Random Matrix Advances in Large Dimensional Statistics, Machine Learning and Neural Nets

(EUSIPCO'2019, A Coruna, Spain)

Romain COUILLET, Malik TIOMOKO, Mohamed SEDDIK

CentraleSupélec, L2S, University of ParisSaclay, France
GSTATS IDEX DataScience Chair, GIPSA-lab, University Grenoble–Alpes, France.

September 2nd, 2019

CentraleSupélec

gipsa-lab

Outline

Outline

Outline

Context

Baseline scenario: $x_1, \ldots, x_n \in \mathbb{R}^p$ (or $\mathbb{C}^p$) i.i.d. with $E[x_1] = 0$, $E[x_1 x_1^\mathsf{T}] = C_p$:

Baseline scenario: $x_1, \ldots, x_n \in \mathbb{R}^p$ (or $\mathbb{C}^p$) i.i.d. with $E[x_1] = 0$, $E[x_1 x_1^\mathsf{T}] = C_p$:

- If $x_1 \sim \mathcal{N}(0, C_p)$, ML estimator for C_p is the sample covariance matrix (SCM)

$$\hat{C}_p = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^\mathsf{T}.$$

Context

Baseline scenario: $x_1, \ldots, x_n \in \mathbb{R}^p$ (or $\mathbb{C}^p$) i.i.d. with $E[x_1] = 0$, $E[x_1 x_1^\mathsf{T}] = C_p$:

- If $x_1 \sim \mathcal{N}(0, C_p)$, ML estimator for C_p is the sample covariance matrix (SCM)

$$\hat{C}_p = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^\mathsf{T}.$$

- If $n \to \infty$, then, strong law of large numbers

$$\hat{C}_p \xrightarrow{\text{a.s.}} C_p.$$

  or equivalently, in spectral norm

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

Context

Baseline scenario: $x_1, \ldots, x_n \in \mathbb{R}^p$ (or $\mathbb{C}^p$) i.i.d. with $E[x_1] = 0$, $E[x_1 x_1^\mathsf{T}] = C_p$:

- If $x_1 \sim \mathcal{N}(0, C_p)$, ML estimator for C_p is the sample covariance matrix (SCM)

$$\hat{C}_p = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^\mathsf{T}.$$

- If $n \to \infty$, then, strong law of large numbers

$$\hat{C}_p \xrightarrow{\text{a.s.}} C_p.$$

  or equivalently, in spectral norm

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

Random Matrix Regime

- No longer valid if $p, n \to \infty$ with $p/n \to c \in (0, \infty)$,

$$\left\| \hat{C}_p - C_p \right\| \not\to 0.$$

Context

Baseline scenario: $x_1, \ldots, x_n \in \mathbb{R}^p$ (or $\mathbb{C}^p$) i.i.d. with $E[x_1] = 0$, $E[x_1 x_1^\mathsf{T}] = C_p$:

- If $x_1 \sim \mathcal{N}(0, C_p)$, ML estimator for C_p is the sample covariance matrix (SCM)

$$\hat{C}_p = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^\mathsf{T}.$$

- If $n \to \infty$, then, strong law of large numbers

$$\hat{C}_p \xrightarrow{\text{a.s.}} C_p.$$

or equivalently, in spectral norm

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

Random Matrix Regime

- No longer valid if $p, n \to \infty$ with $p/n \to c \in (0, \infty)$,

$$\left\| \hat{C}_p - C_p \right\| \not\to 0.$$

- For practical p, n with $p \simeq n$, leads to dramatically wrong conclusions

Context

Baseline scenario: $x_1, \ldots, x_n \in \mathbb{R}^p$ (or $\mathbb{C}^p$) i.i.d. with $E[x_1] = 0$, $E[x_1 x_1^\mathsf{T}] = C_p$:

- If $x_1 \sim \mathcal{N}(0, C_p)$, ML estimator for C_p is the sample covariance matrix (SCM)

$$\hat{C}_p = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^\mathsf{T}.$$

- If $n \to \infty$, then, strong law of large numbers

$$\hat{C}_p \xrightarrow{\text{a.s.}} C_p.$$

  or equivalently, in spectral norm

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

Random Matrix Regime

- No longer valid if $p, n \to \infty$ with $p/n \to c \in (0, \infty)$,

$$\left\| \hat{C}_p - C_p \right\| \not\to 0.$$

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

Setting: $x_i \in \mathbb{R}^p$ i.i.d., $x_1 \sim \mathcal{CN}(0, I_p)$

Setting: $x_i \in \mathbb{R}^p$ i.i.d., $x_1 \sim \mathcal{CN}(0, I_p)$

- assume $p = p(n)$ such that $p/n \to c > 1$

Setting: $x_i \in \mathbb{R}^p$ i.i.d., $x_1 \sim \mathcal{CN}(0, I_p)$

- assume $p = p(n)$ such that $p/n \to c > 1$
- then, joint point-wise convergence

$$\max_{1\leq i,j\leq p} \left| \left[\hat{C}_p - I_p\right]_{ij} \right| = \max_{1\leq i,j\leq p} \left| \frac{1}{n} X_{j,\cdot} X_{i,\cdot}^{\mathsf{T}} - \boldsymbol{\delta}_{ij} \right| \xrightarrow{\text{a.s.}} 0.$$

Setting: $x_i \in \mathbb{R}^p$ i.i.d., $x_1 \sim \mathcal{CN}(0, I_p)$

- assume $p = p(n)$ such that $p/n \to c > 1$
- then, joint point-wise convergence

$$\max_{1\leq i,j\leq p} \left| \left[\hat{C}_p - I_p \right]_{ij} \right| = \max_{1\leq i,j\leq p} \left| \frac{1}{n} X_{j,\cdot} X_{i,\cdot}^\mathsf{T} - \boldsymbol{\delta}_{ij} \right| \xrightarrow{\text{a.s.}} 0.$$

- however, eigenvalue mismatch

$$0 = \lambda_1(\hat{C}_p) = \ldots = \lambda_{p-n}(\hat{C}_p) \leq \lambda_{p-n+1}(\hat{C}_p) \leq \ldots \leq \lambda_p(\hat{C}_p)$$
$$1 = \lambda_1(I_p) = \ldots = \lambda_{p-n}(I_p) = \lambda_{p-n+1}(\hat{C}_p) = \ldots = \lambda_p(I_p)$$

The Large Dimensional Fallacies

Setting: $x_i \in \mathbb{R}^p$ i.i.d., $x_1 \sim \mathcal{CN}(0, I_p)$

- assume $p = p(n)$ such that $p/n \to c > 1$
- then, joint point-wise convergence

$$\max_{1 \leq i,j \leq p} \left| \left[\hat{C}_p - I_p \right]_{ij} \right| = \max_{1 \leq i,j \leq p} \left| \frac{1}{n} X_{j,\cdot} X_{i,\cdot}^{\mathsf{T}} - \boldsymbol{\delta}_{ij} \right| \xrightarrow{\text{a.s.}} 0.$$

- however, eigenvalue mismatch

$$0 = \lambda_1(\hat{C}_p) = \ldots = \lambda_{p-n}(\hat{C}_p) \leq \lambda_{p-n+1}(\hat{C}_p) \leq \ldots \leq \lambda_p(\hat{C}_p)$$
$$1 = \lambda_1(I_p) = \ldots = \lambda_{p-n}(I_p) = \lambda_{p-n+1}(\hat{C}_p) = \ldots = \lambda_p(I_p)$$

$\Rightarrow$ no convergence in spectral norm.

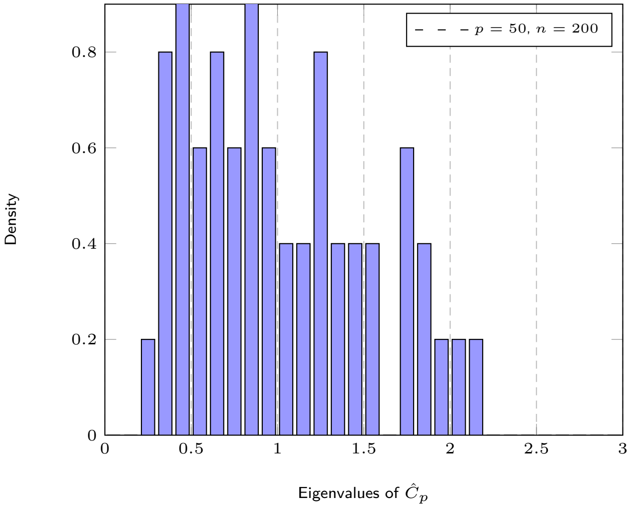


Figure: Histogram of the eigenvalues of $\hat{C}_p$ for $c = 1/4$, $C_p = I_p$.

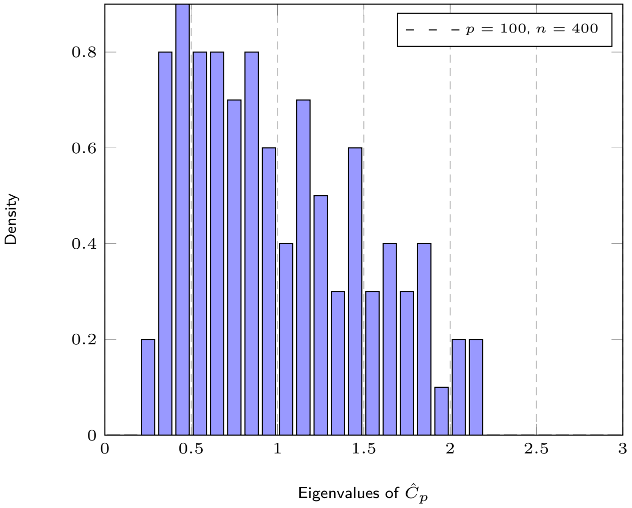


Figure: Histogram of the eigenvalues of $\hat{C}_p$ for $c = 1/4$, $C_p = I_p$.

The Marčenko–Pastur law

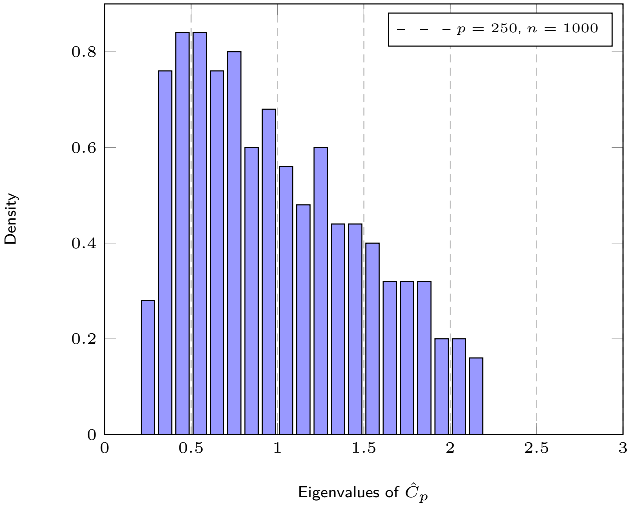


Figure: Histogram of the eigenvalues of $\hat{C}_p$ for $c = 1/4$, $C_p = I_p$.

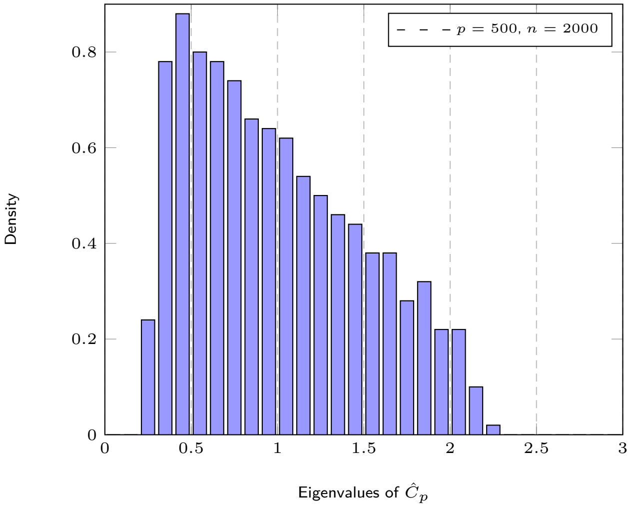


Figure: Histogram of the eigenvalues of $\hat{C}_p$ for $c = 1/4$, $C_p = I_p$.

The Marčenko–Pastur law

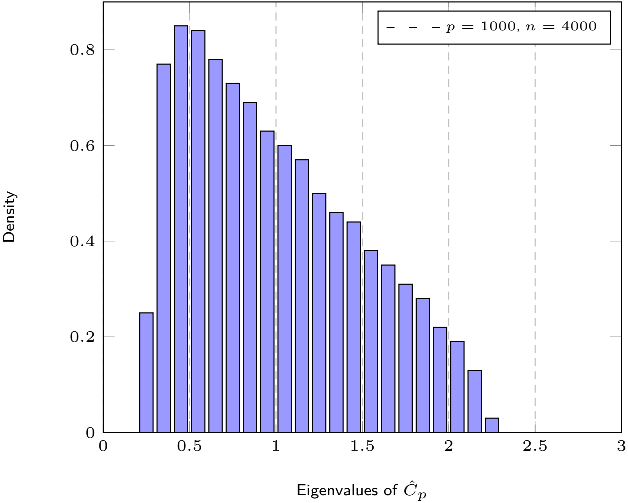


Figure: Histogram of the eigenvalues of $\hat{C}_p$ for $c = 1/4$, $C_p = I_p$.

The Marčenko–Pastur law

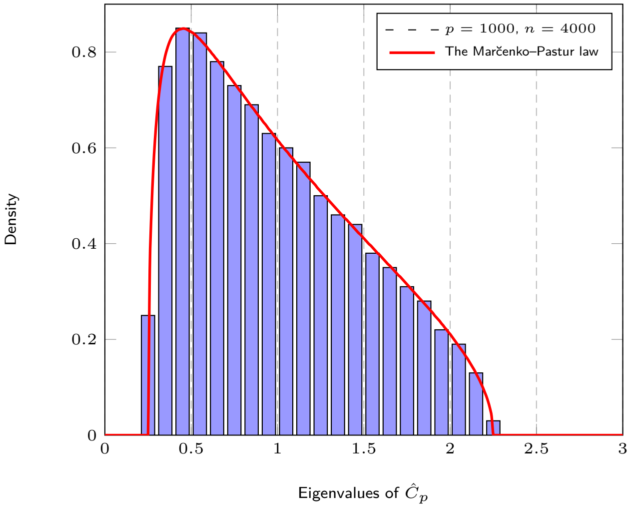


Figure: Histogram of the eigenvalues of $\hat{C}_p$ for $c = 1/4$, $C_p = I_p$.

Definition (Empirical Spectral Distribution)

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

$$\mu_p = \frac{1}{p} \sum_{i=1}^{p} \boldsymbol{\delta}_{\lambda_i(A_p)}.$$

Definition (Empirical Spectral Distribution)

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

$$\mu_p = \frac{1}{p} \sum_{i=1}^{p} \boldsymbol{\delta}_{\lambda_i(A_p)}.$$

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

$X_p \in \mathbb{R}^{p \times n}$ *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* $\frac{1}{n} X_p X_p^\mathsf{T}$ *satisfies*

$$\mu_p \xrightarrow{\text{a.s.}} \mu_{(c)}$$

in distribution (i.e., $\int f(t)\mu_p(dt) \xrightarrow{\text{a.s.}} \int f(t)\mu_{(c)}(dt)$ *for all bounded continuous* f*), where*

- $\mu_c(\{0\}) = \max\{0, 1 - c^{-1}\}$

The Marčenko–Pastur law

Definition (Empirical Spectral Distribution)

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

$$\mu_p = \frac{1}{p} \sum_{i=1}^{p} \boldsymbol{\delta}_{\lambda_i(A_p)}.$$

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

$X_p \in \mathbb{R}^{p \times n}$ 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 $\frac{1}{n} X_p X_p^\mathsf{T}$ satisfies

$$\mu_p \xrightarrow{\text{a.s.}} \mu_{(c)}$$

in distribution (i.e., $\int f(t)\mu_p(dt) \xrightarrow{\text{a.s.}} \int f(t)\mu_{(c)}(dt)$ for all bounded continuous f), where

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

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

The Marčenko–Pastur law

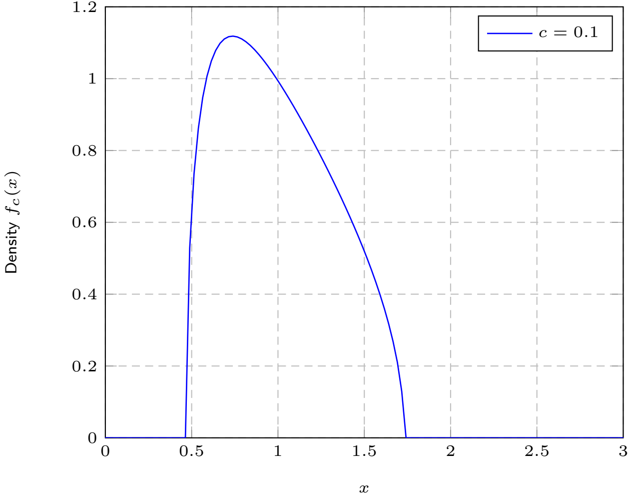


Figure: Marčenko-Pastur law for different limit ratios $c = \lim_{p \to \infty} p/n$.

The Marčenko–Pastur law

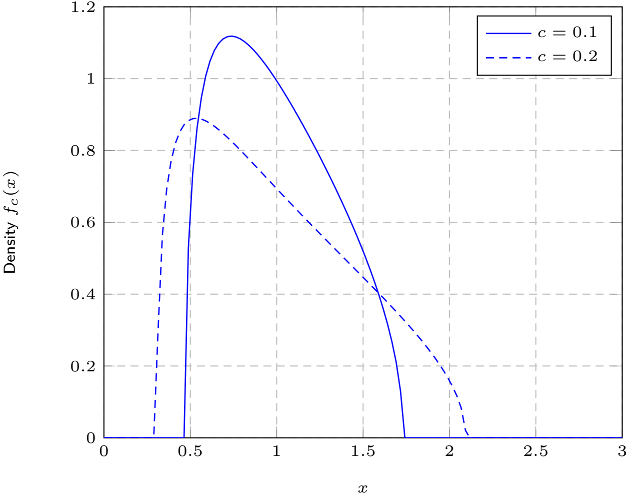


Figure: Marčenko-Pastur law for different limit ratios $c = \lim_{p\to\infty} p/n$.

The Marčenko–Pastur law

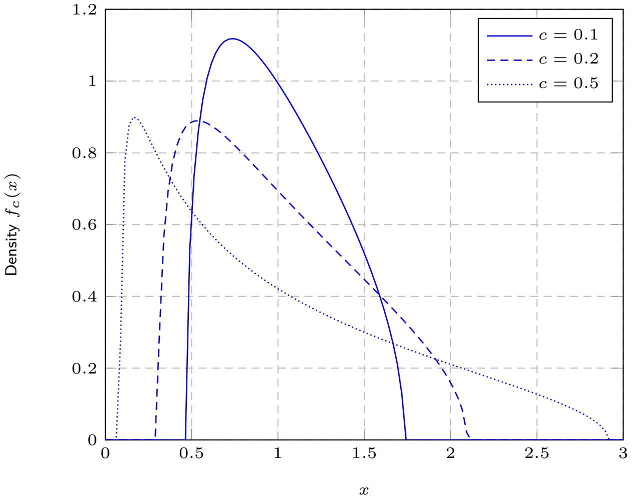


Figure: Marčenko-Pastur law for different limit ratios $c = \lim_{p\to\infty} p/n$.

Outline

Definition (Stieltjes Transform)

For μ real probability measure of support $\operatorname{supp}(\mu)$, Stieltjes transform m_μ defined, for $z \in \mathbb{C} \setminus \operatorname{supp}(\mu)$, as

$$m_\mu(z) = \int \frac{1}{t - z} \mu(dt).$$

Definition (Stieltjes Transform)

For μ real probability measure of support $\operatorname{supp}(\mu)$, Stieltjes transform m_μ defined, for $z \in \mathbb{C} \setminus \operatorname{supp}(\mu)$, as

$$m_\mu(z) = \int \frac{1}{t-z}\mu(dt).$$

Property (Inverse Stieltjes Transform)

For $a < b$ continuity points of μ,

$$\mu([a,b]) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_a^b \Im[m_\mu(x + \imath\varepsilon)]dx$$

Definition (Stieltjes Transform)

For μ real probability measure of support $\operatorname{supp}(\mu)$, Stieltjes transform m_μ defined, for $z \in \mathbb{C} \setminus \operatorname{supp}(\mu)$, as

$$m_\mu(z) = \int \frac{1}{t-z} \mu(dt).$$

Property (Inverse Stieltjes Transform)

For $a < b$ continuity points of μ,

$$\mu([a,b]) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_a^b \Im[m_\mu(x + \imath\varepsilon)] dx$$

Besides, if μ has a density f at x,

$$f(x) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \Im[m_\mu(x + \imath\varepsilon)].$$

Property (Relation to e.s.d.)

If μ e.s.d. of Hermitian $A \in \mathbb{R}^{p \times p}$, (i.e., $\mu = \frac{1}{p} \sum_{i=1}^{p} \boldsymbol{\delta}_{\lambda_i(A)}$)

$$m_\mu(z) = \frac{1}{p} \operatorname{tr} \left(A - zI_p\right)^{-1}$$

Property (Relation to e.s.d.)

If μ e.s.d. of Hermitian $A \in \mathbb{R}^{p \times p}$, (i.e., $\mu = \frac{1}{p} \sum_{i=1}^{p} \boldsymbol{\delta}_{\lambda_i(A)}$)

$$m_\mu(z) = \frac{1}{p} \operatorname{tr} (A - zI_p)^{-1}$$

Proof:

$$m_\mu(z) = \int \frac{\mu(dt)}{t - z} = \frac{1}{p} \sum_{i=1}^{p} \frac{1}{\lambda_i(A) - z} = \frac{1}{p} \operatorname{tr} \left(\operatorname{diag}\{\lambda_i(A)\} - zI_p\right)^{-1}$$
$$= \frac{1}{p} \operatorname{tr} (A - zI_p)^{-1} .$$

Property (Relation to e.s.d.)

If μ e.s.d. of Hermitian $A \in \mathbb{R}^{p\times p}$, (i.e., $\mu = \frac{1}{p}\sum_{i=1}^{p} \boldsymbol{\delta}_{\lambda_i(A)}$)

$$m_\mu(z) = \frac{1}{p}\operatorname{tr}\,(A - zI_p)^{-1}$$

Proof:

$$m_\mu(z) = \int \frac{\mu(dt)}{t-z} = \frac{1}{p}\sum_{i=1}^{p}\frac{1}{\lambda_i(A)-z} = \frac{1}{p}\operatorname{tr}\,(\operatorname{diag}\{\lambda_i(A)\} - zI_p)^{-1}$$
$$= \frac{1}{p}\operatorname{tr}\,(A - zI_p)^{-1}\,.$$

Fundamental object: the resolvent of A

$$Q_A(z) \equiv (A - zI_p)^{-1}.$$

Property (Stieltjes transform of Gram matrices)

For $X \in \mathbb{C}^{p \times n}$, and

- μ e.s.d. of XX^T
- $\tilde{\mu}$ e.s.d. of $X^\mathsf{T}X$

Then

$$m_\mu(z) = \frac{n}{p} m_{\tilde{\mu}}(z) - \frac{p-n}{p}\frac{1}{z}.$$

Property (Stieltjes transform of Gram matrices)

For $X \in \mathbb{C}^{p\times n}$, and

- μ e.s.d. of XX^T
- $\tilde{\mu}$ e.s.d. of $X^\mathsf{T}X$

Then

$$m_\mu(z) = \frac{n}{p} m_{\tilde{\mu}}(z) - \frac{p-n}{p}\frac{1}{z}.$$

Proof:

$$m_\mu(z) = \frac{1}{p}\sum_{i=1}^{p} \frac{1}{\lambda_i(XX^\mathsf{T}) - z} = \frac{1}{p}\sum_{i=1}^{n} \frac{1}{\lambda_i(X^\mathsf{T}X) - z} + \frac{1}{p}(p-n)\frac{1}{0-z}.$$

Three fundamental lemmas in all proofs.

Lemma (Resolvent Identity)

For $A, B \in \mathbb{R}^{p \times p}$ invertible,

$$A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}.$$

Proof: Simply left-multiply by A and right-multiply by B on both sides.

Three fundamental lemmas in all proofs.

Lemma (Resolvent Identity)

For $A, B \in \mathbb{R}^{p \times p}$ invertible,

$$A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}.$$

Proof: Simply left-multiply by A and right-multiply by B on both sides.

Corollary

For $t \in \mathbb{C}$, $x \in \mathbb{R}^p$, $A \in \mathbb{R}^{p \times p}$, with A and $A + txx^\mathsf{T}$ invertible,

$$(A + txx^\mathsf{T})^{-1}x = \frac{A^{-1}x}{1 + tx^\mathsf{T}A^{-1}x}.$$

Proof Intuition: Left-multiply by $(A + tcc^\mathsf{T})$ on both sides.

Three fundamental lemmas in all proofs.

Lemma (Rank-one perturbation)

For $A, B \in \mathbb{R}^{p\times p}$ Hermitian nonnegative definite, e.s.d. μ of A, $t > 0$, $x \in \mathbb{R}^p$, $z \in \mathbb{C} \setminus \operatorname{supp}(\mu)$,

$$\left| \frac{1}{p} \operatorname{tr} B \left(A + txx^{\mathsf{T}} - zI_p\right)^{-1} - \frac{1}{p} \operatorname{tr} B \left(A - zI_p\right)^{-1} \right| \leq \frac{1}{p} \frac{\|B\|}{\operatorname{dist}(z, \operatorname{supp}(\mu))}$$

Three fundamental lemmas in all proofs.

Lemma (Rank-one perturbation)

For $A, B \in \mathbb{R}^{p \times p}$ Hermitian nonnegative definite, e.s.d. μ of A, $t > 0$, $x \in \mathbb{R}^p$, $z \in \mathbb{C} \setminus \operatorname{supp}(\mu)$,

$$\left| \frac{1}{p} \operatorname{tr} B \left(A + t x x^{\mathsf{T}} - z I_p \right)^{-1} - \frac{1}{p} \operatorname{tr} B \left(A - z I_p \right)^{-1} \right| \leq \frac{1}{p} \frac{\|B\|}{\operatorname{dist}(z, \operatorname{supp}(\mu))}$$

In particular, as $p \to \infty$, if $\limsup_p \|B\| < \infty$,

$$\frac{1}{p} \operatorname{tr} B \left(A + t x x^{\mathsf{T}} - z I_p \right)^{-1} - \frac{1}{p} \operatorname{tr} B \left(A - z I_p \right)^{-1} \to 0.$$

Three fundamental lemmas in all proofs.

Lemma (Rank-one perturbation)

For $A, B \in \mathbb{R}^{p\times p}$ Hermitian nonnegative definite, e.s.d. μ of A, $t > 0$, $x \in \mathbb{R}^p$, $z \in \mathbb{C} \setminus \operatorname{supp}(\mu)$,

$$\left| \frac{1}{p}\operatorname{tr} B \left(A + txx^\mathsf{T} - zI_p\right)^{-1} - \frac{1}{p}\operatorname{tr} B \left(A - zI_p\right)^{-1} \right| \leq \frac{1}{p} \frac{\|B\|}{\operatorname{dist}(z, \operatorname{supp}(\mu))}$$

In particular, as $p \to \infty$, if $\limsup_p \|B\| < \infty$,

$$\frac{1}{p}\operatorname{tr} B \left(A + txx^\mathsf{T} - zI_p\right)^{-1} - \frac{1}{p}\operatorname{tr} B \left(A - zI_p\right)^{-1} \to 0.$$

Proof Intuition: Based on Weyl's interlacing identity (eigenvalues of A and $A + txx^\mathsf{T}$ are interlaced).

Three fundamental lemmas in all proofs.

Lemma (Trace Lemma)

For

- $x \in \mathbb{R}^p$ with i.i.d. entries with zero mean, unit variance, finite $2k$ order moment,
- $A \in \mathbb{R}^{p \times p}$ deterministic (or independent of x),

then

$$E\left[\left|\frac{1}{p}x^{\mathsf{T}}Ax - \frac{1}{p}\operatorname{tr} A\right|^k\right] \leq K\frac{\|A\|^p}{p^{k/2}}.$$

Three fundamental lemmas in all proofs.

Lemma (Trace Lemma)

For

- $x \in \mathbb{R}^p$ with i.i.d. entries with zero mean, unit variance, finite $2k$ order moment,
- $A \in \mathbb{R}^{p \times p}$ deterministic (or independent of x),

then

$$E\left[\left|\frac{1}{p}x^\mathsf{T}Ax - \frac{1}{p}\mathrm{tr}\, A\right|^k\right] \leq K\frac{\|A\|^p}{p^{k/2}}.$$

In particular, if $\limsup_p \|A\| < \infty$, and x has entries with finite eighth-order moment,

$$\frac{1}{p}x^\mathsf{T}Ax - \frac{1}{p}\mathrm{tr}\, A \xrightarrow{\text{a.s.}} 0$$

(by Markov inequality and Borel Cantelli lemma).

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

$X_p \in \mathbb{R}^{p\times n}$ *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* $\frac{1}{n}X_pX_p^\mathsf{T}$ *satisfies*

$$\mu_p \xrightarrow{\text{a.s.}} \mu_{(c)}$$

weakly, where

- $\mu_{(c)}(\{0\}) = \max\{0, 1-c^{-1}\}$

Theorem (Marčenko–Pastur Law **[Marčenko,Pastur'67]**)
$X_p \in \mathbb{R}^{p\times n}$ 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 $\frac{1}{n}X_pX_p^\mathsf{T}$ satisfies

$$\mu_p \xrightarrow{\text{a.s.}} \mu_{(c)}$$

weakly, where

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

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

Stieltjes transform approach.

Stieltjes transform approach.

Proof

- With μ_p e.s.d. of $\frac{1}{n}X_pX_p^\mathsf{T}$,

$$m_{\mu_p}(z) = \frac{1}{p}\mathrm{tr}\left(\frac{1}{n}X_pX_p^\mathsf{T} - zI_p\right)^{-1} = \frac{1}{p}\sum_{i=1}^{p}\left[\left(\frac{1}{n}X_pX_p^\mathsf{T} - zI_p\right)^{-1}\right]_{ii}.$$

Stieltjes transform approach.

Proof

- With μ_p e.s.d. of $\frac{1}{n}X_pX_p^\mathsf{T}$,

$$m_{\mu_p}(z) = \frac{1}{p}\mathrm{tr}\left(\frac{1}{n}X_pX_p^\mathsf{T} - zI_p\right)^{-1} = \frac{1}{p}\sum_{i=1}^{p}\left[\left(\frac{1}{n}X_pX_p^\mathsf{T} - zI_p\right)^{-1}\right]_{ii}.$$

- Write

$$X_p = \begin{bmatrix} y^\mathsf{T} \\ Y_{p-1} \end{bmatrix} \in \mathbb{R}^{p\times n}$$

Stieltjes transform approach.

Proof

- With μ_p e.s.d. of $\frac{1}{n}X_pX_p^\mathsf{T}$,

$$m_{\mu_p}(z) = \frac{1}{p}\mathrm{tr}\left(\frac{1}{n}X_pX_p^\mathsf{T} - zI_p\right)^{-1} = \frac{1}{p}\sum_{i=1}^{p}\left[\left(\frac{1}{n}X_pX_p^\mathsf{T} - zI_p\right)^{-1}\right]_{ii}.$$

- Write

$$X_p = \begin{bmatrix} y^\mathsf{T} \\ Y_{p-1} \end{bmatrix} \in \mathbb{R}^{p\times n}$$

so that, for $\Im[z] > 0$,

$$\left(\frac{1}{n}X_pX_p^\mathsf{T} - zI_p\right)^{-1} = \begin{pmatrix} \frac{1}{n}y^\mathsf{T}y - z & \frac{1}{n}y^\mathsf{T}Y_{p-1} \\ \frac{1}{n}Y_{p-1}y & \frac{1}{n}Y_{p-1}Y_{p-1}^\mathsf{T} - zI_{p-1} \end{pmatrix}^{-1}.$$

Proof (continued)

- From block matrix inverse formula

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(A - BD^{-1}C)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix}$$

we have

$$\left[\left(\frac{1}{n} X_p X_p^{\mathsf{T}} - z I_p \right)^{-1} \right]_{11} = \frac{1}{-z - z \frac{1}{n} y^{\mathsf{T}} (\frac{1}{n} Y_{p-1}^{\mathsf{T}} Y_{p-1} - z I_n)^{-1} y}.$$

Proof (continued)

- From block matrix inverse formula

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(A - BD^{-1}C)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix}$$

we have

$$\left[\left(\frac{1}{n} X_p X_p^{\mathsf{T}} - z I_p \right)^{-1} \right]_{11} = \frac{1}{-z - z \frac{1}{n} y^{\mathsf{T}} (\frac{1}{n} Y_{p-1}^{\mathsf{T}} Y_{p-1} - z I_n)^{-1} y}.$$

- By Trace Lemma, as $p, n \to \infty$

$$\left[\left(\frac{1}{n} X_p X_p^{\mathsf{T}} - z I_p \right)^{-1} \right]_{11} - \frac{1}{-z - z \frac{1}{n} \operatorname{tr} (\frac{1}{n} Y_{p-1}^{\mathsf{T}} Y_{p-1} - z I_n)^{-1}} \xrightarrow{\text{a.s.}} 0.$$

Proof (continued)

- By Rank-1 Perturbation Lemma ($X_p^\mathsf{T} X_p = Y_{p-1}^\mathsf{T} Y_{p-1} + yy^\mathsf{T}$), as $p, n \to \infty$

$$\left[\left(\frac{1}{n} X_p X_p^\mathsf{T} - z I_p \right)^{-1} \right]_{11} - \frac{1}{-z - z \frac{1}{n} \operatorname{tr} \left(\frac{1}{n} X_p^\mathsf{T} X_p - z I_n \right)^{-1}} \xrightarrow{\text{a.s.}} 0.$$

Proof (continued)

- By Rank-1 Perturbation Lemma ($X_p^{\mathsf{T}} X_p = Y_{p-1}^{\mathsf{T}} Y_{p-1} + yy^{\mathsf{T}}$), as $p, n \to \infty$

$$\left[\left(\frac{1}{n} X_p X_p^{\mathsf{T}} - z I_p \right)^{-1} \right]_{11} - \frac{1}{-z - z \frac{1}{n} \operatorname{tr} \left(\frac{1}{n} X_p^{\mathsf{T}} X_p - z I_n \right)^{-1}} \xrightarrow{\text{a.s.}} 0.$$

- Since $\frac{1}{n} \operatorname{tr} \left(\frac{1}{n} X_p^{\mathsf{T}} X_p - z I_n \right)^{-1} = \frac{1}{n} \operatorname{tr} \left(\frac{1}{n} X_p X_p^{\mathsf{T}} - z I_p \right)^{-1} - \frac{n-p}{n} \frac{1}{z}$,

$$\left[\left(\frac{1}{n} X_p X_p^{\mathsf{T}} - z I_p \right)^{-1} \right]_{11} - \frac{1}{1 - \frac{p}{n} - z - z \frac{1}{n} \operatorname{tr} \left(\frac{1}{n} X_p X_p^{\mathsf{T}} - z I_p \right)^{-1}} \xrightarrow{\text{a.s.}} 0.$$

Proof (continued)

- By Rank-1 Perturbation Lemma ($X_p^\mathsf{T} X_p = Y_{p-1}^\mathsf{T} Y_{p-1} + yy^\mathsf{T}$), as $p, n \to \infty$

$$\left[\left(\frac{1}{n} X_p X_p^\mathsf{T} - z I_p \right)^{-1} \right]_{11} - \frac{1}{-z - z \frac{1}{n} \operatorname{tr} \left(\frac{1}{n} X_p^\mathsf{T} X_p - z I_n \right)^{-1}} \xrightarrow{\text{a.s.}} 0.$$

- Since $\frac{1}{n} \operatorname{tr} \left(\frac{1}{n} X_p^\mathsf{T} X_p - z I_n \right)^{-1} = \frac{1}{n} \operatorname{tr} \left(\frac{1}{n} X_p X_p^\mathsf{T} - z I_p \right)^{-1} - \frac{n-p}{n} \frac{1}{z}$,

$$\left[\left(\frac{1}{n} X_p X_p^\mathsf{T} - z I_p \right)^{-1} \right]_{11} - \frac{1}{1 - \frac{p}{n} - z - z \frac{1}{n} \operatorname{tr} \left(\frac{1}{n} X_p X_p^\mathsf{T} - z I_p \right)^{-1}} \xrightarrow{\text{a.s.}} 0.$$

- Repeating for entries $(2,2), \ldots, (p,p)$, and averaging, we get (for $\Im[z] > 0$)

$$m_{\mu_p}(z) - \frac{1}{1 - \frac{p}{n} - z - z \frac{p}{n} m_{\mu_p}(z)} \xrightarrow{\text{a.s.}} 0.$$

Proof (continued)

- Then $m_{\mu_p}(z) \xrightarrow{\text{a.s.}} m(z)$ solution to

$$m(z) = \frac{1}{1 - c - z - czm(z)}$$

Proof (continued)

- Then $m_{\mu_p}(z) \xrightarrow{\text{a.s.}} m(z)$ solution to

$$m(z) = \frac{1}{1 - c - z - czm(z)}$$

i.e., (with branch of $\sqrt{f(z)}$ such that $m(z) \to 0$ as $|z| \to \infty$)

$$m(z) = \frac{1-c}{2cz} - \frac{1}{2c} + \frac{\sqrt{\left(z - (1+\sqrt{c})^2\right)\left(z - (1-\sqrt{c})^2\right)}}{2cz}.$$

Proof (continued)

- Then $m_{\mu_p}(z) \xrightarrow{\text{a.s.}} m(z)$ solution to

$$m(z) = \frac{1}{1 - c - z - czm(z)}$$

i.e., (with branch of $\sqrt{f(z)}$ such that $m(z) \to 0$ as $|z| \to \infty$)

$$m(z) = \frac{1-c}{2cz} - \frac{1}{2c} + \frac{\sqrt{\left(z-(1+\sqrt{c})^2\right)\left(z-(1-\sqrt{c})^2\right)}}{2cz}.$$

- Finally, by inverse Stieltjes Transform, for $x > 0$,

$$\lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \Im[m(x + \imath\varepsilon)] = \frac{\sqrt{\left((1+\sqrt{c})^2 - x\right)\left(x-(1-\sqrt{c})^2\right)}}{2\pi cx} 1_{\{x \in [(1-\sqrt{c})^2, (1+\sqrt{c})^2]\}}.$$

And for $x = 0$,

$$\lim_{\varepsilon \downarrow 0} \imath\varepsilon \Im[m(\imath\varepsilon)] = \left(1 - c^{-1}\right) 1_{\{c>1\}}.$$

Theorem (Sample Covariance Matrix Model **[Silverstein,Bai'95]**)

Let $Y_p = C_p^{\frac{1}{2}} X_p \in \mathbb{R}^{p \times n}$, *with*

- $C_p \in \mathbb{C}^{p \times p}$ *nonnegative definite with e.s.d.* $\nu_p \to \nu$ *weakly,*
- $X_p \in \mathbb{C}^{p \times n}$ *has i.i.d. entries of zero mean and unit variance.*

As $p, n \to \infty$, $p/n \to c \in (0, \infty)$, $\tilde{\mu}_p$ *e.s.d. of* $\frac{1}{n} Y_p^{\mathsf{T}} Y_p \in \mathbb{R}^{n \times n}$ *satisfies*

$$\tilde{\mu}_p \xrightarrow{\text{a.s.}} \tilde{\mu}$$

weakly, with $m_{\tilde{\mu}}(z)$, $\Im[z] > 0$, *unique solution with* $\Im[m_{\tilde{\mu}}(z)] > 0$ *of*

$$m_{\tilde{\mu}}(z) = \left(-z + c \int \frac{t}{1 + t m_{\tilde{\mu}}(z)} \nu(dt) \right)^{-1}.$$

Theorem (Sample Covariance Matrix Model [Silverstein,Bai'95])

Let $Y_p = C_p^{\frac{1}{2}} X_p \in \mathbb{R}^{p\times n}$*, with*

- $C_p \in \mathbb{C}^{p\times p}$ *nonnegative definite with e.s.d.* $\nu_p \to \nu$ *weakly,*
- $X_p \in \mathbb{C}^{p\times n}$ *has i.i.d. entries of zero mean and unit variance.*

As $p,n\to\infty$*,* $p/n \to c \in (0,\infty)$*,* $\tilde{\mu}_p$ *e.s.d. of* $\frac{1}{n} Y_p^{\mathsf{T}} Y_p \in \mathbb{R}^{n\times n}$ *satisfies*

$$\tilde{\mu}_p \xrightarrow{\text{a.s.}} \tilde{\mu}$$

weakly, with $m_{\tilde{\mu}}(z)$*,* $\Im[z]>0$*, unique solution with* $\Im[m_{\tilde{\mu}}(z)]>0$ *of*

$$m_{\tilde{\mu}}(z) = \left(-z + c\int \frac{t}{1+t m_{\tilde{\mu}}(z)}\nu(dt)\right)^{-1}.$$

Moreover, $\tilde{\mu}$ *is continuous on* $\mathbb{R}^+$ *and real analytic wherever positive.*

Theorem (Sample Covariance Matrix Model **[Silverstein,Bai'95]**)

Let $Y_p = C_p^{\frac{1}{2}} X_p \in \mathbb{R}^{p \times n}$, *with*

- $C_p \in \mathbb{C}^{p \times p}$ *nonnegative definite with e.s.d.* $\nu_p \to \nu$ *weakly,*
- $X_p \in \mathbb{C}^{p \times n}$ *has i.i.d. entries of zero mean and unit variance.*

As $p, n \to \infty$, $p/n \to c \in (0, \infty)$, $\tilde{\mu}_p$ *e.s.d. of* $\frac{1}{n} Y_p^\mathsf{T} Y_p \in \mathbb{R}^{n \times n}$ *satisfies*

$$\tilde{\mu}_p \xrightarrow{\text{a.s.}} \tilde{\mu}$$

weakly, with $m_{\tilde{\mu}}(z)$, $\Im[z] > 0$, *unique solution with* $\Im[m_{\tilde{\mu}}(z)] > 0$ *of*

$$m_{\tilde{\mu}}(z) = \left(-z + c \int \frac{t}{1 + t m_{\tilde{\mu}}(z)} \nu(dt) \right)^{-1}.$$

Moreover, $\tilde{\mu}$ *is continuous on* $\mathbb{R}^+$ *and real analytic wherever positive.*

Immediate corollary: For μ_p e.s.d. of $\frac{1}{n} Y_p Y_p^\mathsf{T} = \frac{1}{n} \sum_{i=1}^n C_p^{\frac{1}{2}} x_i x_i^\mathsf{T} C_p^{\frac{1}{2}}$,

$$\mu_p \xrightarrow{\text{a.s.}} \mu$$

weakly, with $\tilde{\mu} = c\mu + (1 - c)\boldsymbol{\delta}_0$.

