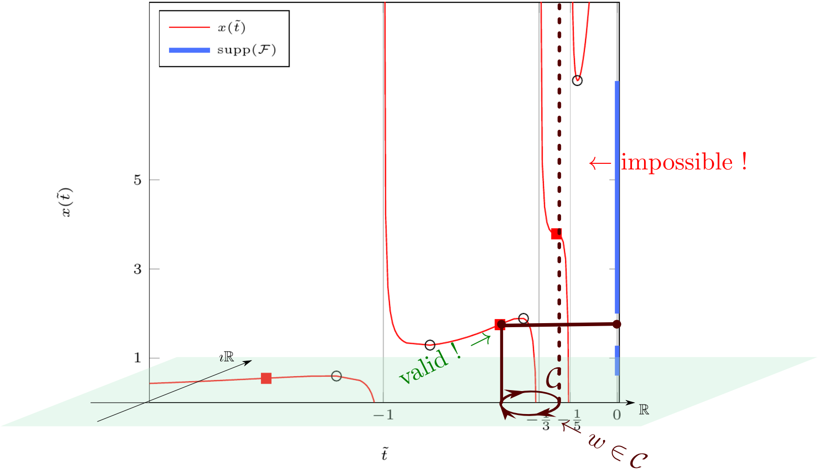

- only works if spectrum is "disjoint"!

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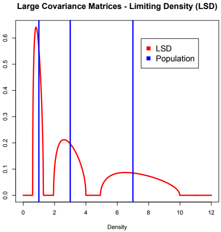
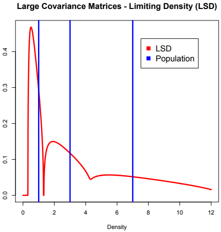
  Limiting density for $c = .1$, $c = .3$, $c = .6$



can evaluate 1, 3, 7



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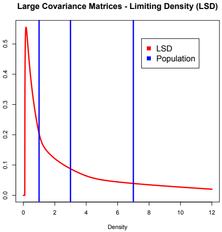

cannot evaluate any.

- or can't we ??? (see lab session)

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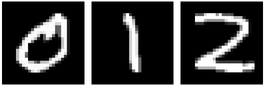

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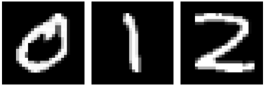

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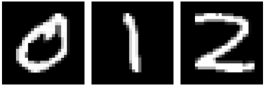

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where

$K = \{\kappa(x_i,x_j)\}_{i,j=1}^n$ and $D = \operatorname{diag}(\{\sum_{j=1}^n K_{ij}\}_{i=1}^n)$ (degrees of the "graph" K).

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$$\operatorname{tr} F^\mathsf{T} (D-K) F = \frac{1}{2} \sum_{i=1}^{k} \sum_{j\bar{j}} K_{j\bar{j}} (F_{ji} - F_{\bar{j}i})^2 \quad \text{(prove it!)}$$

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Position of the problem

Relaxation into spectral clustering:

- problem is discrete, NP-complete.
- solution: relaxing $\mathcal{F}$ into $\{F \in \mathbb{R}^{n\times k},\ F^\mathsf{T} F = I_k\}$

$$\min_{F,\ F^\mathsf{T} F = I_k} \operatorname{tr} F^\mathsf{T}(D-K)F$$

- this is an eigenvector problem!
  $\Rightarrow$ Solution F is concatenation of k "smallest" eigenvectors of $D-K$.
- gives spectral clustering algorithm:
  1. retrieve k smallest eigenvectors of $D-K$ into $V=[v_1,\ldots,v_k]\in\mathbb{R}^{n\times k}$
  2. cluster the (small dimensional!) rows $V_{i\cdot}\in\mathbb{R}^n$ with k-means
  3. the k classes obtained are the estimates of $\mathcal{C}_1,\ldots,\mathcal{C}_k$.

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We will see this will be a problem in large dimensions!

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Refinement: implies also

$$D^{-\frac{1}{2}} K D^{-\frac{1}{2}} (D^{\frac{1}{2}} j_a) = D^{\frac{1}{2}} j_a$$

more stable in practice.

