

A Random Matrix Approach to Machine Learning

(XII Brunel – Bielefeld Workshop on RMT)

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CentraleSupélec

Spectral Clustering Methods and Random Matrices

Community Detection on Graphs

Kernel Spectral Clustering

Kernel Spectral Clustering: Subspace Clustering

Semi-supervised Learning

Support Vector Machines

Neural Networks: Extreme Learning Machines

Random Matrices and Robust Estimation

Perspectives

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Context: Two-step classification of n objects based on similarity $A \in \mathbb{R}^{n \times n}$:

1. extraction of eigenvectors $U = [u_1, \dots, u_\ell]$ with “dominant” eigenvalues

Reminder on Spectral Clustering Methods

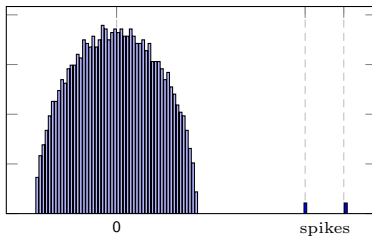
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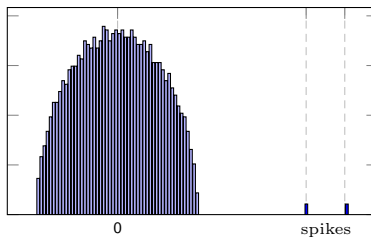
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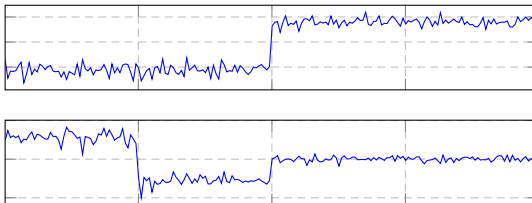
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⇓ **Eigenvectors** ⇓
(in practice, **shuffled!!**)



Reminder on Spectral Clustering Methods

Eigenv. 1

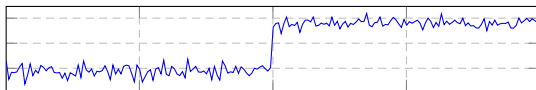


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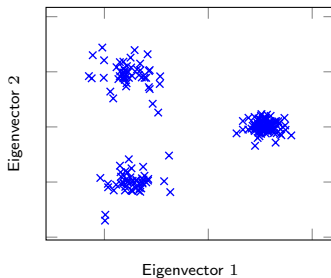
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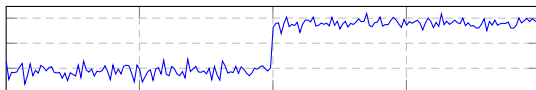


↓ ℓ -dimensional representation ↓
(shuffling no longer matters!)



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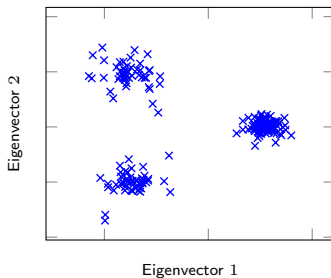
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↓
EM or k-means clustering.

The Random Matrix Approach

A two-step method:

1. If A_n is not a “standard” random matrix, retrieve \tilde{A}_n such that

$$\left\| A_n - \tilde{A}_n \right\| \xrightarrow{\text{a.s.}} 0$$

in operator norm as $n \rightarrow \infty$.

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 - ▶ eigenvectors of isolated eigenvalues.
2. From \tilde{A} , perform spiked model analysis:
 - ▶ exhibit phase transition phenomenon
 - ▶ “read” the content of isolated eigenvectors of \tilde{A} .

The Random Matrix Approach

The Spike Analysis:

For “noisy plateaus”-looking isolated eigenvectors u_1, \dots, u_ℓ of \tilde{A} , write

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

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\Rightarrow Can be done using complex analysis calculus, e.g.

$$\begin{aligned} (\alpha_i^a)^2 &= \frac{1}{n_a} j_a^\top u_i u_i^\top j_a \\ &= \frac{1}{2\pi i} \oint_{\gamma_a} \frac{1}{n_a} j_a^\top (\tilde{A} - zI_n)^{-1} j_a dz. \end{aligned}$$