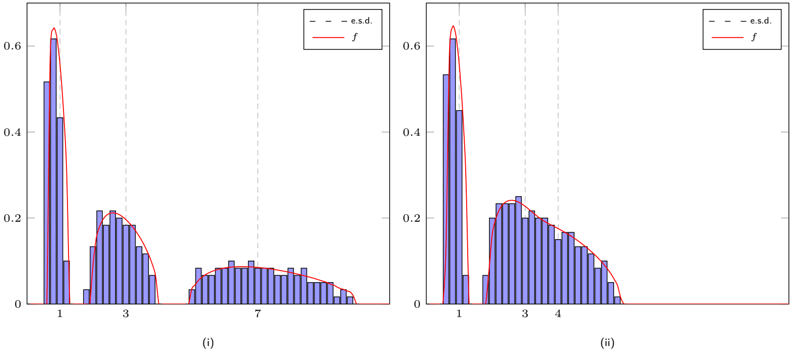


Figure: Histogram of the eigenvalues of $\frac{1}{n} Y_p Y_p^{\mathsf{T}}$, $n = 3000$, $p = 300$, with C_p diagonal with evenly weighted masses in (i) $1, 3, 7$, (ii) $1, 3, 4$.

Sometimes, μ_p does not converge!

Sometimes, μ_p does not converge!

- if ν_p does not converge

Sometimes, μ_p does not converge!

- if ν_p does not converge
- if p/n does not converge

Sometimes, μ_p does not converge!

- if ν_p does not converge
- if p/n does not converge
- if eigenvectors of deterministic matrices play a role!

Sometimes, μ_p does not converge!

- if ν_p does not converge
- if p/n does not converge
- if eigenvectors of deterministic matrices play a role!

Deterministic equivalents: sequence $\bar{\mu}_p$ of deterministic measures, with

$$\mu_p - \bar{\mu}_p \xrightarrow{\text{a.s.}} 0$$

Sometimes, μ_p does not converge!

- if ν_p does not converge
- if p/n does not converge
- if eigenvectors of deterministic matrices play a role!

Deterministic equivalents: sequence $\bar{\mu}_p$ of deterministic measures, with

$$\mu_p - \bar{\mu}_p \xrightarrow{\text{a.s.}} 0$$

or equivalently, deterministic sequence of m_p with

$$m_{\mu_p} - m_p \xrightarrow{\text{a.s.}} 0.$$

Theorem (Doubly-correlated i.i.d. matrices)

Let $B_p = C_p^{\frac{1}{2}} X_p T_p X_p^\mathsf{T} C_p^{\frac{1}{2}}$, *with e.s.d.* μ_p, $X_p \in \mathbb{R}^{p \times n}$ *with i.i.d. entries of zero mean, variance* $1/n$, C_p *Hermitian nonnegative definite,* T_p *diagonal nonnegative,* $\limsup_p \max(\|C_p\|, \|T_p\|) < \infty$. *Denote* $c = p/n$.
Then, as $p, n \to \infty$ *with bounded ratio* c, *for* $z \in \mathbb{C} \setminus \mathbb{R}^-$,

$$m_{\mu_p}(z) - m_p(z) \xrightarrow{\text{a.s.}} 0, \quad m_p(z) = \frac{1}{p} \operatorname{tr} \left(-zI_p + \bar{e}_p(z) C_p\right)^{-1}$$

with $\bar{e}(z)$ *unique solution in* $\{z \in \mathbb{C}^+, \bar{e}_p(z) \in \mathbb{C}^+\}$ *or* $\{z \in \mathbb{R}^-, \bar{e}_p(z) \in \mathbb{R}^+\}$ *of*

$$\begin{aligned} e_p(z) &= \frac{1}{p} \operatorname{tr} C_p \left(-zI_p + \bar{e}_p(z) C_p\right)^{-1} \\ \bar{e}_p(z) &= \frac{1}{n} \operatorname{tr} T_p \left(I_n + c e_p(z) T_p\right)^{-1}. \end{aligned}$$

Side note on other models.
Similar results for multiple matrix models:

Side note on other models.
Similar results for multiple matrix models:

- **Information-plus-noise**: $Y_p = A_p + X_p$, A_p deterministic
- **Variance profile**: $Y_p = P_p \odot X_p$ (entry-wise product)
- **Per-column covariance**: $Y_p = [y_1, \ldots, y_n]$, $y_i = C_{p,i}^{\frac{1}{2}} x_i$
- etc.

Outline

Theorem (No Eigenvalue Outside the Support **[Silverstein,Bai'98]**)

Let $Y_p = C_p^{\frac{1}{2}} X_p \in \mathbb{R}^{p \times n}$*, with*

- $C_p \in \mathbb{R}^{p \times p}$ *nonnegative definite with e.s.d.* $\nu_p \to \nu$ *weakly,*

No Eigenvalue Outside the Support

Theorem (No Eigenvalue Outside the Support **[Silverstein,Bai'98]**)

Let $Y_p = C_p^{\frac{1}{2}} X_p \in \mathbb{R}^{p \times n}$*, with*

- $C_p \in \mathbb{R}^{p \times p}$ *nonnegative definite with e.s.d.* $\nu_p \to \nu$ *weakly,*
- $X_p \in \mathbb{R}^{p \times n}$ *has i.i.d. entries of zero mean and unit variance,*

Theorem (No Eigenvalue Outside the Support [Silverstein,Bai'98])

Let $Y_p = C_p^{\frac{1}{2}} X_p \in \mathbb{R}^{p \times n}$, *with*

- $C_p \in \mathbb{R}^{p \times p}$ *nonnegative definite with e.s.d.* $\nu_p \to \nu$ *weakly,*
- $X_p \in \mathbb{R}^{p \times n}$ *has i.i.d. entries of zero mean and unit variance,*
- $E[|X_p|_{ij}^4] < \infty$,

Theorem (No Eigenvalue Outside the Support **[Silverstein,Bai'98]**)

Let $Y_p = C_p^{\frac{1}{2}} X_p \in \mathbb{R}^{p \times n}$, *with*

- $C_p \in \mathbb{R}^{p \times p}$ *nonnegative definite with e.s.d.* $\nu_p \to \nu$ *weakly,*
- $X_p \in \mathbb{R}^{p \times n}$ *has i.i.d. entries of zero mean and unit variance,*
- $E[|X_p|_{ij}^4] < \infty$,
- $\max_i \operatorname{dist}(\lambda_i(C_p), \operatorname{supp}(\nu)) \to 0$.

No Eigenvalue Outside the Support

Theorem (No Eigenvalue Outside the Support **[Silverstein,Bai'98]**)

Let $Y_p = C_p^{\frac{1}{2}} X_p \in \mathbb{R}^{p \times n}$, *with*

- $C_p \in \mathbb{R}^{p \times p}$ *nonnegative definite with e.s.d.* $\nu_p \to \nu$ *weakly,*
- $X_p \in \mathbb{R}^{p \times n}$ *has i.i.d. entries of zero mean and unit variance,*
- $E[|X_p|_{ij}^4] < \infty$,
- $\max_i \operatorname{dist}(\lambda_i(C_p), \operatorname{supp}(\nu)) \to 0$.

Let $\tilde{\mu}$ *be the limiting e.s.d. of* $\frac{1}{n} Y_p^\mathsf{T} Y_p$ *as before. Let* $[a, b] \subset \mathbb{R}^\mathsf{T} \setminus \operatorname{supp}(\tilde{\nu})$. *Then,*

$$\left\{ \lambda_i \left(\frac{1}{n} Y_p^\mathsf{T} Y_p \right) \right\}_{i=1}^{n} \cap [a, b] = \emptyset$$

for all large n, *almost surely.*

Theorem (No Eigenvalue Outside the Support **[Silverstein,Bai'98]**)

Let $Y_p = C_p^{\frac{1}{2}} X_p \in \mathbb{R}^{p \times n}$*, with*

- $C_p \in \mathbb{R}^{p \times p}$ *nonnegative definite with e.s.d.* $\nu_p \to \nu$ *weakly,*
- $X_p \in \mathbb{R}^{p \times n}$ *has i.i.d. entries of zero mean and unit variance,*
- $E[|X_p|_{ij}^4] < \infty$,
- $\max_i \operatorname{dist}(\lambda_i(C_p), \operatorname{supp}(\nu)) \to 0$.

Let $\tilde{\mu}$ *be the limiting e.s.d. of* $\frac{1}{n} Y_p^\mathsf{T} Y_p$ *as before. Let* $[a, b] \subset \mathbb{R}^\mathsf{T} \setminus \operatorname{supp}(\tilde{\nu})$*. Then,*

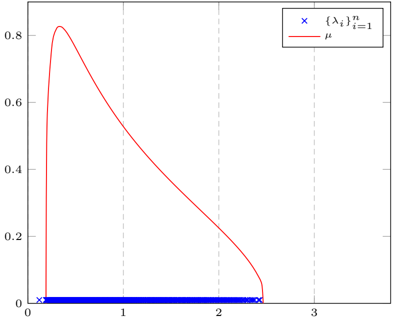
$$\left\{ \lambda_i \left(\frac{1}{n} Y_p^\mathsf{T} Y_p \right) \right\}_{i=1}^{n} \cap [a, b] = \emptyset$$

for all large n*, almost surely.*

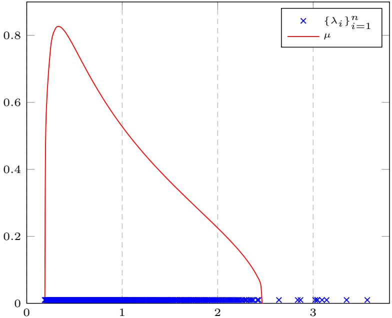
In practice: This means that eigenvalues of $\frac{1}{n} Y_p^\mathsf{T} Y_p$ cannot be bound at macroscopic distance from the bulk, for p, n large.

Breaking the rules. If we break

- **Rule 1**: Infinitely many eigenvalues may wander away from $\mathrm{supp}(\mu)$.



$E[X_{ij}^4] < \infty$



$E[X_{ij}^4] = \infty$

If we break:

- **Rule 2**: C_p may create isolated eigenvalues in $\frac{1}{n}Y_pY_p^\mathsf{T}$, called spikes.

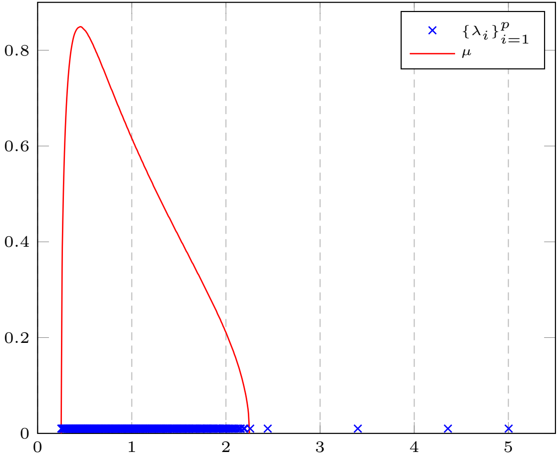


Figure: Eigenvalues of $\frac{1}{n}Y_pY_p^\mathsf{T}$, $C_p = \text{diag}(\underbrace{1,\ldots,1}_{p-4},2,3,4,5)$, $p=500$, $n=2000$.

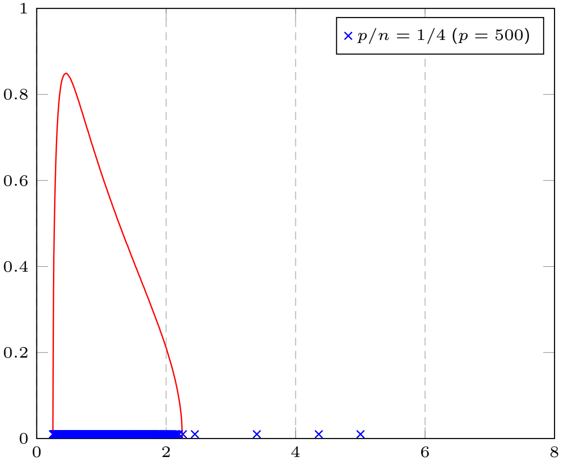


Figure: Eigenvalues of $\frac{1}{n}Y_pY_p^\mathsf{T}$, $C_p = \text{diag}(\underbrace{1,\ldots,1}_{p-4},2,3,4,5)$.

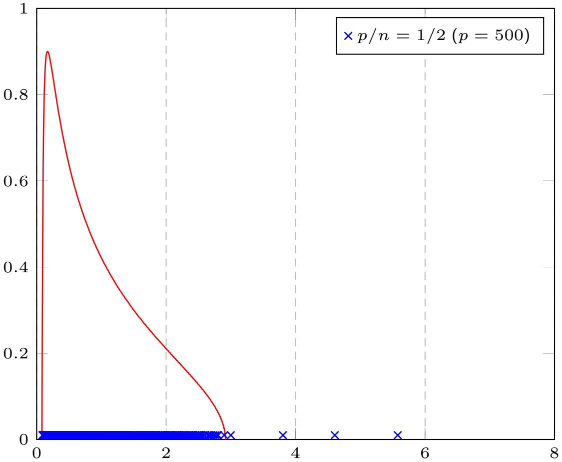


Figure: Eigenvalues of $\frac{1}{n} Y_p Y_p^{\mathsf{T}}$, $C_p = \text{diag}(\underbrace{1, \ldots, 1}_{p-4}, 2, 3, 4, 5)$.

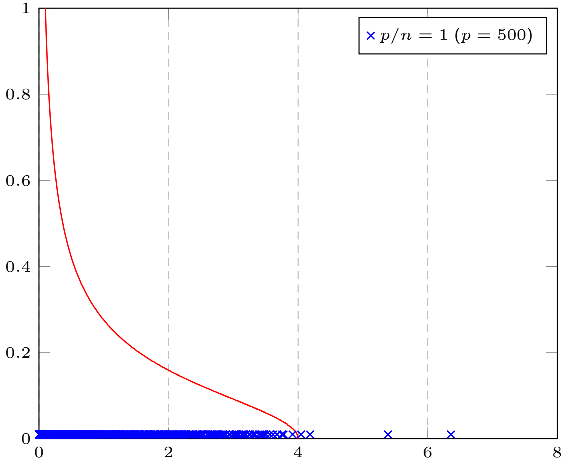


Figure: Eigenvalues of $\frac{1}{n}Y_pY_p^\mathsf{T}$, $C_p = \text{diag}(\underbrace{1,\ldots,1}_{p-4}, 2, 3, 4, 5)$.

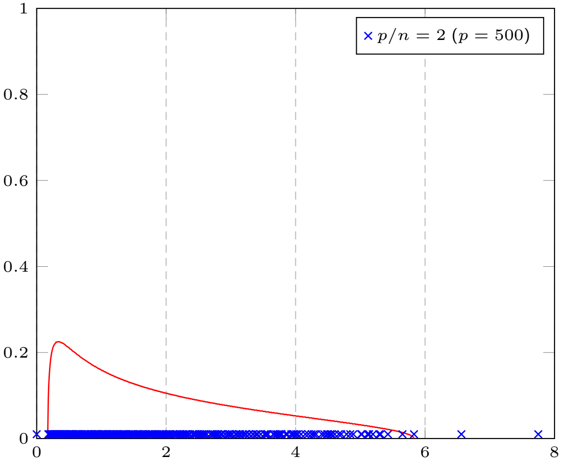


Figure: Eigenvalues of $\frac{1}{n}Y_pY_p^{\mathsf{T}}$, $C_p = \mathrm{diag}(\underbrace{1,\ldots,1}_{p-4},2,3,4,5)$.

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,* $E[|X_p|_{ij}^4] < \infty$.
- $C_p = I_p + P$, $P = U \Omega U^{\mathsf{T}}$, *where, for* K *fixed,*

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

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,* $E[|X_p|_{ij}^4] < \infty$.
- $C_p = I_p + P$, $P = U\Omega U^{\mathsf{T}}$, *where, for* K *fixed,*

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

Then, as $p, n \to \infty$, $p/n \to c \in (0, \infty)$, *denoting* $\lambda_i = \lambda_i(\frac{1}{n} Y_p Y_p^{\mathsf{T}})$,

- *if* $\omega_m > \sqrt{c}$,

$$\lambda_m \xrightarrow{\text{a.s.}} 1 + \omega_m + c\frac{1 + \omega_m}{\omega_m} > (1 + \sqrt{c})^2$$

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,* $E[|X_p|_{ij}^4] < \infty$.
- $C_p = I_p + P$, $P = U\Omega U^\mathsf{T}$, *where, for* K *fixed,*

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

Then, as $p, n \to \infty$, $p/n \to c \in (0, \infty)$, *denoting* $\lambda_i = \lambda_i(\frac{1}{n} Y_p Y_p^\mathsf{T})$,

- *if* $\omega_m > \sqrt{c}$,

$$\lambda_m \xrightarrow{\text{a.s.}} 1 + \omega_m + c\frac{1 + \omega_m}{\omega_m} > (1 + \sqrt{c})^2$$

- *if* $\omega_m \in (0, \sqrt{c}]$,

$$\lambda_m \xrightarrow{\text{a.s.}} (1 + \sqrt{c})^2$$

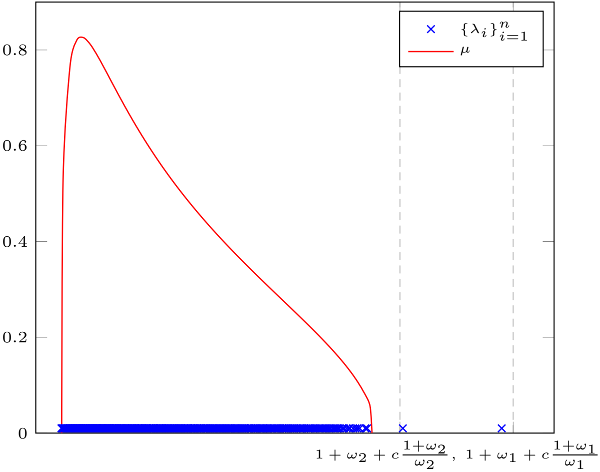


Figure: Eigenvalues of $\frac{1}{n}Y_pY_p^{\mathsf{T}}$, $C_p = \text{diag}(\underbrace{1,\ldots,1}_{p-2},2,3)$, $p=500$, $n=1500$.

Proof

- **Two ingredients**: Algebraic calculus + trace lemma

Proof

- **Two ingredients**: Algebraic calculus + trace lemma
- **Find eigenvalues away from eigenvalues of $\frac{1}{n}X_pX_p^\mathsf{T}$**:

$$
\begin{aligned}
0 &= \det\left(\frac{1}{n}Y_pY_p^\mathsf{T} - \lambda I_p\right), \quad Y_p = C_p^{\frac{1}{2}} X_p \\
&= \det(C_p)\det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda C_p^{-1}\right) \\
&= \det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p + \lambda(I_p - C_p^{-1})\right) \\
&= \det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)\det\left(I_p + \lambda(I_p - C_p^{-1})\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)^{-1}\right).
\end{aligned}
$$

Proof

- **Two ingredients**: Algebraic calculus + trace lemma
- **Find eigenvalues away from eigenvalues of $\frac{1}{n}X_pX_p^\mathsf{T}$**:

$$\begin{aligned}
0 &= \det\left(\frac{1}{n}Y_pY_p^\mathsf{T} - \lambda I_p\right), \quad Y_p = C_p^{\frac{1}{2}}X_p \\
&= \det(C_p)\det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda C_p^{-1}\right) \\
&= \det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p + \lambda(I_p - C_p^{-1})\right) \\
&= \det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)\det\left(I_p + \lambda(I_p - C_p^{-1})\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)^{-1}\right).
\end{aligned}$$

- **Use low rank property**: $(C_p = I_p + P = I_p + U\Omega U^\mathsf{T})$

$$I_p - C_p^{-1} = I_p - (I_p + U\Omega U^\mathsf{T})^{-1} = U(I_K + \Omega^{-1})^{-1}U^\mathsf{T},\ \Omega \in \mathbb{C}^{K\times K}.$$

Hence

$$0 = \det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)\det\left(I_p + \lambda U(I_K + \Omega^{-1})^{-1}U^\mathsf{T}\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)^{-1}\right).$$

Proof

- **Two ingredients**: Algebraic calculus + trace lemma
- **Find eigenvalues away from eigenvalues of** $\frac{1}{n}X_pX_p^{\mathsf{T}}$:

$$
\begin{aligned}
0 &= \det\left(\frac{1}{n}Y_pY_p^{\mathsf{T}} - \lambda I_p\right), \quad Y_p = C_p^{\frac{1}{2}}X_p \\
&= \det(C_p)\det\left(\frac{1}{n}X_pX_p^{\mathsf{T}} - \lambda C_p^{-1}\right) \\
&= \det\left(\frac{1}{n}X_pX_p^{\mathsf{T}} - \lambda I_p + \lambda(I_p - C_p^{-1})\right) \\
&= \det\left(\frac{1}{n}X_pX_p^{\mathsf{T}} - \lambda I_p\right)\det\left(I_p + \lambda(I_p - C_p^{-1})\left(\frac{1}{n}X_pX_p^{\mathsf{T}} - \lambda I_p\right)^{-1}\right).
\end{aligned}
$$

- **Use low rank property**: $(C_p = I_p + P = I_p + U\Omega U^{\mathsf{T}})$

$$
I_p - C_p^{-1} = I_p - (I_p + U\Omega U^{\mathsf{T}})^{-1} = U(I_K + \Omega^{-1})^{-1}U^{\mathsf{T}},\ \Omega \in \mathbb{C}^{K\times K}.
$$

Hence

$$
0 = \det\left(\frac{1}{n}X_pX_p^{\mathsf{T}} - \lambda I_p\right)\det\left(I_p + \lambda U(I_K + \Omega^{-1})^{-1}U^{\mathsf{T}}\left(\frac{1}{n}X_pX_p^{\mathsf{T}} - \lambda I_p\right)^{-1}\right).
$$

Proof (2)

- **Sylverster's identity** $(\det(I + AB) = \det(I + BA))$,

$$0 = \det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)\det\left(I_K + \lambda(I_K + \Omega^{-1})^{-1}U^\mathsf{T}\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)^{-1}U\right)$$

Proof (2)

- **Sylverster's identity** $(\det(I + AB) = \det(I + BA))$,

$$0 = \det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)\det\left(I_K + \lambda(I_K + \Omega^{-1})^{-1}U^\mathsf{T}\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)^{-1}U\right)$$

- **No eigenvalue outside the support [Bai,Sil'98]**: $\det(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p)$ has no zero beyond $(1+\sqrt{c})^2$ for all large n a.s.

Proof (2)

- **Sylverster's identity** ($\det(I + AB) = \det(I + BA)$),

$$0 = \det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)\det\left(I_K + \lambda(I_K + \Omega^{-1})^{-1}U^\mathsf{T}\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)^{-1}U\right)$$

- **No eigenvalue outside the support [Bai,Sil'98]**: $\det(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p)$ has no zero beyond $(1+\sqrt{c})^2$ for all large n a.s.
- **Extension of Trace Lemma**: for each $z \in \mathbb{C} \setminus \operatorname{supp}(\mu)$,

$$U^\mathsf{T}\left(\frac{1}{n}X_pX_p^\mathsf{T} - zI_p\right)^{-1}U \xrightarrow{\text{a.s.}} m_\mu(z)I_K.$$

(X_p being "almost-unitarily invariant", U made of "i.i.d.-like" random vectors)

Proof (2)

- **Sylverster's identity** ($\det(I + AB) = \det(I + BA)$),

$$0 = \det\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)\det\left(I_K + \lambda(I_K + \Omega^{-1})^{-1}U^\mathsf{T}\left(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p\right)^{-1}U\right)$$

- **No eigenvalue outside the support [Bai,Sil'98]**: $\det(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p)$ has no zero beyond $(1 + \sqrt{c})^2$ for all large n a.s.
- **Extension of Trace Lemma**: for each $z \in \mathbb{C} \setminus \operatorname{supp}(\mu)$,

$$U^\mathsf{T}\left(\frac{1}{n}X_pX_p^\mathsf{T} - zI_p\right)^{-1}U \xrightarrow{\text{a.s.}} m_\mu(z)I_K.$$

  (X_p being "almost-unitarily invariant", U made of "i.i.d.-like" random vectors)
- As a result, for all large n a.s.,

$$\begin{aligned}0 &= \det\left(I_K + \lambda(I_K + \Omega^{-1})^{-1}U^\mathsf{T}(\frac{1}{n}X_pX_p^\mathsf{T} - \lambda I_p)^{-1}U\right)\\ &\simeq \prod_{k=1}^{K}\left(1 + \frac{\lambda}{1+\omega_k^{-1}}m_\mu(\lambda)\right) = \prod_{k=1}^{K}\left(1 + \frac{\omega_k}{1+\omega_k}\lambda m_\mu(\lambda)\right)\end{aligned}$$

Proof (3)

- **Limiting solutions:** zeros of

$$\lambda m_\mu(\lambda) = -\frac{1+\omega_m}{\omega_m}.$$

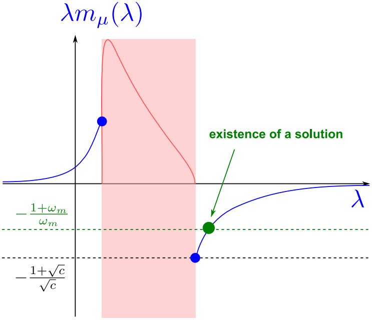
Proof (3)

- **Limiting solutions:** zeros of

$$\lambda m_\mu(\lambda) = -\frac{1+\omega_m}{\omega_m}.$$

- Marčenko–Pastur law properties $(m_\mu(z) = (1-c-z-czm_\mu(z))^{-1})$:
  - $\lambda \mapsto \lambda m_\mu(\lambda) = \int \frac{\lambda}{t-\lambda}\mu(dt)$ maps $((1+\sqrt{c})^2, \infty)$ onto $(-\frac{1+\sqrt{c}}{\sqrt{c}}, 0^-)$
  - Solution only when $\omega_m > \sqrt{c}$:

$$\lambda = 1 + \omega_m + c\frac{1+\omega_m}{\omega_m}.$$



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

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

- X_p *with i.i.d. zero mean, unit variance, finite fourth order moment entries*
- $C_p = I_p + P$*,* $P = \sum_{i=1}^{K} \omega_i u_i u_i^{\mathsf{T}}$*,* $\omega_1 > \ldots > \omega_M > 0$*.*

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

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

- X_p *with i.i.d. zero mean, unit variance, finite fourth order moment entries*
- $C_p = I_p + P$, $P = \sum_{i=1}^{K} \omega_i u_i u_i^\mathsf{T}$, $\omega_1 > \ldots > \omega_M > 0$.

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

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

In particular,

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

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

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

- X_p *with i.i.d. zero mean, unit variance, finite fourth order moment entries*
- $C_p = I_p + P$, $P = \sum_{i=1}^K \omega_i u_i u_i^\mathsf{T}$, $\omega_1 > \ldots > \omega_M > 0$.

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

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

In particular,

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

Proof: Based on Cauchy integral + similar ingredients as eigenvalue proof

$$a^\mathsf{T} \hat{u}_i \hat{u}_i^\mathsf{T} b = \frac{1}{2\pi\imath} \oint_{\mathcal{C}_i} a^\mathsf{T} \left(\frac{1}{n} Y_p Y_p^\mathsf{T} - zI_p \right)^{-1} b \, dz$$

for $\mathcal{C}_m$ contour circling around λ_i only.

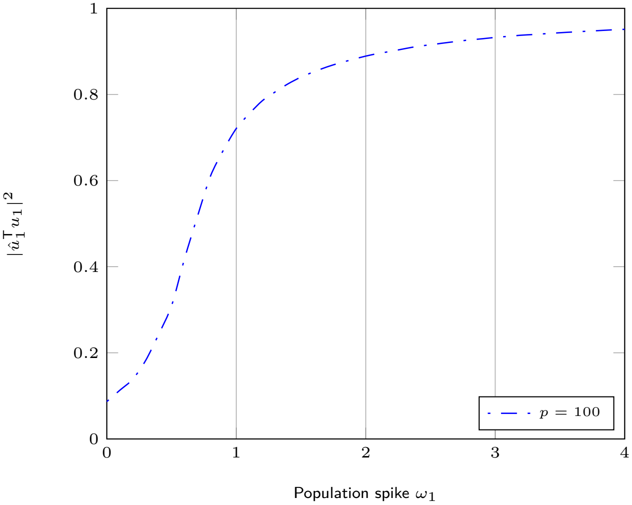


Figure: Simulated versus limiting $|\hat{u}_1^\mathsf{T} u_1|^2$ for $Y_p = C_p^{\frac{1}{2}} X_p$, $C_p = I_p + \omega_1 u_1 u_1^\mathsf{T}$, $p/n = 1/3$, varying ω_1.

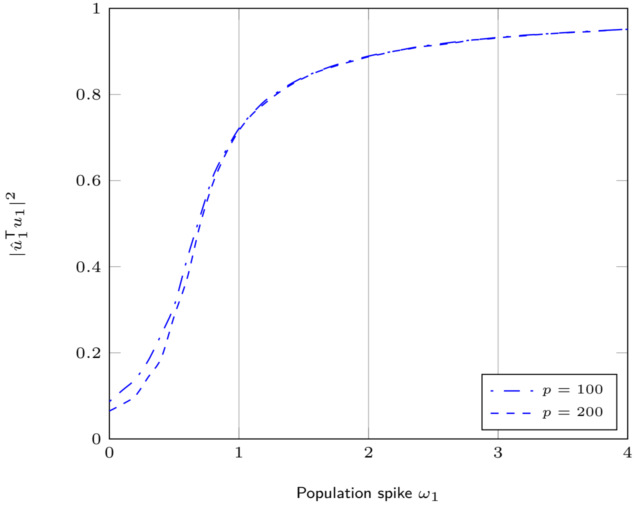


Figure: Simulated versus limiting $|\hat{u}_1^{\mathsf{T}} u_1|^2$ for $Y_p = C_p^{\frac{1}{2}} X_p$, $C_p = I_p + \omega_1 u_1 u_1^{\mathsf{T}}$, $p/n = 1/3$, varying ω_1.

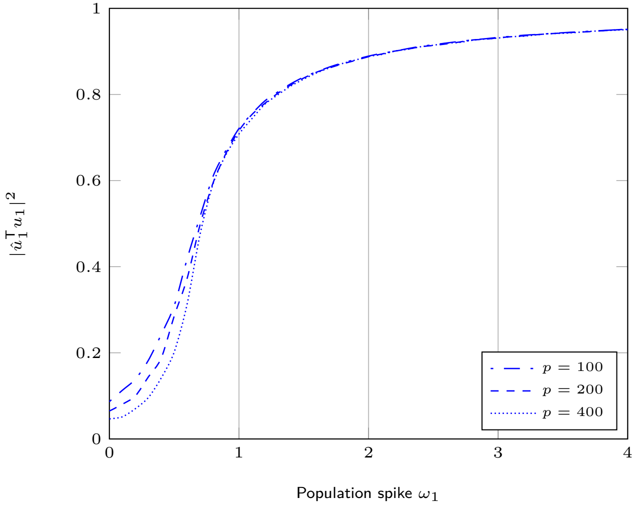


Figure: Simulated versus limiting $|\hat{u}_1^\mathsf{T} u_1|^2$ for $Y_p = C_p^{\frac{1}{2}} X_p$, $C_p = I_p + \omega_1 u_1 u_1^\mathsf{T}$, $p/n = 1/3$, varying ω_1.

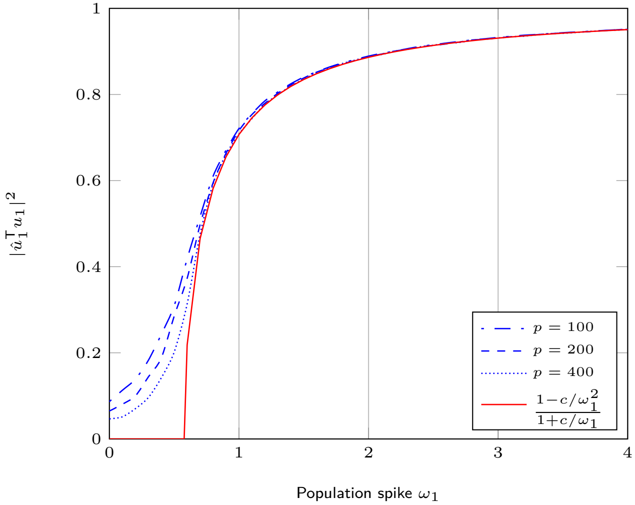


Figure: Simulated versus limiting $|\hat{u}_1^\mathsf{T} u_1|^2$ for $Y_p = C_p^{\frac{1}{2}} X_p$, $C_p = I_p + \omega_1 u_1 u_1^\mathsf{T}$, $p/n = 1/3$, varying ω_1.

Theorem (Fluctuations of Eigenvalues **[Baik,BenArous,Péché'05]**)

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

- X_p *with i.i.d. real or complex Gaussian zero mean, unit variance entries,*
- $C_p = I_p + P$, $P = \sum_{i=1}^{K} \omega_i u_i u_i^{\mathsf{T}}$, $\omega_1 > \ldots > \omega_K > 0$ *(*$K \geq 0$*).*

Theorem (Fluctuations of Eigenvalues [Baik,BenArous,Péché'05])

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

- X_p *with i.i.d. real or complex Gaussian zero mean, unit variance entries,*
- $C_p = I_p + P$, $P = \sum_{i=1}^{K} \omega_i u_i u_i^{\mathsf{T}}$, $\omega_1 > \ldots > \omega_K > 0$ *(*$K \geq 0$*).*

Then, as $p, n \to \infty$, $p/n \to c < 1$,

- *If* $\omega_1 < \sqrt{c}$ *(or* $K = 0$*),*

$$p^{\frac{2}{3}} \frac{\lambda_1 - (1+\sqrt{c})^2}{(1+\sqrt{c})^{\frac{4}{3}} c^{\frac{1}{2}}} \xrightarrow{\mathcal{L}} T, \text{ (real or complex Tracy–Widom law)}$$

Tracy–Widom Theorem

Theorem (Fluctuations of Eigenvalues **[Baik,BenArous,Péché'05]**)

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

- X_p *with i.i.d. real or complex Gaussian zero mean, unit variance entries,*
- $C_p = I_p + P$, $P = \sum_{i=1}^{K} \omega_i u_i u_i^{\mathsf{T}}$, $\omega_1 > \ldots > \omega_K > 0$ *(*$K \geq 0$*).*

Then, as $p, n \to \infty$, $p/n \to c < 1$,

- *If* $\omega_1 < \sqrt{c}$ *(or* $K = 0$*),*

$$p^{\frac{2}{3}} \frac{\lambda_1 - (1+\sqrt{c})^2}{(1+\sqrt{c})^{\frac{4}{3}} c^{\frac{1}{2}}} \xrightarrow{\mathcal{L}} T, \quad \text{(real or complex Tracy–Widom law)}$$

- *If* $\omega_1 > \sqrt{c}$,

$$\left(\frac{(1+\omega_1)^2}{c} - \frac{(1+\omega_1)^2}{\omega_1^2} \right)^{\frac{1}{2}} p^{\frac{1}{2}} \left[\lambda_1 - \left(1 + \omega_1 + c \frac{1+\omega_1}{\omega_1} \right) \right] \xrightarrow{\mathcal{L}} \mathcal{N}(0,1).$$

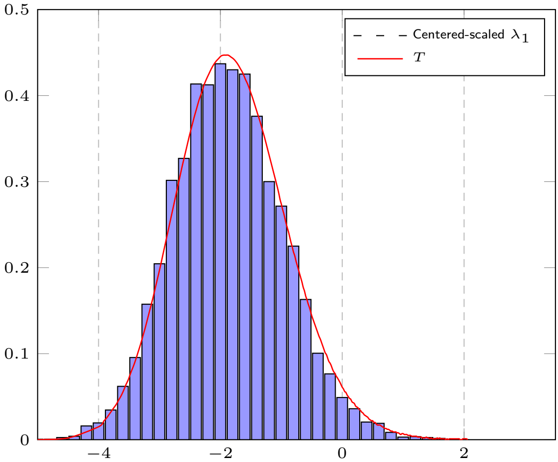


Figure: Distribution of $p^{\frac{2}{3}}c^{-\frac{1}{2}}(1+\sqrt{c})^{-\frac{4}{3}}\left[\lambda_1(\frac{1}{n}X_pX_p^{\mathsf{T}})-(1+\sqrt{c})^2\right]$ versus real Tracy–Widom (T), $p=500$, $n=1500$.

Other Spiked Models

Similar results for multiple matrix models:

- $Y_p = \frac{1}{n}XX^\mathsf{T} + P$, P deterministic and low rank
- $Y_p = \frac{1}{n}X^\mathsf{T}(I + P)X$
- $Y_p = \frac{1}{n}(X + P)^\mathsf{T}(X + P)$
- $Y_p = \frac{1}{n}TX^\mathsf{T}(I + P)XT$
- etc.

Theorem

Let $X_n \in \mathbb{R}^{n\times n}$ Hermitian with e.s.d. μ_n such that $\frac{1}{\sqrt{n}}[X_n]_{i>j}$ are i.i.d. with zero mean and unit variance. Then, as $n \to \infty$,

$$\mu_n \xrightarrow{\text{a.s.}} \mu$$

with $\mu(dt) = \frac{1}{2\pi}\sqrt{(4-t^2)^+}dt$. In particular, m_μ satisfies

$$m_\mu(z) = \frac{1}{-z - m_\mu(z)}.$$

The Semi-circle law

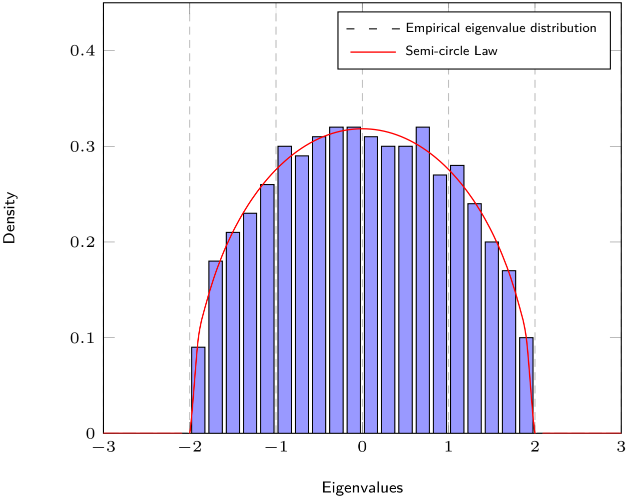


Figure: Histogram of the eigenvalues of Wigner matrices and the semi-circle law, for $n = 500$

Theorem

Let $X_n \in \mathbb{C}^{n\times n}$ with e.s.d. μ_n be such that $\frac{1}{\sqrt{n}}[X_n]_{ij}$ are i.i.d. entries with zero mean and unit variance. Then, as $n \to \infty$,

$$\mu_n \xrightarrow{\text{a.s.}} \mu$$

with μ a complex-supported measure with $\mu(dz) = \frac{1}{2\pi}\delta_{|z|\leq 1}dz$.

The Circular law

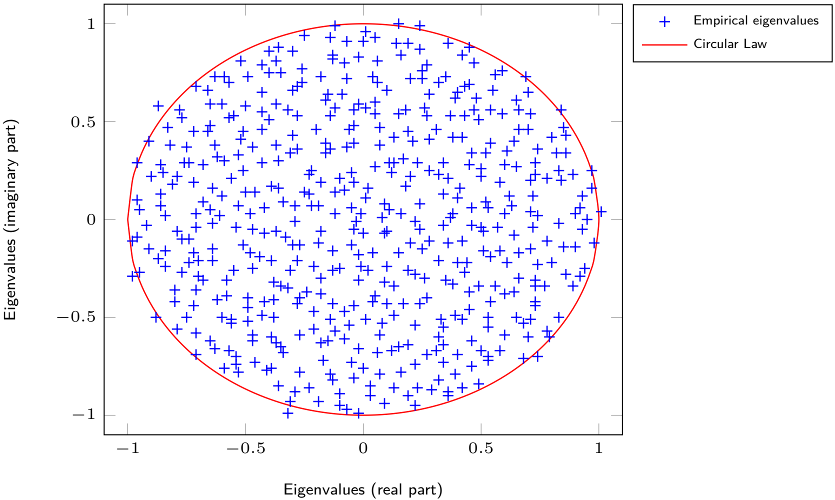


Figure: Eigenvalues of X_n with i.i.d. standard Gaussian entries, for $n = 500$.