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From theory to practice: **not at all what was expected!!**

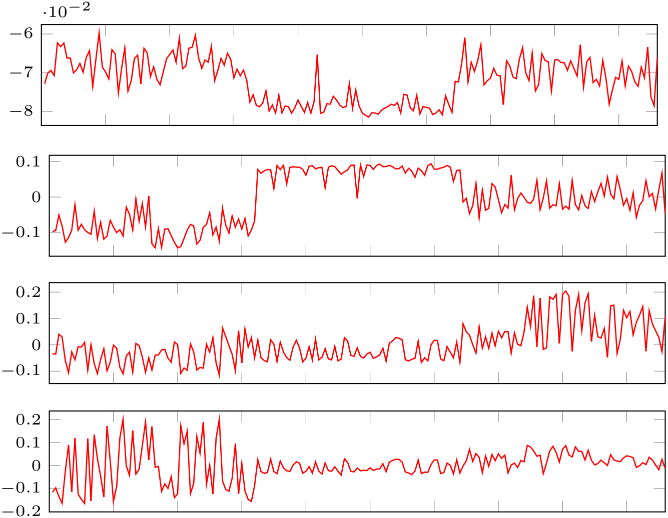

Figure: 4 dominant eigenvectors of $L = D^{-\frac{1}{2}} K D^{-\frac{1}{2}}$ (**red**); MNIST data (0, 1, 2).

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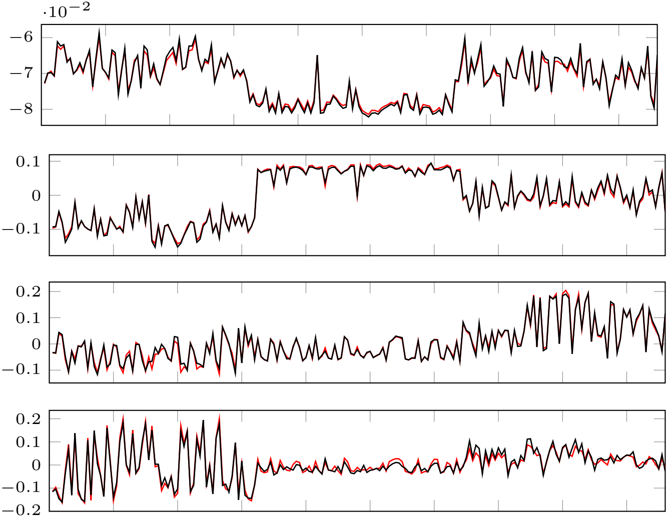

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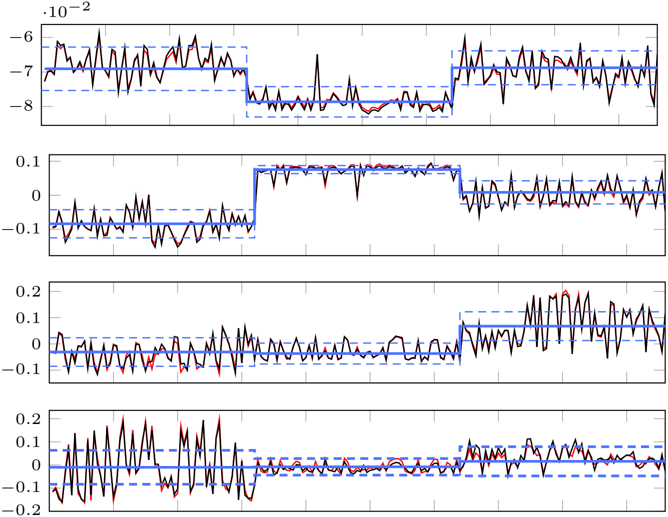

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Only non-trivial if $\|\mu_1 - \mu_2\| = 2\|\mu\| = O(1)$! (with respect to p)

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- *Conclusion*: non-trivial conditions:

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Can we do better???

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- **asymptotic non-triviality conditions:** for $\mu^\circ = \sum_{a=1}^k \frac{n_a}{n}\mu_a$ and $C^\circ = \sum_{a=1}^k \frac{n_a}{n}C_a$

$$\|\mu_a - \mu^\circ\| = O(1) \quad \operatorname{tr}(C_a - C_a) = O(\sqrt{p}) \quad \|C_a\| = O(1)$$

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Key idea: Taylor expansion of K_{ij} around $f(\tau_p)$!

Position of the problem

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

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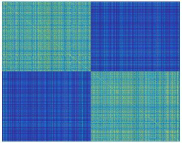
$p = 4$, $n = 1000$

$K =$  $v_2 =$ 

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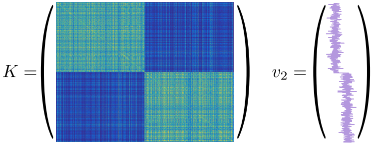
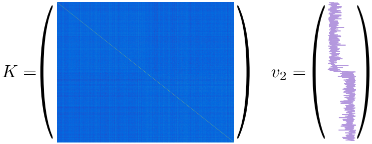


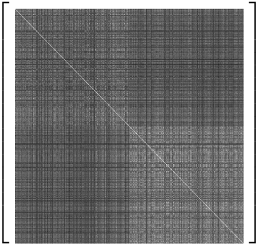
$p = \mathbf{400},\ n = 1000$

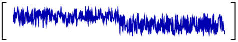


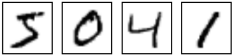
Position of the problem

And for real data?