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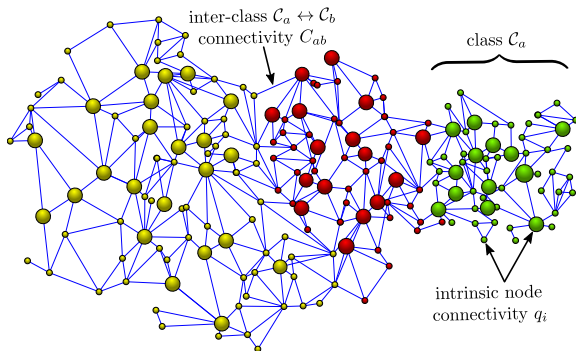
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- ▶ adjacency matrix A with $A_{ij} \sim \text{Bernoulli}(q_i q_j C_{ab})$.



Study of spectral methods:

- ▶ standard methods based on **adjacency** A , **modularity** $A - \frac{dd^T}{2m}$, **normalized adjacency** $D^{-1}AD^{-1}$, etc. (adapted to **dense nets**)
- ▶ refined methods based on **Bethe Hessian** $(r^2 - 1)I_n - rA + D$ (adapted to **sparse nets!**)

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Improvement to realistic graphs:

- ▶ observation of **failure of standard methods** above
- ▶ improvement by new methods.

Limitations of Adjacency/Modularity Approach

Scenario: 3 classes with μ bi-modal (e.g., $\mu = \frac{3}{4}\delta_{0.1} + \frac{1}{4}\delta_{0.5}$)

→ Leading eigenvectors of A (or modularity $A - \frac{dd^T}{2m}$) **biased by q_i distribution.**

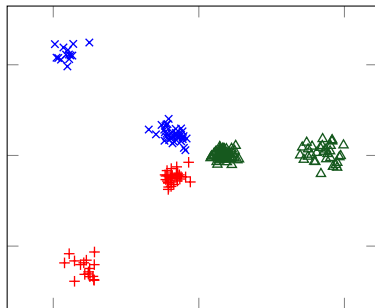
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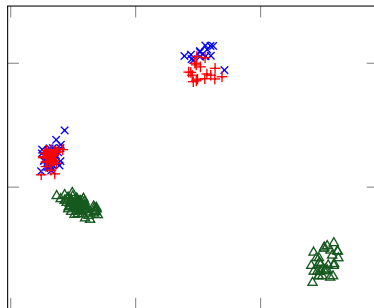
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(Modularity)



(Bethe Hessian)

Regularized Modularity Approach

Connectivity Model: $P(i \sim j) = q_i q_j C_{ab}$ for $i \in \mathcal{C}_a, j \in \mathcal{C}_b$.

Dense Regime Assumptions: **Non trivial regime** when, as $n \rightarrow \infty$,

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For $\alpha \in [0, 1]$, (and with $D = \text{diag}(A1_n) = \text{diag}(d)$ the degree matrix)

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- ▶ we find **consistent estimator** $\hat{\alpha}_{\text{opt}}$ from A alone.
- ▶ we claim **optimal eigenvector regularization** $D^{\alpha-1}u$, u eigenvector of L_α .
 \Rightarrow **Never proposed before!**

Asymptotic Equivalence

Theorem (Limiting Random Matrix Equivalent)

For each $\alpha \in [0, 1]$, as $n \rightarrow \infty$, $\|L_\alpha - \tilde{L}_\alpha\| \rightarrow 0$ almost surely, where

$$L_\alpha = (2m)^\alpha \frac{1}{\sqrt{n}} D^{-\alpha} \left[A - \frac{dd^\top}{d^\top 1_n} \right] D^{-\alpha}$$
$$\tilde{L}_\alpha = \frac{1}{\sqrt{n}} D_q^{-\alpha} X D_q^{-\alpha} + U \Lambda U^\top$$

with $D_q = \text{diag}(\{q_i\})$, X zero-mean random matrix,

$$U = \begin{bmatrix} D_q^{1-\alpha} \frac{J}{\sqrt{n}} & \frac{1}{nm_\mu} D_q^{-\alpha} X 1_n \end{bmatrix}, \text{ rank } k+1$$
$$\Lambda = \begin{bmatrix} (I_k - 1_k c^\top) M (I_k - c 1_k^\top) & -1_k \\ 1_k^\top & 0 \end{bmatrix}$$

and $J = [j_1, \dots, j_k]$, $j_a = [0, \dots, 0, 1_{n_a}^\top, 0, \dots, 0]^\top \in \mathbb{R}^n$ canonical vector of class \mathcal{C}_a .