Bibliographical references: Maths Book and Tutorial References I

From most accessible to least:

- Couillet, R., & Debbah, M. (2011). Random matrix methods for wireless communications. Cambridge University Press.
- Tao, T. (2012). Topics in random matrix theory (Vol. 132). Providence, RI: American Mathematical Society.
- Bai, Z., & Silverstein, J. W. (2010). Spectral analysis of large dimensional random matrices (Vol. 20). New York: Springer.
- Pastur, L. A., Shcherbina, M., & Shcherbina, M. (2011). Eigenvalue distribution of large random matrices (Vol. 171). Providence, RI: American Mathematical Society.
- Anderson, G. W., Guionnet, A., & Zeitouni, O. (2010). An introduction to random matrices (Vol. 118). Cambridge university press.

Large range of applications:

Large range of applications:

- ***Wireless communications:*** capacity of large communication channels $H \in \mathbb{C}^{p \times n}$, optimal precoding in mu-MIMO, power allocation in large networks, sensing in cognitive radios, etc.

Large range of applications:

- ***Wireless communications:*** capacity of large communication channels $H \in \mathbb{C}^{p \times n}$, optimal precoding in mu-MIMO, power allocation in large networks, sensing in cognitive radios, etc.
- ***Array processing:*** improved MUSIC methods for large arrays ($p \sim n$), optimal beamforming (MVDR), detection filters (ANMF), etc.

Large range of applications:

- ***Wireless communications:*** capacity of large communication channels $H \in \mathbb{C}^{p \times n}$, optimal precoding in mu-MIMO, power allocation in large networks, sensing in cognitive radios, etc.
- ***Array processing:*** improved MUSIC methods for large arrays ($p \sim n$), optimal beamforming (MVDR), detection filters (ANMF), etc.
- ***Statistical finance:*** portfolio optimization (Markowitz, GMVP) for large portfolios and short time windows.

From classical applications...

Large range of applications:

- ***Wireless communications:*** capacity of large communication channels $H \in \mathbb{C}^{p \times n}$, optimal precoding in mu-MIMO, power allocation in large networks, sensing in cognitive radios, etc.
- ***Array processing:*** improved MUSIC methods for large arrays ($p \sim n$), optimal beamforming (MVDR), detection filters (ANMF), etc.
- ***Statistical finance:*** portfolio optimization (Markowitz, GMVP) for large portfolios and short time windows.
- ***Brain signal processing:*** EEG covariance estimation on short windows.

From classical applications...

Large range of applications:

- ***Wireless communications:*** capacity of large communication channels $H \in \mathbb{C}^{p \times n}$, optimal precoding in mu-MIMO, power allocation in large networks, sensing in cognitive radios, etc.
- ***Array processing:*** improved MUSIC methods for large arrays ($p \sim n$), optimal beamforming (MVDR), detection filters (ANMF), etc.
- ***Statistical finance:*** portfolio optimization (Markowitz, GMVP) for large portfolios and short time windows.
- ***Brain signal processing:*** EEG covariance estimation on short windows.

Any application where $p \sim n$ "rather large"

(convergence speed in up to $O(n)$ and not $O(\sqrt{n})$ as usual!)

Large range of applications:

- ***Wireless communications:*** capacity of large communication channels $H \in \mathbb{C}^{p \times n}$, optimal precoding in mu-MIMO, power allocation in large networks, sensing in cognitive radios, etc.
- ***Array processing:*** improved MUSIC methods for large arrays ($p \sim n$), optimal beamforming (MVDR), detection filters (ANMF), etc.
- ***Statistical finance:*** portfolio optimization (Markowitz, GMVP) for large portfolios and short time windows.
- ***Brain signal processing:*** EEG covariance estimation on short windows.

Any application where $p \sim n$ "rather large"

(convergence speed in up to $O(n)$ and not $O(\sqrt{n})$ as usual!)

BUT mostly linear settings...

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(Wx_l)$, non-linear features, etc.

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(W x_l)$, non-linear features, etc.
- ***Often non-explicit solutions:*** robust statistics (fixed-point matrices), SVM margin constraints, logistic regression, etc.

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(Wx_l)$, non-linear features, etc.
- ***Often non-explicit solutions:*** robust statistics (fixed-point matrices), SVM margin constraints, logistic regression, etc.

CENTRAL ISSUE: Given that basic sample covariance matrices are not consistent for large n, p, what happens to machine learning methods?

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(Wx_l)$, non-linear features, etc.
- ***Often non-explicit solutions:*** robust statistics (fixed-point matrices), SVM margin constraints, logistic regression, etc.

CENTRAL ISSUE: Given that basic sample covariance matrices are not consistent for large n, p, what happens to machine learning methods?

- we will see that **small-dimensional intuitions dramatically fail**

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(Wx_l)$, non-linear features, etc.
- ***Often non-explicit solutions:*** robust statistics (fixed-point matrices), SVM margin constraints, logistic regression, etc.

CENTRAL ISSUE: Given that basic sample covariance matrices are not consistent for large n, p, what happens to machine learning methods?

- we will see that **small-dimensional intuitions dramatically fail**
- some **classical and widely-used algorithms become ineffective**

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(Wx_l)$, non-linear features, etc.
- ***Often non-explicit solutions:*** robust statistics (fixed-point matrices), SVM margin constraints, logistic regression, etc.

CENTRAL ISSUE: Given that basic sample covariance matrices are not consistent for large n, p, what happens to machine learning methods?

- we will see that **small-dimensional intuitions dramatically fail**
- some **classical and widely-used algorithms become ineffective**
- **BUT** random matrix theory provides a renewed understanding.

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(Wx_l)$, non-linear features, etc.
- ***Often non-explicit solutions:*** robust statistics (fixed-point matrices), SVM margin constraints, logistic regression, etc.

CENTRAL ISSUE: Given that basic sample covariance matrices are not consistent for large n, p, what happens to machine learning methods?

- we will see that **small-dimensional intuitions dramatically fail**
- some **classical and widely-used algorithms become ineffective**
- **BUT** random matrix theory provides a renewed understanding.

TUTORIAL: first answers to

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(Wx_l)$, non-linear features, etc.
- ***Often non-explicit solutions:*** robust statistics (fixed-point matrices), SVM margin constraints, logistic regression, etc.

CENTRAL ISSUE: Given that basic sample covariance matrices are not consistent for large n, p, what happens to machine learning methods?

- we will see that **small-dimensional intuitions dramatically fail**
- some **classical and widely-used algorithms become ineffective**
- **BUT** random matrix theory provides a renewed understanding.

TUTORIAL: first answers to **understand**,

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(Wx_l)$, non-linear features, etc.
- ***Often non-explicit solutions:*** robust statistics (fixed-point matrices), SVM margin constraints, logistic regression, etc.

CENTRAL ISSUE: Given that basic sample covariance matrices are not consistent for large n, p, what happens to machine learning methods?

- we will see that **small-dimensional intuitions dramatically fail**
- some **classical and widely-used algorithms become ineffective**
- **BUT** random matrix theory provides a renewed understanding.

TUTORIAL: first answers to **understand**, **improve**, and

Specificities in statistical and machine learning:

- ***Matrix of non-linear entries:*** kernel matrices $K = \{\kappa(x_i, x_j)\}_{i,j=1}^n$, activation functions in neural nets $x_{l+1} = \sigma(Wx_l)$, non-linear features, etc.
- ***Often non-explicit solutions:*** robust statistics (fixed-point matrices), SVM margin constraints, logistic regression, etc.

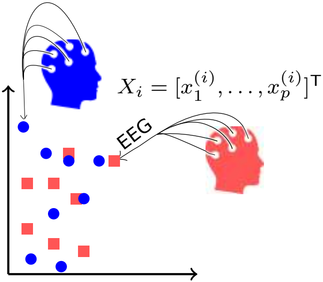
CENTRAL ISSUE: Given that basic sample covariance matrices are not consistent for large n, p, what happens to machine learning methods?

- we will see that **small-dimensional intuitions dramatically fail**
- some **classical and widely-used algorithms become ineffective**
- **BUT** random matrix theory provides a renewed understanding.

TUTORIAL: first answers to **understand**, **improve**, and **change paradigm**.

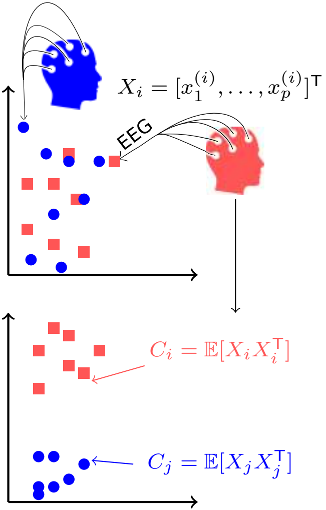
Outline

- Hard classification on raw data X_i:
  Need Features



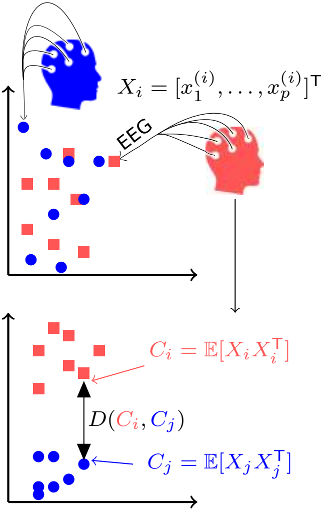
Motivation example: EEG-based clustering

- Hard classification on raw data X_i: Need Features
- Relevant Feature: Covariance C_i



Motivation example: EEG-based clustering

- Hard classification on raw data X_i: Need Features
- Relevant Feature: Covariance C_i
- Distance between features: $D(C_i, C_j)$



Context

Observations:

- two data vector classes $x_i^{(1)} \in \mathcal{C}_1$ and $x_i^{(2)} \in \mathcal{C}_2$

Context

Observations:

- two data vector classes $x_i^{(1)} \in \mathcal{C}_1$ and $x_i^{(2)} \in \mathcal{C}_2$
- $X_a = [x_1^{(a)}, \ldots, x_{n_a}^{(a)}]$, $x_i^{(a)} \in \mathbb{R}^p$ with $E[x_i^{(a)}] = 0$, $E[x_i^{(a)} x_i^{(a)\mathsf{T}}] = C_a$.

Context

Observations:

- two data vector classes $x_i^{(1)} \in \mathcal{C}_1$ and $x_i^{(2)} \in \mathcal{C}_2$
- $X_a = [x_1^{(a)}, \ldots, x_{n_a}^{(a)}]$, $x_i^{(a)} \in \mathbb{R}^p$ with $E[x_i^{(a)}] = 0$, $E[x_i^{(a)} x_i^{(a)\mathsf{T}}] = C_a$.

Objective:

- From the data $x_i^{(a)}$, estimate some distance function

$$D \equiv D(C_1, C_2).$$

Observations:

- two data vector classes $x_i^{(1)} \in \mathcal{C}_1$ and $x_i^{(2)} \in \mathcal{C}_2$
- $X_a = [x_1^{(a)}, \ldots, x_{n_a}^{(a)}]$, $x_i^{(a)} \in \mathbb{R}^p$ with $E[x_i^{(a)}] = 0$, $E[x_i^{(a)} x_i^{(a)\mathsf{T}}] = C_a$.

Objective:

- From the data $x_i^{(a)}$, estimate some distance function

$$D \equiv D(C_1, C_2).$$

- Classical approach:

$$\hat{D} \equiv D(\hat{C}_1, \hat{C}_2), \quad \text{with } \hat{C}_a = \frac{1}{n_a} \sum_{i=1}^{n_a} x_i^{(a)} x_i^{(a)\mathsf{T}} = \frac{1}{n_a} X_a X_a^{\mathsf{T}}.$$

Context

Observations:

- two data vector classes $x_i^{(1)} \in \mathcal{C}_1$ and $x_i^{(2)} \in \mathcal{C}_2$
- $X_a = [x_1^{(a)}, \ldots, x_{n_a}^{(a)}]$, $x_i^{(a)} \in \mathbb{R}^p$ with $E[x_i^{(a)}] = 0$, $E[x_i^{(a)} x_i^{(a)\mathsf{T}}] = C_a$.

Objective:

- From the data $x_i^{(a)}$, estimate some distance function

$$D \equiv D(C_1, C_2).$$

- Classical approach:

$$\hat{D} \equiv D(\hat{C}_1, \hat{C}_2), \quad \text{with } \hat{C}_a = \frac{1}{n_a} \sum_{i=1}^{n_a} x_i^{(a)} x_i^{(a)\mathsf{T}} = \frac{1}{n_a} X_a X_a^{\mathsf{T}}.$$

$\longrightarrow$ **Often justified by Law of Large Numbers**: $\hat{D} \xrightarrow{\text{a.s.}} D$ as $n \to \infty$.

In practice though...

Example:

- The Fisher distance

$$D(C_1, C_2) = \frac{1}{p} \left\| \log^2(C_1^{-\frac{1}{2}} C_2 C_1^{-\frac{1}{2}}) \right\|_F^2$$

Example:

- The Fisher distance

$$D(C_1, C_2) = \frac{1}{p} \left\| \log^2(C_1^{-\frac{1}{2}} C_2 C_1^{-\frac{1}{2}}) \right\|_F^2 = \frac{1}{p} \sum_{i=1}^{p} \log^2 \left(\lambda_i (C_1^{-1} C_2) \right)$$

In practice though...

Example:

- The Fisher distance

$$D(C_1, C_2) = \frac{1}{p} \left\| \log^2 (C_1^{-\frac{1}{2}} C_2 C_1^{-\frac{1}{2}}) \right\|_F^2 = \frac{1}{p} \sum_{i=1}^{p} \log^2 \left(\lambda_i (C_1^{-1} C_2) \right) = \int \log^2(t) \nu_p(dt)$$

with $\nu_p = \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i (C_1^{-1} C_2)}$.

In practice though...

Example:

- The Fisher distance

$$D(C_1, C_2) = \frac{1}{p} \left\| \log^2(C_1^{-\frac{1}{2}} C_2 C_1^{-\frac{1}{2}}) \right\|_F^2 = \frac{1}{p} \sum_{i=1}^{p} \log^2 \left(\lambda_i(C_1^{-1} C_2) \right) = \int \log^2(t) \nu_p(dt)$$

  with $\nu_p = \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(C_1^{-1} C_2)}$.

- for $n_1 = 1024$, $n_2 = 2048$, different p (here $[C_1^{-\frac{1}{2}} C_2 C_1^{-\frac{1}{2}}]_{ij} = .3^{|i-j|}$):

In practice though...

Example:

- The Fisher distance

$$D(C_1, C_2) = \frac{1}{p} \left\| \log^2 (C_1^{-\frac{1}{2}} C_2 C_1^{-\frac{1}{2}}) \right\|_F^2 = \frac{1}{p} \sum_{i=1}^{p} \log^2 \left(\lambda_i (C_1^{-1} C_2) \right) = \int \log^2(t) \nu_p(dt)$$

with $\nu_p = \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(C_1^{-1}C_2)}$.

- for $n_1 = 1024$, $n_2 = 2048$, different p (here $[C_1^{-\frac{1}{2}} C_2 C_1^{-\frac{1}{2}}]_{ij} = .3^{|i-j|}$):

p	Fisher distance	Classical estimator
2	0.0980	0.1002
4	0.1456	0.1520
8	0.1694	0.1820
16	0.1812	0.2081
32	0.1872	0.2363
64	0.1901	**0.2892**
128	0.1916	**0.3955**
256	0.1924	**0.6338**
512	0.1927	**1.2715**

(error $< 5\%$) **(error $> 50\%$)** **(error $> 100\%$)** **(error $> 500\%$)**

In practice though...

Example:

- The Fisher distance

$$D(C_1,C_2)=\frac{1}{p}\left\|\log^2(C_1^{-\frac{1}{2}}C_2C_1^{-\frac{1}{2}})\right\|_F^2=\frac{1}{p}\sum_{i=1}^p\log^2\left(\lambda_i(C_1^{-1}C_2)\right)=\int\log^2(t)\nu_p(dt)$$

with $\nu_p=\frac{1}{p}\sum_{i=1}^p\delta_{\lambda_i(C_1^{-1}C_2)}$.

- for $n_1=1024$, $n_2=2048$, different p (here $[C_1^{-\frac{1}{2}}C_2C_1^{-\frac{1}{2}}]_{ij}=.3^{|i-j|}$):

p	Fisher distance	Classical estimator	RMT estimator
2	0.0980	0.1002	0.0973
4	0.1456	0.1520	0.1461
8	0.1694	0.1820	0.1703
16	0.1812	0.2081	0.1845
32	0.1872	0.2363	0.1886
64	0.1901	**0.2892**	0.1920
128	0.1916	**0.3955**	0.1934
256	0.1924	**0.6338**	0.1942
512	0.1927	**1.2715**	0.1953

(error $<$ 5%) **(error $>$ 50%)** **(error $>$ 100%)** **(error $>$ 500%)**

Explanation for failure

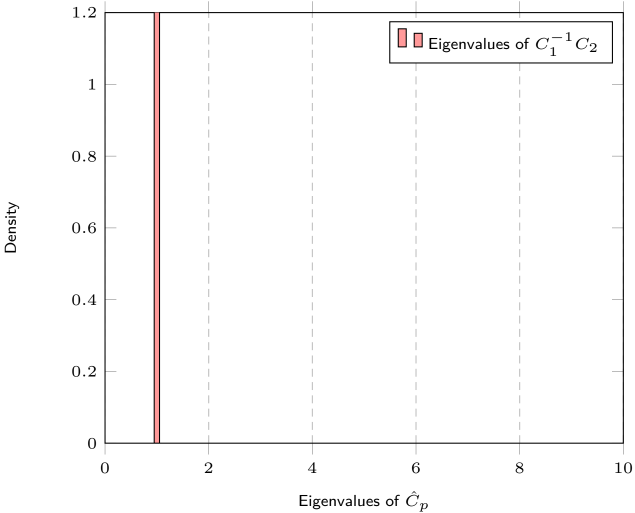


Figure: Population and Sample Eigenvalues for $n_1 = 1024$, $n_2 = 2048$, varying p, $C_1 = C_2$.

Explanation for failure

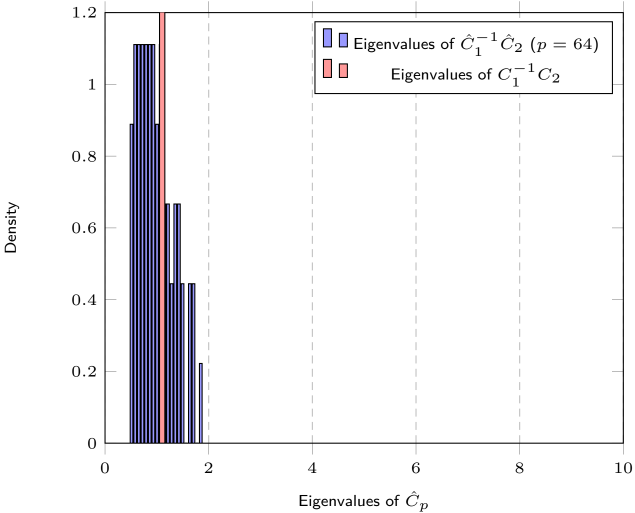


Figure: Population and Sample Eigenvalues for $n_1 = 1024$, $n_2 = 2048$, varying p, $C_1 = C_2$.

Explanation for failure

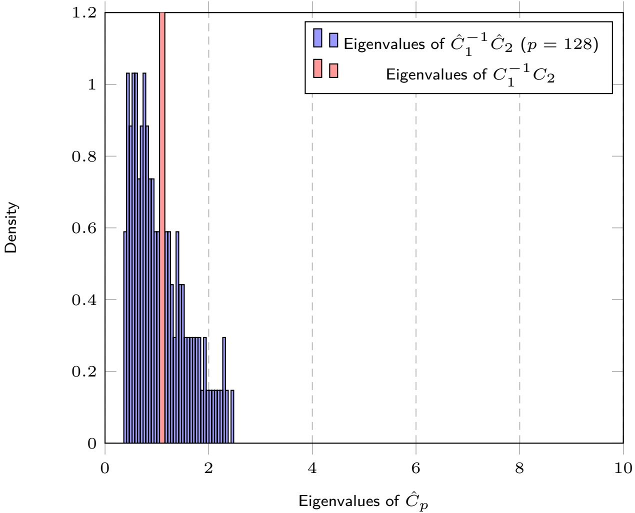


Figure: Population and Sample Eigenvalues for $n_1 = 1024$, $n_2 = 2048$, varying p, $C_1 = C_2$.

Explanation for failure

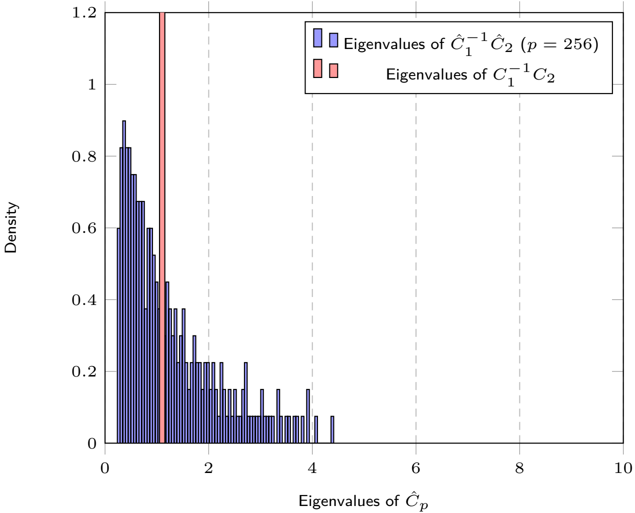


Figure: Population and Sample Eigenvalues for $n_1 = 1024$, $n_2 = 2048$, varying p, $C_1 = C_2$.

Explanation for failure

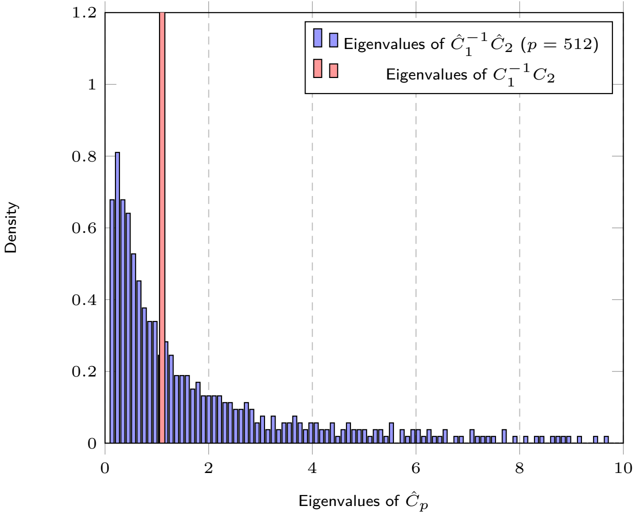


Figure: Population and Sample Eigenvalues for $n_1 = 1024$, $n_2 = 2048$, varying p, $C_1 = C_2$.

Setup

Assumptions

- **[Spatial independence]** $x_i^{(a)} = C_a^{\frac{1}{2}} \tilde{x}_i^{(a)}$, $\tilde{x}_i^{(a)} \in \mathbb{R}^p$ with i.i.d. zero mean, unit variance, finite $4 + \varepsilon$ order moment.

Setup

Assumptions

- **[Spatial independence]** $x_i^{(a)} = C_a^{\frac{1}{2}} \tilde{x}_i^{(a)}$, $\tilde{x}_i^{(a)} \in \mathbb{R}^p$ with i.i.d. zero mean, unit variance, finite $4 + \varepsilon$ order moment.

- **[RMT regime]** As $n_a \to \infty$,

$$\frac{p}{n_a} = c_a \to c_a^\infty \in (0, 1).$$

- **[Studied distances]** for f a complex-analytic extensible function,

$$D(C_1, C_2) = \int f(t) \nu_p(dt)$$

Setup

Assumptions

- **[Spatial independence]** $x_i^{(a)} = C_a^{\frac{1}{2}} \tilde{x}_i^{(a)}$, $\tilde{x}_i^{(a)} \in \mathbb{R}^p$ with i.i.d. zero mean, unit variance, finite $4+\varepsilon$ order moment.
- **[RMT regime]** As $n_a \to \infty$,

$$\frac{p}{n_a} = c_a \to c_a^\infty \in (0,1).$$

- **[Studied distances]** for f a complex-analytic extensible function,

$$D(C_1, C_2) = \int f(t)\nu_p(dt), \quad \nu_p = \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i(C_1^{-1}C_2)}.$$

Assumptions

- **[Spatial independence]** $x_i^{(a)} = C_a^{\frac{1}{2}} \tilde{x}_i^{(a)}$, $\tilde{x}_i^{(a)} \in \mathbb{R}^p$ with i.i.d. zero mean, unit variance, finite $4 + \varepsilon$ order moment.
- **[RMT regime]** As $n_a \to \infty$,

$$\frac{p}{n_a} = c_a \to c_a^\infty \in (0,1).$$

- **[Studied distances]** for f a complex-analytic extensible function,

$$D(C_1, C_2) = \int f(t) \nu_p(dt), \quad \nu_p = \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(C_1^{-1} C_2)}.$$

Examples

- *Fisher geodesic distance*: $f(t) = \log^2(t)$
- *Bhattacharyya distance*: $f(t) = -\frac{1}{4}\log(t) + \frac{1}{2}\log(1+t) - \frac{1}{2}\log(2)$
- *Kullback-Leibler divergence for Gaussian:* $f(t) = \frac{1}{2}t - \frac{1}{2}\log(t) - \frac{1}{2}$
- *Rényi divergence for Gaussian:* $f(t) = \frac{-1}{2(\alpha-1)}\log(\alpha + (1-\alpha)t) + \frac{1}{2}\log(t)$

Notations:

RMT-improved estimator

Notations:

- **Population eigenvalue distribution**: $\nu_p = \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(C_1^{-1} C_2)}$

RMT-improved estimator

Notations:

- **Population eigenvalue distribution**: $\nu_p = \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i(C_1^{-1}C_2)}$
- **Sample eigenvalue distribution**: $\mu_p = \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i(\hat{C}_1{}^{-1}\hat{C}_2)}$

RMT-improved estimator

Notations:

- **Population eigenvalue distribution**: $\nu_p = \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i(C_1^{-1}C_2)}$
- **Sample eigenvalue distribution**: $\mu_p = \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i(\hat{C}_1{}^{-1}\hat{C}_2)} \equiv \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i}$

RMT-improved estimator

Notations:

- **Population eigenvalue distribution**: $\nu_p = \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i(C_1^{-1}C_2)}$
- **Sample eigenvalue distribution**: $\mu_p = \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i(\hat{C_1}^{-1}\hat{C_2})} \equiv \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i}$
- Recall **Stieltjes transform** $m_\theta(z)$, $z \in \mathbb{C} \setminus \mathrm{Supp}(\theta)$, of measure θ:

$$m_\theta(z) = \int \frac{1}{\lambda - z} d\theta(\lambda)$$

RMT-improved estimator

Notations:

- **Population eigenvalue distribution**: $\nu_p = \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i(C_1^{-1}C_2)}$
- **Sample eigenvalue distribution**: $\mu_p = \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i(\hat{C}_1{}^{-1}\hat{C}_2)} \equiv \frac{1}{p}\sum_{i=1}^{p} \delta_{\lambda_i}$
- Recall **Stieltjes transform** $m_\theta(z)$, $z \in \mathbb{C} \setminus \mathrm{Supp}(\theta)$, of measure θ:

$$m_\theta(z) = \int \frac{1}{\lambda - z} d\theta(\lambda)$$

e.g., $m_{\mu_p}(z) = \frac{1}{p}\sum_{i=1}^{p} \frac{1}{\lambda_i - z}$.

Notations:

- **Population eigenvalue distribution**: $\nu_p = \frac{1}{p}\sum_{i=1}^p \delta_{\lambda_i(C_1^{-1}C_2)}$
- **Sample eigenvalue distribution**: $\mu_p = \frac{1}{p}\sum_{i=1}^p \delta_{\lambda_i(\hat{C}_1{}^{-1}\hat{C}_2)} \equiv \frac{1}{p}\sum_{i=1}^p \delta_{\lambda_i}$
- Recall **Stieltjes transform** $m_\theta(z)$, $z \in \mathbb{C} \setminus \mathrm{Supp}(\theta)$, of measure θ:

$$m_\theta(z) = \int \frac{1}{\lambda - z} d\theta(\lambda)$$

e.g., $m_{\mu_p}(z) = \frac{1}{p}\sum_{i=1}^p \frac{1}{\lambda_i - z}$.

Theorem (Estimation via contour integral)

For $z \in \mathbb{C} \setminus \mathrm{Supp}(\mu_p)$*, let*

$$\varphi_p(z) \equiv z + c_1 z^2 m_{\mu_p}(z)$$
$$\psi_p(z) \equiv 1 - c_2 - c_2 z m_{\mu_p}(z).$$

Notations:

- **Population eigenvalue distribution**: $\nu_p = \frac{1}{p}\sum_{i=1}^p \delta_{\lambda_i(C_1^{-1}C_2)}$
- **Sample eigenvalue distribution**: $\mu_p = \frac{1}{p}\sum_{i=1}^p \delta_{\lambda_i(\hat{C}_1{}^{-1}\hat{C}_2)} \equiv \frac{1}{p}\sum_{i=1}^p \delta_{\lambda_i}$
- Recall **Stieltjes transform** $m_\theta(z)$, $z \in \mathbb{C}\setminus \mathrm{Supp}(\theta)$, of measure θ:

$$m_\theta(z) = \int \frac{1}{\lambda - z} d\theta(\lambda)$$

e.g., $m_{\mu_p}(z) = \frac{1}{p}\sum_{i=1}^p \frac{1}{\lambda_i - z}$.

Theorem (Estimation via contour integral)

For $z \in \mathbb{C}\setminus \mathrm{Supp}(\mu_p)$, *let*

$$\varphi_p(z) \equiv z + c_1 z^2 m_{\mu_p}(z)$$
$$\psi_p(z) \equiv 1 - c_2 - c_2 z m_{\mu_p}(z).$$

Then, for any (positively oriented) contour $\Gamma \subset \{z \in \mathbb{C}, \Re[z] > 0\}$ *surrounding* $\mathrm{Supp}(\mu_p)$.

$$\int f d\nu_p - \frac{1}{2\pi\imath}\oint_\Gamma f\left(\frac{\varphi_p(z)}{\psi_p(z)}\right)\left(\frac{\varphi_p'(z)}{\varphi_p(z)} - \frac{\psi_p'(z)}{\psi_p(z)}\right)\frac{\psi_p(z)}{c_2} dz \xrightarrow{\text{a.s.}} 0.$$

Idea of proof

From [Bai-Silverstein'95][1], limiting spectra of C and $\hat{C}$ related through Stieljes transform.

[1] **SIL95**.

Idea of proof

From [Bai-Silverstein'95][1], limiting spectra of C and $\hat{C}$ related through Stieljes transform.
Besides, by Cauchy's integral,

$$\int f(t)\nu_p(dt) = \int \left[\frac{-1}{2\pi \imath} \oint_\Gamma \frac{f(z)}{t-z} dz \right] \nu_p(dt)$$

[1] **SIL95**.

Idea of proof

From [Bai-Silverstein'95][1], limiting spectra of C and $\hat{C}$ related through Stieljes transform.
Besides, by Cauchy's integral,

$$\int f(t)\nu_p(dt) = \int \left[\frac{-1}{2\pi\imath} \oint_\Gamma \frac{f(z)}{t-z} dz \right] \nu_p(dt) = \frac{-1}{2\pi\imath} \oint_\Gamma f(z) \underbrace{\left[\int \frac{1}{t-z} \nu_p(dt) \right]}_{=m_{\nu_p}(z)} dz.$$

[1] **SIL95**.

From [Bai-Silverstein'95][1], limiting spectra of C and $\hat{C}$ related through Stieljes transform.
Besides, by Cauchy's integral,

$$\int f(t)\nu_p(dt) = \int \left[\frac{-1}{2\pi\imath}\oint_\Gamma \frac{f(z)}{t-z}dz\right]\nu_p(dt) = \frac{-1}{2\pi\imath}\oint_\Gamma f(z)\underbrace{\left[\int \frac{1}{t-z}\nu_p(dt)\right]}_{=m_{\nu_p}(z)}dz.$$

$$\begin{tikzcd}
\int f(t)\nu_p(dt) \arrow[rr, dash, "\times"] \arrow[d, leftrightarrow] & & \int h(t)\mu_p(dt) \arrow[d, leftrightarrow] \\
\oint H(m_{\nu_p}(z))dz \arrow[r, leftrightarrow] & \oint G(m_{\zeta_p}(z))dz \arrow[r, leftrightarrow] & \oint F(m_{\mu_p}(z))dz \\
C_2^{-\frac{1}{2}}C_1C_2^{-\frac{1}{2}} & \hat{C}_2^{-\frac{1}{2}}C_1\hat{C}_2^{-\frac{1}{2}} & \hat{C}_2^{-\frac{1}{2}}\hat{C}_1\hat{C}_2^{-\frac{1}{2}}
\end{tikzcd}$$

[1] **SIL95**.

Evaluation of the complex integrals

Object of interest: Evaluate in closed-form

$$\frac{1}{2\pi\imath}\oint_{\Gamma} f\left(\frac{\varphi_p(z)}{\psi_p(z)}\right)\left(\frac{\varphi_p'(z)}{\varphi_p(z)}-\frac{\psi_p'(z)}{\psi_p(z)}\right)\frac{\psi_p(z)}{c_2}dz.$$

Evaluation of the complex integrals

Object of interest: Evaluate in closed-form

$$\frac{1}{2\pi\imath}\oint_\Gamma f\left(\frac{\varphi_p(z)}{\psi_p(z)}\right)\left(\frac{\varphi_p'(z)}{\varphi_p(z)}-\frac{\psi_p'(z)}{\psi_p(z)}\right)\frac{\psi_p(z)}{c_2}dz.$$

Reminder: functions of interest

- *Fisher geodesic distance*: $f(t)=\log^2(t)$
- *Bhattacharyya distance*: $f(t)=-\frac{1}{4}\log(t)+\frac{1}{2}\log(1+t)-\frac{1}{2}\log(2)$
- *Kullback-Leibler divergence for Gaussian:* $f(t)=\frac{1}{2}t-\frac{1}{2}\log(t)-\frac{1}{2}$
- *Rényi divergence for Gaussian:* $f(t)=\frac{-1}{2(\alpha-1)}\log(\alpha+(1-\alpha)t)+\frac{1}{2}\log(t)$

Evaluation of the complex integrals

Object of interest: Evaluate in closed-form

$$\frac{1}{2\pi\imath}\oint_\Gamma f\left(\frac{\varphi_p(z)}{\psi_p(z)}\right)\left(\frac{\varphi_p'(z)}{\varphi_p(z)}-\frac{\psi_p'(z)}{\psi_p(z)}\right)\frac{\psi_p(z)}{c_2}dz.$$

Reminder: functions of interest

- *Fisher geodesic distance*: $f(t)=\log^2(t)$
- *Bhattacharyya distance*: $f(t)=-\frac{1}{4}\log(t)+\frac{1}{2}\log(1+t)-\frac{1}{2}\log(2)$
- *Kullback-Leibler divergence for Gaussian:* $f(t)=\frac{1}{2}t-\frac{1}{2}\log(t)-\frac{1}{2}$
- *Rényi divergence for Gaussian:* $f(t)=\frac{-1}{2(\alpha-1)}\log(\alpha+(1-\alpha)t)+\frac{1}{2}\log(t)$

Cases of interest:

- Entire functions (e.g., $f(t)=t$): **residue calculus**

Evaluation of the complex integrals

Object of interest: Evaluate in closed-form

$$\frac{1}{2\pi\imath}\oint_\Gamma f\left(\frac{\varphi_p(z)}{\psi_p(z)}\right)\left(\frac{\varphi_p'(z)}{\varphi_p(z)}-\frac{\psi_p'(z)}{\psi_p(z)}\right)\frac{\psi_p(z)}{c_2}dz.$$

Reminder: functions of interest

- *Fisher geodesic distance*: $f(t) = \log^2(t)$
- *Bhattacharyya distance*: $f(t) = -\frac{1}{4}\log(t) + \frac{1}{2}\log(1+t) - \frac{1}{2}\log(2)$
- *Kullback-Leibler divergence for Gaussian:* $f(t) = \frac{1}{2}t - \frac{1}{2}\log(t) - \frac{1}{2}$
- *Rényi divergence for Gaussian:* $f(t) = \frac{-1}{2(\alpha-1)}\log(\alpha + (1-\alpha)t) + \frac{1}{2}\log(t)$

Cases of interest:

- Entire functions (e.g., $f(t) = t$): **residue calculus**
- Functions with **branch cuts**: $f(t) = \log(t)$, $f(t) = \log(1+st)$, $f(t) = \log^2(t)$, etc.
  $\longrightarrow$ **Much more technical!**

Sketch of Proof

The case $f(t) = \log^k(t)$

- Much less trivial due to **branch cuts of** $\log(z)$**!!**

$$\log(z) \equiv \log(|z|) + \imath \arg(z), \quad \arg(z) \in (-\pi, \pi].$$

The case $f(t) = \log^k(t)$

- Much less trivial due to **branch cuts of** $\log(z)$**!!**

$$\log(z) \equiv \log(|z|) + \imath \arg(z), \quad \arg(z) \in (-\pi, \pi].$$

- Singularities arise when $\log(\varphi_p(z)/\psi_p(z))$ discontinuous.

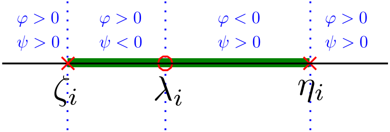
The case $f(t) = \log^k(t)$

- Much less trivial due to **branch cuts of** $\log(z)$**!!**

$$\log(z) \equiv \log(|z|) + \imath \arg(z), \quad \arg(z) \in (-\pi, \pi].$$

- Singularities arise when $\log(\varphi_p(z)/\psi_p(z))$ discontinuous.

- The situation in image...

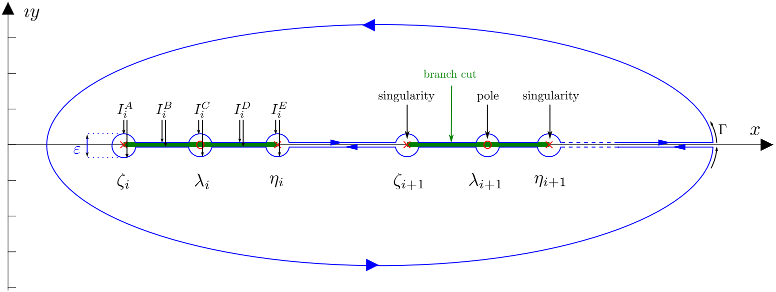


with

- ζ_i zeros of ψ_p
- η_i zeros of φ_p.

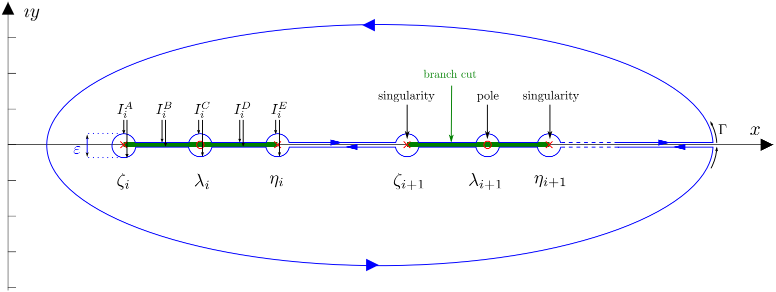
The case $f(t) = \log^k(t)$ **(continued)**

- Integration method: avoid branch cuts:



The case $f(t) = \log^k(t)$ **(continued)**

- Integration method: avoid branch cuts:



- Detailed method:
  - careful control of integrals on circles I_i^A, I_i^C, I_i^E (Jordan's identity does not apply!)
  - linear integrals on segments, up to integrability... **easy for** $\log(t)$**, difficult for** $\log^2(t)$**!**

Corollary (Case $f(t) = t$)

Under the same assumptions,

$$\int t\nu_p(dt) - (1 - c_1) \int t\mu_p(dt) \xrightarrow{\text{a.s.}} 0.$$

Corollary (Case $f(t) = t$)

Under the same assumptions,

$$\int t\nu_p(dt) - (1 - c_1) \int t\mu_p(dt) \xrightarrow{\text{a.s.}} 0.$$

(i.e., $\frac{1}{p} \operatorname{tr} C_1^{-1} C_2 \simeq (1 - \frac{p}{n_1}) \frac{1}{p} \operatorname{tr} \hat{C}_1^{-1} \hat{C}_2$)

Corollary (Case $f(t) = t$)

Under the same assumptions,

$$\int t\nu_p(dt) - (1-c_1)\int t\mu_p(dt) \xrightarrow{\text{a.s.}} 0.$$

(i.e., $\frac{1}{p}\operatorname{tr} C_1^{-1}C_2 \simeq (1-\frac{p}{n_1})\frac{1}{p}\operatorname{tr} \hat{C}_1^{-1}\hat{C}_2$)

$\longrightarrow$ Just a scaling factor!

Corollary (Case $f(t) = t$)

Under the same assumptions,

$$\int t\nu_p(dt) - (1 - c_1) \int t\mu_p(dt) \xrightarrow{\text{a.s.}} 0.$$

(i.e., $\frac{1}{p} \operatorname{tr} C_1^{-1} C_2 \simeq (1 - \frac{p}{n_1}) \frac{1}{p} \operatorname{tr} \hat{C}_1^{-1} \hat{C}_2$)

$\longrightarrow$ Just a scaling factor!