MNIST
raw
$p = 784,\ n = 500$
$\downarrow$

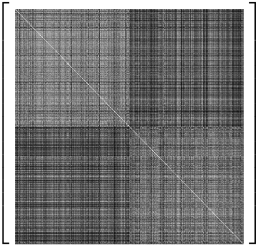
$\mathbf{K} =$ 

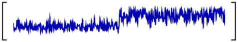
$\mathbf{v}_2 =$ 



(ici, classes "5" et "0")

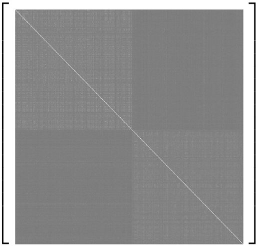
ImageNet
VGG-features
$p = 3084,\ n = 500$
$\downarrow$

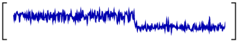
$\mathbf{K} =$ 

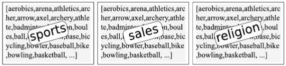
$\mathbf{v}_2 =$ 

(ici, classes "bird" et "plane")

20NewsGroup
BERT embedding
$p = 300,\ n = 500$
$\downarrow$

$\mathbf{K} =$ 

$\mathbf{v}_2 =$ 



(ici, classes "sports" et "sales")

Taylor expansion

The Taylor expansion: For simplicity, consider the simpler case (with $\|\mu_i\| = O(1)$)

$$K = \left\{ \frac{1}{p} x_i^\mathsf{T} x_j \right\}_{i,j=1}^n \quad \text{(so we forget the terms } \|x_i\|^2/p \text{ and } \|x_j\|^2/p\text{)}$$

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- just develop (for, say, $x_i \sim \mathcal{N}(\mu_a, C_a)$ and $x_j \sim \mathcal{N}(\mu_b, C_b)$):

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- just develop (for, say, $x_i \sim \mathcal{N}(\mu_a, C_a)$ and $x_j \sim \mathcal{N}(\mu_b, C_b)$):

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Taylor expansion

The Taylor expansion: For simplicity, consider the simpler case (with $\|\mu_i\| = O(1)$)

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- **key difficulty**: moving from entries Taylor expansion to matrix Taylor expansion!

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$$\frac{1}{\sqrt{n}} X \in \mathbb{R}^{n \times n} \quad X_{ij} = X_{ji} \sim \mathcal{N}(0,1) = O(1)?$$

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$$\frac{1}{\sqrt{n}} X \in \mathbb{R}^{n \times n} \quad X_{ij} = X_{ji} = 1? \quad \Rightarrow O(\sqrt{p})! \quad \text{(rank-1 matrix)}$$

Taylor expansion

Continuing the expansion: with $\mathcal{C}_a \ni x_i = \mu_a + w_i$,

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in which

$\|\frac{1}{p}W^\mathsf{T}W\| = O(1)$ (SCM model!) and $\|\frac{1}{p}(MJ^\mathsf{T})^\mathsf{T}(MJ^\mathsf{T})\| = \|\frac{1}{p}J\underbrace{M^\mathsf{T}M}_{=O(1)}J^\mathsf{T}\| = O(1)$

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so finally

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$$= O_{\|\cdot\|}(1) + O_{\|\cdot\|}(p^{-\frac{1}{2}})$$

Main result

Summing up:

$$K = f(0) \underbrace{1_n 1_n^{\mathsf{T}}}_{=O_{\|\cdot\|}(n)} + f'(0) \underbrace{\frac{1}{p}(W + MJ^{\mathsf{T}})^{\mathsf{T}}(W + MJ^{\mathsf{T}})}_{=O_{\|\cdot\|}(1)} + \frac{f''(0)}{2} \underbrace{\frac{1}{p} JTJ^{\mathsf{T}}}_{=O_{\|\cdot\|}(1)} + o_{\|\cdot\|}(1)$$

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- this is ... **a spiked model!!**

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Back to $D^{-\frac{1}{2}} K D^{-\frac{1}{2}}$: can be studied similarly, just more painful!

Main result: comparison to simulations

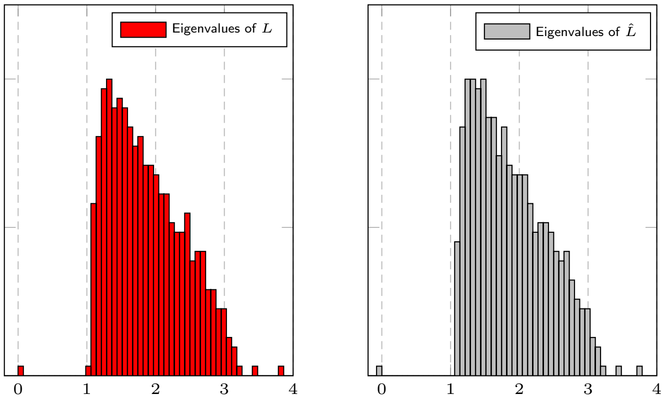

Figure: Eigenvalues of $L = D^{-\frac{1}{2}} K D^{-\frac{1}{2}}$ versus **Taylor expansion** $\hat{L}$, $k = 3$, $p = 2048$, $n = 512$, $c_1 = c_2 = 1/4$, $c_3 = 1/2$, $[\mu_a]_j = 4\boldsymbol{\delta}_{aj}$, $C_a = (1 + 2(a-1)/\sqrt{p})I_p$, $f(x) = \exp(-x/2)$ **(Gaussian kernel)**.

Main result: comparison to **real data** simulations

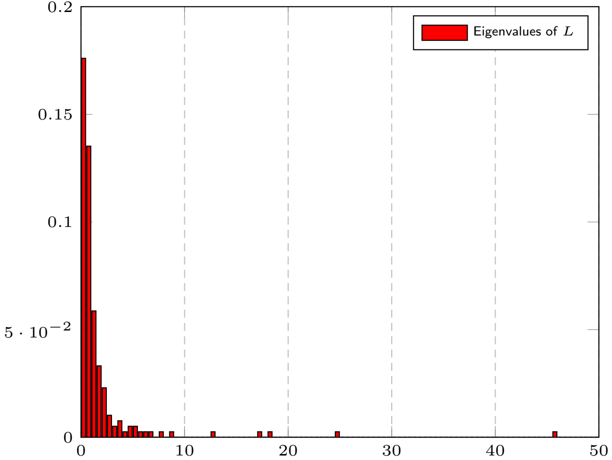

Figure: Eigenvalues of L (red) and **(equivalent Gaussian model)** $\hat{L}$ (white), MNIST data, $p = 784$, $n = 192$.

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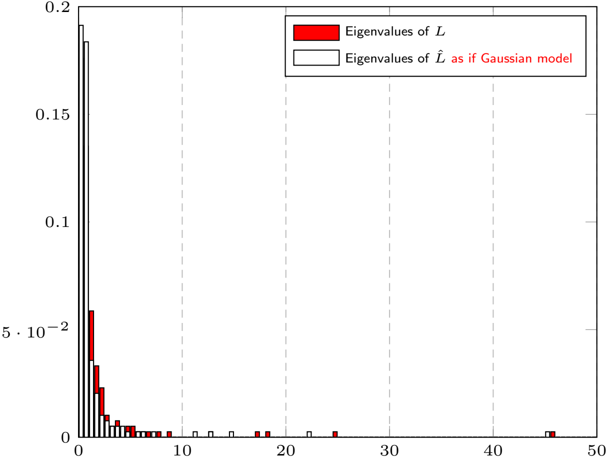