Corollary (Case $f(t) = \log(t)$)

Under the same assumptions,

$$\int \log(t)\nu_p(dt) - \left[\int \log(t)\mu_p(dt) - \frac{1 - c_1}{c_1} \log(1 - c_1) + \frac{1 - c_2}{c_2} \log(1 - c_2) \right] \xrightarrow{\text{a.s.}} 0.$$

Corollary (Case $f(t) = t$)

Under the same assumptions,

$$\int t\nu_p(dt) - (1 - c_1) \int t\mu_p(dt) \xrightarrow{\text{a.s.}} 0.$$

(i.e., $\frac{1}{p} \operatorname{tr} C_1^{-1} C_2 \simeq (1 - \frac{p}{n_1}) \frac{1}{p} \operatorname{tr} \hat{C}_1^{-1} \hat{C}_2$)

$\longrightarrow$ Just a scaling factor!

Corollary (Case $f(t) = \log(t)$)

Under the same assumptions,

$$\int \log(t)\nu_p(dt) - \left[\int \log(t)\mu_p(dt) - \frac{1 - c_1}{c_1} \log(1 - c_1) + \frac{1 - c_2}{c_2} \log(1 - c_2) \right] \xrightarrow{\text{a.s.}} 0.$$

(i.e., $\frac{1}{p} \log\det(C_1^{-1} C_2) \simeq \frac{1}{p} \log\det(\hat{C}_1^{-1} \hat{C}_2) - \frac{n_1 - p}{n_1} \log(1 - \frac{p}{n_1}) + \frac{n_2 - p}{n_2} \log(1 - \frac{p}{n_2})$)

Application to specific functions

Corollary (Case $f(t) = t$)

Under the same assumptions,

$$\int t\nu_p(dt) - (1-c_1)\int t\mu_p(dt) \xrightarrow{\text{a.s.}} 0.$$

(i.e., $\frac{1}{p}\operatorname{tr} C_1^{-1}C_2 \simeq (1-\frac{p}{n_1})\frac{1}{p}\operatorname{tr}\hat{C}_1^{-1}\hat{C}_2$)

$\longrightarrow$ Just a scaling factor!

Corollary (Case $f(t) = \log(t)$)

Under the same assumptions,

$$\int \log(t)\nu_p(dt) - \left[\int \log(t)\mu_p(dt) - \frac{1-c_1}{c_1}\log(1-c_1) + \frac{1-c_2}{c_2}\log(1-c_2)\right] \xrightarrow{\text{a.s.}} 0.$$

(i.e., $\frac{1}{p}\log\det(C_1^{-1}C_2) \simeq \frac{1}{p}\log\det(\hat{C}_1^{-1}\hat{C}_2) - \frac{n_1-p}{n_1}\log(1-\frac{p}{n_1}) + \frac{n_2-p}{n_2}\log(1-\frac{p}{n_2})$)

$\longrightarrow$ Just a bias term!

Corollary (Case $f(t) = \log(1+st)$)

Denoting $\kappa_0 < 0$ unique negative solution to $1 + s\frac{\varphi_p(x)}{\psi_p(x)} = 0$,

$$\int \log(1+st)d\nu_p(t) - \left[\frac{c_1+c_2-c_1c_2}{c_1c_2}\log\left(\frac{c_1+c_2-c_1c_2}{(1-c_1)(c_2-sc_1\kappa_0)}\right) + \frac{1}{c_2}\log\left(-s\kappa_0(1-c_1)\right) + \int \log\left(1-\frac{t}{\kappa_0}\right)d\mu_p(t)\right] \xrightarrow{\text{a.s.}} 0.$$

Corollary (Case $f(t) = \log(1+st)$)

Denoting $\kappa_0 < 0$ unique negative solution to $1 + s\frac{\varphi_p(x)}{\psi_p(x)} = 0$,

$$\int \log(1+st)d\nu_p(t) - \left[\frac{c_1+c_2-c_1c_2}{c_1c_2}\log\left(\frac{c_1+c_2-c_1c_2}{(1-c_1)(c_2-sc_1\kappa_0)}\right)\right.$$
$$\left.+\frac{1}{c_2}\log\left(-s\kappa_0(1-c_1)\right) + \int \log\left(1-\frac{t}{\kappa_0}\right)d\mu_p(t)\right] \xrightarrow{\text{a.s.}} 0.$$

$\longrightarrow$ Highly non-trivial!

Corollary (Case $f(t) = \log^2(t)$)

$$
\begin{aligned}
&\frac{1}{2\pi\imath} \oint_\Gamma \log^2\left(\frac{\varphi_p(z)}{\psi_p(z)}\right)\left(\frac{\varphi_p'(z)}{\varphi_p(z)} - \frac{\psi_p'(z)}{\psi_p(z)}\right)\frac{\psi_p(z)}{c_2} dz \\
&= \frac{c_1 + c_2 - c_1 c_2}{c_1 c_2}\left[\sum_{i=1}^p \left\{\log^2\left((1-c_1)\eta_i\right) - \log^2\left((1-c_1)\lambda_i\right)\right\}\right. \\
&\left. +2\sum_{1\leq i,j\leq p}\left\{\mathrm{Li}_2\left(1-\frac{\zeta_i}{\lambda_j}\right) - \mathrm{Li}_2\left(1-\frac{\eta_i}{\lambda_j}\right) + \mathrm{Li}_2\left(1-\frac{\eta_i}{\eta_j}\right) - \mathrm{Li}_2\left(1-\frac{\zeta_i}{\eta_j}\right)\right\}\right] \\
&- \frac{1-c_2}{c_2}\left[\log^2(1-c_2) - \log^2(1-c_1) + \sum_{i=1}^p \left\{\log^2\left(\eta_i\right) - \log^2\left(\zeta_i\right)\right\}\right] \\
&- \frac{1}{p}\left[2\sum_{1\leq i,j\leq p}\left\{\mathrm{Li}_2\left(1-\frac{\zeta_i}{\lambda_j}\right) - \mathrm{Li}_2\left(1-\frac{\eta_i}{\lambda_j}\right)\right\} - \sum_{i=1}^p \log^2\left((1-c_1)\lambda_i\right)\right]
\end{aligned}
$$

Corollary (Case $f(t) = \log^2(t)$)

$$\frac{1}{2\pi\imath}\oint_\Gamma \log^2\left(\frac{\varphi_p(z)}{\psi_p(z)}\right)\left(\frac{\varphi_p'(z)}{\varphi_p(z)} - \frac{\psi_p'(z)}{\psi_p(z)}\right)\frac{\psi_p(z)}{c_2}dz$$

$$= \frac{c_1+c_2-c_1c_2}{c_1c_2}\left[\sum_{i=1}^{p}\left\{\log^2\left((1-c_1)\eta_i\right) - \log^2\left((1-c_1)\lambda_i\right)\right\}\right.$$

$$\left. +2\sum_{1\leq i,j\leq p}\left\{\mathrm{Li}_2\left(1-\frac{\zeta_i}{\lambda_j}\right) - \mathrm{Li}_2\left(1-\frac{\eta_i}{\lambda_j}\right) + \mathrm{Li}_2\left(1-\frac{\eta_i}{\eta_j}\right) - \mathrm{Li}_2\left(1-\frac{\zeta_i}{\eta_j}\right)\right\}\right]$$

$$-\frac{1-c_2}{c_2}\left[\log^2(1-c_2) - \log^2(1-c_1) + \sum_{i=1}^{p}\left\{\log^2\left(\eta_i\right) - \log^2\left(\zeta_i\right)\right\}\right]$$

$$-\frac{1}{p}\left[2\sum_{1\leq i,j\leq p}\left\{\mathrm{Li}_2\left(1-\frac{\zeta_i}{\lambda_j}\right) - \mathrm{Li}_2\left(1-\frac{\eta_i}{\lambda_j}\right)\right\} - \sum_{i=1}^{p}\log^2\left((1-c_1)\lambda_i\right)\right]$$

$\longrightarrow$ Involves dilogarithm functions!

Spectral clustering with feature C_i

Setting:

- "m" observations, $X_1, \ldots, X_m$ with $X_i = [x_1^{(i)}, ..., x_{n_i}^{(i)}]$
- Two classes: $C_i = C^{(1)}$ for $i \leq m/2$, $C_i = C^{(2)}$ for $i > m/2$.

Objective:

- Classify observations X_i based on $C^{(1)}$ and $C^{(2)}$.

Method:

- Spectral clustering with kernel

$$K_{ij} = D(C_i, C_j)$$

estimated by $D(\hat{C}_i, \hat{C}_j)$ versus RMT estimator.

Simulation: random n_i

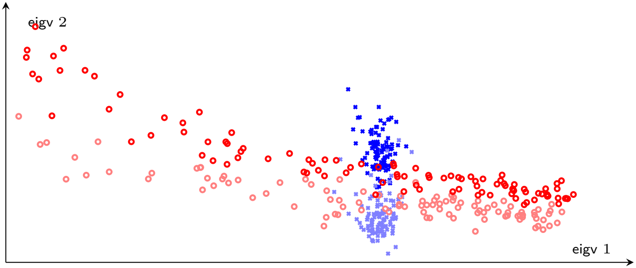


Figure: Eigenvectors 1 and 2 of K for traditional (red circles) versus RMT estimator (blue crosses).

Classical

- Wide spread of eigenvectors
- Small inter space
- $\rightarrow$ Poor clustering

RMT estimator

- Well centered eigenvector
- Large inter space
- $\rightarrow$ Good clustering

Simulation: outlier $n_1 = ... = n_{m-1}$, $n_m = n_1/2$

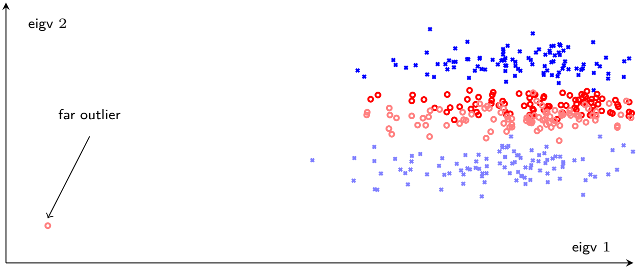


Figure: Eigenvectors 1 and 2 of K for traditional (red circles) versus RMT estimator (blue crosses).

Classical

- Isolated outlier
- Adversarial effect of outlier ("draws" eigenvector to itself)
- Effect increased by more outliers

RMT estimator

- No outlier effect
- Large inter space

Observations:

- $X = [x_1, \ldots, x_n]$, $x_i \in \mathbb{R}^p$ with $\mathbb{E}[x_i] = 0$, $\mathbb{E}[x_i x_i^\mathsf{T}] = C$.

Observations:

- $X = [x_1, \ldots, x_n]$, $x_i \in \mathbb{R}^p$ with $\mathbb{E}[x_i] = 0$, $\mathbb{E}[x_i x_i^\mathsf{T}] = C$.

Objective:

- From the data x_i, estimate C.

Observations:

- $X = [x_1, \ldots, x_n]$, $x_i \in \mathbb{R}^p$ with $\mathbb{E}[x_i] = 0$, $\mathbb{E}[x_i x_i^\mathsf{T}] = C$.

Objective:

- From the data x_i, estimate C.

State of the Art:

- Sample Covariance Matrix (SCM):

$$\hat{C} = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^\mathsf{T} = \frac{1}{n} X X^\mathsf{T}.$$

Application to covariance matrix estimation

Observations:

- $X = [x_1, \ldots, x_n]$, $x_i \in \mathbb{R}^p$ with $\mathbb{E}[x_i] = 0$, $\mathbb{E}[x_i x_i^\mathsf{T}] = C$.

Objective:

- From the data x_i, estimate C.

State of the Art:

- Sample Covariance Matrix (SCM):

$$\hat{C} = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^\mathsf{T} = \frac{1}{n} X X^\mathsf{T}.$$

$\longrightarrow$ **Often justified by Law of Large Numbers**: $n \to \infty$.

Application to covariance matrix estimation

Observations:

- $X = [x_1, \ldots, x_n]$, $x_i \in \mathbb{R}^p$ with $\mathbb{E}[x_i] = 0$, $\mathbb{E}[x_i x_i^\mathsf{T}] = C$.

Objective:

- From the data x_i, estimate C.

State of the Art:

- Sample Covariance Matrix (SCM):

$$\hat{C} = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^\mathsf{T} = \frac{1}{n} X X^\mathsf{T}.$$

  $\longrightarrow$ **Often justified by Law of Large Numbers**: $n \to \infty$.
- Numerical inversion of asymptotic spectrum (QuEST).
  1. Bai-Silverstein equation: Estimate $\lambda(\hat{C})$ from $\lambda(C)$ in "large p, n" regime.
  2. Need for non trivial inversion of the equation.

Application to covariance matrix estimation (continued)

- Elementary idea

$$C \equiv \operatorname{argmin}_{M \succ 0} \delta(M, C)$$

where $\delta(M, C)$ can be the Fisher, Bhattacharyya, KL, Rényi divergence.

Application to covariance matrix estimation (continued)

- Elementary idea
$$C \equiv \operatorname{argmin}_{M \succ 0} \delta(M, C)$$
where $\delta(M, C)$ can be the Fisher, Bhattacharyya, KL, Rényi divergence.
- Divergence $\delta(M, C) = \int f(t) d\nu_p(t)$ inaccessible, $\nu_p \equiv \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(M^{-1}C)}$.

Application to covariance matrix estimation (continued)

- Elementary idea

$$C \equiv \operatorname{argmin}_{M \succ 0} \delta(M, C)$$

  where $\delta(M,C)$ can be the Fisher, Bhattacharyya, KL, Rényi divergence.

- Divergence $\delta(M,C) = \int f(t) d\nu_p(t)$ inaccessible, $\nu_p \equiv \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(M^{-1}C)}$.

- Random Matrix improved estimate $\boxed{\hat{\delta}(M,X)}$ of $\delta(M,C)$ using $\mu_p \equiv \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(M^{-1}\hat{C})}$.

$$\begin{tikzcd}
\int f(t)\nu_p(dt) \arrow[r, dash, "\times" marking] \arrow[d, leftrightarrow] & \int h(t)\mu_p(dt) \arrow[d, leftrightarrow] \\
\oint H(m_{\nu_p}(z))dz \arrow[r, leftrightarrow] & \boxed{\oint G(m_{\mu_p}(z))dz}
\end{tikzcd}$$

Application to covariance matrix estimation (continued)

- Elementary idea
$$C \equiv \operatorname{argmin}_{M \succ 0} \delta(M, C)$$
where $\delta(M, C)$ can be the Fisher, Bhattacharyya, KL, Rényi divergence.
- Divergence $\delta(M, C) = \int f(t) d\nu_p(t)$ inaccessible, $\nu_p \equiv \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(M^{-1}C)}$.
- Random Matrix improved estimate $\boxed{\hat{\delta}(M, X)}$ of $\delta(M, C)$ using $\mu_p \equiv \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(M^{-1}\hat{C})}$.

$$\begin{tikzcd}
\int f(t)\nu_p(dt) \arrow[r, no head, "\times" description] \arrow[d, leftrightarrow] & \int h(t)\mu_p(dt) \arrow[d, leftrightarrow] \\
\oint H(m_{\nu_p}(z))dz \arrow[r, leftrightarrow] & \boxed{\oint G(m_{\mu_p}(z))dz}
\end{tikzcd}$$

- $\hat{\delta}(M, X) < 0$ with non zero probability.

Application to covariance matrix estimation (continued)

- Elementary idea

$$C \equiv \operatorname{argmin}_{M \succ 0} \delta(M, C)$$

  where $\delta(M, C)$ can be the Fisher, Bhattacharyya, KL, Rényi divergence.

- Divergence $\delta(M, C) = \int f(t) d\nu_p(t)$ inaccessible, $\nu_p \equiv \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(M^{-1}C)}$.

- Random Matrix improved estimate $\boxed{\hat{\delta}(M, X)}$ of $\delta(M, C)$ using $\mu_p \equiv \frac{1}{p} \sum_{i=1}^{p} \delta_{\lambda_i(M^{-1}\hat{C})}$.

$$\begin{tikzcd}
\int f(t) \nu_p(dt) \arrow[rr, dash, "\times" marking] \arrow[d, leftrightarrow] & & \int h(t) \mu_p(dt) \arrow[d, leftrightarrow] \\
\oint H(m_{\nu_p}(z)) dz \arrow[rr, leftrightarrow] & & \boxed{\oint G(m_{\mu_p}(z)) dz}
\end{tikzcd}$$

- $\hat{\delta}(M, X) < 0$ with non zero probability.
- RMT estimation

$$\boxed{\check{C} \equiv \operatorname{argmin}_{M \succ 0} h(M), \quad h(M) = \hat{\delta}(M, X)^2}$$

- Gradient descent over the Positive Definite manifold.

Algorithm 1 RMT estimation algorithm.

Require $M_0 \in C_n^{++}$.

Repeat $M \leftarrow M^{\frac{1}{2}} \exp\left(-tM^{-\frac{1}{2}} \nabla h_X(M) M^{-\frac{1}{2}}\right) M^{\frac{1}{2}}$.

Until Convergence.

Return $\check{C} = M$.

- 2 Data classes $x_1^{(1)}, \ldots, x_{n_1}^{(1)} \sim N(\mu_1, C_1)$ and $x_1^{(2)}, \ldots, x_{n_2}^{(2)} \sim N(\mu_2, C_2)$.
- Classify point x using Linear Discriminant Analysis based on the sign of

$$\delta_x^{\mathrm{LDA}} = (\hat{\mu}_1 - \hat{\mu}_2)^{\mathsf{T}} \check{C}^{-1} x + \frac{1}{2} \hat{\mu}_2^{\mathsf{T}} \check{C}^{-1} \hat{\mu}_2 - \frac{1}{2} \hat{\mu}_1^{\mathsf{T}} \check{C}^{-1} \hat{\mu}_1.$$

- Estimate $\check{C} \equiv \frac{n_1}{n_1+n_2} \check{C}_1 + \frac{n_2}{n_1+n_2} \check{C}_2$.

- 2 Data classes $x_1^{(1)}, \ldots, x_{n_1}^{(1)} \sim N(\mu_1, C_1)$ and $x_1^{(2)}, \ldots, x_{n_2}^{(2)} \sim N(\mu_2, C_2)$.
- Classify point x using Linear Discriminant Analysis based on the sign of

$$\delta_x^{\mathrm{LDA}} = (\hat{\mu}_1 - \hat{\mu}_2)^{\mathsf{T}} \check{C}^{-1} x + \frac{1}{2} \hat{\mu}_2^{\mathsf{T}} \check{C}^{-1} \hat{\mu}_2 - \frac{1}{2} \hat{\mu}_1^{\mathsf{T}} \check{C}^{-1} \hat{\mu}_1.$$

- Estimate $\check{C} \equiv \frac{n_1}{n_1+n_2} \check{C}_1 + \frac{n_2}{n_1+n_2} \check{C}_2$.

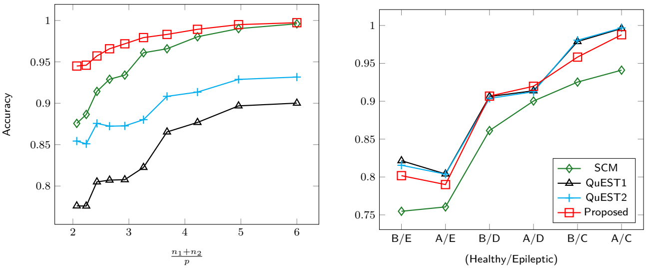
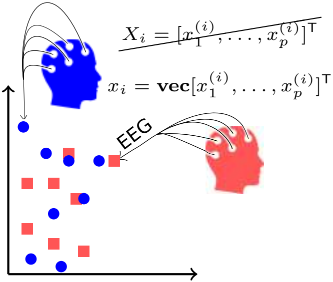


Figure: Mean accuracy obtained over 10 realizations of LDA classification. (Left) C_1 and C_2 Toeplitz-0.2/Toeplitz-0.4, and (Right) real EEG data.

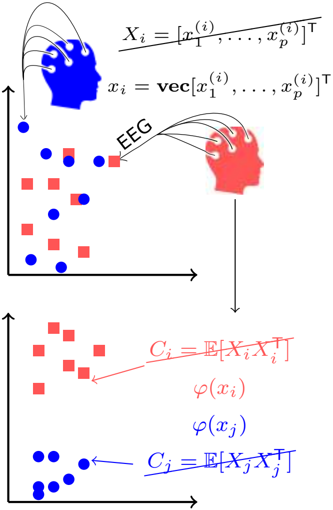
Outline

- Hard classification on raw data x_i:
  Need Features



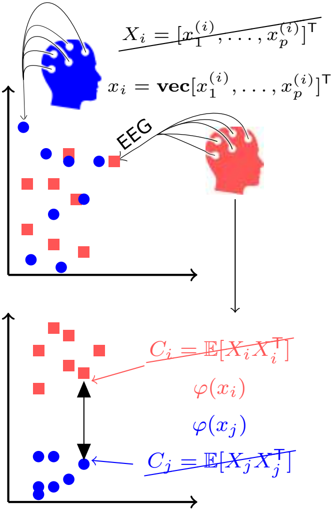
Reconsider clustering

- Hard classification on raw data x_i:
  Need Features
- ~~Relevant Feature: Covariance C_i~~
  $\rightarrow$Learn features from data



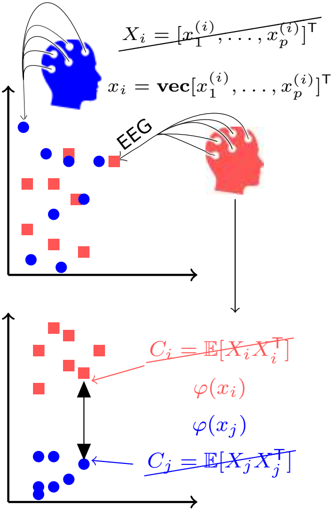
Reconsider clustering

- Hard classification on raw data x_i:
  Need Features
- ~~Relevant Feature: Covariance C_i~~
  $\rightarrow$Learn features from data
- $D(C_i, C_j) \leftrightarrow \varphi(x_i)^\mathsf{T}\varphi(x_j)$

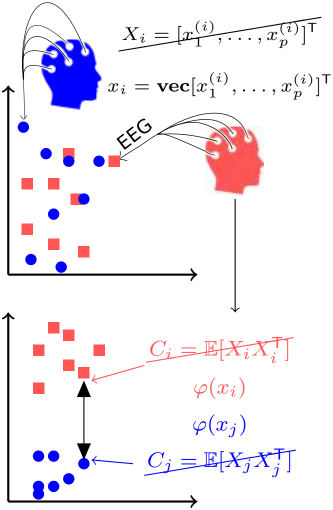


Reconsider clustering

- Hard classification on raw data x_i: Need Features
- ~~Relevant Feature: Covariance C_i~~ $\rightarrow$Learn features from data
- $D(C_i, C_j) \leftrightarrow \varphi(x_i)^\mathsf{T}\varphi(x_j)$
- Kernel trick $\varphi(x_i)^\mathsf{T}\varphi(x_j) \rightarrow f(\|x_i - x_j\|^2)$ or $f({x_i}^\mathsf{T} x_j)$



- Hard classification on raw data x_i: Need Features
- ~~Relevant Feature: Covariance C_i~~ $\rightarrow$Learn features from data
- $D(C_i, C_j) \leftrightarrow \varphi(x_i)^\mathsf{T}\varphi(x_j)$
- Kernel trick $\varphi(x_i)^\mathsf{T}\varphi(x_j) \to f(\|x_i - x_j\|^2)$ or $f({x_i}^\mathsf{T} x_j)$
- Asymptotic performance of kernel methods?



Outline

Problem Statement

- Dataset $x_1, \ldots, x_n \in \mathbb{R}^p$
- Objective: "cluster" data in k similarity classes $\mathcal{C}_1, \ldots, \mathcal{C}_k$.

Problem Statement

- Dataset $x_1, \ldots, x_n \in \mathbb{R}^p$
- Objective: "cluster" data in k similarity classes $\mathcal{C}_1, \ldots, \mathcal{C}_k$.

- Kernel spectral clustering based on kernel matrix

$$\boxed{K = \{\kappa(x_i, x_j)\}_{i,j=1}^n}$$

Problem Statement

- Dataset $x_1, \ldots, x_n \in \mathbb{R}^p$
- Objective: "cluster" data in k similarity classes $\mathcal{C}_1, \ldots, \mathcal{C}_k$.

- Kernel spectral clustering based on kernel matrix

$$\boxed{K = \{\kappa(x_i, x_j)\}_{i,j=1}^n}$$

- Usually, $\kappa(x, y) = f(x^\mathsf{T} y)$ or $\kappa(x, y) = f(\|x - y\|^2)$

Kernel spectral clustering

Intuition (from small dimensions)

$$K = \left(\begin{array}{ccc} \kappa(x_i,x_j) \gg 1 & \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \ll 1 \\ \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \gg 1 & \kappa(x_i,x_j) \ll 1 \\ \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \gg 1 \end{array}\right) \begin{array}{l} \updownarrow \mathcal{C}_1 \\ \updownarrow \mathcal{C}_2 \\ \updownarrow \mathcal{C}_3 \end{array}$$

- K essentially low rank with class structure in eigenvectors.

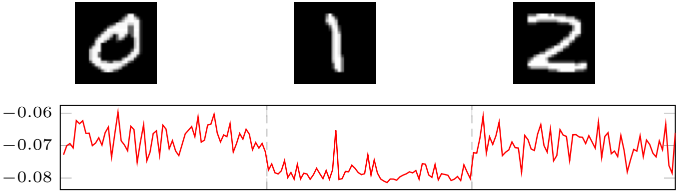
Kernel spectral clustering

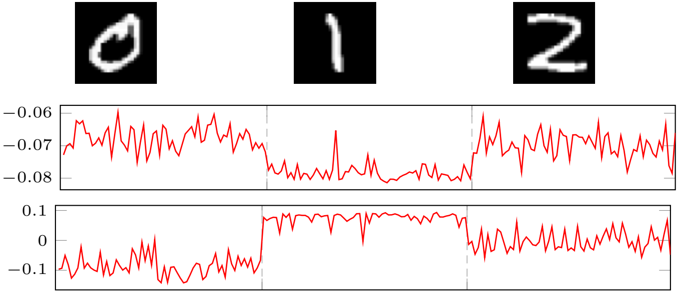
Intuition (from small dimensions)

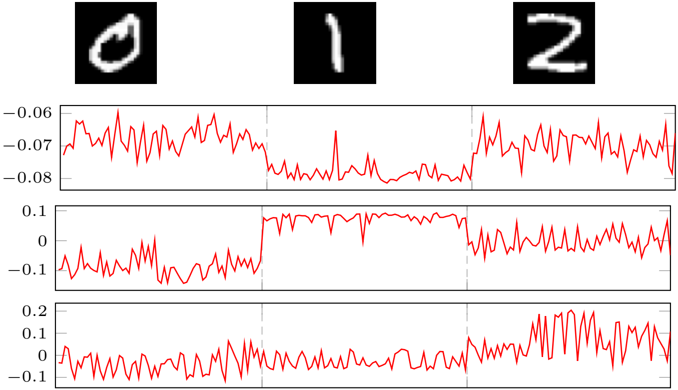
$$K = \begin{array}{c}\left(\begin{array}{ccc} \kappa(x_i,x_j) \gg 1 & \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \ll 1 \\ \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \gg 1 & \kappa(x_i,x_j) \ll 1 \\ \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \ll 1 & \kappa(x_i,x_j) \gg 1 \end{array}\right)\end{array} \begin{array}{l}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

- K essentially low rank with class structure in eigenvectors.
- **Ng–Weiss–Jordan key remark**: $D^{-\frac{1}{2}}KD^{-\frac{1}{2}}(D^{\frac{1}{2}}j_a) \simeq D^{\frac{1}{2}}j_a$ (j_a canonical vector of $\mathcal{C}_a$)

Kernel Spectral Clustering




−0.06
−0.07
−0.08
0.1
0
−0.1


−0.06
−0.07
−0.08
0.1
0
−0.1
0.2
0.1
0
−0.1

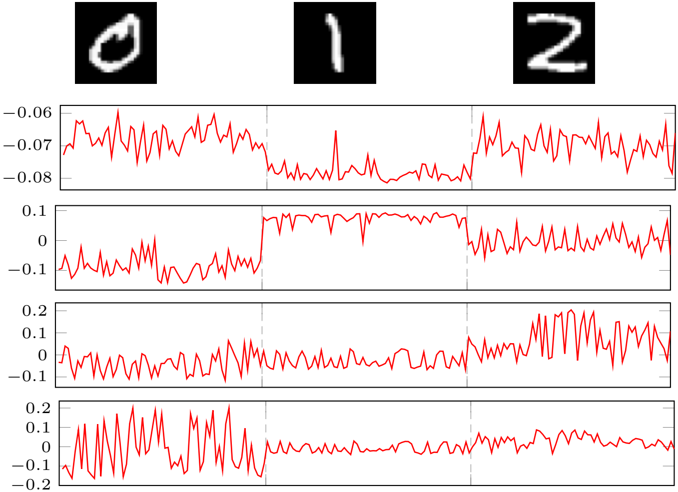


Figure: Leading four eigenvectors of $D^{-\frac{1}{2}}KD^{-\frac{1}{2}}$ for MNIST data, RBF kernel $(f(t) = \exp(-t^2/2))$.

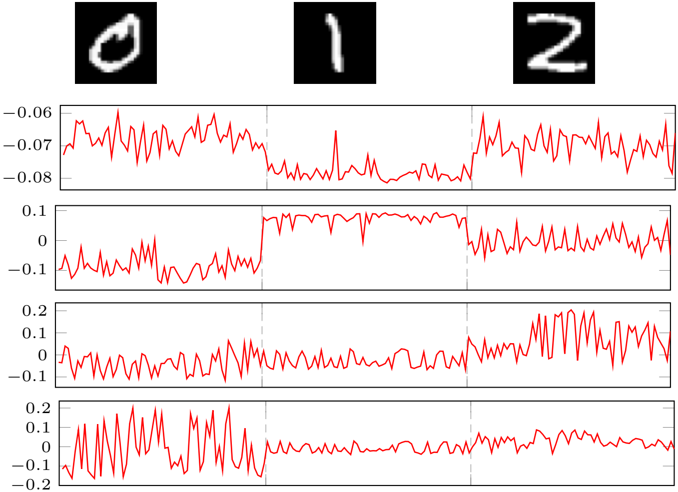


Figure: Leading four eigenvectors of $D^{-\frac{1}{2}}KD^{-\frac{1}{2}}$ for MNIST data, RBF kernel ($f(t) = \exp(-t^2/2)$).

- **Important Remark:** eigenvectors informative **BUT** far from $D^{\frac{1}{2}}j_a$!

Model and Assumptions

Gaussian mixture model:

- $x_1, \ldots, x_n \in \mathbb{R}^p$,
- k classes $\mathcal{C}_1, \ldots, \mathcal{C}_k$,
- $x_1, \ldots, x_{n_1} \in \mathcal{C}_1, \ldots, x_{n-n_k+1}, \ldots, x_n \in \mathcal{C}_k$,
- $x_i \sim \mathcal{N}(\mu_{g_i}, C_{g_i})$.

Gaussian mixture model:

- $x_1, \ldots, x_n \in \mathbb{R}^p$,
- k classes $\mathcal{C}_1, \ldots, \mathcal{C}_k$,
- $x_1, \ldots, x_{n_1} \in \mathcal{C}_1, \ldots, x_{n-n_k+1}, \ldots, x_n \in \mathcal{C}_k$,
- $x_i \sim \mathcal{N}(\mu_{g_i}, C_{g_i})$.

Assumption (Growth Rate)

As $n \to \infty$,

1. **Data scaling**: $\frac{p}{n} \to c_0 \in (0, \infty)$, $\frac{n_a}{n} \to c_a \in (0,1)$,
2. **Mean scaling**: *with* $\mu^\circ \triangleq \sum_{a=1}^k \frac{n_a}{n}\mu_a$ *and* $\mu_a^\circ \triangleq \mu_a - \mu^\circ$, *then* $\|\mu_a^\circ\| = O(1)$
3. **Covariance scaling**: *with* $C^\circ \triangleq \sum_{a=1}^k \frac{n_a}{n} C_a$ *and* $C_a^\circ \triangleq C_a - C^\circ$, *then*

$$\|C_a\| = O(1), \quad \mathrm{tr}\, C_a^\circ = O(\sqrt{p}), \quad \mathrm{tr}\, C_a^\circ C_b^\circ = O(p)$$

Gaussian mixture model:

- $x_1, \ldots, x_n \in \mathbb{R}^p$,
- k classes $\mathcal{C}_1, \ldots, \mathcal{C}_k$,
- $x_1, \ldots, x_{n_1} \in \mathcal{C}_1, \ldots, x_{n-n_k+1}, \ldots, x_n \in \mathcal{C}_k$,
- $x_i \sim \mathcal{N}(\mu_{g_i}, C_{g_i})$.

Assumption (Growth Rate)

As $n \to \infty$,

1. **Data scaling**: $\frac{p}{n} \to c_0 \in (0, \infty)$, $\frac{n_a}{n} \to c_a \in (0, 1)$,
2. **Mean scaling**: *with* $\mu^\circ \triangleq \sum_{a=1}^{k} \frac{n_a}{n} \mu_a$ *and* $\mu_a^\circ \triangleq \mu_a - \mu^\circ$, *then* $\|\mu_a^\circ\| = O(1)$
3. **Covariance scaling**: *with* $C^\circ \triangleq \sum_{a=1}^{k} \frac{n_a}{n} C_a$ *and* $C_a^\circ \triangleq C_a - C^\circ$, *then*

$$\|C_a\| = O(1), \quad \operatorname{tr} C_a^\circ = O(\sqrt{p}), \quad \operatorname{tr} C_a^\circ C_b^\circ = O(p)$$

For 2 classes, this is

$$\|\mu_1 - \mu_2\| = O(1), \quad \operatorname{tr}(C_1 - C_2) = O(\sqrt{p}), \quad \|C_i\| = O(1), \quad \operatorname{tr}([C_1 - C_2]^2) = O(p).$$

Model and Assumptions

Gaussian mixture model:

- $x_1, \ldots, x_n \in \mathbb{R}^p$,
- k classes $\mathcal{C}_1, \ldots, \mathcal{C}_k$,
- $x_1, \ldots, x_{n_1} \in \mathcal{C}_1, \ldots, x_{n-n_k+1}, \ldots, x_n \in \mathcal{C}_k$,
- $x_i \sim \mathcal{N}(\mu_{g_i}, C_{g_i})$.

Assumption (Growth Rate)

As $n \to \infty$,

1. **Data scaling**: $\frac{p}{n} \to c_0 \in (0, \infty)$, $\frac{n_a}{n} \to c_a \in (0, 1)$,
2. **Mean scaling**: *with* $\mu^\circ \triangleq \sum_{a=1}^k \frac{n_a}{n} \mu_a$ *and* $\mu_a^\circ \triangleq \mu_a - \mu^\circ$, *then* $\|\mu_a^\circ\| = O(1)$
3. **Covariance scaling**: *with* $C^\circ \triangleq \sum_{a=1}^k \frac{n_a}{n} C_a$ *and* $C_a^\circ \triangleq C_a - C^\circ$, *then*

$$\|C_a\| = O(1), \quad \mathrm{tr}\, C_a^\circ = O(\sqrt{p}), \quad \mathrm{tr}\, C_a^\circ C_b^\circ = O(p)$$

For 2 classes, this is

$$\|\mu_1 - \mu_2\| = O(1), \quad \mathrm{tr}\,(C_1 - C_2) = O(\sqrt{p}), \quad \|C_i\| = O(1), \quad \mathrm{tr}\,([C_1 - C_2]^2) = O(p).$$

Remark: [Neyman–Pearson optimality]

- $x \sim \mathcal{N}(\pm\mu, I_p)$ (known μ) decidable iif $\|\mu\| \geq O(1)$.
- $x \sim \mathcal{N}(0, (1 \pm \varepsilon) I_p)$ (known ε) decidable iif $\|\epsilon\| \geq O(p^{-\frac{1}{2}})$.

Model and Assumptions

Kernel Matrix:

- Kernel matrix of interest:

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

for some sufficiently smooth nonnegative f ($f(\frac{1}{p} x_i^\mathsf{T} x_j)$ simpler).

Kernel Matrix:

- Kernel matrix of interest:

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

  for some sufficiently smooth nonnegative f ($f(\frac{1}{p} x_i^\mathsf{T} x_j)$ simpler).

- We study the normalized Laplacian:

$$L = nD^{-\frac{1}{2}} \left(K - \frac{dd^\mathsf{T}}{d^\mathsf{T} 1_n} \right) D^{-\frac{1}{2}}$$

  with $d = K1_n$, $D = \mathrm{diag}(d)$.
  (more stable both theoretically and in practice)

- **Key Remark:** Under growth rate assumptions,

$$\boxed{\max_{1\leq i\neq j\leq n}\left\{\left|\frac{1}{p}\left\|x_i-x_j\right\|^2-\tau\right|\right\}\xrightarrow{\text{a.s.}}0.}$$

where $\tau=\frac{1}{p}\operatorname{tr} C^\circ$.

- **Key Remark:** Under growth rate assumptions,

$$\boxed{\max_{1\leq i\neq j\leq n}\left\{\left|\frac{1}{p}\left\|x_i-x_j\right\|^2-\tau\right|\right\}\xrightarrow{\text{a.s.}}0.}$$

where $\tau=\frac{1}{p}\operatorname{tr}C^\circ$.

$\Rightarrow$ Suggests that (up to diagonal) $K\simeq f(\tau)1_n1_n^{\mathsf{T}}$!

- **Key Remark:** Under growth rate assumptions,

$$\boxed{\max_{1\leq i\neq j\leq n}\left\{\left|\frac{1}{p}\|x_i-x_j\|^2-\tau\right|\right\}\xrightarrow{\text{a.s.}}0.}$$

where $\tau=\frac{1}{p}\operatorname{tr}C^\circ$.
$\Rightarrow$ Suggests that (up to diagonal) $K\simeq f(\tau)1_n1_n^\mathsf{T}$!

- In fact, **information hidden in low order fluctuations**! from "matrix-wise" Taylor expansion of K:

$$K=\underbrace{f(\tau)1_n1_n^\mathsf{T}}_{O_{\|\cdot\|}(n)}+\underbrace{\sqrt{n}K_1}_{\text{low rank, } O_{\|\cdot\|}(\sqrt{n})}+\underbrace{K_2}_{\text{informative terms, } O_{\|\cdot\|}(1)}$$

Random Matrix Equivalent

- **Key Remark:** Under growth rate assumptions,

$$\boxed{\max_{1\leq i\neq j\leq n}\left\{\left|\frac{1}{p}\|x_i-x_j\|^2-\tau\right|\right\}\xrightarrow{\text{a.s.}}0.}$$

  where $\tau=\frac{1}{p}\operatorname{tr}C^\circ$.
  $\Rightarrow$ Suggests that (up to diagonal) $K\simeq f(\tau)1_n1_n^\mathsf{T}$!

- In fact, **information hidden in low order fluctuations**! from "matrix-wise" Taylor expansion of K:

$$K=\underbrace{f(\tau)1_n1_n^\mathsf{T}}_{O_{\|\cdot\|}(n)}+\underbrace{\sqrt{n}K_1}_{\text{low rank, }O_{\|\cdot\|}(\sqrt{n})}+\underbrace{K_2}_{\text{informative terms, }O_{\|\cdot\|}(1)}$$

$$\boxed{\text{Clearly not the (small dimension) expected behavior.}}$$

Theorem (Random Matrix Equivalent **[Couillet, Benaych'2015]**)
As $n, p \to \infty$, $\left\| L - \hat{L} \right\| \xrightarrow{\text{a.s.}} 0$, *where*

$$L = nD^{-\frac{1}{2}} \left(K - \frac{dd^{\mathsf{T}}}{d^{\mathsf{T}} 1_n} \right) D^{-\frac{1}{2}}, \text{ avec } K_{ij} = f\left(\frac{1}{p} \|x_i - x_j\|^2 \right)$$

$$\hat{L} = -2 \frac{f'(\tau)}{f(\tau)} \frac{1}{p} PW^{\mathsf{T}} WP + \frac{1}{p} JBJ^{\mathsf{T}} + *$$

et $W = [w_1, \ldots, w_n] \in \mathbb{R}^{p \times n}$ *(*$x_i = \mu_a + w_i$*)*, $P = I_n - \frac{1}{n} 1_n 1_n^{\mathsf{T}}$,

Theorem (Random Matrix Equivalent **[Couillet, Benaych'2015]**)
As $n, p \to \infty$, $\left\| L - \hat{L} \right\| \xrightarrow{\text{a.s.}} 0$, *where*

$$L = nD^{-\frac{1}{2}} \left(K - \frac{dd^{\mathsf{T}}}{d^{\mathsf{T}} 1_n} \right) D^{-\frac{1}{2}}, \text{ avec } K_{ij} = f\left(\frac{1}{p} \| x_i - x_j \|^2 \right)$$

$$\hat{L} = -2 \frac{f'(\tau)}{f(\tau)} \frac{1}{p} P W^{\mathsf{T}} W P + \frac{1}{p} J B J^{\mathsf{T}} + *$$

et $W = [w_1, \ldots, w_n] \in \mathbb{R}^{p \times n}$ *(*$x_i = \mu_a + w_i$*)*, $P = I_n - \frac{1}{n} 1_n 1_n^{\mathsf{T}}$,

$$J = [j_1, \ldots, j_k], \; j_a^{\mathsf{T}} = (0 \ldots 0, 1_{n_a}, 0, \ldots, 0)$$

$$B = -2 \frac{f'(\tau)}{f(\tau)} M^{\mathsf{T}} M + \left(\frac{f''(\tau)}{f(\tau)} - \frac{5 f'(\tau)^2}{4 f(\tau)^2} \right) t t^{\mathsf{T}} + 2 \frac{f''(\tau)}{f(\tau)} T + *.$$

Recall $M = [\mu_1^\circ, \ldots, \mu_k^\circ]$, $t = [\frac{1}{\sqrt{p}} \operatorname{tr} C_1^\circ, \ldots, \frac{1}{\sqrt{p}} \operatorname{tr} C_k^\circ]^{\mathsf{T}}$, $T = \left\{ \frac{1}{p} \operatorname{tr} C_a^\circ C_b^\circ \right\}_{a,b=1}^{k}$.