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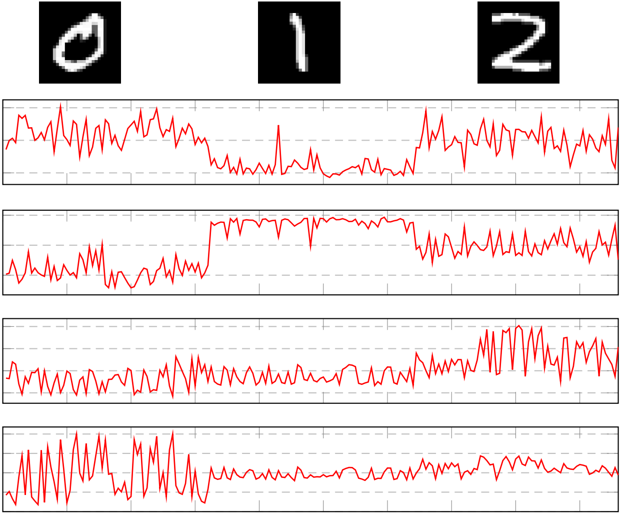
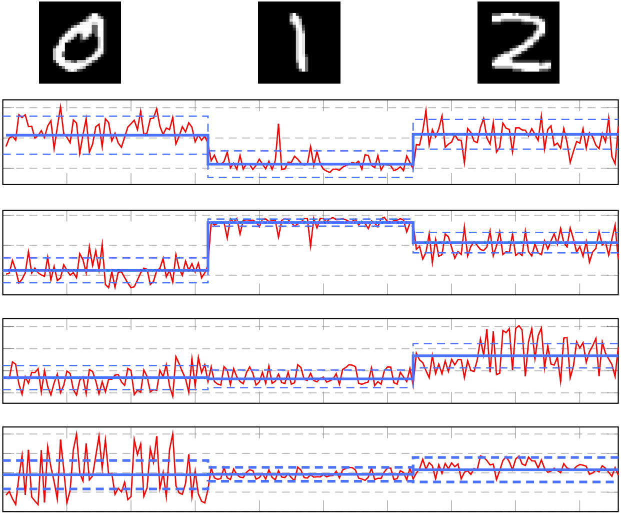


Figure: Leading four eigenvectors of $D^{-\frac{1}{2}}KD^{-\frac{1}{2}}$ for MNIST data (**red**) and theoretical findings (**blue**).

Main result: comparison to **real data** simulations



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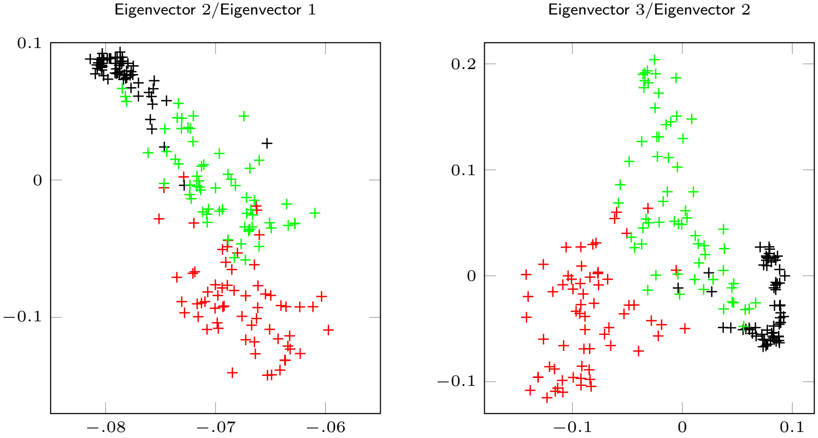
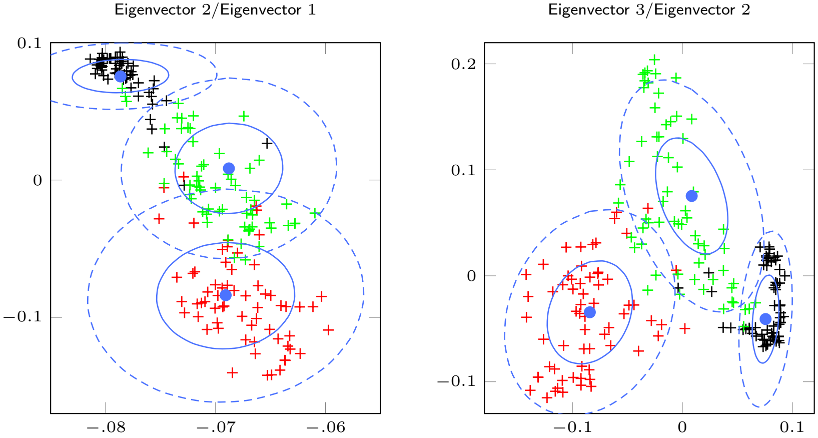


Figure: 2D representation of eigenvectors of L, for the MNIST dataset. Theoretical means and 1- and 2-standard deviations in **blue**. Class 1 in **red**, Class 2 in **black**, Class 3 in **green**.

Main result: comparison to **real data** simulations



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Going further: the surprising $f'(\tau) = 0$ case

Remember:

$$K = f(0) \underbrace{1_n 1_n^\mathsf{T}}_{=O_{\|\cdot\|}(n)} + f'(0) \underbrace{\frac{1}{p}(W + MJ^\mathsf{T})^\mathsf{T}(W + MJ^\mathsf{T})}_{=O_{\|\cdot\|}(1)} + \frac{f''(0)}{2} \underbrace{\frac{1}{p}JTJ^\mathsf{T}}_{=O_{\|\cdot\|}(1)} + o_{\|\cdot\|}(1)$$

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- what if $f'(0) = 0$?

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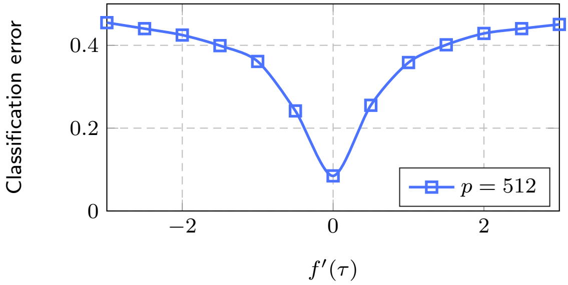

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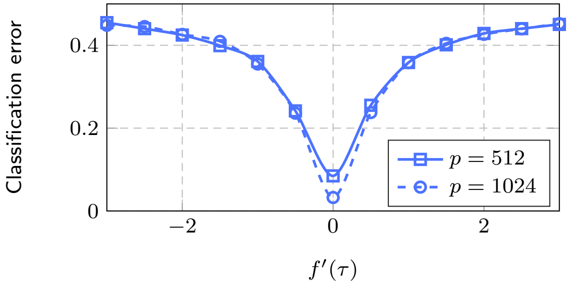

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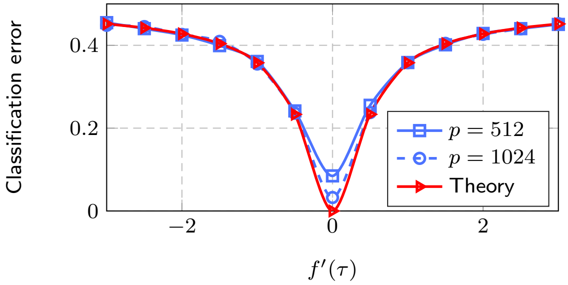

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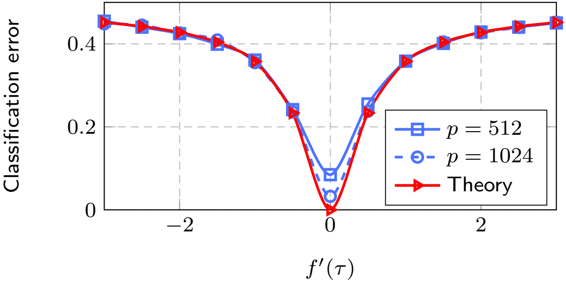

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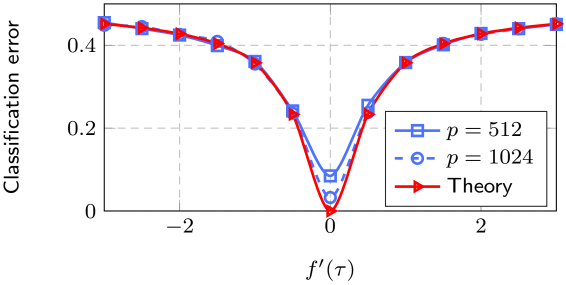

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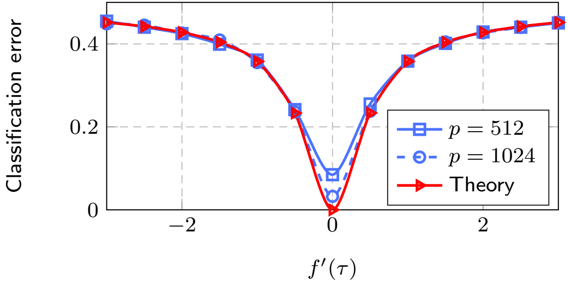

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- **Key remark**: what is the shape of this "optimal" $f(t)$???

Outline

Notion of Concentrated Vectors

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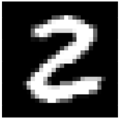 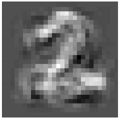

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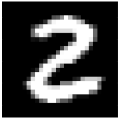 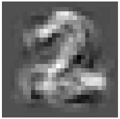

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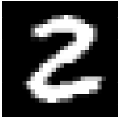

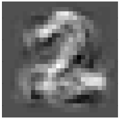

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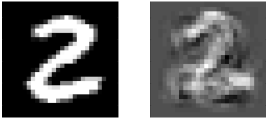

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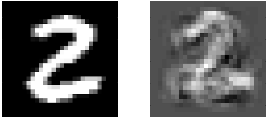

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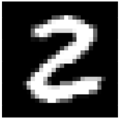 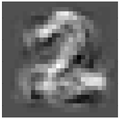

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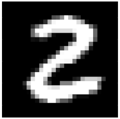
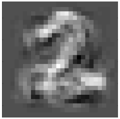

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"Concentrated vectors are stable through Lipschitz maps."