Theorem (Random Matrix Equivalent **[Couillet, Benaych'2015]**)
As $n,p\to\infty$, $\left\|L-\hat{L}\right\| \xrightarrow{\text{a.s.}} 0$, where

$$L = nD^{-\frac{1}{2}}\left(K - \frac{dd^{\mathsf{T}}}{d^{\mathsf{T}}1_n}\right)D^{-\frac{1}{2}},\ \text{avec}\ K_{ij} = f\left(\frac{1}{p}\|x_i-x_j\|^2\right)$$

$$\hat{L} = -2\frac{f'(\tau)}{f(\tau)}\frac{1}{p}PW^{\mathsf{T}}WP + \frac{1}{p}JBJ^{\mathsf{T}} + *$$

et $W=[w_1,\ldots,w_n]\in\mathbb{R}^{p\times n}$ *($x_i=\mu_a+w_i$)*, $P=I_n-\frac{1}{n}1_n1_n^{\mathsf{T}}$,

$$J = [j_1,\ldots,j_k],\ j_a^{\mathsf{T}} = (0\ldots 0, 1_{n_a}, 0,\ldots,0)$$

$$B = -2\frac{f'(\tau)}{f(\tau)}M^{\mathsf{T}}M + \left(\frac{f''(\tau)}{f(\tau)} - \frac{5f'(\tau)^2}{4f(\tau)^2}\right)tt^{\mathsf{T}} + 2\frac{f''(\tau)}{f(\tau)}T + *.$$

Recall $M=[\mu_1^\circ,\ldots,\mu_k^\circ]$, $t=[\frac{1}{\sqrt{p}}\mathrm{tr}\,C_1^\circ,\ldots,\frac{1}{\sqrt{p}}\mathrm{tr}\,C_k^\circ]^{\mathsf{T}}$, $T=\left\{\frac{1}{p}\mathrm{tr}\,C_a^\circ C_b^\circ\right\}_{a,b=1}^k$.

Fundamental conclusions:

Theorem (Random Matrix Equivalent [Couillet, Benaych'2015])
As $n, p \to \infty$, $\left\| L - \hat{L} \right\| \xrightarrow{\text{a.s.}} 0$, *where*

$$L = nD^{-\frac{1}{2}} \left(K - \frac{dd^\mathsf{T}}{d^\mathsf{T} 1_n} \right) D^{-\frac{1}{2}}, \text{ avec } K_{ij} = f\left(\frac{1}{p} \|x_i - x_j\|^2 \right)$$

$$\hat{L} = -2\frac{f'(\tau)}{f(\tau)} \frac{1}{p} PW^\mathsf{T} WP + \frac{1}{p} JBJ^\mathsf{T} + *$$

et $W = [w_1, \ldots, w_n] \in \mathbb{R}^{p \times n}$ *(*$x_i = \mu_a + w_i$*)*, $P = I_n - \frac{1}{n} 1_n 1_n^\mathsf{T}$,

$$J = [j_1, \ldots, j_k], \ j_a^\mathsf{T} = (0 \ldots 0, 1_{n_a}, 0, \ldots, 0)$$

$$B = -2\frac{f'(\tau)}{f(\tau)} M^\mathsf{T} M + \left(\frac{f''(\tau)}{f(\tau)} - \frac{5f'(\tau)^2}{4f(\tau)^2} \right) tt^\mathsf{T} + 2\frac{f''(\tau)}{f(\tau)} T + *.$$

Recall $M = [\mu_1^\circ, \ldots, \mu_k^\circ]$, $t = [\frac{1}{\sqrt{p}} \mathrm{tr}\, C_1^\circ, \ldots, \frac{1}{\sqrt{p}} \mathrm{tr}\, C_k^\circ]^\mathsf{T}$, $T = \left\{ \frac{1}{p} \mathrm{tr}\, C_a^\circ C_b^\circ \right\}_{a,b=1}^k$.

Fundamental conclusions:

- asymptotic **kernel impact** only through $f'(\tau)$ and $f''(\tau)$, **that's all!**

Theorem (Random Matrix Equivalent [Couillet, Benaych'2015])
As $n, p \to \infty$, $\left\| L - \hat{L} \right\| \xrightarrow{\text{a.s.}} 0$, where

$$L = nD^{-\frac{1}{2}} \left(K - \frac{dd^{\mathsf{T}}}{d^{\mathsf{T}} 1_n} \right) D^{-\frac{1}{2}}, \text{ avec } K_{ij} = f\left(\frac{1}{p} \|x_i - x_j\|^2 \right)$$

$$\hat{L} = -2 \frac{f'(\tau)}{f(\tau)} \frac{1}{p} PW^{\mathsf{T}} WP + \frac{1}{p} JBJ^{\mathsf{T}} + *$$

et $W = [w_1, \ldots, w_n] \in \mathbb{R}^{p \times n}$ *(*$x_i = \mu_a + w_i$*)*, $P = I_n - \frac{1}{n} 1_n 1_n^{\mathsf{T}}$,

$$J = [j_1, \ldots, j_k], \; j_a^{\mathsf{T}} = (0 \ldots 0, 1_{n_a}, 0, \ldots, 0)$$

$$B = -2 \frac{f'(\tau)}{f(\tau)} M^{\mathsf{T}} M + \left(\frac{f''(\tau)}{f(\tau)} - \frac{5 f'(\tau)^2}{4 f(\tau)^2} \right) tt^{\mathsf{T}} + 2 \frac{f''(\tau)}{f(\tau)} T + *.$$

Recall $M = [\mu_1^\circ, \ldots, \mu_k^\circ]$, $t = [\frac{1}{\sqrt{p}} \operatorname{tr} C_1^\circ, \ldots, \frac{1}{\sqrt{p}} \operatorname{tr} C_k^\circ]^{\mathsf{T}}$, $T = \left\{ \frac{1}{p} \operatorname{tr} C_a^\circ C_b^\circ \right\}_{a,b=1}^{k}$.

Fundamental conclusions:

- asymptotic **kernel impact** only through $f'(\tau)$ and $f''(\tau)$, **that's all!**
- spectral clustering **reads** $M^{\mathsf{T}} M$, tt^{T} and T, **that's all!**

Isolated eigenvalues: Gaussian inputs

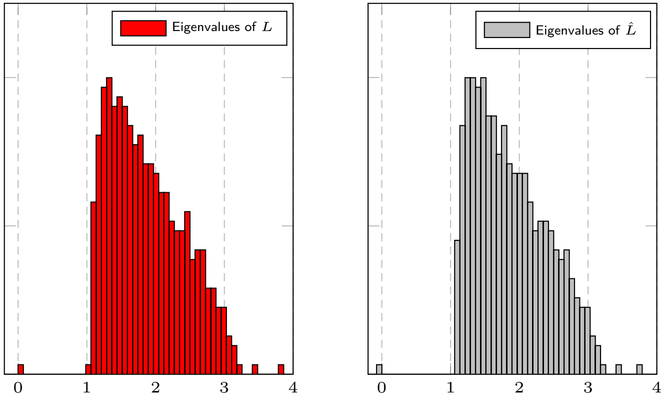


Figure: Eigenvalues of L and $\hat{L}$, $k = 3$, $p = 2048$, $n = 512$, $c_1 = c_2 = 1/4$, $c_3 = 1/2$, $[\mu_a]_j = 4\boldsymbol{\delta}_{aj}$, $C_a = (1 + 2(a-1)/\sqrt{p})I_p$, $f(x) = \exp(-x/2)$.

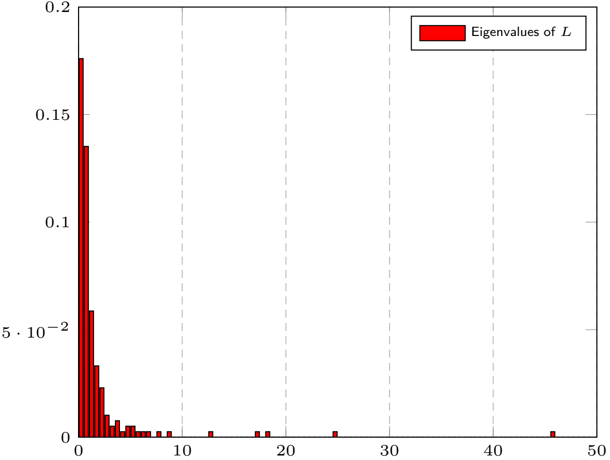


Figure: Eigenvalues of L (red) and (equivalent Gaussian model) $\hat{L}$ (white), MNIST data, $p = 784$, $n = 192$.

Theoretical Findings versus MNIST

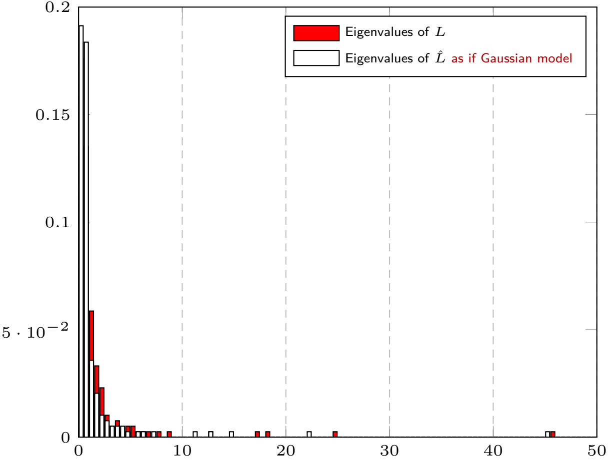


Figure: Eigenvalues of L (red) and (equivalent Gaussian model) $\hat{L}$ (white), MNIST data, $p = 784$, $n = 192$.

Theoretical Findings versus MNIST

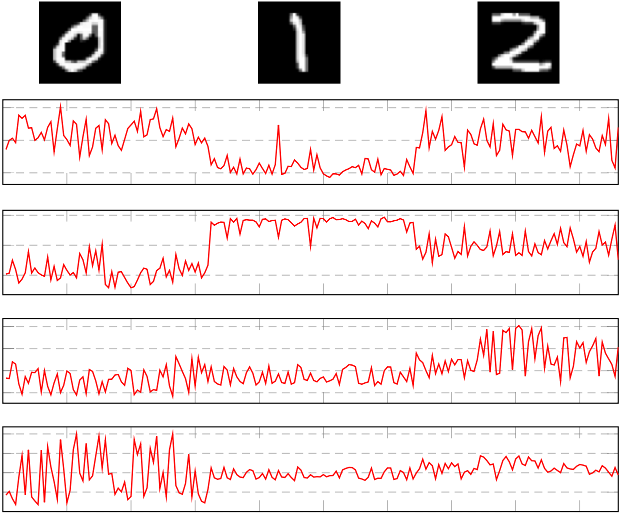


Figure: Leading four eigenvectors of $D^{-\frac{1}{2}} K D^{-\frac{1}{2}}$ for MNIST data (**red**) and theoretical findings (**blue**).

Theoretical Findings versus MNIST

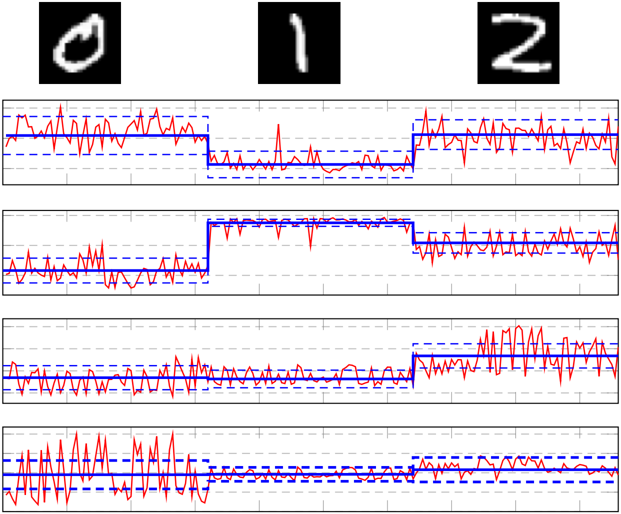


Figure: Leading four eigenvectors of $D^{-\frac{1}{2}} K D^{-\frac{1}{2}}$ for MNIST data (**red**) and theoretical findings (**blue**).

Theoretical Findings versus MNIST

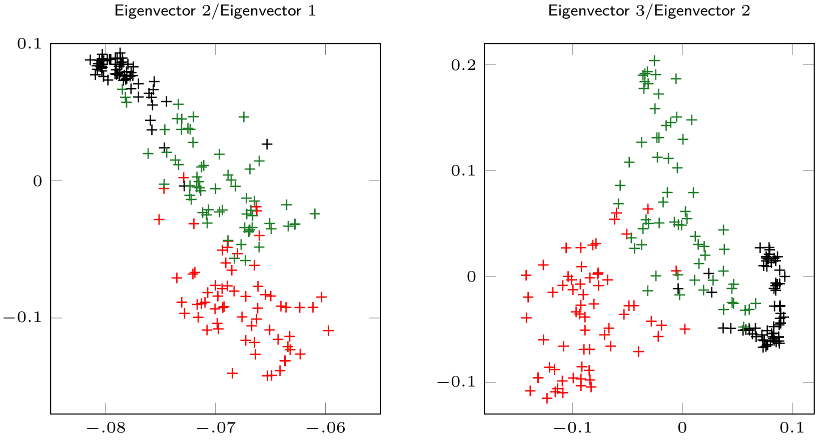


Figure: 2D representation of eigenvectors of L, for the MNIST dataset. Theoretical means and 1- and 2-standard deviations in **blue**. Class 1 in **red**, Class 2 in **black**, Class 3 in **green**.

Theoretical Findings versus MNIST

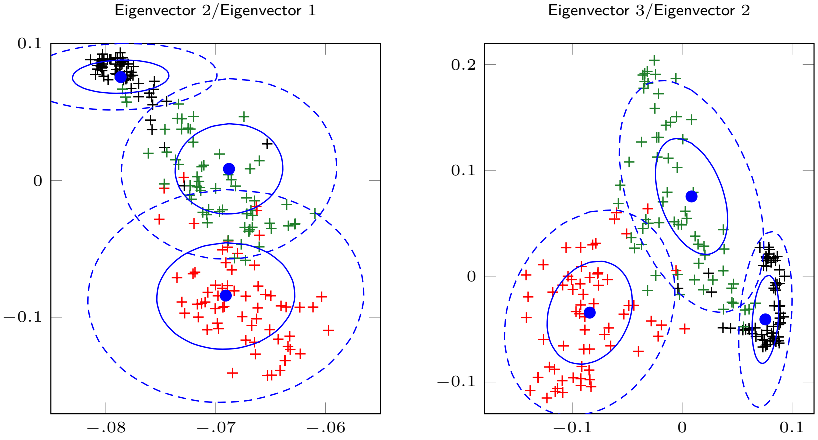


Figure: 2D representation of eigenvectors of L, for the MNIST dataset. Theoretical means and 1- and 2-standard deviations in **blue**. Class 1 in **red**, Class 2 in **black**, Class 3 in **green**.

The surprising $f'(\tau) = 0$ case

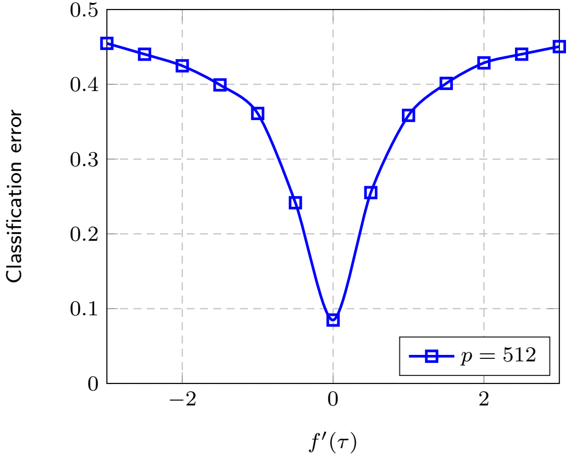


Figure: Polynomial kernel with $f(\tau) = 4$, $f''(\tau) = 2$, $x_i \in \mathcal{N}(0, C_a)$, with $C_1 = I_p$, $[C_2]_{i,j} = .4^{|i-j|}$, $c_0 = \frac{1}{4}$.

The surprising $f'(\tau) = 0$ case

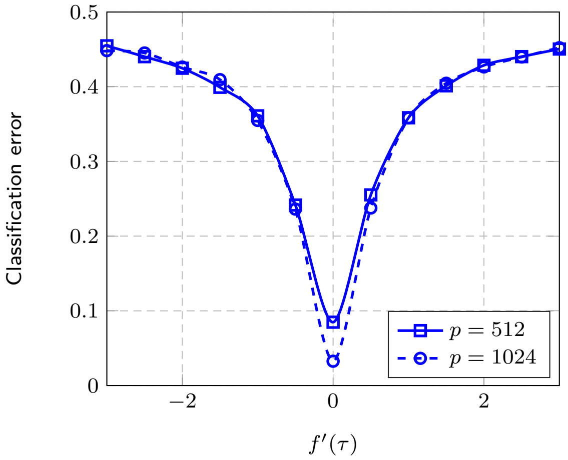


Figure: Polynomial kernel with $f(\tau) = 4$, $f''(\tau) = 2$, $x_i \in \mathcal{N}(0, C_a)$, with $C_1 = I_p$, $[C_2]_{i,j} = .4^{|i-j|}$, $c_0 = \frac{1}{4}$.

The surprising $f'(\tau) = 0$ case

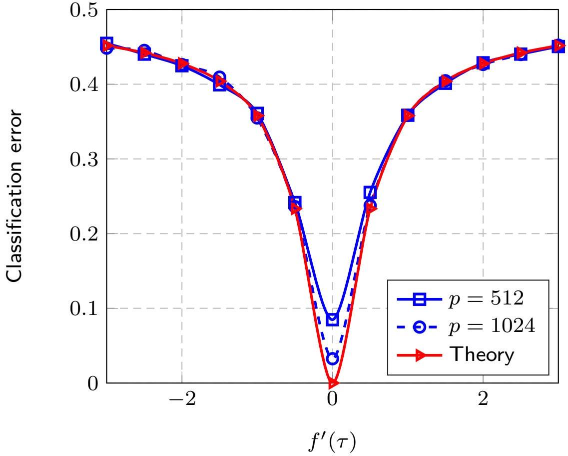


Figure: Polynomial kernel with $f(\tau) = 4$, $f''(\tau) = 2$, $x_i \in \mathcal{N}(0, C_a)$, with $C_1 = I_p$, $[C_2]_{i,j} = .4^{|i-j|}$, $c_0 = \frac{1}{4}$.

The surprising $f'(\tau) = 0$ case

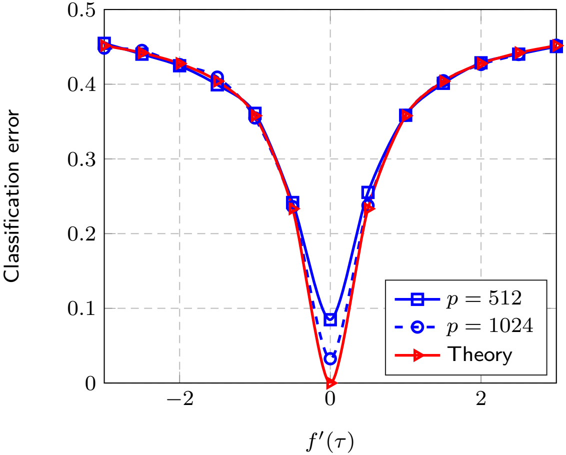


Figure: Polynomial kernel with $f(\tau) = 4$, $f''(\tau) = 2$, $x_i \in \mathcal{N}(0, C_a)$, with $C_1 = I_p$, $[C_2]_{i,j} = .4^{|i-j|}$, $c_0 = \frac{1}{4}$.

- **Trivial classification** when $t = 0$, $M = 0$ and $\|T\| = O(1)$.

Problem: Cluster large data $x_1, \ldots, x_n \in \mathbb{R}^p$ based on "spanned subspaces".

Problem: Cluster large data $x_1, \ldots, x_n \in \mathbb{R}^p$ based on "spanned subspaces".

Method:

- Still assume $x_1, \ldots, x_n$ belong to k classes $\mathcal{C}_1, \ldots, \mathcal{C}_k$.
- Zero-mean Gaussian model for the data: for $x_i \in \mathcal{C}_k$,

$$x_i \sim \mathcal{N}(0, C_k).$$

Problem: Cluster large data $x_1, \ldots, x_n \in \mathbb{R}^p$ based on "spanned subspaces".

Method:

- Still assume $x_1, \ldots, x_n$ belong to k classes $\mathcal{C}_1, \ldots, \mathcal{C}_k$.
- Zero-mean Gaussian model for the data: for $x_i \in \mathcal{C}_k$,

$$x_i \sim \mathcal{N}(0, C_k).$$

- Performance of $L = nD^{-\frac{1}{2}} \left(K - \frac{1_n 1_n^\mathsf{T}}{1_n^\mathsf{T} D 1_n} \right) D^{-\frac{1}{2}}$, with

$$K = \left\{ f\left(\|\bar{x}_i - \bar{x}_j\|^2 \right) \right\}_{1 \leq i,j \leq n}, \quad \bar{x} = \frac{x}{\|x\|}$$

  in the regime $n, p \to \infty$.
  (alternatively, we can ask $\frac{1}{p} \mathrm{tr}\, C_i = 1$ for all $1 \leq i \leq k$)

Assumption 1 [Classes]. Vectors $x_1, \ldots, x_n \in \mathbb{R}^p$ i.i.d. from k-class Gaussian mixture, with $x_i \in \mathcal{C}_k \Leftrightarrow x_i \sim \mathcal{N}(0, C_k)$ (sorted by class for simplicity).

Assumption 1 [Classes]. Vectors $x_1, \ldots, x_n \in \mathbb{R}^p$ i.i.d. from k-class Gaussian mixture, with $x_i \in \mathcal{C}_k \Leftrightarrow x_i \sim \mathcal{N}(0, C_k)$ (sorted by class for simplicity).

Assumption 2a [Growth Rates]. As $n \to \infty$, for each $a \in \{1, \ldots, k\}$,

1. $\frac{n}{p} \to c_0 \in (0, \infty)$
2. $\frac{n_a}{n} \to c_a \in (0, \infty)$
3. $\frac{1}{p} \operatorname{tr} C_a = 1$ and $\operatorname{tr} C_a^\circ C_b^\circ = O(p)$, with $C_a^\circ = C_a - C^\circ$, $C^\circ = \sum_{b=1}^k c_b C_b$.

Assumption 1 [Classes]. Vectors $x_1, \ldots, x_n \in \mathbb{R}^p$ i.i.d. from k-class Gaussian mixture, with $x_i \in \mathcal{C}_k \Leftrightarrow x_i \sim \mathcal{N}(0, C_k)$ (sorted by class for simplicity).

Assumption 2a [Growth Rates]. As $n \to \infty$, for each $a \in \{1, \ldots, k\}$,

1. $\frac{n}{p} \to c_0 \in (0, \infty)$
2. $\frac{n_a}{n} \to c_a \in (0, \infty)$
3. $\frac{1}{p} \operatorname{tr} C_a = 1$ and $\operatorname{tr} C_a^\circ C_b^\circ = O(p)$, with $C_a^\circ = C_a - C^\circ$, $C^\circ = \sum_{b=1}^k c_b C_b$.

Theorem (Corollary of Previous Section)

Let f smooth with $f'(2) \neq 0$. Then, under Assumptions 2a,

$$L = nD^{-\frac{1}{2}} \left(K - \frac{1_n 1_n^\mathsf{T}}{1_n^\mathsf{T} D 1_n} \right) D^{-\frac{1}{2}}, \text{ with } K = \left\{ f\left(\|\bar{x}_i - \bar{x}_j\|^2 \right) \right\}_{i,j=1}^n \quad (\bar{x} = x / \|x\|)$$

exhibits phase transition phenomenon

Assumption 1 [Classes]. Vectors $x_1, \ldots, x_n \in \mathbb{R}^p$ i.i.d. from k-class Gaussian mixture, with $x_i \in \mathcal{C}_k \Leftrightarrow x_i \sim \mathcal{N}(0, C_k)$ (sorted by class for simplicity).

Assumption 2a [Growth Rates]. As $n \to \infty$, for each $a \in \{1, \ldots, k\}$,

1. $\frac{n}{p} \to c_0 \in (0, \infty)$
2. $\frac{n_a}{n} \to c_a \in (0, \infty)$
3. $\frac{1}{p} \operatorname{tr} C_a = 1$ and $\operatorname{tr} C_a^\circ C_b^\circ = O(p)$, with $C_a^\circ = C_a - C^\circ$, $C^\circ = \sum_{b=1}^k c_b C_b$.

Theorem (Corollary of Previous Section)

Let f smooth with $f'(2) \neq 0$. Then, under Assumptions 2a,

$$L = nD^{-\frac{1}{2}} \left(K - \frac{1_n 1_n^\mathsf{T}}{1_n^\mathsf{T} D 1_n} \right) D^{-\frac{1}{2}}, \text{ with } K = \left\{ f\left(\|\bar{x}_i - \bar{x}_j\|^2 \right) \right\}_{i,j=1}^n \quad (\bar{x} = x/\|x\|)$$

exhibits phase transition phenomenon, i.e., leading eigenvectors of L asymptotically contain structural information about $\mathcal{C}_1, \ldots, \mathcal{C}_k$ if and only if

$$T = \left\{ \frac{1}{p} \operatorname{tr} C_a^\circ C_b^\circ \right\}_{a,b=1}^k$$

has sufficiently large eigenvalues (here $M = 0$, $t = 0$).

Assumption 2b [Growth Rates]. As $n \to \infty$, for each $a \in \{1, \ldots, k\}$,

1. $\frac{n}{p} \to c_0 \in (0, \infty)$
2. $\frac{n_a}{n} \to c_a \in (0, \infty)$
3. $\frac{1}{p}\operatorname{tr} C_a = 1$ and $\cancel{\operatorname{tr} C_a^\circ C_b^\circ = O(p)}$, with $C_a^\circ = C_a - C^\circ$, $C^\circ = \sum_{b=1}^k c_b C_b$.

Assumption 2b [Growth Rates]. As $n \to \infty$, for each $a \in \{1, \ldots, k\}$,

1. $\frac{n}{p} \to c_0 \in (0, \infty)$
2. $\frac{n_a}{n} \to c_a \in (0, \infty)$
3. $\frac{1}{p}\operatorname{tr} C_a = 1$ and $\operatorname{tr} C_a^\circ C_b^\circ = O(\sqrt{p})$, with $C_a^\circ = C_a - C^\circ$, $C^\circ = \sum_{b=1}^k c_b C_b$.

(in this regime, previous kernels clearly fail)

Remark: [Neyman–Pearson optimality]

- *if $C_i = I_p \pm E$ with $\|E\| \to 0$,* **detectability iif** $\frac{1}{p} tr\,(C_1 - C_2)^2 \geq O(p^{-\frac{1}{2}})$.

Assumption 2b [Growth Rates]. As $n \to \infty$, for each $a \in \{1, \ldots, k\}$,

1. $\frac{n}{p} \to c_0 \in (0, \infty)$
2. $\frac{n_a}{n} \to c_a \in (0, \infty)$
3. $\frac{1}{p}\operatorname{tr} C_a = 1$ and $\operatorname{tr} C_a^\circ C_b^\circ = O(\sqrt{p})$, with $C_a^\circ = C_a - C^\circ$, $C^\circ = \sum_{b=1}^k c_b C_b$.

(in this regime, previous kernels clearly fail)

Remark: [Neyman–Pearson optimality]

- *if* $C_i = I_p \pm E$ *with* $\|E\| \to 0$, **detectability iif** $\frac{1}{p}\mathit{tr}\,(C_1 - C_2)^2 \geq O(p^{-\frac{1}{2}})$.

Theorem (Random Equivalent for $f'(2) = 0$)

Let f be smooth with $f'(2) = 0$ and

$$\mathcal{L} \equiv \sqrt{p}\frac{f(2)}{2f''(2)}\left[L - \frac{f(0) - f(2)}{f(2)}P\right], \quad P = I_n - \frac{1}{n}1_n 1_n^\mathsf{T}.$$

Then, under Assumptions 2b,

$$\mathcal{L} = P\Phi P + \left\{\frac{1}{\sqrt{p}}\mathit{tr}\,(C_a^\circ C_b^\circ)\frac{1_{n_a}1_{n_b}^\mathsf{T}}{p}\right\}_{a,b=1}^k + o_{\|\cdot\|}(1)$$

where $\Phi_{ij} = \boldsymbol{\delta}_{i \neq j}\sqrt{p}\left[(x_i^\mathsf{T} x_j)^2 - E[(x_i^\mathsf{T} x_j)^2]\right]$.

Spectral Clustering: The case $f'(\tau) = 0$

The case $f'(2) = 0$

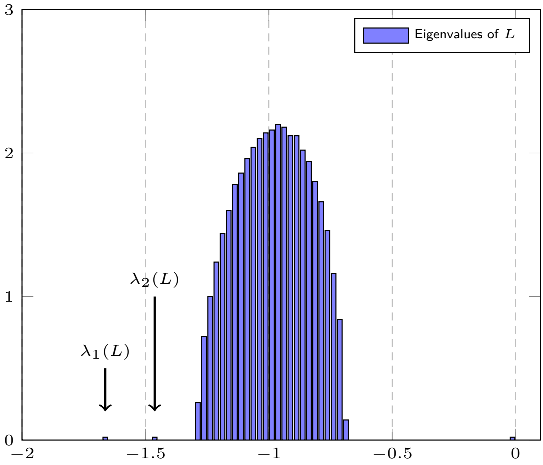
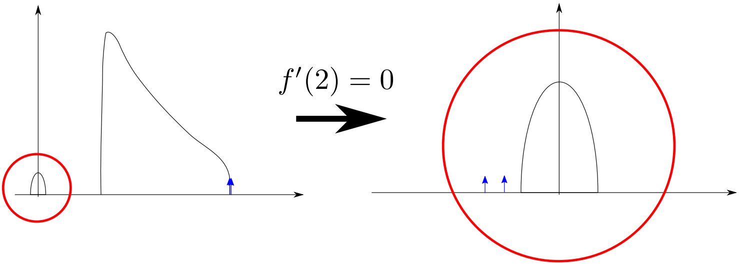


Figure: Eigenvalues of L, $p = 1000$, $n = 2000$, $k = 3$, $c_1 = c_2 = 1/4$, $c_3 = 1/2$, $C_i \propto I_p + (p/8)^{-\frac{5}{4}} W_i W_i^{\mathsf{T}}$, $W_i \in \mathbb{R}^{p\times(p/8)}$ of i.i.d. $\mathcal{N}(0,1)$ entries, $f(t) = \exp(-(t-2)^2)$.

⇒ **No longer a Marcenko–Pastur like bulk, but rather a semi-circle bulk!**



$f'(2) = 0$

Roadmap. We now need to:

- study the spectrum of Φ

Roadmap. We now need to:

- study the spectrum of Φ
- study the isolated eigenvalues of $\mathcal{L}$ (and the phase transition)

Roadmap. We now need to:

- study the spectrum of Φ
- study the isolated eigenvalues of $\mathcal{L}$ (and the phase transition)
- retrieve information from the eigenvectors.

Roadmap. We now need to:

- study the spectrum of Φ
- study the isolated eigenvalues of $\mathcal{L}$ (and the phase transition)
- retrieve information from the eigenvectors.

Theorem (Semi-circle law for Φ)

Let $\mu_n = \frac{1}{n}\sum_{i=1}^n \boldsymbol{\delta}_{\lambda_i(\mathcal{L})}$. Then, under Assumption 2b,

$$\mu_n \xrightarrow{\text{a.s.}} \mu$$

with μ the semi-circle distribution

$$\mu(dt) = \frac{1}{2\pi c_0 \omega^2}\sqrt{(4c_0\omega^2 - t^2)^+}dt, \quad \omega = \lim_{p\to\infty} \sqrt{2}\frac{1}{p}\operatorname{tr}(C^\circ)^2.$$

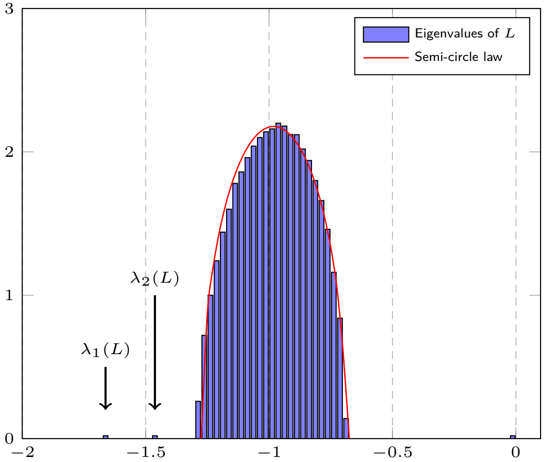


Figure: Eigenvalues of L, $p = 1000$, $n = 2000$, $k = 3$, $c_1 = c_2 = 1/4$, $c_3 = 1/2$, $C_i \propto I_p + (p/8)^{-\frac{5}{4}} W_i W_i^{\mathsf{T}}$, $W_i \in \mathbb{R}^{p \times (p/8)}$ of i.i.d. $\mathcal{N}(0,1)$ entries, $f(t) = \exp(-(t-2)^2)$.

Denote now

$$\mathcal{T} \equiv \lim_{p\to\infty} \left\{ \frac{\sqrt{c_a c_b}}{\sqrt{p}} \operatorname{tr} C_a^\circ C_b^\circ \right\}_{a,b=1}^{k}.$$

Denote now

$$\mathcal{T} \equiv \lim_{p\to\infty} \left\{ \frac{\sqrt{c_a c_b}}{\sqrt{p}} \operatorname{tr} C_a^\circ C_b^\circ \right\}_{a,b=1}^{k}.$$

Theorem (Isolated Eigenvalues)

Let $\nu_1 \geq \ldots \geq \nu_k$ eigenvalues of $\mathcal{T}$. Then, if $\sqrt{c_0}|\nu_i| > \omega$, $\mathcal{L}$ has an isolated eigenvalue λ_i satisfying

$$\lambda_i \xrightarrow{\text{a.s.}} \rho_i \equiv c_0 \nu_i + \frac{\omega^2}{\nu_i}.$$

Theorem (Isolated Eigenvectors)

For each isolated eigenpair (λ_i, u_i) *of* $\mathcal{L}$ *corresponding to* (ν_i, v_i) *of* $\mathcal{T}$*, write*

$$u_i = \sum_{a=1}^{k} \alpha_i^a \frac{j_a}{\sqrt{n_a}} + \sigma_i^a w_i^a$$

with $j_a = [0_{n_1}^\mathsf{T}, \ldots, 1_{n_a}^\mathsf{T}, \ldots, 0_{n_k}^\mathsf{T}]^\mathsf{T}$, $(w_i^a)^\mathsf{T} j_a = 0$, $\mathrm{supp}(w_i^a) = \mathrm{supp}(j_a)$, $\|w_i^a\| = 1$.
Then, under Assumptions 1–2b,

$$\alpha_i^a \alpha_i^b \xrightarrow{\text{a.s.}} \left(1 - \frac{1}{c_0} \frac{\omega^2}{\nu_i^2}\right) [v_i v_i^\mathsf{T}]_{ab}$$

$$(\sigma_i^a)^2 \xrightarrow{\text{a.s.}} \frac{c_a}{c_0} \frac{\omega^2}{\nu_i^2}$$

and the fluctuations of u_i, u_j, $i \neq j$, *are asymptotically uncorrelated.*

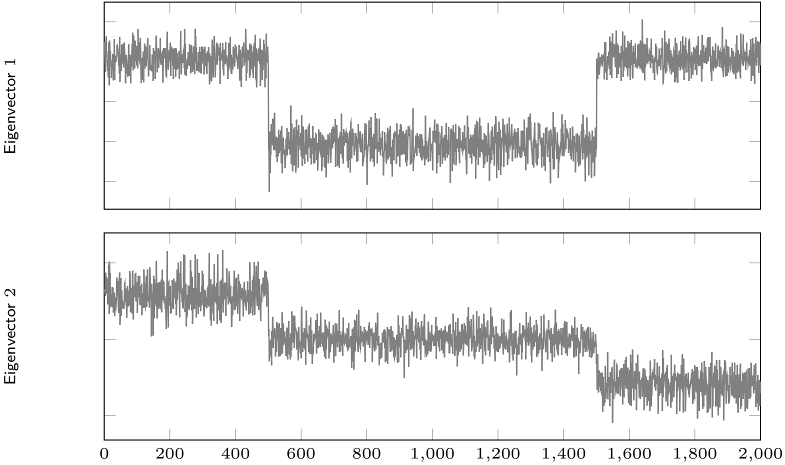


Figure: Leading two eigenvectors of $\mathcal{L}$ (or equivalently of L) versus deterministic approximations of $\alpha_i^a \pm \sigma_i^a$.

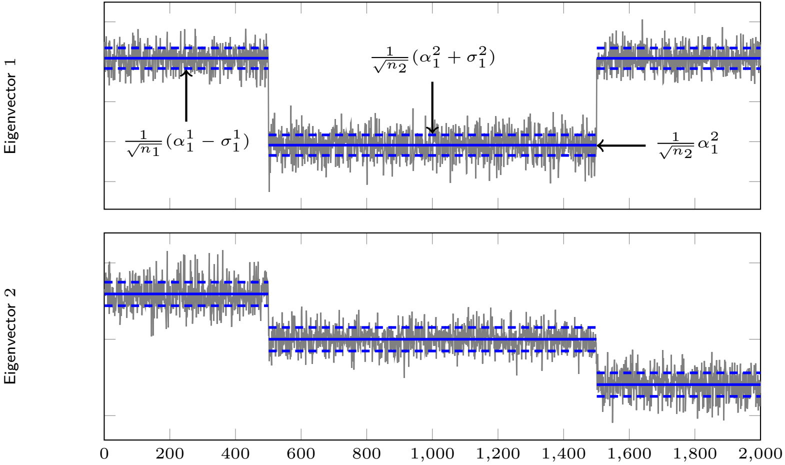


Figure: Leading two eigenvectors of $\mathcal{L}$ (or equivalently of L) versus deterministic approximations of $\alpha_i^a \pm \sigma_i^a$.

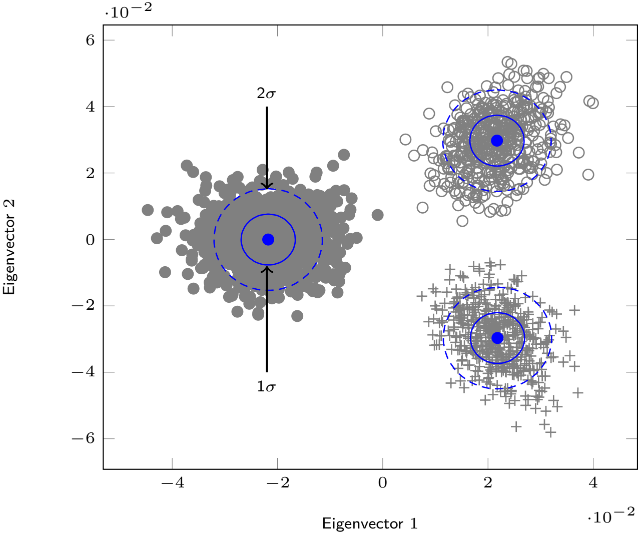


Figure: Leading two eigenvectors of $\mathcal{L}$ (or equivalently of L) versus deterministic approximations of $\alpha_i^a \pm \sigma_i^a$.

Setting.

- p dimensional vector observations.
- m data sources.
- $E[x_i] = 0$, $E[x_i x_i^\mathsf{T}] = C_i$.

Setting.

- p dimensional vector observations.
- m data sources.
- $E[x_i] = 0$, $E[x_i x_i^\mathsf{T}] = C_i$.
- n_i independent observations $x_i^{(1)}, \ldots, x_i^{(n_i)}$ for source i.

Setting.

- p dimensional vector observations.
- m data sources.
- $E[x_i] = 0$, $E[x_i x_i^\mathsf{T}] = C_i$.
- n_i independent observations $x_i^{(1)}, \ldots, x_i^{(n_i)}$ for source i.

Objective. Cluster sources based on covariance C_i.

Setting.

- p dimensional vector observations.
- m data sources.
- $E[x_i] = 0$, $E[x_i x_i^\mathsf{T}] = C_i$.
- n_i independent observations $x_i^{(1)}, \ldots, x_i^{(n_i)}$ for source i.

Objective. Cluster sources based on covariance C_i.

Applications examples. Massive MIMO scheduling / EEG classification / etc.

Setting.

- p dimensional vector observations.
- m data sources.
- $E[x_i] = 0$, $E[x_i x_i^\mathsf{T}] = C_i$.
- n_i independent observations $x_i^{(1)}, \ldots, x_i^{(n_i)}$ for source i.

Objective. Cluster sources based on covariance C_i.

Applications examples. Massive MIMO scheduling / EEG classification / etc.

Algorithm.

1. Build kernel matrix K, then $\mathcal{L}$, based on mn_i vectors $x_1^{(1)}, \ldots, x_m^{(n_i)}$ (as if mn_i values to cluster).

Setting.

- p dimensional vector observations.
- m data sources.
- $E[x_i] = 0$, $E[x_i x_i^\mathsf{T}] = C_i$.
- n_i independent observations $x_i^{(1)}, \ldots, x_i^{(n_i)}$ for source i.

Objective. Cluster sources based on covariance C_i.

Applications examples. Massive MIMO scheduling / EEG classification / etc.

Algorithm.

1. Build kernel matrix K, then $\mathcal{L}$, based on mn_i vectors $x_1^{(1)}, \ldots, x_m^{(n_i)}$ (as if mn_i values to cluster).
2. Extract dominant isolated eigenvectors $u_1, \ldots, u_\kappa$

Setting.

- p dimensional vector observations.
- m data sources.
- $E[x_i] = 0$, $E[x_i x_i^\mathsf{T}] = C_i$.
- n_i independent observations $x_i^{(1)}, \ldots, x_i^{(n_i)}$ for source i.

Objective. Cluster sources based on covariance C_i.

Applications examples. Massive MIMO scheduling / EEG classification / etc.

Algorithm.

1. Build kernel matrix K, then $\mathcal{L}$, based on mn_i vectors $x_1^{(1)}, \ldots, x_m^{(n_i)}$ (as if mn_i values to cluster).
2. Extract dominant isolated eigenvectors $u_1, \ldots, u_\kappa$
3. For each i, create $\tilde{u}_i = \frac{1}{n_i}(I_m \otimes 1_{n_i}^\mathsf{T})u_i$, i.e., average eigenvectors along time.

Setting.

- p dimensional vector observations.
- m data sources.
- $E[x_i] = 0$, $E[x_i x_i^{\mathsf{T}}] = C_i$.
- n_i independent observations $x_i^{(1)}, \ldots, x_i^{(n_i)}$ for source i.

Objective. Cluster sources based on covariance C_i.

Applications examples. Massive MIMO scheduling / EEG classification / etc.

Algorithm.

1. Build kernel matrix K, then $\mathcal{L}$, based on mn_i vectors $x_1^{(1)}, \ldots, x_m^{(n_i)}$ (as if mn_i values to cluster).
2. Extract dominant isolated eigenvectors $u_1, \ldots, u_\kappa$
3. For each i, create $\tilde{u}_i = \frac{1}{n_i}(I_m \otimes 1_{n_i}^{\mathsf{T}})u_i$, i.e., average eigenvectors along time.
4. Perform k-class clustering on vectors $\tilde{u}_1, \ldots, \tilde{u}_\kappa$.

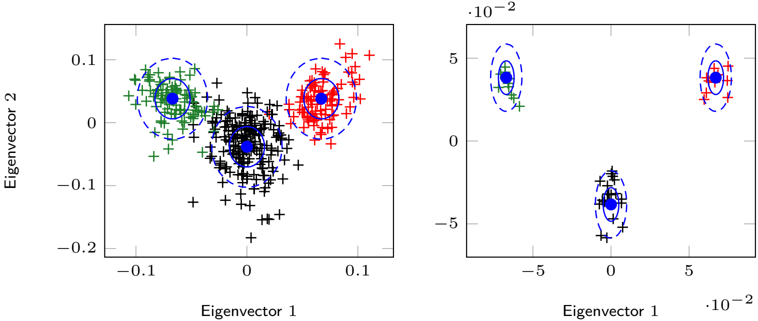


Figure: **Clustering data vectors with close covariances application**: Leading two eigenvectors before (left figure) and after (right figure) n_i-averaging. Setting: $p = 400$, $m = 40$, $n_i = 10$, $k = 3$, $c_1 = c_3 = 1/4$, $c_2 = 1/2$.Kernel function $f(t) = \exp(-(t-2)^2)$.

Spectral Clustering: The case $f'(\tau) = 0$

Application Example: Clustering data vectors with close covariances

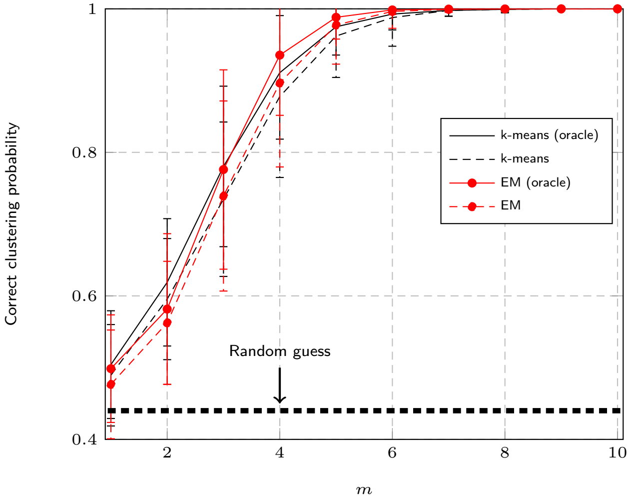


Figure: Overlap for different m, using the k-means or EM starting from actual centroid solutions (oracle) or randomly.

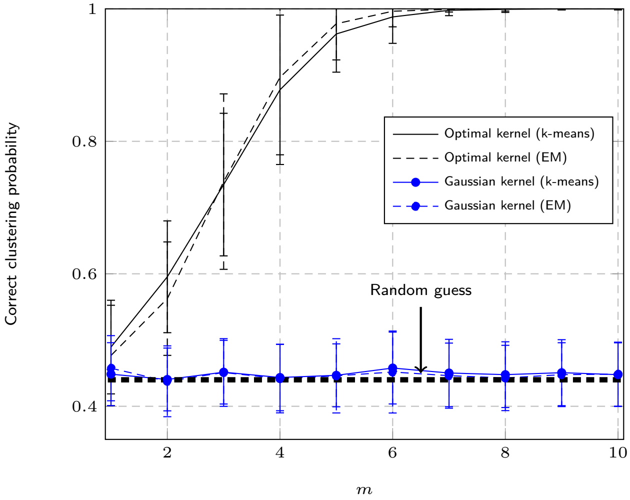


Figure: Overlap for optimal kernel $f(t)$ (here $f(t) = \exp(-(t-2)^2)$) and Gaussian kernel $f(t) = \exp(-t^2)$, for different m, using the k-means or EM.

Conclusion of previous analyses:

- kernel $f(\frac{1}{p}\|x_i - x_j\|^2)$ with $f'(\tau) \neq 0$:
  - optimal in $\|\mu_a^\circ\| = O(1)$, $\frac{1}{p}\operatorname{tr} C_a^\circ = O(p^{-\frac{1}{2}})$
  - suboptimal in $\frac{1}{p}\operatorname{tr} C_a^\circ C_b^\circ = O(1)$

$\longrightarrow$ **Model type:** Marčenko–Pastur + spikes.

Conclusion of previous analyses:

- kernel $f(\frac{1}{p}\|x_i - x_j\|^2)$ with $f'(\tau) \neq 0$:
  - optimal in $\|\mu_a^\circ\| = O(1)$, $\frac{1}{p}\operatorname{tr} C_a^\circ = O(p^{-\frac{1}{2}})$
  - suboptimal in $\frac{1}{p}\operatorname{tr} C_a^\circ C_b^\circ = O(1)$

  $\longrightarrow$ **Model type:** Marčenko–Pastur + spikes.

- kernel $f(\frac{1}{p}\|x_i - x_j\|^2)$ with $f'(\tau) = 0$:
  - suboptimal in $\|\mu_a^\circ\| \gg O(1)$ (**kills the means**)
  - better in discriminating covariance (stress on t and T)

  $\longrightarrow$ **Model type:** smaller order semi-circle law + spikes.

Conclusion of previous analyses:

- kernel $f(\frac{1}{p}\|x_i - x_j\|^2)$ with $f'(\tau) \neq 0$:
  - optimal in $\|\mu_a^\circ\| = O(1)$, $\frac{1}{p}\operatorname{tr} C_a^\circ = O(p^{-\frac{1}{2}})$
  - suboptimal in $\frac{1}{p}\operatorname{tr} C_a^\circ C_b^\circ = O(1)$

$\longrightarrow$ **Model type:** Marčenko–Pastur + spikes.

- kernel $f(\frac{1}{p}\|x_i - x_j\|^2)$ with $f'(\tau) = 0$:
  - suboptimal in $\|\mu_a^\circ\| \gg O(1)$ (**kills the means**)
  - better in discriminating covariance (stress on t and T)

$\longrightarrow$ **Model type:** smaller order semi-circle law + spikes.

Jointly optimal solution:

- evenly weighing Marčenko–Pastur and semi-circle laws

Conclusion of previous analyses:

- kernel $f(\frac{1}{p}\|x_i - x_j\|^2)$ with $f'(\tau) \neq 0$:
  - optimal in $\|\mu_a^\circ\| = O(1)$, $\frac{1}{p}\operatorname{tr} C_a^\circ = O(p^{-\frac{1}{2}})$
  - suboptimal in $\frac{1}{p}\operatorname{tr} C_a^\circ C_b^\circ = O(1)$

$\longrightarrow$ **Model type:** Marčenko–Pastur + spikes.

- kernel $f(\frac{1}{p}\|x_i - x_j\|^2)$ with $f'(\tau) = 0$:
  - suboptimal in $\|\mu_a^\circ\| \gg O(1)$ (**kills the means**)
  - better in discriminating covariance (stress on t and T)

$\longrightarrow$ **Model type:** smaller order semi-circle law + spikes.

Jointly optimal solution:

- evenly weighing Marčenko–Pastur and semi-circle laws
- the "α-β" kernel:

$$f'(\tau) = \frac{\alpha}{\sqrt{p}}, \quad \frac{1}{2}f''(\tau) = \beta.$$

- We consider now an **improved growth rate setting**.

Assumption (Optimal Growth Rate)

As $n \to \infty$,

1. **Data scaling**: $\frac{p}{n} \to c_0 \in (0, \infty)$, $\frac{n_a}{n} \to c_a \in (0, 1)$,
2. **Mean scaling**: *with* $\mu^\circ \triangleq \sum_{a=1}^{k} \frac{n_a}{n} \mu_a$ *and* $\mu_a^\circ \triangleq \mu_a - \mu^\circ$, *then* $\|\mu_a^\circ\| = O(1)$
3. **Covariance scaling**: *with* $C^\circ \triangleq \sum_{a=1}^{k} \frac{n_a}{n} C_a$ *and* $C_a^\circ \triangleq C_a - C^\circ$, *then*

$$\|C_a\| = O(1), \quad \mathrm{tr}\, C_a^\circ = O(\sqrt{p}), \quad \mathrm{tr}\, C_a^\circ C_b^\circ = O(\sqrt{p}).$$

- We consider now an **improved growth rate setting**.

Assumption (Optimal Growth Rate)

As $n \to \infty$,

1. **Data scaling**: $\frac{p}{n} \to c_0 \in (0, \infty)$, $\frac{n_a}{n} \to c_a \in (0,1)$,
2. **Mean scaling**: *with* $\mu^\circ \triangleq \sum_{a=1}^k \frac{n_a}{n}\mu_a$ *and* $\mu_a^\circ \triangleq \mu_a - \mu^\circ$, *then* $\|\mu_a^\circ\| = O(1)$
3. **Covariance scaling**: *with* $C^\circ \triangleq \sum_{a=1}^k \frac{n_a}{n} C_a$ *and* $C_a^\circ \triangleq C_a - C^\circ$, *then*

$$\|C_a\| = O(1), \quad \operatorname{tr} C_a^\circ = O(\sqrt{p}), \quad \operatorname{tr} C_a^\circ C_b^\circ = O(\sqrt{p}).$$

Kernel:

- For technical simplicity, we consider

$$\boxed{\tilde{K} = PKP = P\left\{ f\left(\frac{1}{p}(x^\circ)^\mathsf{T}(x_j^\circ)\right)\right\}_{i,j=1}^n P}, \quad P = I_n - \frac{1}{n}1_n 1_n^\mathsf{T}.$$

i.e., τ replaced by 0.

Theorem

As $n \to \infty$,

$$\left\| \sqrt{p} \left(PKP + \left(f(0) + \tau f'(0) \right) P \right) - \hat{\mathcal{K}} \right\| \xrightarrow{\text{a.s.}} 0$$

with, for $\alpha = \sqrt{p} f'(0) = O(1)$ *and* $\beta = \frac{1}{2} f''(0) = O(1)$,

$$\begin{aligned}
\hat{\mathcal{K}} &= \alpha P W^{\mathsf{T}} W P + \beta P \Phi P + U A U^{\mathsf{T}} \\
A &= \begin{bmatrix} \alpha M^{\mathsf{T}} M + \beta T & \alpha I_k \\ \alpha I_k & 0 \end{bmatrix} \\
U &= \left[\frac{J}{\sqrt{p}}, P W^{\mathsf{T}} M \right] \\
\frac{\Phi}{\sqrt{p}} &= \left\{ ((\omega_i^\circ)^{\mathsf{T}} \omega_j^\circ)^2 \boldsymbol{\delta}_{i \neq j} \right\}_{i,j=1}^{n} - \left\{ \frac{\mathrm{tr}(C_a C_b)}{p^2} 1_{n_a} 1_{n_b}^{\mathsf{T}} \right\}_{a,b=1}^{k}.
\end{aligned}$$

Theorem

As $n \to \infty$,

$$\left\| \sqrt{p} \left(PKP + \left(f(0) + \tau f'(0) \right) P \right) - \hat{\mathcal{K}} \right\| \xrightarrow{\text{a.s.}} 0$$

with, for $\alpha = \sqrt{p} f'(0) = O(1)$ *and* $\beta = \frac{1}{2} f''(0) = O(1)$,

$$\hat{\mathcal{K}} = \alpha P W^\mathsf{T} W P + \beta P \Phi P + U A U^\mathsf{T}$$
$$A = \begin{bmatrix} \alpha M^\mathsf{T} M + \beta T & \alpha I_k \\ \alpha I_k & 0 \end{bmatrix}$$
$$U = \left[\frac{J}{\sqrt{p}}, P W^\mathsf{T} M \right]$$
$$\frac{\Phi}{\sqrt{p}} = \left\{ ((\omega_i^\circ)^\mathsf{T} \omega_j^\circ)^2 \boldsymbol{\delta}_{i \neq j} \right\}_{i,j=1}^n - \left\{ \frac{\mathit{tr}(C_a C_b)}{p^2} 1_{n_a} 1_{n_b}^\mathsf{T} \right\}_{a,b=1}^k .$$

Role of α**,** β:

- Weighs Marčenko–Pastur versus semi-circle parts.

Theorem (Eigenvalues Bulk)

As $p \to \infty$,

$$\nu_n \triangleq \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{\delta}_{\lambda_i(\hat{K})} \xrightarrow{\text{a.s.}} \nu$$

with ν having Stieltjes transform $m(z)$ solution of

$$\frac{1}{m(z)} = -z + \frac{\alpha}{p} \mathit{tr} C^\circ \left(I_k + \frac{\alpha m(z)}{c_0} C^\circ \right)^{-1} - \frac{2\beta^2}{c_0} \omega^2 m(z)$$

where $\omega = \lim_{p\to\infty} \frac{1}{p} \mathit{tr} (C^\circ)^2$.

Kernel Spectral Clustering: The case $f'(\tau) = \frac{\alpha}{\sqrt{p}}$

Limiting eigenvalue distribution

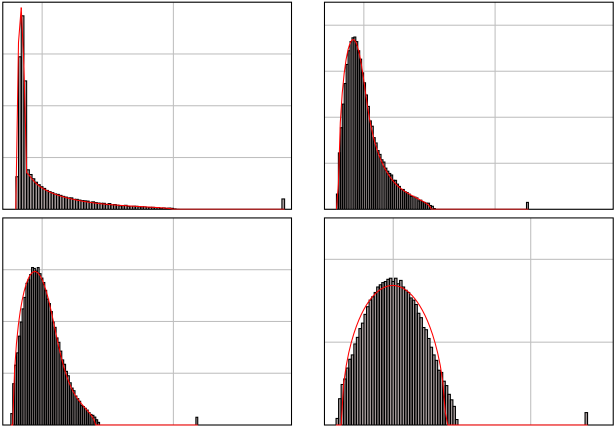


Figure: Eigenvalues of K (up to recentering) versus limiting law, $p = 2048$, $n = 4096$, $k = 2$, $n_1 = n_2$, $\boldsymbol{\mu}_i = 3\boldsymbol{\delta}_i$, $f(x) = \frac{1}{2}\beta\left(x + \frac{1}{\sqrt{p}}\frac{\alpha}{\beta}\right)^2$. **(Top left)**: $\alpha = 8, \beta = 1$, **(Top right)**: $\alpha = 4, \beta = 3$, **(Bottom left)**: $\alpha = 3, \beta = 4$, **(Bottom right)**: $\alpha = 1, \beta = 8$.

- MNIST is "means-dominant" but not that much!

Datasets	$\\|\boldsymbol{\mu}_1^\circ - \boldsymbol{\mu}_2^\circ\\|^2$	$\frac{1}{\sqrt{p}} \operatorname{tr} (\mathbf{C}_1 - \mathbf{C}_2)^2$	$\frac{1}{p} \operatorname{tr} (\mathbf{C}_1 - \mathbf{C}_2)^2$
MNIST (digits 1, 7)	613	1990	71.1
MNIST (digits 3, 6)	441	1119	39.9
MNIST (digits 3, 8)	212	652	23.5

- MNIST is "means-dominant" but not that much!

Datasets	$\|\mu_1^\circ - \mu_2^\circ\|^2$	$\frac{1}{\sqrt{p}} \operatorname{tr}(\mathbf{C}_1 - \mathbf{C}_2)^2$	$\frac{1}{p} \operatorname{tr}(\mathbf{C}_1 - \mathbf{C}_2)^2$
MNIST (digits $1, 7$)	613	1990	71.1
MNIST (digits $3, 6$)	441	1119	39.9
MNIST (digits $3, 8$)	212	652	23.5

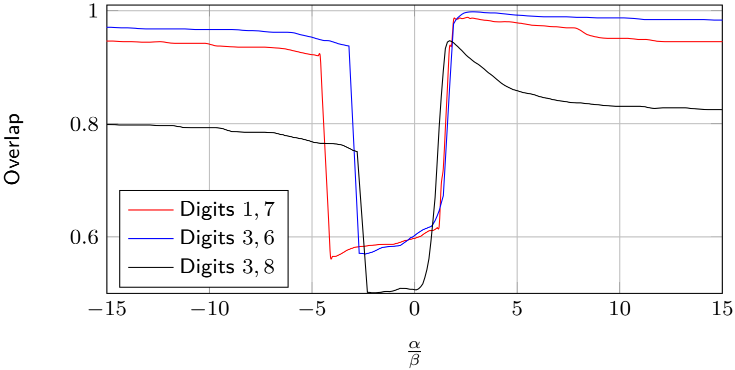


Figure: Spectral clustering of the MNIST database for varying $\frac{\alpha}{\beta}$.

- EEG data are "variance-dominant"

Datasets	$\|\boldsymbol{\mu}_1^\circ - \boldsymbol{\mu}_2^\circ\|^2$	$\frac{1}{\sqrt{p}} \operatorname{tr} (\mathbf{C}_1 - \mathbf{C}_2)^2$	$\frac{1}{p} \operatorname{tr} (\mathbf{C}_1 - \mathbf{C}_2)^2$
EEG (sets A, E)	2.4	10.9	1.1

- EEG data are "variance-dominant"

Datasets	$\|\mu_1^\circ - \mu_2^\circ\|^2$	$\frac{1}{\sqrt{p}} \operatorname{tr}(\mathbf{C}_1 - \mathbf{C}_2)^2$	$\frac{1}{p} \operatorname{tr}(\mathbf{C}_1 - \mathbf{C}_2)^2$
EEG (sets A, E)	2.4	10.9	1.1

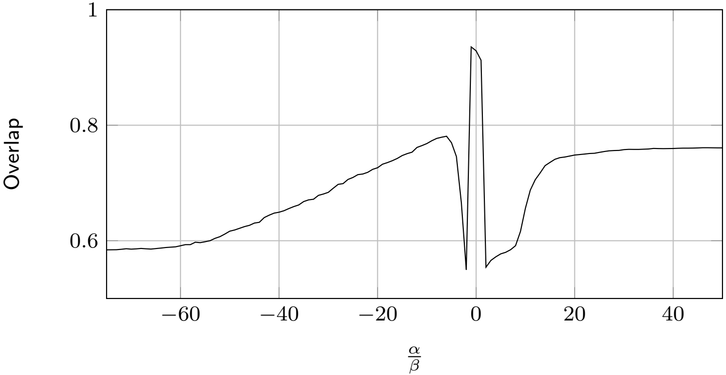


Figure: Spectral clustering of the EEG database for varying $\frac{\alpha}{\beta}$.

Outline

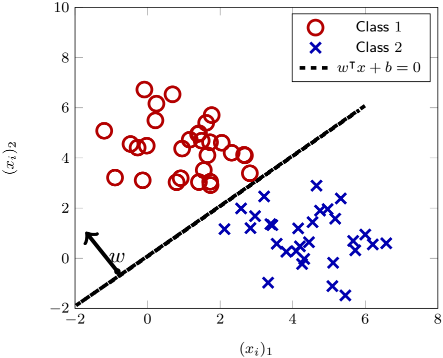
Outline

LS-SVM Problem Statement

Optimization problem: find separating hyperplane (linear separability case)

$$\operatorname*{arg\,min}_{w} \quad J(w,e) = \|w\|^2 + \frac{\gamma}{n}\sum_{i=1}^{n} e_i^2$$

$$\text{such that} \quad y_i = w^\intercal x_i + b + e_i \quad \text{for } i = 1,\ldots,n$$

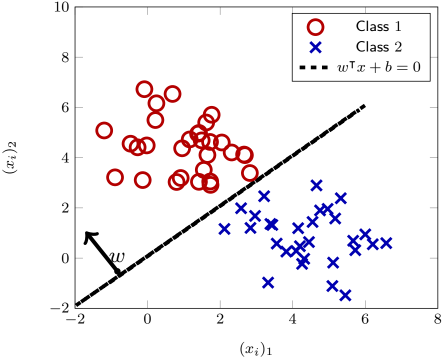


LS-SVM Problem Statement

Optimization problem: find separating hyperplane (linear separability case)

$$\arg\min_{w} \quad J(w,e) = \|w\|^2 + \frac{\gamma}{n}\sum_{i=1}^{n} e_i^2$$

$$\text{such that} \quad y_i = w^\mathsf{T} x_i + b + e_i \quad \text{for } i = 1,\ldots,n$$



Advantage of LS-SVM

Explicit form, as opposed to SVM ⇒ easier to analyze.

LS-SVM Problem Statement

When no linear separability:
$\Rightarrow$ Kernel method

LS-SVM Problem Statement

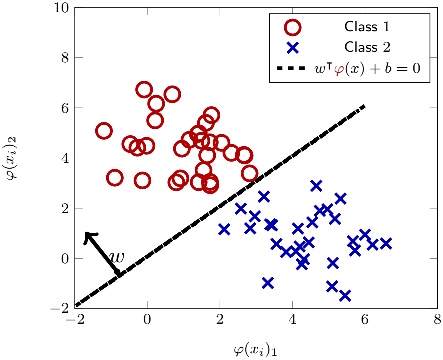
When no linear separability:
$\Rightarrow$ Kernel method

To solve the optimization problem:

$$\arg\min_{w} \quad J(w,e) = \|w\|^2 + \frac{\gamma}{n}\sum_{i=1}^{n} e_i^2$$

$$\text{such that} \quad y_i = w^\mathsf{T}\varphi(x_i) + b + e_i$$

$$\text{for } i = 1,\ldots,n$$



- **Training**: Solution given by $w = \sum_{i=1}^{n} \alpha_i \varphi(x_i)$, where

$$\begin{cases} \alpha & = S\left(I_n - \frac{1_n 1_n^\intercal S}{1_n^\intercal S 1_n}\right) y = S\left(y - b 1_n\right) \\ b & = \frac{1_n^\intercal S y}{1_n^\intercal S 1_n} \end{cases}$$

with $S \equiv \left(K + \frac{n}{\gamma} I_n\right)^{-1}$ resolvent of kernel matrix:

$$K \equiv \{\varphi(x_i)^\intercal \varphi(x_j)\}_{i,j=1}^{n}$$

LS-SVM Training and Inference

- **Training**: Solution given by $w = \sum_{i=1}^{n} \alpha_i \varphi(x_i)$, where

$$\begin{cases} \alpha &= S\left(I_n - \frac{1_n 1_n^{\mathsf{T}} S}{1_n^{\mathsf{T}} S 1_n}\right) y = S\left(y - b 1_n\right) \\ b &= \frac{1_n^{\mathsf{T}} S y}{1_n^{\mathsf{T}} S 1_n} \end{cases}$$

with $S \equiv \left(K + \frac{n}{\gamma} I_n\right)^{-1}$ resolvent of kernel matrix:

$$K \equiv \{\varphi(x_i)^{\mathsf{T}} \varphi(x_j)\}_{i,j=1}^{n}$$

LS-SVM Training and Inference

- **Training**: Solution given by $w = \sum_{i=1}^{n} \alpha_i \varphi(x_i)$, where

$$\begin{cases} \alpha &= S\left(I_n - \frac{1_n 1_n^\mathsf{T} S}{1_n^\mathsf{T} S 1_n}\right) y = S\left(y - b 1_n\right) \\ b &= \frac{1_n^\mathsf{T} S y}{1_n^\mathsf{T} S 1_n} \end{cases}$$

with $S \equiv \left(K + \frac{n}{\gamma} I_n\right)^{-1}$ resolvent of kernel matrix:

$$K \equiv \{\varphi(x_i)^\mathsf{T} \varphi(x_j)\}_{i,j=1}^{n} \underbrace{=}_{\textbf{kernel trick}} \left\{ f\left(\frac{\|x_i - x_j\|^2}{p} \right) \right\}_{i,j=1}^{n}$$

for some *translation invariant* kernel function $f : \mathbb{R}_+ \mapsto \mathbb{R}_+$, $y \equiv [y_1, \ldots, y_n]^\mathsf{T}$ and $\alpha \equiv [\alpha_1, \ldots, \alpha_n]^\mathsf{T}$.

LS-SVM Training and Inference

- **Training**: Solution given by $w = \sum_{i=1}^{n} \alpha_i \varphi(x_i)$, where

$$\begin{cases} \alpha & = S\left(I_n - \frac{1_n 1_n^\mathsf{T} S}{1_n^\mathsf{T} S 1_n}\right) y = S\left(y - b1_n\right) \\ b & = \frac{1_n^\mathsf{T} S y}{1_n^\mathsf{T} S 1_n} \end{cases}$$

with $S \equiv \left(K + \frac{n}{\gamma} I_n\right)^{-1}$ resolvent of kernel matrix:

$$K \equiv \{\varphi(x_i)^\mathsf{T} \varphi(x_j)\}_{i,j=1}^{n} \underbrace{=}_{\textbf{kernel trick}} \left\{ f\left(\frac{\|x_i - x_j\|^2}{p}\right)\right\}_{i,j=1}^{n}$$

for some *translation invariant* kernel function $f : \mathbb{R}_+ \mapsto \mathbb{R}_+$, $y \equiv [y_1, \ldots, y_n]^\mathsf{T}$ and $\alpha \equiv [\alpha_1, \ldots, \alpha_n]^\mathsf{T}$.

- **Inference**: Decision for new x

$$g(x) = \alpha^\mathsf{T} k(x) + b \text{ where } k(x) = \left\{ f\left(\|x_j - x\|^2 / p\right)\right\}_{j=1}^{n} \in \mathbb{R}^n$$

LS-SVM Training and Inference

- **Training**: Solution given by $w = \sum_{i=1}^n \alpha_i \varphi(x_i)$, where

$$\begin{cases} \alpha &= S\left(I_n - \frac{1_n 1_n^\mathsf{T} S}{1_n^\mathsf{T} S 1_n}\right) y = S\left(y - b1_n\right) \\ b &= \frac{1_n^\mathsf{T} S y}{1_n^\mathsf{T} S 1_n} \end{cases}$$

with $S \equiv \left(K + \frac{n}{\gamma} I_n\right)^{-1}$ resolvent of kernel matrix:

$$K \equiv \{\varphi(x_i)^\mathsf{T}\varphi(x_j)\}_{i,j=1}^n \underbrace{=}_{\textbf{kernel trick}} \left\{ f\left(\frac{\|x_i - x_j\|^2}{p}\right)\right\}_{i,j=1}^n$$

for some *translation invariant* kernel function $f : \mathbb{R}_+ \mapsto \mathbb{R}_+$, $y \equiv [y_1, \ldots, y_n]^\mathsf{T}$ and $\alpha \equiv [\alpha_1, \ldots, \alpha_n]^\mathsf{T}$.

- **Inference**: Decision for new x

$$g(x) = \alpha^\mathsf{T} k(x) + b \text{ where } k(x) = \left\{ f\left(\|x_j - x\|^2/p\right)\right\}_{j=1}^n \in \mathbb{R}^n$$

- **In practice, $\operatorname{sign}(g(x))$ to predict the class.**

- **Large dimension**: $n, p \to \infty$ and $\frac{p}{n} \to c_0$

RMT Analysis: Growth Rate Assumptions

- **Large dimension**: $n, p \to \infty$ and $\frac{p}{n} \to c_0$
- **Gaussian mixture model**: for $a \in \{1, 2\}$:

$$x_i \sim \mathcal{N}(\mu_a, C_a)$$

- **Large dimension**: $n, p \to \infty$ and $\frac{p}{n} \to c_0$
- **Gaussian mixture model**: for $a \in \{1, 2\}$:

$$x_i \sim \mathcal{N}(\mu_a, C_a)$$

- **Non-trivial regime**: to ensure $P(x_i \to \mathcal{C}_b \mid x_i \in \mathcal{C}_a) \not\to 0$ nor 1

RMT Analysis: Growth Rate Assumptions

- **Large dimension**: $n, p \to \infty$ and $\frac{p}{n} \to c_0$
- **Gaussian mixture model**: for $a \in \{1, 2\}$:

$$x_i \sim \mathcal{N}(\mu_a, C_a)$$

- **Non-trivial regime**: to ensure $P(x_i \to \mathcal{C}_b \mid x_i \in \mathcal{C}_a) \not\to 0$ nor 1
  - $\|\mu_2 - \mu_1\| = \mathcal{O}(1)$

- **Large dimension**: $n, p \to \infty$ and $\frac{p}{n} \to c_0$
- **Gaussian mixture model**: for $a \in \{1, 2\}$:

$$x_i \sim \mathcal{N}(\mu_a, C_a)$$

- **Non-trivial regime**: to ensure $P(x_i \to \mathcal{C}_b \mid x_i \in \mathcal{C}_a) \not\to 0$ nor 1
  - $\|\mu_2 - \mu_1\| = \mathcal{O}(1)$
  - $\|C_a\| = \mathcal{O}(1)$ and tr $(C_2 - C_1) = \mathcal{O}(\sqrt{n})$

RMT Analysis: Growth Rate Assumptions

- **Large dimension**: $n, p \to \infty$ and $\frac{p}{n} \to c_0$
- **Gaussian mixture model**: for $a \in \{1, 2\}$:

$$x_i \sim \mathcal{N}(\mu_a, C_a)$$

- **Non-trivial regime**: to ensure $P(x_i \to \mathcal{C}_b \mid x_i \in \mathcal{C}_a) \not\to 0$ nor 1
  - $\|\mu_2 - \mu_1\| = \mathcal{O}(1)$
  - $\|C_a\| = \mathcal{O}(1)$ and tr $(C_2 - C_1) = \mathcal{O}(\sqrt{n})$
- **Notations**:

RMT Analysis: Growth Rate Assumptions

- **Large dimension**: $n, p \to \infty$ and $\frac{p}{n} \to c_0$
- **Gaussian mixture model**: for $a \in \{1, 2\}$:

$$x_i \sim \mathcal{N}(\mu_a, C_a)$$

- **Non-trivial regime**: to ensure $P(x_i \to \mathcal{C}_b \mid x_i \in \mathcal{C}_a) \not\to 0$ nor 1
  - $\|\mu_2 - \mu_1\| = \mathcal{O}(1)$
  - $\|C_a\| = \mathcal{O}(1)$ and tr $(C_2 - C_1) = \mathcal{O}(\sqrt{n})$
- **Notations**:
  - $C^\circ \equiv c_1 C_1 + c_2 C_2$, $c_1 \equiv \frac{n_1}{n}$ and $c_2 \equiv \frac{n_2}{n} = 1 - c_1$

- **Large dimension**: $n, p \to \infty$ and $\frac{p}{n} \to c_0$
- **Gaussian mixture model**: for $a \in \{1, 2\}$:

$$x_i \sim \mathcal{N}(\mu_a, C_a)$$

- **Non-trivial regime**: to ensure $P(x_i \to \mathcal{C}_b \mid x_i \in \mathcal{C}_a) \not\to 0$ nor 1
  - $\|\mu_2 - \mu_1\| = \mathcal{O}(1)$
  - $\|C_a\| = \mathcal{O}(1)$ and tr $(C_2 - C_1) = \mathcal{O}(\sqrt{n})$
- **Notations**:
  - $C^\circ \equiv c_1 C_1 + c_2 C_2$, $c_1 \equiv \frac{n_1}{n}$ and $c_2 \equiv \frac{n_2}{n} = 1 - c_1$
  - **Key Notation**: $\tau \equiv \frac{2}{p} \operatorname{tr} C^\circ$

Reminder: kernel matrix

$$K_{i,j} = f\left(\frac{\|x_i - x_j\|^2}{p}\right)$$

For $x_i \in \mathcal{C}_a$ and $x_j \in \mathcal{C}_b$: $\frac{1}{p}\|x_i - x_j\|^2 = \tau + \mathcal{O}(n^{-1/2})$, thus for $K_{i,j}$

$$K_{i,j} = f\left(\tau + \mathcal{O}(n^{-1/2})\right) = f(\tau) + f'(\tau)[\ldots] + f''(\tau)[\ldots] + \ldots$$

or in matrix form

$$K = f(\tau)1_n 1_n^\intercal + f'(\tau)[\ldots] + f''(\tau)[\ldots] + \ldots$$

Reminder: kernel matrix

$$K_{i,j} = f\left(\frac{\|x_i - x_j\|^2}{p}\right)$$

For $x_i \in \mathcal{C}_a$ and $x_j \in \mathcal{C}_b$: $\frac{1}{p}\|x_i - x_j\|^2 = \tau + \mathcal{O}(n^{-1/2})$, thus for $K_{i,j}$

$$K_{i,j} = f\left(\tau + \mathcal{O}(n^{-1/2})\right) = f(\tau) + f'(\tau)[\ldots] + f''(\tau)[\ldots] + \ldots$$

or in matrix form

$$K = f(\tau)1_n 1_n^\mathsf{T} + f'(\tau)[\ldots] + f''(\tau)[\ldots] + \ldots$$

Consequence

Asymptotic statistics of K, thus of

$$g(x) = \alpha^\mathsf{T} k(x) + b$$

Reminder: kernel matrix

$$K_{i,j} = f\left(\frac{\|x_i - x_j\|^2}{p}\right)$$

For $x_i \in \mathcal{C}_a$ and $x_j \in \mathcal{C}_b$: $\frac{1}{p}\|x_i - x_j\|^2 = \tau + \mathcal{O}(n^{-1/2})$, thus for $K_{i,j}$

$$K_{i,j} = f\left(\tau + \mathcal{O}(n^{-1/2})\right) = f(\tau) + f'(\tau)[\ldots] + f''(\tau)[\ldots] + \ldots$$

or in matrix form

$$K = f(\tau)1_n 1_n^\intercal + f'(\tau)[\ldots] + f''(\tau)[\ldots] + \ldots$$

Consequence

Asymptotic statistics of K, thus of

$$g(x) = \alpha^\intercal k(x) + b$$

$$\begin{cases} \alpha & = S\left(I_n - \frac{1_n 1_n^\intercal S}{1_n^\intercal S 1_n}\right) y = S\left(y - b1_n\right) \\ b & = \frac{1_n^\intercal S y}{1_n^\intercal S 1_n} \end{cases}, \quad S \equiv \left(K + \frac{n}{\gamma} I_n\right)^{-1}$$

Theorem ([Liao,C'19])

Under previous assumptions, for $x \in \mathcal{C}_a$, $a \in \{1, 2\}$

$$n\left(g(x) - G_a\right) \xrightarrow{d} 0$$

where $G_a \sim \mathcal{N}(\mathrm{E}_a, \mathrm{Var}_a)$

Theorem ([Liao,C'19])

Under previous assumptions, for $x \in \mathcal{C}_a$, $a \in \{1,2\}$

$$n\left(g(x) - G_a\right) \xrightarrow{d} 0$$

where $G_a \sim \mathcal{N}(\mathrm{E}_a, \mathrm{Var}_a)$ *with*

$$\mathrm{E}_a = \begin{cases} c_2 - c_1 - \frac{2}{p} c_2 \cdot c_1 c_2 \gamma \mathfrak{D} \ , & a = 1 \\ c_2 - c_1 + \frac{2}{p} 2c_1 \cdot c_1 c_2 \gamma \mathfrak{D} \ , & a = 2 \end{cases}$$

$$\mathrm{Var}_a = \frac{8}{p^2} \gamma^2 c_1^2 c_2^2 \left(\mathcal{V}_1^a + \mathcal{V}_2^a + \mathcal{V}_3^a\right)$$

Theorem ([Liao,C'19])

Under previous assumptions, for $x \in \mathcal{C}_a$, $a \in \{1,2\}$

$$n\left(g(x) - G_a\right) \xrightarrow{d} 0$$

where $G_a \sim \mathcal{N}(\mathrm{E}_a, \mathrm{Var}_a)$ *with*

$$\mathrm{E}_a = \begin{cases} c_2 - c_1 - \frac{2}{p} c_2 \cdot c_1 c_2 \gamma \mathfrak{D}\ , & a = 1 \\ c_2 - c_1 + \frac{2}{p} 2c_1 \cdot c_1 c_2 \gamma \mathfrak{D}\ , & a = 2 \end{cases}$$

$$\mathrm{Var}_a = \frac{8}{p^2} \gamma^2 c_1^2 c_2^2 \left(\mathcal{V}_1^a + \mathcal{V}_2^a + \mathcal{V}_3^a\right)$$

and

$$\mathfrak{D} = -2 f'(\tau) \|\mu_2 - \mu_1\|^2 + \frac{f''(\tau)}{p} \left(\mathrm{tr}\,(C_2 - C_1)\right)^2 + \frac{2 f''(\tau)}{p} \mathrm{tr}\left((C_2 - C_1)^2\right)$$

$$\mathcal{V}_1^a = \frac{\left(f''(\tau)\right)^2}{p^2} \left(\mathrm{tr}\,(C_2 - C_1)\right)^2 \mathrm{tr}\, C_a^2$$

$$\mathcal{V}_2^a = 2\left(f'(\tau)\right)^2 (\mu_2 - \mu_1)^\mathsf{T} C_a (\mu_2 - \mu_1)$$

$$\mathcal{V}_3^a = \frac{2\left(f'(\tau)\right)^2}{n} \left(\frac{\mathrm{tr}\, C_1 C_a}{c_1} + \frac{\mathrm{tr}\, C_2 C_a}{c_2}\right)$$

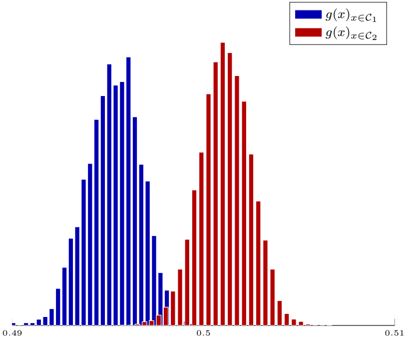


Figure: Gaussian approximation of $g(x)$, $n = 256, p = 512$, $c_1 = 1/4, c_2 = 3/4$, $\gamma = 1$, Gaussian kernel with $\sigma^2 = 1$, $x \sim \mathcal{N}(\mu_a, C_a)$ with $\mu_a = [0_{a-1}; 3; 0_{p-a}]$, $C_1 = I_p$ and $\{C_2\}_{i,j} = .4^{|i-j|}(1 + \frac{5}{\sqrt{p}})$.

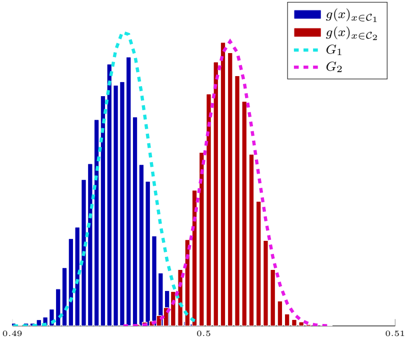


Figure: Gaussian approximation of $g(x)$, $n = 256, p = 512$, $c_1 = 1/4, c_2 = 3/4$, $\gamma = 1$, Gaussian kernel with $\sigma^2 = 1$, $x \sim \mathcal{N}(\mu_a, C_a)$ with $\mu_a = [0_{a-1}; 3; 0_{p-a}]$, $C_1 = I_p$ and $\{C_2\}_{i,j} = .4^{|i-j|}(1 + \frac{5}{\sqrt{p}})$.