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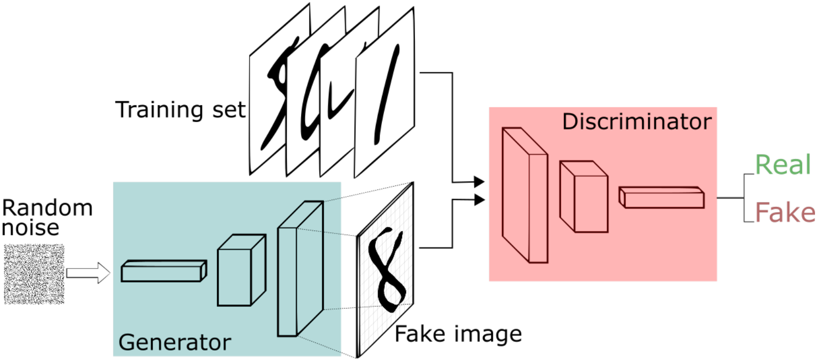
GAN data: An Example of Concentrated Vectors



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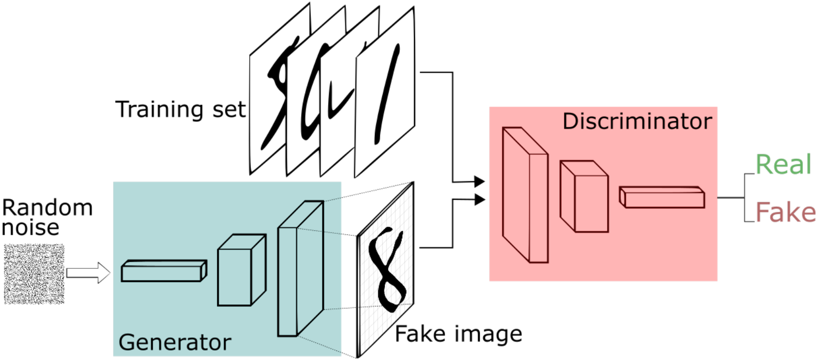

Generated image $= \mathcal{G}$(Gaussian) (with $\mathcal{G}$ Lipschitz!)

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Figure: Images generated by the BigGAN model [Brock *et al*, ICLR'19].

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New assumption: k **concentrated random vector classes**,

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Behavior of Gram Matrices for Concentrated Vectors

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$$\left\|\mathbb{E}[Q(z)] - \bar{Q}(z)\right\| = \mathcal{O}\left(\sqrt{\frac{\log p}{p}}\right)$$

where $\bar{Q}(z)$ **only depends on** $\mu_1, \ldots, \mu_k$, $C_1, \ldots, C_k$.

- **Exactly** the same result as for Gaussian mixture!

Behavior of Gram Matrices for Concentrated Vectors

Theorem (Universality result)

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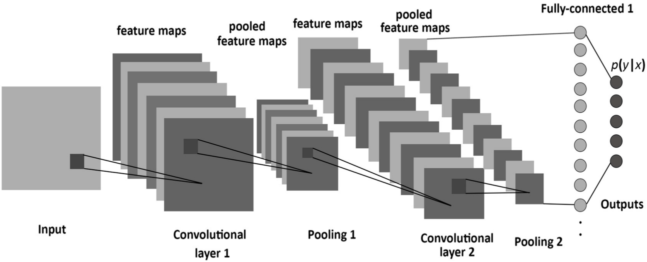
- only means (but this is huge!) that **ML algorithms treat GAN data as if Gaussian**

Application to CNN Representations of GAN Images



- CNN representations correspond to the **one before last** layer.