Simulations on Gaussian data

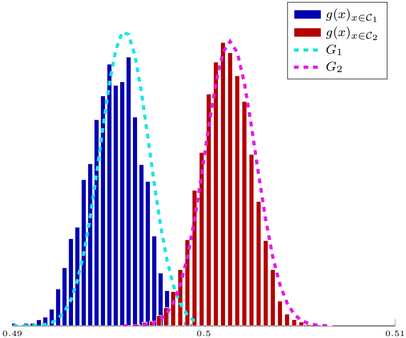


Figure: Gaussian approximation of $g(x)$, $n = 256, p = 512$, $c_1 = 1/4, c_2 = 3/4$, $\gamma = 1$, Gaussian kernel with $\sigma^2 = 1$, $x \sim \mathcal{N}(\mu_a, C_a)$ with $\mu_a = [0_{a-1}; 3; 0_{p-a}]$, $C_1 = I_p$ and $\{C_2\}_{i,j} = .4^{|i-j|}(1 + \frac{5}{\sqrt{p}})$.

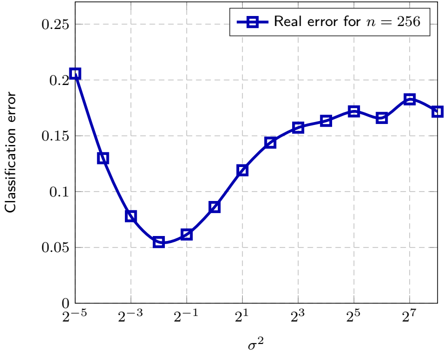


Figure: Performance of LS-SVM, $c_0 = 2$, $c_1 = c_2 = 1/2$, $\gamma = 1$, Gaussian kernel $f(t) = \exp(-\frac{t}{2\sigma^2})$. $x \sim \mathcal{N}(\mu_a, C_a)$, with $\mu_a = [0_{a-1}; 2; 0_{p-a}]$, $C_1 = I_p$ and $\{C_2\}_{i,j} = .4^{|i-j|}(1 + \frac{4}{\sqrt{p}})$.

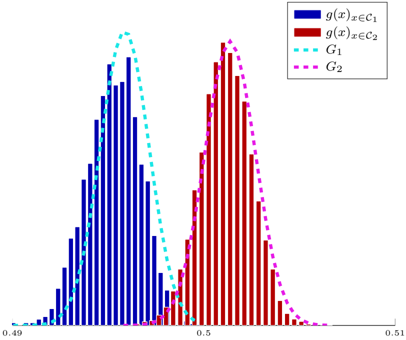


Figure: Gaussian approximation of $g(x)$, $n = 256, p = 512$, $c_1 = 1/4, c_2 = 3/4$, $\gamma = 1$, Gaussian kernel with $\sigma^2 = 1$, $x \sim \mathcal{N}(\mu_a, C_a)$ with $\mu_a = [0_{a-1}; 3; 0_{p-a}]$, $C_1 = I_p$ and $\{C_2\}_{i,j} = .4^{|i-j|}(1 + \frac{5}{\sqrt{p}})$.

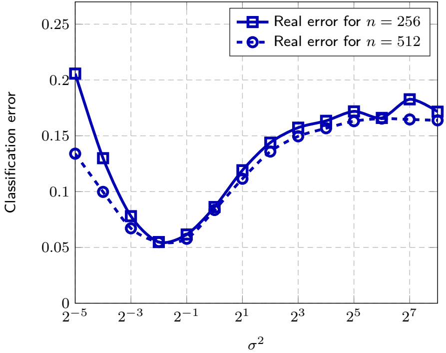


Figure: Performance of LS-SVM, $c_0 = 2$, $c_1 = c_2 = 1/2$, $\gamma = 1$, Gaussian kernel $f(t) = \exp(-\frac{t}{2\sigma^2})$. $x \sim \mathcal{N}(\mu_a, C_a)$, with $\mu_a = [0_{a-1}; 2; 0_{p-a}]$, $C_1 = I_p$ and $\{C_2\}_{i,j} = .4^{|i-j|}(1 + \frac{4}{\sqrt{p}})$.

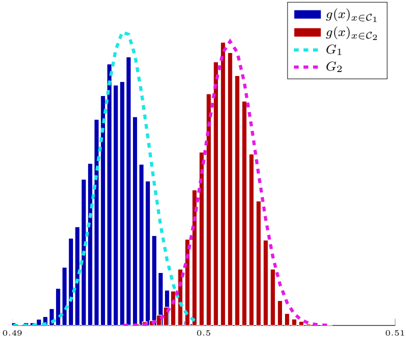


Figure: Gaussian approximation of $g(x)$, $n = 256, p = 512$, $c_1 = 1/4, c_2 = 3/4$, $\gamma = 1$, Gaussian kernel with $\sigma^2 = 1$, $x \sim \mathcal{N}(\mu_a, C_a)$ with $\mu_a = [0_{a-1}; 3; 0_{p-a}]$, $C_1 = I_p$ and $\{C_2\}_{i,j} = .4^{|i-j|}(1 + \frac{5}{\sqrt{p}})$.

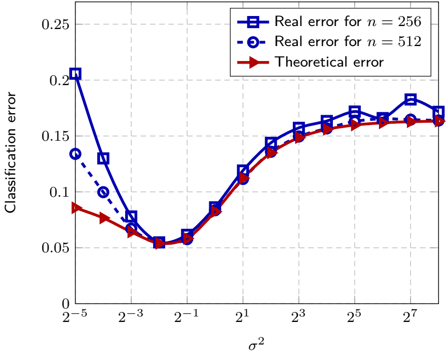
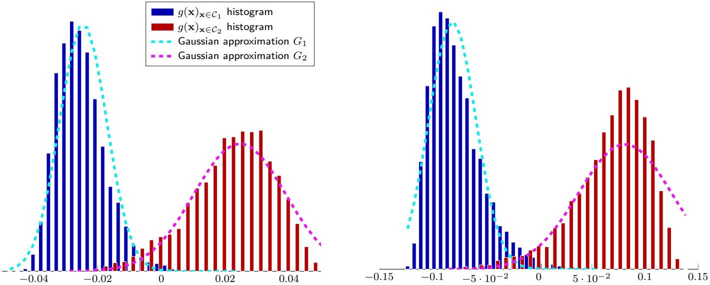


Figure: Performance of LS-SVM, $c_0 = 2$, $c_1 = c_2 = 1/2$, $\gamma = 1$, Gaussian kernel $f(t) = \exp(-\frac{t}{2\sigma^2})$. $x \sim \mathcal{N}(\mu_a, C_a)$, with $\mu_a = [0_{a-1}; 2; 0_{p-a}]$, $C_1 = I_p$ and $\{C_2\}_{i,j} = .4^{|i-j|}(1 + \frac{4}{\sqrt{p}})$.



(a) with 0dB noise (b) without noise

Figure: Gaussian approximation of $g(\mathbf{x})$, $n = 256, p = 784$, $c_1 = c_2 = 1/2$, $\gamma = 1$, Gaussian kernel with $\sigma^2 = 1$, MNIST data (numbers 1 and 7) without and with 0dB noise.

Outline

SSL Problem Statement

Context: Similar to clustering:

- Classify $x_1, \ldots, x_n \in \mathbb{R}^p$ in k classes, with n_l labelled and n_u unlabelled data.

SSL Problem Statement

Context: Similar to clustering:

- Classify $x_1, \ldots, x_n \in \mathbb{R}^p$ in k classes, with n_l labelled and n_u unlabelled data.
- Problem statement: give scores F_{ia} ($d_i = [K 1_n]_i$)

$$F = \operatorname{argmin}_{F \in \mathbb{R}^{n \times k}} \sum_{a=1}^{k} \sum_{i,j} K_{ij} (F_{ia} \qquad - F_{ja} \qquad)^2$$

such that $F_{ia} = \boldsymbol{\delta}_{\{x_i \in \mathcal{C}_a\}}$, for all labelled x_i.

Context: Similar to clustering:

- Classify $x_1, \ldots, x_n \in \mathbb{R}^p$ in k classes, with n_l labelled and n_u unlabelled data.
- Problem statement: give scores F_{ia} ($d_i = [K1_n]_i$)

$$F = \operatorname{argmin}_{F \in \mathbb{R}^{n \times k}} \sum_{a=1}^{k} \sum_{i,j} K_{ij} (F_{ia} d_i^{\alpha-1} - F_{ja} d_j^{\alpha-1})^2$$

such that $F_{ia} = \boldsymbol{\delta}_{\{x_i \in \mathcal{C}_a\}}$, for all labelled x_i.

SSL Problem Statement

Context: Similar to clustering:

- Classify $x_1, \ldots, x_n \in \mathbb{R}^p$ in k classes, with n_l labelled and n_u unlabelled data.
- Problem statement: give scores F_{ia} ($d_i = [K1_n]_i$)

$$F = \operatorname{argmin}_{F \in \mathbb{R}^{n \times k}} \sum_{a=1}^{k} \sum_{i,j} K_{ij} (F_{ia} d_i^{\alpha-1} - F_{ja} d_j^{\alpha-1})^2$$

such that $F_{ia} = \boldsymbol{\delta}_{\{x_i \in \mathcal{C}_a\}}$, for all labelled x_i.

- **Solution**: for $F^{(u)} \in \mathbb{R}^{n_u \times k}$, $F^{(l)} \in \mathbb{R}^{n_l \times k}$ scores of unlabelled/labelled data,

$$F^{(u)} = \left(I_{n_u} - D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1} \right)^{-1} D_{(u)}^{-\alpha} K_{(u,l)} D_{(l)}^{\alpha-1} F^{(l)}$$

where we naturally decompose

$$K = \begin{bmatrix} K_{(l,l)} & K_{(l,u)} \\ K_{(u,l)} & K_{(u,u)} \end{bmatrix}$$

$$D = \begin{bmatrix} D_{(l)} & 0 \\ 0 & D^{(u)} \end{bmatrix} = \operatorname{diag}\{K1_n\}.$$

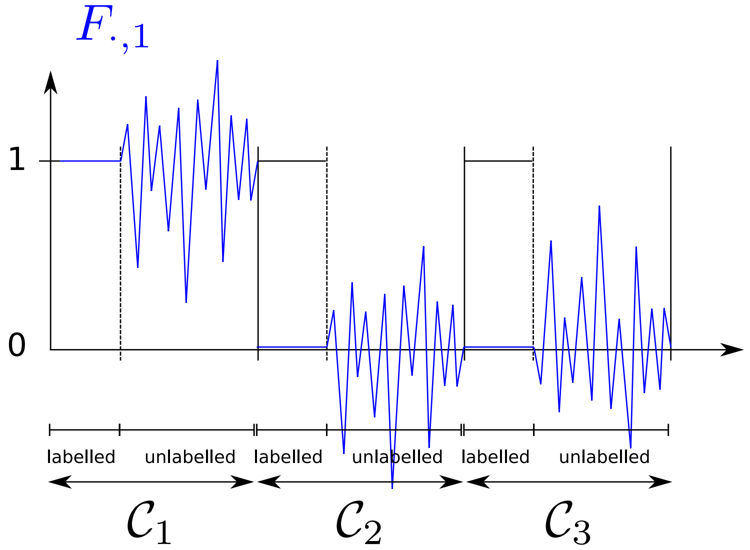


Figure: Typical expected performance output

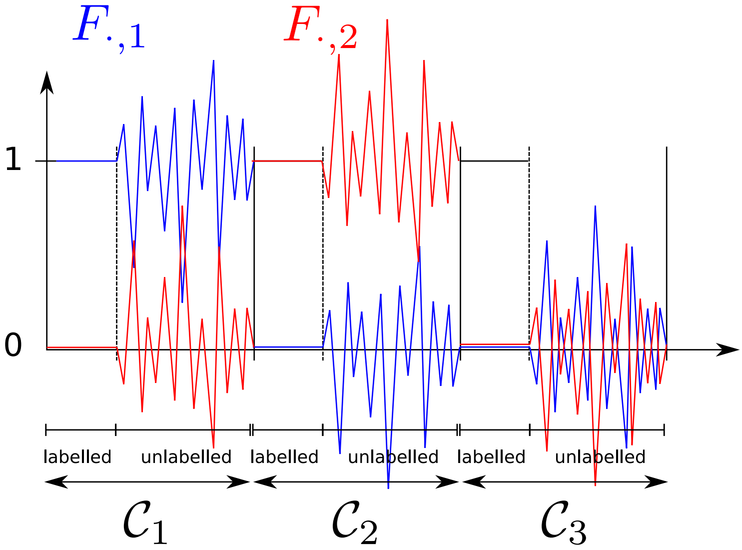


Figure: Typical expected performance output

The finite-dimensional intuition: What we expect

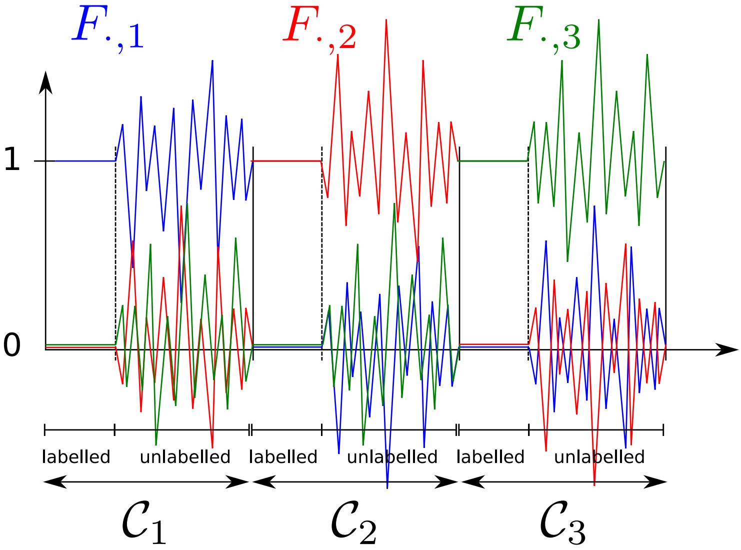
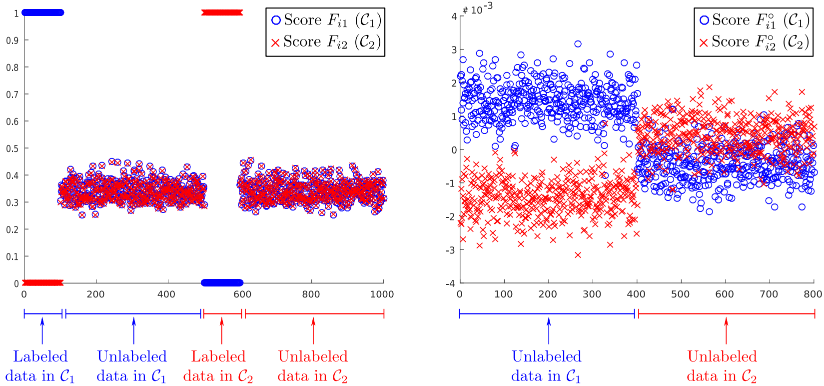


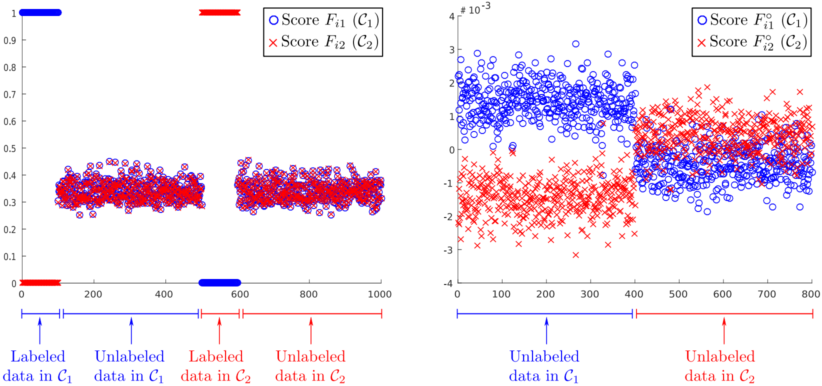
Figure: Typical expected performance output

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).



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).



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

MNIST Data Example

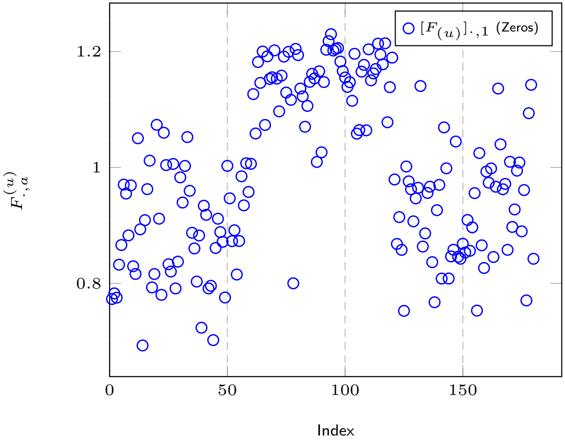


Figure: Vectors $[F^{(u)}]_{\cdot,a}$, $a = 1, 2, 3$, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

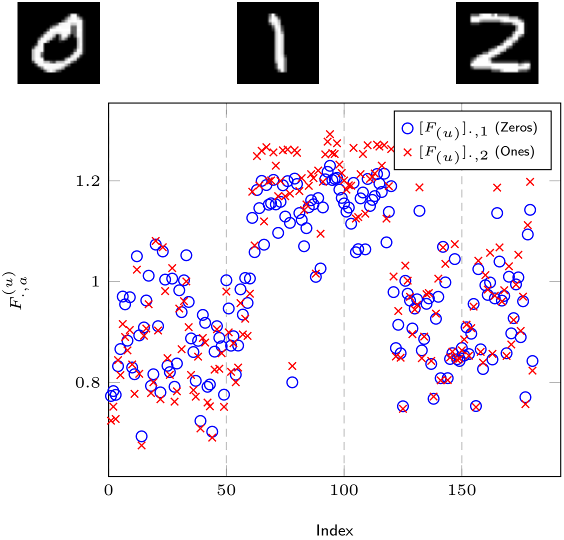


Figure: Vectors $[F^{(u)}]_{\cdot,a}$, $a = 1, 2, 3$, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

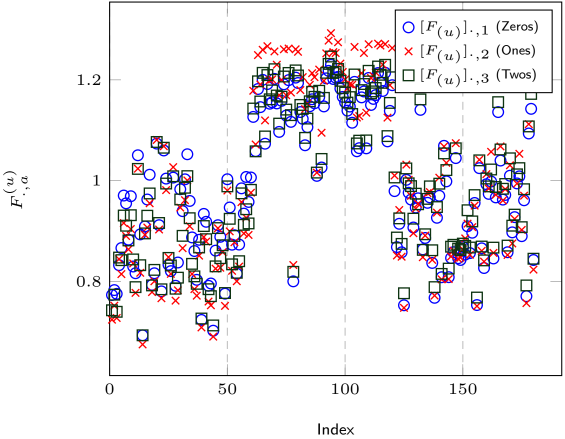


Figure: Vectors $[F^{(u)}]_{\cdot,a}$, $a = 1, 2, 3$, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

Method: Assume $n_l/n \to c_l \in (0,1)$

- We aim at characterizing

$$F^{(u)} = \left(I_{n_u} - D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1} \right)^{-1} D_{(u)}^{-\alpha} K_{(u,l)} D_{(l)}^{\alpha-1} F^{(l)}$$

Method: Assume $n_l/n \to c_l \in (0,1)$

- We aim at characterizing

$$F^{(u)} = \left(I_{n_u} - D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1} \right)^{-1} D_{(u)}^{-\alpha} K_{(u,l)} D_{(l)}^{\alpha-1} F^{(l)}$$

- Taylor expansion of K as $n, p \to \infty$,

$$K_{(u,u)} = f(\tau) 1_{n_u} 1_{n_u}^{\mathsf{T}} + O_{\|\cdot\|}(n^{-\frac{1}{2}})$$
$$D_{(u)} = n f(\tau) I_{n_u} + O(n^{\frac{1}{2}})$$

and similarly for $K_{(u,l)}$, $D_{(l)}$.

Method: Assume $n_l/n \to c_l \in (0,1)$

- We aim at characterizing

$$F^{(u)} = \left(I_{n_u} - D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1}\right)^{-1} D_{(u)}^{-\alpha} K_{(u,l)} D_{(l)}^{\alpha-1} F^{(l)}$$

- Taylor expansion of K as $n, p \to \infty$,

$$K_{(u,u)} = f(\tau) 1_{n_u} 1_{n_u}^{\mathsf{T}} + O_{\|\cdot\|}(n^{-\frac{1}{2}})$$
$$D_{(u)} = n f(\tau) I_{n_u} + O(n^{\frac{1}{2}})$$

  and similarly for $K_{(u,l)}$, $D_{(l)}$.

- So that

$$\left(I_{n_u} - D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1}\right)^{-1} = \left(I_{n_u} - \frac{1_{n_u} 1_{n_u}^{\mathsf{T}}}{n} + O_{\|\cdot\|}(n^{-\frac{1}{2}})\right)^{-1}$$

  easily Taylor expanded.

Results: Assuming $n_l/n \to c_l \in (0,1)$, by previous Taylor expansion,

- In the first order,

$$F_{\cdot,a}^{(u)} = C\frac{n_{l,a}}{n}\Big[\underbrace{v}_{O(1)} + \underbrace{\alpha\frac{t_a 1_{n_u}}{\sqrt{n}}}_{O(n^{-\frac{1}{2}})}\Big] + \underbrace{O(n^{-1})}_{\text{Informative terms}}$$

where $v = O(1)$ random vector (entry-wise) and $t_a = \frac{1}{\sqrt{p}}\operatorname{tr} C_a^{\circ}$.

Main Results

Results: Assuming $n_l/n \to c_l \in (0,1)$, by previous Taylor expansion,

- In the first order,

$$F_{\cdot,a}^{(u)} = C\frac{n_{l,a}}{n}\left[\underbrace{v}_{O(1)} + \underbrace{\alpha\frac{t_a 1_{n_u}}{\sqrt{n}}}_{O(n^{-\frac{1}{2}})}\right] + \underbrace{O(n^{-1})}_{\text{Informative terms}}$$

where $v = O(1)$ random vector (entry-wise) and $t_a = \frac{1}{\sqrt{p}}\operatorname{tr} C_a^\circ$.

- Consequences:

Results: Assuming $n_l/n \to c_l \in (0,1)$, by previous Taylor expansion,

- In the first order,

$$F^{(u)}_{\cdot,a} = C\frac{n_{l,a}}{n}\left[\underbrace{v}_{O(1)} + \underbrace{\alpha\frac{t_a 1_{n_u}}{\sqrt{n}}}_{O(n^{-\frac{1}{2}})}\right] + \underbrace{O(n^{-1})}_{\text{Informative terms}}$$

  where $v = O(1)$ random vector (entry-wise) and $t_a = \frac{1}{\sqrt{p}}\operatorname{tr} C_a^\circ$.

- Consequences:
  - Random non-informative bias v

Main Results

Results: Assuming $n_l/n \to c_l \in (0,1)$, by previous Taylor expansion,

- In the first order,

$$F_{\cdot,a}^{(u)} = C\frac{n_{l,a}}{n}\Bigg[\underbrace{v}_{O(1)} + \underbrace{\alpha\frac{t_a 1_{n_u}}{\sqrt{n}}}_{O(n^{-\frac{1}{2}})}\Bigg] + \underbrace{O(n^{-1})}_{\text{Informative terms}}$$

  where $v = O(1)$ random vector (entry-wise) and $t_a = \frac{1}{\sqrt{p}}\operatorname{tr} C_a^{\circ}$.

- Consequences:
  - Random non-informative bias v
  - Strong Impact of $n_{l,a}$

$$\boxed{F_{\cdot,a}^{(u)} \text{ to be scaled by } n_{l,a}}$$

Main Results

Results: Assuming $n_l/n \to c_l \in (0,1)$, by previous Taylor expansion,

- In the first order,

$$F^{(u)}_{\cdot,a} = C\frac{n_{l,a}}{n}\Big[\underbrace{v}_{O(1)} + \underbrace{\alpha\frac{t_a 1_{n_u}}{\sqrt{n}}}_{O(n^{-\frac{1}{2}})}\Big] + \underbrace{O(n^{-1})}_{\text{Informative terms}}$$

  where $v = O(1)$ random vector (entry-wise) and $t_a = \frac{1}{\sqrt{p}}\operatorname{tr} C^{\circ}_a$.

- Consequences:
  - Random non-informative bias v
  - Strong Impact of $n_{l,a}$

$$\boxed{F^{(u)}_{\cdot,a} \text{ to be scaled by } n_{l,a}}$$

  - Additional per-class bias $\alpha t_a 1_{n_u}$

$$\boxed{\alpha = 0 + \frac{\beta}{\sqrt{p}}.}$$

Main Results

As a consequence of the remarks above, we take

$$\alpha = \frac{\beta}{\sqrt{p}}$$

and define

$$\hat{F}^{(u)}_{i,a} = \frac{np}{n_{l,a}} F^{(u)}_{ia}.$$

As a consequence of the remarks above, we take

$$\alpha = \frac{\beta}{\sqrt{p}}$$

and define

$$\hat{F}_{i,a}^{(u)} = \frac{np}{n_{l,a}} F_{ia}^{(u)}.$$

Theorem

For $x_i \in \mathcal{C}_b$ unlabelled,

$$\boxed{\hat{F}_{i,\cdot} - G_b \to 0,\ G_b \sim \mathcal{N}(m_b, \Sigma_b)}$$

where $m_b \in \mathbb{R}^k$, $\Sigma_b \in \mathbb{R}^{k\times k}$ given by

$$(m_b)_a = -\frac{2f'(\tau)}{f(\tau)}\tilde{M}_{ab} + \frac{f''(\tau)}{f(\tau)}\tilde{t}_a\tilde{t}_b + \frac{2f''(\tau)}{f(\tau)}\tilde{T}_{ab} - \frac{f'(\tau)^2}{f(\tau)^2}t_a t_b + \beta\frac{n}{n_l}\frac{f'(\tau)}{f(\tau)}t_a + B_b$$

$$(\Sigma_b)_{a_1a_2} = \frac{2\mathit{tr}\,C_b^2}{p}\left(\frac{f'(\tau)^2}{f(\tau)^2} - \frac{f''(\tau)}{f(\tau)}\right)^2 t_{a_1}t_{a_2} + \frac{4f'(\tau)^2}{f(\tau)^2}\left([M^\mathsf{T} C_b M]_{a_1a_2} + \frac{\delta_{a_1}^{a_2}p}{n_{l,a_1}}T_{ba_1}\right)$$

with t, T, M as before, $\tilde{X}_a = X_a - \sum_{d=1}^k \frac{n_{l,d}}{n_l}X_d^\circ$ and B_b bias independent of a.

Corollary (Asymptotic Classification Error)

For $k = 2$ classes and $a \neq b$,

$$P(\hat{F}_{i,a} > \hat{F}_{ib} \mid x_i \in \mathcal{C}_b) - Q\left(\frac{(m_b)_b - (m_b)_a}{\sqrt{[1,-1]\Sigma_b[1,-1]^{\mathsf{T}}}}\right) \to 0.$$

Corollary (Asymptotic Classification Error)

For $k = 2$ classes and $a \neq b$,

$$P(\hat{F}_{i,a} > \hat{F}_{ib} \mid x_i \in \mathcal{C}_b) - Q\left(\frac{(m_b)_b - (m_b)_a}{\sqrt{[1,-1]\Sigma_b[1,-1]^\mathsf{T}}}\right) \to 0.$$

Some consequences:

- non obvious choices of appropriate kernels
- non obvious choice of optimal β (induces a possibly beneficial bias)
- importance of n_l versus n_u.

MNIST Data Example

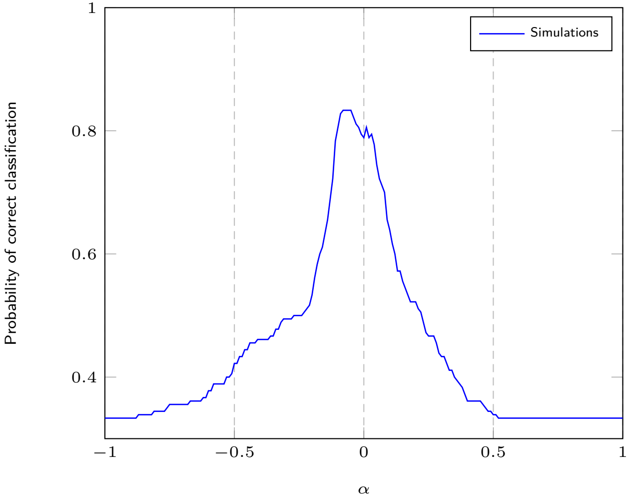


Figure: Performance as a function of α, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

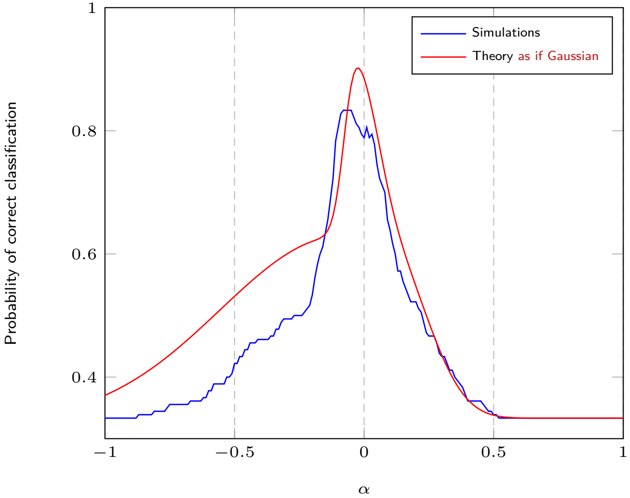


Figure: Performance as a function of α, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

MNIST Data Example

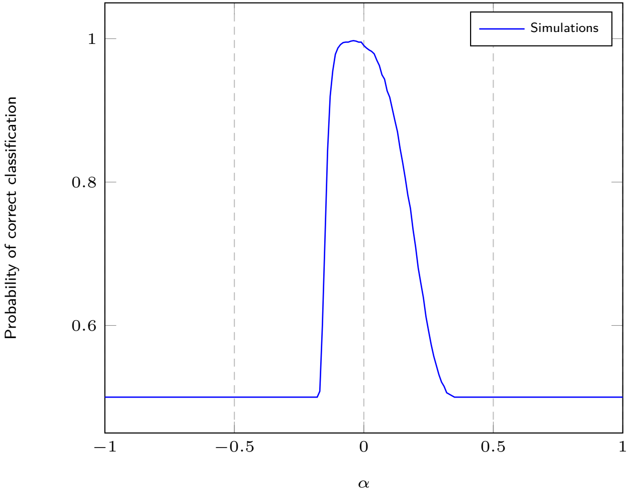


Figure: Performance as a function of α, for 2-class MNIST data (zeros, ones), $n = 1568$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

MNIST Data Example

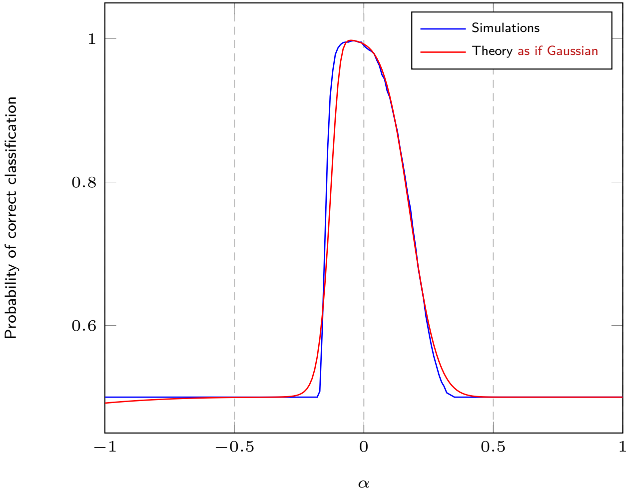


Figure: Performance as a function of α, for 2-class MNIST data (zeros, ones), $n = 1568$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

Reminder:
For $x_i \in \mathcal{C}_b$ unlabelled, $\hat{F}_{i,\cdot} - G_b \to 0$, $G_b \sim \mathcal{N}(m_b, \Sigma_b)$ with

$$(m_b)_a = -\frac{2f'(\tau)}{f(\tau)}\tilde{M}_{ab} + \frac{f''(\tau)}{f(\tau)}\tilde{t}_a\tilde{t}_b + \frac{2f''(\tau)}{f(\tau)}\tilde{T}_{ab} - \frac{f'(\tau)^2}{f(\tau)^2}t_at_b + \beta\frac{n}{n_l}\frac{f'(\tau)}{f(\tau)}t_a + B_b$$

$$(\Sigma_b)_{a_1a_2} = \frac{2\mathrm{tr}\,C_b^2}{p}\left(\frac{f'(\tau)^2}{f(\tau)^2} - \frac{f''(\tau)}{f(\tau)}\right)^2 t_{a_1}t_{a_2} + \frac{4f'(\tau)^2}{f(\tau)^2}\left([M^\mathsf{T}C_bM]_{a_1a_2} + \frac{\delta_{a_1}^{a_2}p}{n_{l,a_1}}T_{ba_1}\right)$$

with t, T, M as before, $\tilde{X}_a = X_a - \sum_{d=1}^k \frac{n_{l,d}}{n_l}X_d^\circ$ and B_b bias independent of a.

Reminder:
For $x_i \in \mathcal{C}_b$ unlabelled, $\hat{F}_{i,\cdot} - G_b \to 0$, $G_b \sim \mathcal{N}(m_b, \Sigma_b)$ with

$$(m_b)_a = -\frac{2f'(\tau)}{f(\tau)}\tilde{M}_{ab} + \frac{f''(\tau)}{f(\tau)}\tilde{t}_a\tilde{t}_b + \frac{2f''(\tau)}{f(\tau)}\tilde{T}_{ab} - \frac{f'(\tau)^2}{f(\tau)^2}t_a t_b + \beta\frac{n}{n_l}\frac{f'(\tau)}{f(\tau)}t_a + B_b$$

$$(\Sigma_b)_{a_1a_2} = \frac{2\operatorname{tr} C_b^2}{p}\left(\frac{f'(\tau)^2}{f(\tau)^2} - \frac{f''(\tau)}{f(\tau)}\right)^2 t_{a_1}t_{a_2} + \frac{4f'(\tau)^2}{f(\tau)^2}\left([M^\mathsf{T} C_b M]_{a_1a_2} + \frac{\delta_{a_1}^{a_2} p}{n_{l,a_1}}T_{ba_1}\right)$$

with t, T, M as before, $\tilde{X}_a = X_a - \sum_{d=1}^k \frac{n_{l,d}}{n_l}X_d^\circ$ and B_b bias independent of a.

The problem with unlabelled data:

- Result **does not** depend on n_u!
  $\longrightarrow$ increasing n_u asymptotically non beneficial.

Reminder:
For $x_i \in \mathcal{C}_b$ unlabelled, $\hat{F}_{i,\cdot} - G_b \to 0$, $G_b \sim \mathcal{N}(m_b, \Sigma_b)$ with

$$(m_b)_a = -\frac{2f'(\tau)}{f(\tau)}\tilde{M}_{ab} + \frac{f''(\tau)}{f(\tau)}\tilde{t}_a\tilde{t}_b + \frac{2f''(\tau)}{f(\tau)}\tilde{T}_{ab} - \frac{f'(\tau)^2}{f(\tau)^2}t_a t_b + \beta\frac{n}{n_l}\frac{f'(\tau)}{f(\tau)}t_a + B_b$$

$$(\Sigma_b)_{a_1 a_2} = \frac{2\operatorname{tr} C_b^2}{p}\left(\frac{f'(\tau)^2}{f(\tau)^2} - \frac{f''(\tau)}{f(\tau)}\right)^2 t_{a_1}t_{a_2} + \frac{4f'(\tau)^2}{f(\tau)^2}\left([M^\mathsf{T} C_b M]_{a_1 a_2} + \frac{\delta_{a_1}^{a_2} p}{n_{l,a_1}}T_{ba_1}\right)$$

with t, T, M as before, $\tilde{X}_a = X_a - \sum_{d=1}^{k}\frac{n_{l,d}}{n_l}X_d^\circ$ and B_b bias independent of a.

The problem with unlabelled data:

- Result **does not** depend on n_u!
  $\longrightarrow$ increasing n_u asymptotically non beneficial.
- Even best Laplacian regularizer **brings SSL to be merely supervised learning**.

Consequences of the finite-dimensional "mismatch"

Exploiting RMT to resurrect SSL

Consequences of the finite-dimensional “mismatch”

- A priori, **the algorithm should not work**

Consequences of the finite-dimensional "mismatch"

- A priori, **the algorithm should not work**
- Indeed "in general" it does not!

Consequences of the finite-dimensional "mismatch"

- A priori, **the algorithm should not work**
- Indeed "in general" it does not!
- But, luckily, after some (not clearly motivated) renormalization, it works again...

Consequences of the finite-dimensional "mismatch"

- A priori, **the algorithm should not work**
- Indeed "in general" it does not!
- But, luckily, after some (not clearly motivated) renormalization, it works again...

- **BUT** it does not use efficiently unlabelled data!

Consequences of the finite-dimensional "mismatch"

- A priori, **the algorithm should not work**
- Indeed "in general" it does not!
- But, luckily, after some (not clearly motivated) renormalization, it works again...

- **BUT** it does not use efficiently unlabelled data!

Chapelle, Schölkopf, Zien, "**Semi-Supervised Learning**", Chapter 4, 2009.

Our concern is this: it is frequently the case that we would be better off just discarding the unlabeled data and employing a supervised method, rather than taking a semi-supervised route. Thus ***we worry about the embarrassing situation where the addition of unlabeled data degrades the performance*** *of a classifier.*

Consequences of the finite-dimensional "mismatch"

- A priori, **the algorithm should not work**
- Indeed "in general" it does not!
- But, luckily, after some (not clearly motivated) renormalization, it works again...

- **BUT** it does not use efficiently unlabelled data!

Chapelle, Schölkopf, Zien, "**Semi-Supervised Learning**", Chapter 4, 2009.

Our concern is this: it is frequently the case that we would be better off just discarding the unlabeled data and employing a supervised method, rather than taking a semi-supervised route. Thus ***we worry about the embarrassing situation where the addition of unlabeled data degrades the performance*** *of a classifier.*

What RMT can do about it

Consequences of the finite-dimensional "mismatch"

- A priori, **the algorithm should not work**
- Indeed "in general" it does not!
- But, luckily, after some (not clearly motivated) renormalization, it works again...

- **BUT** it does not use efficiently unlabelled data!

Chapelle, Schölkopf, Zien, "**Semi-Supervised Learning**", Chapter 4, 2009.

*Our concern is this: it is frequently the case that we would be better off just discarding the unlabeled data and employing a supervised method, rather than taking a semi-supervised route. Thus **we worry about the embarrassing situation where the addition of unlabeled data degrades the performance** of a classifier.*

What RMT can do about it

- Asymptotic performance analysis: **clear understanding of what we see!**

Exploiting RMT to resurrect SSL

Consequences of the finite-dimensional "mismatch"

- A priori, **the algorithm should not work**
- Indeed "in general" it does not!
- But, luckily, after some (not clearly motivated) renormalization, it works again...
- **BUT** it does not use efficiently unlabelled data!

Chapelle, Schölkopf, Zien, "**Semi-Supervised Learning**", Chapter 4, 2009.

*Our concern is this: it is frequently the case that we would be better off just discarding the unlabeled data and employing a supervised method, rather than taking a semi-supervised route. Thus **we worry about the embarrassing situation where the addition of unlabeled data degrades the performance** of a classifier.*

What RMT can do about it

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

Resurrecting SSL by centering (SSL Improved)

Reminder:

$$F = \operatorname{argmin}_{F \in \mathbb{R}^{n \times k}} \sum_{a=1}^{k} \sum_{i,j} K_{ij} (F_{ia} d_i^{\alpha-1} - F_{ja} d_j^{\alpha-1})^2 \quad \text{with } F_{ia}^{(l)} = \boldsymbol{\delta}_{\{x_i \in \mathcal{C}_a\}}$$

$$\Leftrightarrow F^{(u)} = \left(I_{n_u} - D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1} \right)^{-1} D_{(u)}^{-\alpha} K_{(u,l)} D_{(l)}^{\alpha-1} F^{(l)}.$$

Resurrecting SSL by centering (SSL Improved)

Reminder:

$$F = \operatorname{argmin}_{F \in \mathbb{R}^{n \times k}} \sum_{a=1}^{k} \sum_{i,j} K_{ij} (F_{ia} d_i^{\alpha-1} - F_{ja} d_j^{\alpha-1})^2 \quad \text{with } F_{ia}^{(l)} = \boldsymbol{\delta}_{\{x_i \in \mathcal{C}_a\}}$$

$$\Leftrightarrow F^{(u)} = \left(I_{n_u} - D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1} \right)^{-1} D_{(u)}^{-\alpha} K_{(u,l)} D_{(l)}^{\alpha-1} F^{(l)}.$$

Domination of score flattening:

- **Consequence of** $\frac{1}{p}\|\mathbf{x}_i - \mathbf{x}_i\|^2 \to \tau$: $D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1} \simeq \frac{1}{n} 1_{n_u} 1_{n_u}^{\mathsf{T}}$ and **clustering information vanishes** (not so obvious but can be shown).

Resurrecting SSL by centering (SSL Improved)

Reminder:

$$F = \operatorname{argmin}_{F\in\mathbb{R}^{n\times k}} \sum_{a=1}^{k}\sum_{i,j} K_{ij}(F_{ia}d_i^{\alpha-1} - F_{ja}d_j^{\alpha-1})^2 \quad \text{with } F_{ia}^{(l)} = \boldsymbol{\delta}_{\{x_i\in\mathcal{C}_a\}}$$

$$\Leftrightarrow F^{(u)} = \left(I_{n_u} - D_{(u)}^{-\alpha}K_{(u,u)}D_{(u)}^{\alpha-1}\right)^{-1} D_{(u)}^{-\alpha}K_{(u,l)}D_{(l)}^{\alpha-1}F^{(l)}.$$

Domination of score flattening:

- **Consequence of** $\frac{1}{p}\|\mathbf{x}_i-\mathbf{x}_i\|^2 \to \tau$: $D_{(u)}^{-\alpha}K_{(u,u)}D_{(u)}^{\alpha-1} \simeq \frac{1}{n}1_{n_u}1_{n_u}^{\mathsf{T}}$ and **clustering information vanishes** (not so obvious but can be shown).