Application to CNN representations of GAN Images

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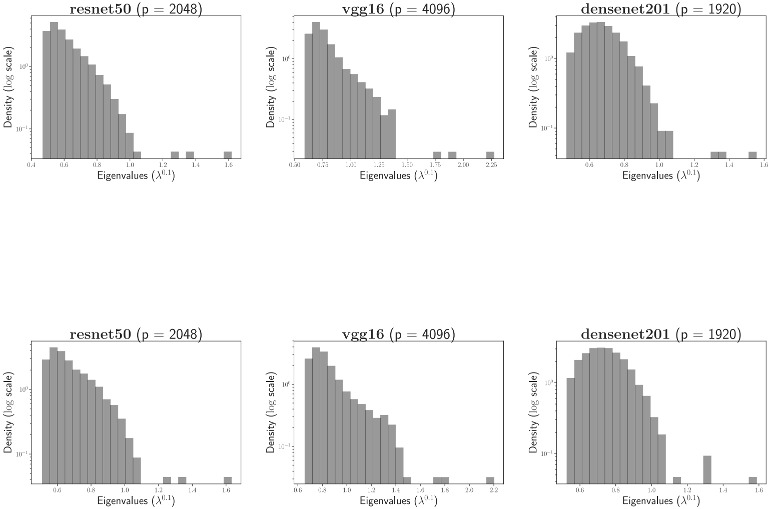
GAN Images

Real Images



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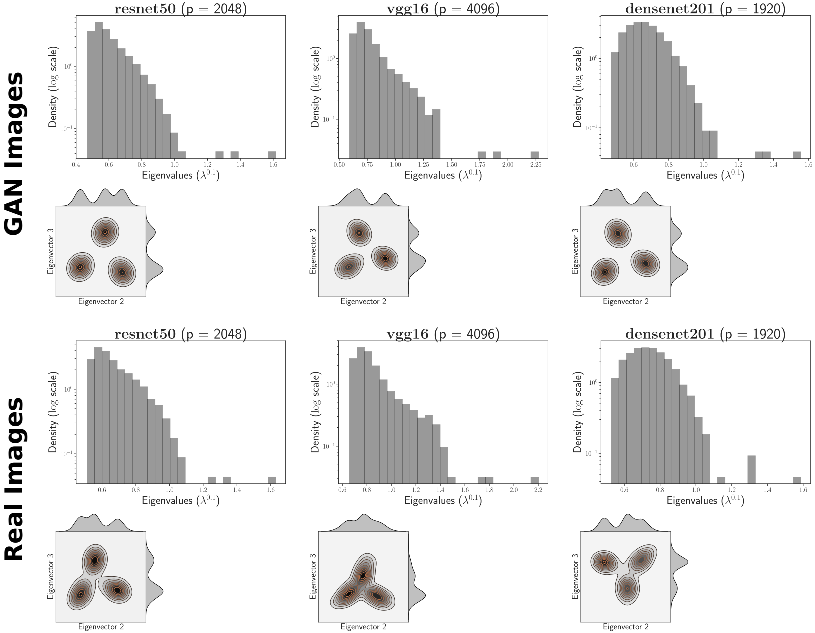

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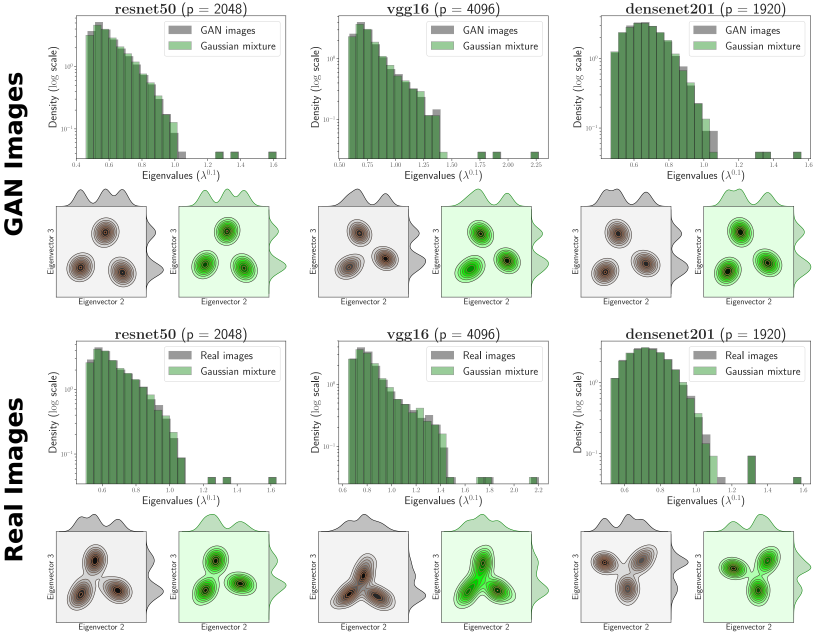

Takeaway message

Random matrix theory **explains the inner working of practical ML algorithms**

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Random matrix theory **explains the inner working of practical ML algorithms**

and this is **provably valid for real data!**