Solution:

- Forgetting finite-dimensional intuition: **"recenter" K to kill flattening**, i.e., use

$$\boxed{\tilde{K} = PKP},\; P = I_n - \frac{1}{n}1_n1_n^{\mathsf{T}}.$$

Theorem ([Mai,C'19] Asymptotic Performance of Improved SSL)

For $x_i \in \mathcal{C}_b$ unlabelled, score vector $\hat{F}_{i,\cdot} \in \mathbb{R}^k$ with $\tilde{K}$ satisfies:

$$\hat{F}_{i,\cdot} - \tilde{G}_b \to 0,\ \tilde{G}_b \sim \mathcal{N}(\tilde{m}_b, \tilde{\Sigma}_b)$$

with $\tilde{m}_b \in \mathbb{R}^k$, $\tilde{\Sigma}_b \in \mathbb{R}^{k\times k}$ still function of $f(\tau), f'(\tau), f''(\tau)$, $\mu_1, \ldots, \mu_k$, $C_1, \ldots, C_k$.

Theorem (**[Mai,C'19]** Asymptotic Performance of Improved SSL)

For $x_i \in \mathcal{C}_b$ unlabelled, score vector $\hat{F}_{i,\cdot} \in \mathbb{R}^k$ with $\tilde{K}$ satisfies:

$$\hat{F}_{i,\cdot} - \tilde{G}_b \to 0, \ \tilde{G}_b \sim \mathcal{N}(\tilde{m}_b, \tilde{\Sigma}_b)$$

with $\tilde{m}_b \in \mathbb{R}^k$, $\tilde{\Sigma}_b \in \mathbb{R}^{k \times k}$ still function of $f(\tau), f'(\tau), f''(\tau)$, $\mu_1, \ldots, \mu_k$, $C_1, \ldots, C_k$.

Most importantly: $\tilde{m}_b, \tilde{\Sigma}_b$ now dependent of n_u (number of unlabelled data).

Theorem ([Mai,C'19] Asymptotic Performance of Improved SSL)

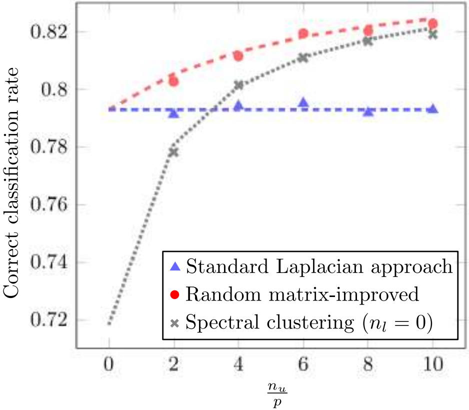
For $x_i \in \mathcal{C}_b$ unlabelled, score vector $\hat{F}_{i,\cdot} \in \mathbb{R}^k$ with $\tilde{K}$ satisfies:

$$\hat{F}_{i,\cdot} - \tilde{G}_b \to 0, \ \tilde{G}_b \sim \mathcal{N}(\tilde{m}_b, \tilde{\Sigma}_b)$$

with $\tilde{m}_b \in \mathbb{R}^k$, $\tilde{\Sigma}_b \in \mathbb{R}^{k\times k}$ still function of $f(\tau), f'(\tau), f''(\tau)$, $\mu_1, \ldots, \mu_k$, $C_1, \ldots, C_k$.

Most importantly: $\tilde{m}_b, \tilde{\Sigma}_b$ now dependent of n_u (number of unlabelled data).

Performances:



Performance as a function of n_u, n_l for $\mathcal{N}(\pm, I_p)$

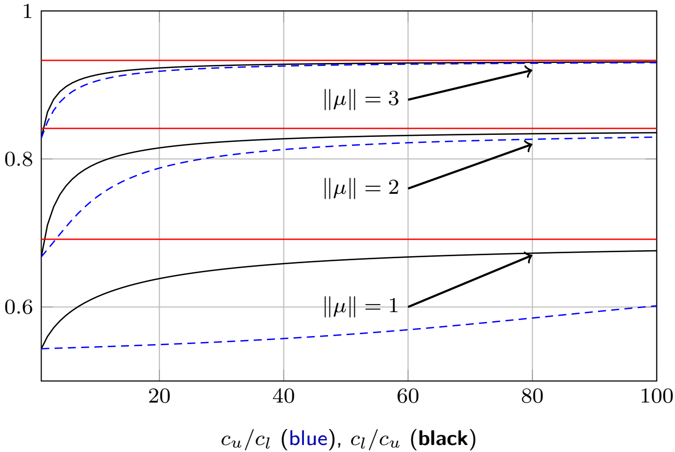
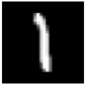


Figure: Correct classification rate, at optimal α, as a function of (i) n_u for fixed $p/n_l = 5$ (blue) and (ii) n_l for fixed $p/n_u = 5$ (black); $c_1 = c_2 = \frac{1}{2}$; different values for $\|\mu\|$. Comparison to optimal Neyman–Pearson performance for known μ (in red).

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 $n_u = 1000$.

Outline

Notion of Concentrated Vectors

- **Observation**: RMT seems to predict ML performances for real data even with Gaussian assumptions!

[2]**Reminder:** $\mathcal{F} : E \to F$ is $\|\mathcal{F}\|_{lip}$-Lipschitz if $\forall (x, y) \in E^2 : \|\mathcal{F}(x) - \mathcal{F}(y)\|_F \leq \|\mathcal{F}\|_{lip} \|x - y\|_E$.

- **Observation**: RMT seems to predict ML performances for real data even with Gaussian assumptions!
- **But** Real data are **unlikely close** to Gaussian.

[2] **Reminder:** $\mathcal{F} : E \to F$ is $\|\mathcal{F}\|_{lip}$-Lipschitz if $\forall (x, y) \in E^2 : \|\mathcal{F}(x) - \mathcal{F}(y)\|_F \leq \|\mathcal{F}\|_{lip} \|x - y\|_E$.

Notion of Concentrated Vectors

- **Observation**: RMT seems to predict ML performances for real data even with Gaussian assumptions!
- **But** Real data are **unlikely close** to Gaussian.
- Gaussian vectors fall within a larger, more useful, class of random vectors!

[2]**Reminder:** $\mathcal{F} : E \to F$ is $\|\mathcal{F}\|_{lip}$-Lipschitz if $\forall (x, y) \in E^2 : \|\mathcal{F}(x) - \mathcal{F}(y)\|_F \leq \|\mathcal{F}\|_{lip} \|x - y\|_E$.

- **Observation**: RMT seems to predict ML performances for real data even with Gaussian assumptions!
- **But** Real data are **unlikely close** to Gaussian.
- Gaussian vectors fall within a larger, more useful, class of random vectors!

Definition

Given a normed space $(E, \|\cdot\|_E)$ and $q \in \mathbb{R}$, a random vector $\mathbf{z} \in E$ is q-exponentially **concentrated** if for any 1-**Lipschitz function**[2] $\mathcal{F} : \mathbb{R}^p \to \mathbb{R}$, there exists $C, c > 0$ s.t.

$$\mathbb{P}\left\{|\mathcal{F}(\mathbf{z}) - \mathbb{E}\mathcal{F}(\mathbf{z})| > t\right\} \leq Ce^{-c\,t^q}$$

[2] **Reminder:** $\mathcal{F} : E \to F$ is $\|\mathcal{F}\|_{lip}$-Lipschitz if $\forall (x, y) \in E^2 : \|\mathcal{F}(x) - \mathcal{F}(y)\|_F \leq \|\mathcal{F}\|_{lip} \|x - y\|_E$.

- **Observation**: RMT seems to predict ML performances for real data even with Gaussian assumptions!
- **But** Real data are **unlikely close** to Gaussian.
- Gaussian vectors fall within a larger, more useful, class of random vectors!

Definition

Given a normed space $(E, \|\cdot\|_E)$ and $q \in \mathbb{R}$, a random vector $\mathbf{z} \in E$ is q-exponentially **concentrated** if for any 1-**Lipschitz function**[2] $\mathcal{F} : \mathbb{R}^p \to \mathbb{R}$, there exists $C, c > 0$ s.t.

$$\mathbb{P}\left\{|\mathcal{F}(\mathbf{z}) - \mathbb{E}\mathcal{F}(\mathbf{z})| > t\right\} \leq Ce^{-c\,t^q} \xrightarrow{\text{denoted}} \boxed{\mathbf{z} \in \mathcal{O}(e^{-\cdot^q})}$$

[2] **Reminder:** $\mathcal{F} : E \to F$ is $\|\mathcal{F}\|_{lip}$-Lipschitz if $\forall (x, y) \in E^2 : \|\mathcal{F}(x) - \mathcal{F}(y)\|_F \leq \|\mathcal{F}\|_{lip} \|x - y\|_E$.

- **Observation**: RMT seems to predict ML performances for real data even with Gaussian assumptions!
- **But** Real data are **unlikely close** to Gaussian.
- Gaussian vectors fall within a larger, more useful, class of random vectors!

Definition

Given a normed space $(E, \|\cdot\|_E)$ and $q \in \mathbb{R}$, a random vector $\mathbf{z} \in E$ is q-exponentially **concentrated** if for any 1-**Lipschitz function**[2] $\mathcal{F} : \mathbb{R}^p \to \mathbb{R}$, there exists $C, c > 0$ s.t.

$$\mathbb{P}\left\{|\mathcal{F}(\mathbf{z}) - \mathbb{E}\mathcal{F}(\mathbf{z})| > t\right\} \leq Ce^{-c\,t^q} \xrightarrow{\text{denoted}} \boxed{\mathbf{z} \in \mathcal{O}(e^{-\cdot^q})}$$

(P1) $X \sim \mathcal{N}(0, I_p)$ is 2-exponentially **concentrated**.

[2]**Reminder:** $\mathcal{F} : E \to F$ is $\|\mathcal{F}\|_{lip}$-Lipschitz if $\forall (x, y) \in E^2 : \|\mathcal{F}(x) - \mathcal{F}(y)\|_F \leq \|\mathcal{F}\|_{lip} \|x - y\|_E$.

- **Observation**: RMT seems to predict ML performances for real data even with Gaussian assumptions!
- **But** Real data are **unlikely close** to Gaussian.
- Gaussian vectors fall within a larger, more useful, class of random vectors!

Definition

Given a normed space $(E, \|\cdot\|_E)$ and $q \in \mathbb{R}$, a random vector $\mathbf{z} \in E$ is q-exponentially **concentrated** if for any 1-**Lipschitz function**[2] $\mathcal{F} : \mathbb{R}^p \to \mathbb{R}$, there exists $C, c > 0$ s.t.

$$\mathbb{P}\left\{|\mathcal{F}(\mathbf{z}) - \mathbb{E}\mathcal{F}(\mathbf{z})| > t\right\} \leq Ce^{-c\,t^q} \xrightarrow{\text{denoted}} \boxed{\mathbf{z} \in \mathcal{O}(e^{-\cdot^q})}$$

(P1) $X \sim \mathcal{N}(0, I_p)$ is 2-exponentially **concentrated**.

(P2) If $X \in \mathcal{O}(e^{-\cdot^q})$ and $\mathcal{G}$ is $\|\mathcal{G}\|_{lip}$-**Lipschitz**, then

$$\mathcal{G}(X) \in \mathcal{O}\left(e^{-(\cdot/\|\mathcal{G}\|_{lip})^q}\right).$$

[2] **Reminder:** $\mathcal{F} : E \to F$ is $\|\mathcal{F}\|_{lip}$-Lipschitz if $\forall (x, y) \in E^2 : \|\mathcal{F}(x) - \mathcal{F}(y)\|_F \leq \|\mathcal{F}\|_{lip} \|x - y\|_E$.

- **Observation**: RMT seems to predict ML performances for real data even with Gaussian assumptions!
- **But** Real data are **unlikely close** to Gaussian.
- Gaussian vectors fall within a larger, more useful, class of random vectors!

Definition

Given a normed space $(E, \|\cdot\|_E)$ and $q \in \mathbb{R}$, a random vector $\mathbf{z} \in E$ is q-exponentially **concentrated** if for any 1-**Lipschitz function**[2] $\mathcal{F} : \mathbb{R}^p \to \mathbb{R}$, there exists $C, c > 0$ s.t.

$$\mathbb{P}\left\{|\mathcal{F}(\mathbf{z}) - \mathbb{E}\mathcal{F}(\mathbf{z})| > t\right\} \leq Ce^{-c\,t^q} \xrightarrow{\text{denoted}} \boxed{\mathbf{z} \in \mathcal{O}(e^{-\cdot^q})}$$

(P1) $X \sim \mathcal{N}(0, I_p)$ is 2-exponentially **concentrated**.

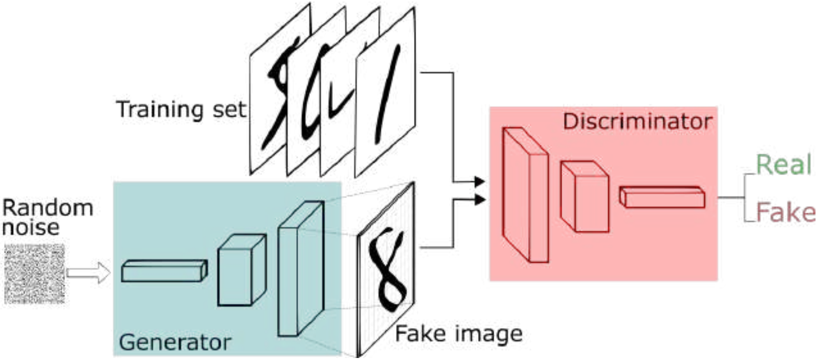
(P2) If $X \in \mathcal{O}(e^{-\cdot^q})$ and $\mathcal{G}$ is $\|\mathcal{G}\|_{lip}$-**Lipschitz**, then

$$\mathcal{G}(X) \in \mathcal{O}\left(e^{-(\cdot/\|\mathcal{G}\|_{lip})^q}\right).$$

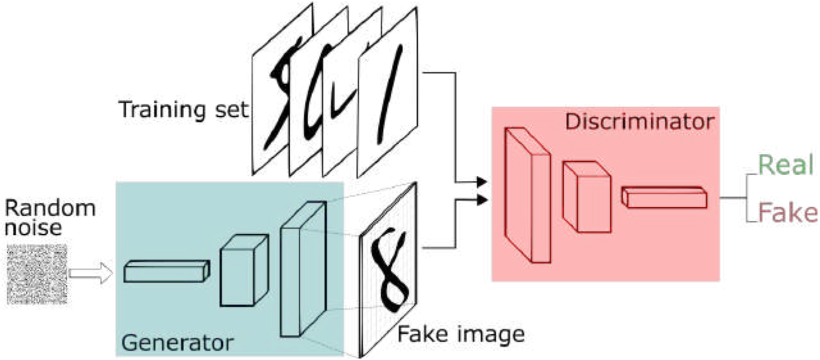
"Concentrated vectors are stable through Lipschitz maps."

[2] **Reminder:** $\mathcal{F} : E \to F$ is $\|\mathcal{F}\|_{lip}$-Lipschitz if $\forall (x, y) \in E^2 : \|\mathcal{F}(x) - \mathcal{F}(y)\|_F \leq \|\mathcal{F}\|_{lip} \|x - y\|_E$.

GAN data: An Example of Concentrated Vectors



GAN data: An Example of Concentrated Vectors



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

We generate data as

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

GAN data: An Example of Concentrated Vectors

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

GAN data: An Example of Concentrated Vectors

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

$$\text{GAN Data} = \mathcal{F}_1 \circ \mathcal{F}_2 \circ \cdots \circ \mathcal{F}_N(\text{Gaussian})$$

GAN data: An Example of Concentrated Vectors

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

$$\text{GAN Data} = \mathcal{F}_1 \circ \mathcal{F}_2 \circ \cdots \circ \mathcal{F}_N(\text{Gaussian})$$

where the $\mathcal{F}_i$'s are either Fully Connected Layers, Convolutional Layers, Pooling Layers and Activation Functions, Residual Connections or Batch Normalizations.

GAN data: An Example of Concentrated Vectors

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

$$\text{GAN Data} = \mathcal{F}_1 \circ \mathcal{F}_2 \circ \cdots \circ \mathcal{F}_N(\text{Gaussian})$$

where the $\mathcal{F}_i$'s are either Fully Connected Layers, Convolutional Layers, Pooling Layers and Activation Functions, Residual Connections or Batch Normalizations.

$\Rightarrow$ The $\mathcal{F}_i$'s are *Lipschitz* operations.

- **Fully Connected Layers and Convolutional Layers** are affine operations:

$$\mathcal{F}_i(x) = W_i x + b_i,$$

and $\|\mathcal{F}_i\|_{lip} = \sup_{u \neq 0} \frac{\|W_i u\|_p}{\|u\|_p}$, for any p-norm.

- **Fully Connected Layers and Convolutional Layers** are affine operations:

$$\mathcal{F}_i(x) = W_i x + b_i,$$

and $\|\mathcal{F}_i\|_{lip} = \sup_{u \neq 0} \frac{\|W_i u\|_p}{\|u\|_p}$, for any p-norm.

- **Pooling Layers and Activation Functions:** Are 1-Lipschitz operations with respect to any p-norm (e.g., ReLU and Max-pooling).

- **Fully Connected Layers and Convolutional Layers** are affine operations:

$$\mathcal{F}_i(x) = W_i x + b_i,$$

  and $\|\mathcal{F}_i\|_{lip} = \sup_{u \neq 0} \frac{\|W_i u\|_p}{\|u\|_p}$, for any p-norm.

- **Pooling Layers and Activation Functions:** Are 1-Lipschitz operations with respect to any p-norm (e.g., ReLU and Max-pooling).

- **Residual Connections:** $\mathcal{F}_i(x) = x + \mathcal{F}_i^{(1)} \circ \cdots \circ \mathcal{F}_i^{(\ell)}(x)$
  where the $\mathcal{F}_i^{(j)}$'s are Lipschitz operations, thus $\mathcal{F}_i$ is a Lipschitz operation with Lipschitz constant bounded by $1 + \prod_{j=1}^{\ell} \|\mathcal{F}_i^{(j)}\|_{lip}$.

- ...

Consider data distributed in k classes $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$ as

$$X = [\underbrace{x_1, \ldots, x_{n_1}}_{\in \mathcal{O}(e^{-\cdot^{q_1}})}, \underbrace{x_{n_1+1}, \ldots, x_{n_2}}_{\in \mathcal{O}(e^{-\cdot^{q_2}})}, \ldots, \underbrace{x_{n-n_k+1}, \ldots, x_n}_{\in \mathcal{O}(e^{-\cdot^{q_k}})}] \in \mathbb{R}^{p \times n}$$

Consider data distributed in k classes $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$ as

$$X = [\underbrace{x_1, \ldots, x_{n_1}}_{\in \mathcal{O}(e^{-\cdot^{q_1}})}, \underbrace{x_{n_1+1}, \ldots, x_{n_2}}_{\in \mathcal{O}(e^{-\cdot^{q_2}})}, \ldots, \underbrace{x_{n-n_k+1}, \ldots, x_n}_{\in \mathcal{O}(e^{-\cdot^{q_k}})}] \in \mathbb{R}^{p \times n}$$

Denote

$$\mu_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i], \;\; C_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i x_i^\intercal]$$

Consider data distributed in k classes $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$ as

$$X = [\underbrace{x_1, \ldots, x_{n_1}}_{\in \mathcal{O}(e^{-\cdot^{q_1}})}, \underbrace{x_{n_1+1}, \ldots, x_{n_2}}_{\in \mathcal{O}(e^{-\cdot^{q_2}})}, \ldots, \underbrace{x_{n-n_k+1}, \ldots, x_n}_{\in \mathcal{O}(e^{-\cdot^{q_k}})}] \in \mathbb{R}^{p \times n}$$

Denote

$$\mu_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i], \;\; C_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i x_i^\intercal]$$

Assumption (Growth rate)

As $p \to \infty$,

Consider data distributed in k classes $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$ as

$$X = [\underbrace{x_1, \ldots, x_{n_1}}_{\in \mathcal{O}(e^{-\cdot^{q_1}})}, \underbrace{x_{n_1+1}, \ldots, x_{n_2}}_{\in \mathcal{O}(e^{-\cdot^{q_2}})}, \ldots, \underbrace{x_{n-n_k+1}, \ldots, x_n}_{\in \mathcal{O}(e^{-\cdot^{q_k}})}] \in \mathbb{R}^{p \times n}$$

Denote

$$\mu_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i], \;\; C_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i x_i^\intercal]$$

Assumption (Growth rate)

As $p \to \infty$,

1. $p/n \to c \in (0, \infty)$.

Consider data distributed in k classes $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$ as

$$X = [\underbrace{x_1, \ldots, x_{n_1}}_{\in \mathcal{O}(e^{-\cdot^{q_1}})}, \underbrace{x_{n_1+1}, \ldots, x_{n_2}}_{\in \mathcal{O}(e^{-\cdot^{q_2}})}, \ldots, \underbrace{x_{n-n_k+1}, \ldots, x_n}_{\in \mathcal{O}(e^{-\cdot^{q_k}})}] \in \mathbb{R}^{p \times n}$$

Denote

$$\mu_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i], \;\; C_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i x_i^\intercal]$$

Assumption (Growth rate)

As $p \to \infty$,

1. $p/n \to c \in (0, \infty)$.
2. *The number of classes k is bounded.*

Mixture of Concentrated Vectors

Consider data distributed in k classes $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$ as

$$X = [\underbrace{x_1, \ldots, x_{n_1}}_{\in \mathcal{O}(e^{-\cdot^{q_1}})}, \underbrace{x_{n_1+1}, \ldots, x_{n_2}}_{\in \mathcal{O}(e^{-\cdot^{q_2}})}, \ldots, \underbrace{x_{n-n_k+1}, \ldots, x_n}_{\in \mathcal{O}(e^{-\cdot^{q_k}})}] \in \mathbb{R}^{p \times n}$$

Denote

$$\mu_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i], \;\; C_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i x_i^\intercal]$$

Assumption (Growth rate)

As $p \to \infty$,

1. $p/n \to c \in (0, \infty)$.
2. *The number of classes k is bounded.*
3. *For any $\ell \in [k]$, $\|\mu_\ell\| = \mathcal{O}(\sqrt{p})$.*

Consider data distributed in k classes $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_k$ as

$$X = [\underbrace{x_1, \ldots, x_{n_1}}_{\in \mathcal{O}(e^{-\cdot^{q_1}})}, \underbrace{x_{n_1+1}, \ldots, x_{n_2}}_{\in \mathcal{O}(e^{-\cdot^{q_2}})}, \ldots, \underbrace{x_{n-n_k+1}, \ldots, x_n}_{\in \mathcal{O}(e^{-\cdot^{q_k}})}] \in \mathbb{R}^{p \times n}$$

Denote

$$\mu_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i], \;\; C_\ell = \mathbb{E}_{x_i \in \mathcal{C}_\ell}[x_i x_i^\intercal]$$

Assumption (Growth rate)

As $p \to \infty$,

1. $p/n \to c \in (0, \infty)$.
2. *The number of classes k is bounded.*
3. *For any $\ell \in [k]$, $\|\mu_\ell\| = \mathcal{O}(\sqrt{p})$.*

Notation

$Q(z) = (X^\intercal X/p + zI_n)^{-1}$.

Theorem

Under the assumptions above, we have $Q(z) \in \mathcal{O}(e^{-(\sqrt{p}\,\cdot)^q})$ *in* $(\mathbb{R}^{n\times n}, \|\cdot\|)$*. Furthermore,*

$$\left\|\mathbb{E}[Q(z)] - \tilde{Q}(z)\right\| = \mathcal{O}\left(\sqrt{\frac{\log p}{p}}\right) \quad \textit{where } \tilde{Q}(z) = \frac{1}{z}\Lambda(z) + \frac{1}{p\,z}J\Omega(z)J^\intercal$$

Theorem

Under the assumptions above, we have $Q(z) \in \mathcal{O}(e^{-(\sqrt{p}\,\cdot)^q})$ *in* $(\mathbb{R}^{n\times n}, \|\cdot\|)$*. Furthermore,*

$$\left\|\mathbb{E}[Q(z)] - \tilde{Q}(z)\right\| = \mathcal{O}\left(\sqrt{\frac{\log p}{p}}\right) \quad \textit{where} \quad \tilde{Q}(z) = \frac{1}{z}\Lambda(z) + \frac{1}{p\,z}J\Omega(z)J^{\intercal}$$

with $\Lambda(z) = \textit{diag}\left\{\frac{1_{n_\ell}}{1+\delta_\ell(z)}\right\}_{\ell=1}^{k}$ *and* $\Omega(z) = \textit{diag}\{\mu_\ell^{\intercal}\tilde{R}(z)\mu_\ell\}_{\ell=1}^{k}$

Theorem

Under the assumptions above, we have $Q(z) \in \mathcal{O}(e^{-(\sqrt{p}\,\cdot)^q})$ in $(\mathbb{R}^{n\times n}, \|\cdot\|)$. Furthermore,

$$\left\|\mathbb{E}[Q(z)] - \tilde{Q}(z)\right\| = \mathcal{O}\left(\sqrt{\frac{\log p}{p}}\right) \quad \textit{where } \tilde{Q}(z) = \frac{1}{z}\Lambda(z) + \frac{1}{p\,z} J\Omega(z)J^{\mathsf{T}}$$

with $\Lambda(z) = \textit{diag}\left\{\frac{1_{n_\ell}}{1+\delta_\ell(z)}\right\}_{\ell=1}^{k}$ *and* $\Omega(z) = \textit{diag}\{\mu_\ell^{\mathsf{T}}\tilde{R}(z)\mu_\ell\}_{\ell=1}^{k}$

$$\tilde{R}(z) = \left(\frac{1}{k}\sum_{\ell=1}^{k}\frac{C_\ell}{1+\delta_\ell(z)} + zI_p\right)^{-1}$$

Theorem

Under the assumptions above, we have $Q(z) \in \mathcal{O}(e^{-(\sqrt{p}\,\cdot)^q})$ *in* $(\mathbb{R}^{n\times n}, \|\cdot\|)$. *Furthermore,*

$$\left\|\mathbb{E}[Q(z)] - \tilde{Q}(z)\right\| = \mathcal{O}\left(\sqrt{\frac{\log p}{p}}\right) \quad \text{where } \tilde{Q}(z) = \frac{1}{z}\Lambda(z) + \frac{1}{p\,z}J\Omega(z)J^\intercal$$

with $\Lambda(z) = \text{diag}\left\{\frac{1_{n_\ell}}{1+\delta_\ell(z)}\right\}_{\ell=1}^k$ *and* $\Omega(z) = \text{diag}\{\mu_\ell^\intercal \tilde{R}(z)\mu_\ell\}_{\ell=1}^k$

$$\tilde{R}(z) = \left(\frac{1}{k}\sum_{\ell=1}^k \frac{C_\ell}{1+\delta_\ell(z)} + zI_p\right)^{-1}$$

with $\delta(z) = [\delta_1(z), \ldots, \delta_k(z)]$ *is the unique fixed point of the system of equations*

$$\delta_\ell(z) = \frac{1}{p}\text{tr}\left(C_\ell\left(\frac{1}{k}\sum_{j=1}^k \frac{C_j}{1+\delta_j(z)} + zI_p\right)^{-1}\right) \quad \text{for each } \ell \in [k].$$

Theorem

Under the assumptions above, we have $Q(z) \in \mathcal{O}(e^{-(\sqrt{p}\,\cdot)^q})$ *in* $(\mathbb{R}^{n\times n}, \|\cdot\|)$. *Furthermore,*

$$\left\| \mathbb{E}[Q(z)] - \tilde{Q}(z) \right\| = \mathcal{O}\left(\sqrt{\frac{\log p}{p}} \right) \quad \textit{where} \quad \tilde{R}(z) = \frac{1}{z}\Lambda(z) + \frac{1}{p\,z} J\Omega(z)J^\intercal$$

with $\Lambda(z) = \textit{diag}\left\{ \frac{1_{n_\ell}}{1+\delta_\ell(z)} \right\}_{\ell=1}^k$ *and* $\Omega(z) = \textit{diag}\{\mu_\ell{}^\intercal \tilde{R}(z)\mu_\ell\}_{\ell=1}^k$

$$\tilde{R}(z) = \left(\frac{1}{k}\sum_{\ell=1}^k \frac{C_\ell}{1+\delta_\ell(z)} + zI_p \right)^{-1}$$

with $\delta(z) = [\delta_1(z), \ldots, \delta_k(z)]$ *is the unique fixed point of the system of equations*

$$\delta_\ell(z) = \textit{tr}\left(C_\ell \left(\frac{1}{k}\sum_{j=1}^k \frac{C_j}{1+\delta_j(z)} + zI_p \right)^{-1} \right) \quad \textit{for each } \ell \in [k].$$

Theorem

Under the assumptions above, we have $Q(z) \in \mathcal{O}(e^{-(\sqrt{p}\,\cdot)^q})$ *in* $(\mathbb{R}^{n\times n}, \|\cdot\|)$. *Furthermore,*

$$\left\|\mathbb{E}[Q(z)] - \tilde{Q}(z)\right\| = \mathcal{O}\left(\sqrt{\frac{\log p}{p}}\right) \quad \textit{where} \quad \tilde{R}(z) = \frac{1}{z}\Lambda(z) + \frac{1}{p\,z} J\Omega(z)J^\intercal$$

with $\Lambda(z) = \textit{diag}\left\{\frac{1_{n_\ell}}{1+\delta_\ell(z)}\right\}_{\ell=1}^k$ *and* $\Omega(z) = \textit{diag}\{\mu_\ell{}^\intercal \tilde{R}(z)\mu_\ell\}_{\ell=1}^k$

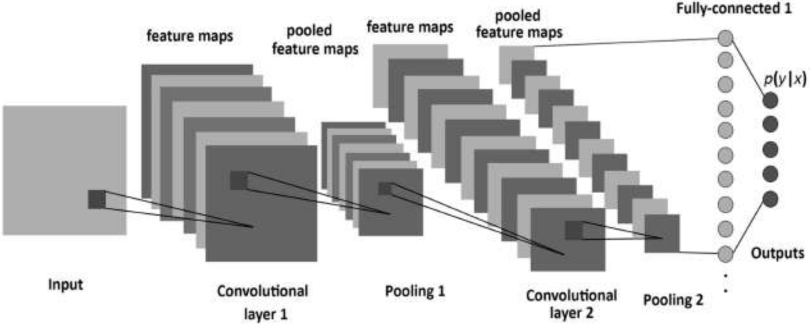
$$\tilde{R}(z) = \left(\frac{1}{k}\sum_{\ell=1}^k \frac{C_\ell}{1+\delta_\ell(z)} + zI_p\right)^{-1}$$

with $\delta(z) = [\delta_1(z), \ldots, \delta_k(z)]$ *is the unique fixed point of the system of equations*

$$\delta_\ell(z) = \textit{tr}\left(C_\ell\left(\frac{1}{k}\sum_{j=1}^k \frac{C_j}{1+\delta_j(z)} + zI_p\right)^{-1}\right) \quad \textit{for each} \quad \ell \in [k].$$

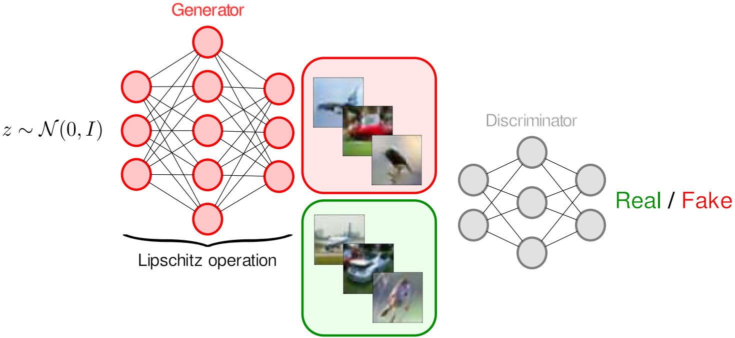
Key Observation: Only first and second order statistics matter!

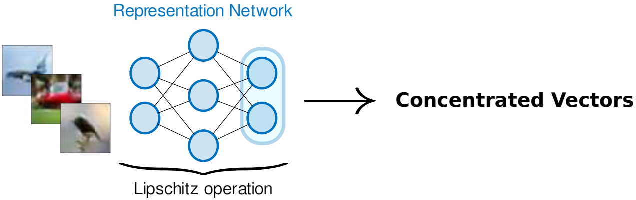
Application to CNN Representations of GAN Images



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

Application to CNN Representations of GAN Images

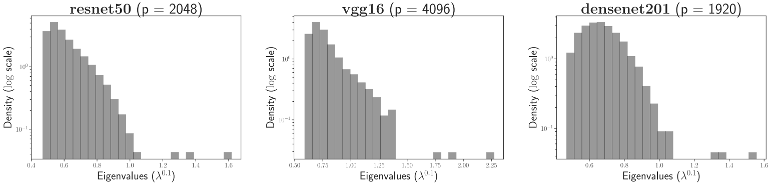




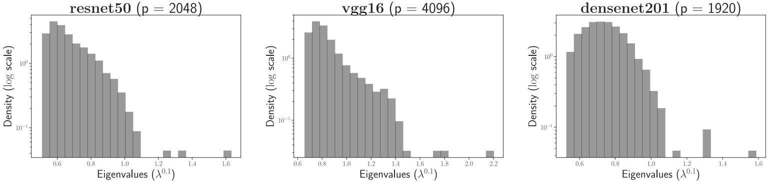

GAN Images
Real Images

Application to CNN representations of GAN Images

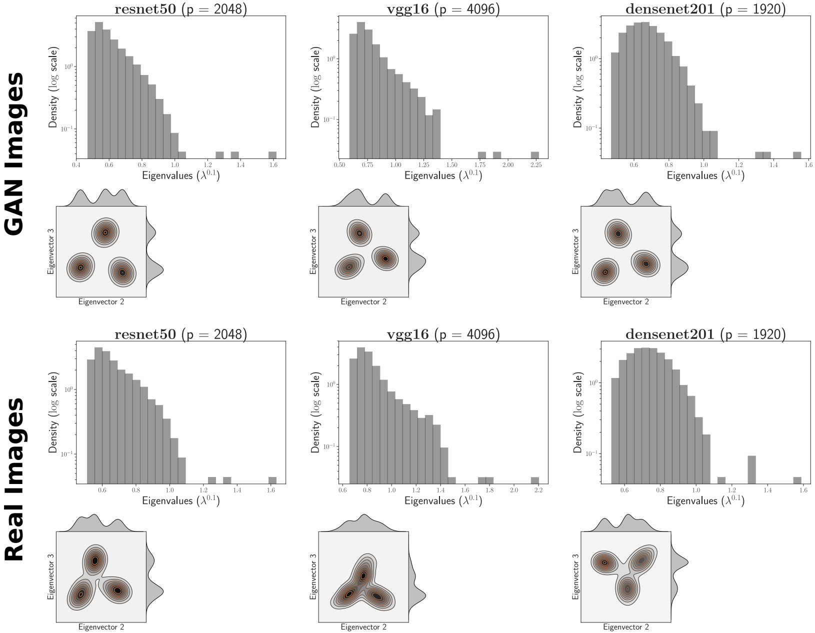
GAN Images



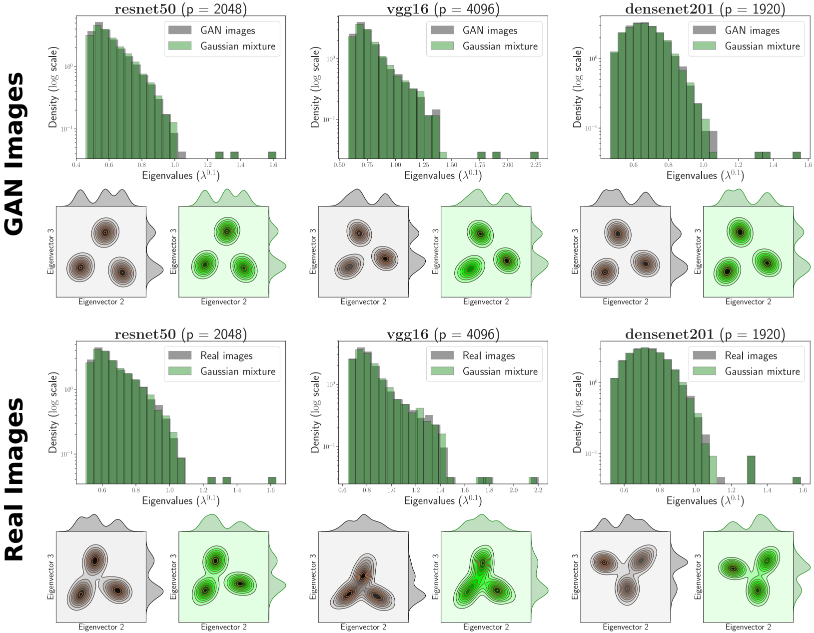
Real Images



Application to CNN representations of GAN Images



Application to CNN representations of GAN Images



Outline

Take-away messages

- Asymptotic "**concentration effect**" for large n, p

Take-away messages

- Asymptotic "**concentration effect**" for large $n, p \Rightarrow$ simplification in analyses **and** models.

Take-away messages

- Asymptotic "**concentration effect**" for large $n, p \Rightarrow$ simplification in analyses **and** models.

- Non-trivial **phase transition** phenomena (ability to detect, estimate) when $p, n \to \infty$.

Take-away messages

- Asymptotic "**concentration effect**" for large $n, p \Rightarrow$ simplification in analyses **and** models.
- Non-trivial **phase transition** phenomena (ability to detect, estimate) when $p, n \to \infty$.
- Access to **limiting performances** and <u>not only bounds</u>!

Take-away messages

- Asymptotic "**concentration effect**" for large $n, p \Rightarrow$ simplification in analyses **and** models.
- Non-trivial **phase transition** phenomena (ability to detect, estimate) when $p, n \to \infty$.
- Access to **limiting performances** and not only bounds! $\Rightarrow$ hyperparameter optimization, algorithm improvement.

Take-away messages

- Asymptotic "**concentration effect**" for large $n, p \Rightarrow$ simplification in analyses **and** models.
- Non-trivial **phase transition** phenomena (ability to detect, estimate) when $p, n \to \infty$.
- Access to **limiting performances** and not only bounds! $\Rightarrow$ hyperparameter optimization, algorithm improvement.
- **Complete intuitive change**

Take-away messages

- Asymptotic "**concentration effect**" for large $n, p \Rightarrow$ simplification in analyses **and** models.
- Non-trivial **phase transition** phenomena (ability to detect, estimate) when $p, n \to \infty$.
- Access to **limiting performances** and not only bounds! $\Rightarrow$ hyperparameter optimization, algorithm improvement.
- **Complete intuitive change** $\Rightarrow$ opens way to renewed methods.

Take-away messages

- Asymptotic "**concentration effect**" for large $n, p \Rightarrow$ simplification in analyses **and** models.
- Non-trivial **phase transition** phenomena (ability to detect, estimate) when $p, n \to \infty$.
- Access to **limiting performances** and <u>not only bounds</u>! $\Rightarrow$ hyperparameter optimization, algorithm improvement.
- **Complete intuitive change** $\Rightarrow$ opens way to renewed methods.
- **Strong coincidence with real datasets**

Take-away messages

- Asymptotic "**concentration effect**" for large $n, p \Rightarrow$ simplification in analyses **and** models.
- Non-trivial **phase transition** phenomena (ability to detect, estimate) when $p, n \to \infty$.
- Access to **limiting performances** and not only bounds! $\Rightarrow$ hyperparameter optimization, algorithm improvement.
- **Complete intuitive change** $\Rightarrow$ opens way to renewed methods.
- **Strong coincidence with real datasets** $\Rightarrow$ easy link between theory and practice.

- Neural nets: loss landscape, gradient descent dynamics and

- Neural nets: loss landscape, gradient descent dynamics and deep learning!

Perspectives and Open Problems

- Neural nets: loss landscape, gradient descent dynamics and deep learning!
- Generalized linear models

Perspectives and Open Problems

- Neural nets: loss landscape, gradient descent dynamics and deep learning!
- Generalized linear models
- More general problems from convex optimization (often of *implicit solution*)

Perspectives and Open Problems

- Neural nets: loss landscape, gradient descent dynamics and deep learning!
- Generalized linear models
- More general problems from convex optimization (often of *implicit solution*)
- More difficult: problem raised from *non-convex* optimization problems

Perspectives and Open Problems

- Neural nets: loss landscape, gradient descent dynamics and deep learning!
- Generalized linear models
- More general problems from convex optimization (often of *implicit solution*)
- More difficult: problem raised from *non-convex* optimization problems
- Transfer learning, active learning, generative networks (GAN)

Perspectives and Open Problems

- Neural nets: loss landscape, gradient descent dynamics and deep learning!
- Generalized linear models
- More general problems from convex optimization (often of *implicit solution*)
- More difficult: problem raised from *non-convex* optimization problems
- Transfer learning, active learning, generative networks (GAN)
- Robust statistics in machine learning

Perspectives and Open Problems

- Neural nets: loss landscape, gradient descent dynamics and deep learning!
- Generalized linear models
- More general problems from convex optimization (often of *implicit solution*)
- More difficult: problem raised from *non-convex* optimization problems
- Transfer learning, active learning, generative networks (GAN)
- Robust statistics in machine learning
- . . .

Thank you.