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- ▶ **eigenvectors correlated to** $D_q^{1-\alpha} J$
 \Rightarrow **Natural regularization by** $D^{\alpha-1} J!$

Eigenvalue Spectrum

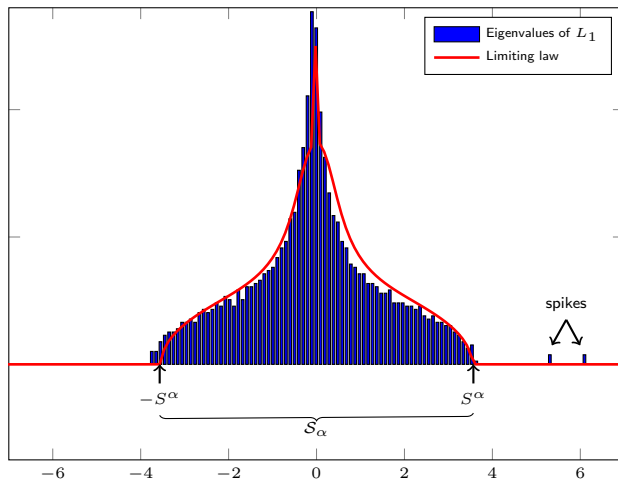


Figure: Eigenvalues of L_1 , $K = 3$, $n = 2000$, $c_1 = 0.3$, $c_2 = 0.3$, $c_3 = 0.4$, $\mu = \frac{1}{2}\delta_{q_1} + \frac{1}{2}\delta_{q_2}$, $q_1 = 0.4$, $q_2 = 0.9$, M defined by $M_{ii} = 12$, $M_{ij} = -4$, $i \neq j$.

Theorem (Phase Transition)

For $\alpha \in [0, 1]$, *isolated eigenvalue* $\lambda_i(L_\alpha)$ if $|\lambda_i(\bar{M})| > \tau^\alpha$, $\bar{M} = (\mathcal{D}(c) - cc^\top)M$,

$$\tau^\alpha = \lim_{x \downarrow S_+^\alpha} -\frac{1}{e_2^\alpha(x)}, \text{ *phase transition threshold*}$$

with $[S_-^\alpha, S_+^\alpha]$ limiting eigenvalue support of $m_\mu^{2\alpha} L_\alpha$ and $e_2^\alpha(x)$ ($|x| > S_+^\alpha$) solution of

$$\begin{aligned} e_1^\alpha(x) &= \int \frac{q^{1-2\alpha}}{-x - q^{1-2\alpha} e_1^\alpha(x) + q^{2-2\alpha} e_2^\alpha(x)} \mu(dq) \\ e_2^\alpha(x) &= \int \frac{q^{2-2\alpha}}{-x - q^{1-2\alpha} e_1^\alpha(x) + q^{2-2\alpha} e_2^\alpha(x)} \mu(dq). \end{aligned}$$

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Clustering still possible when $\lambda_i(\bar{M}) = (\min_\alpha \tau_\alpha) + \varepsilon$.

- **“Optimal”** $\alpha = \alpha_{\text{opt}}$:

$$\alpha_{\text{opt}} = \operatorname{argmin}_{\alpha \in [0,1]} \{\tau_\alpha\}.$$

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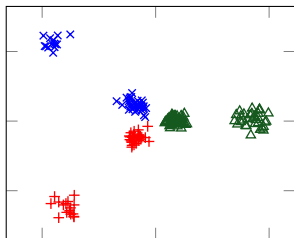
Clustering still possible when $\lambda_i(\bar{M}) = (\min_\alpha \tau_\alpha) + \varepsilon$.

- “Optimal” $\alpha = \alpha_{\text{opt}}$:

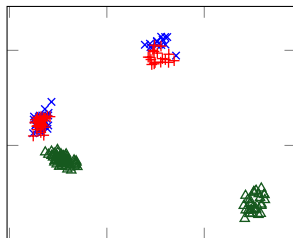
$$\alpha_{\text{opt}} = \operatorname{argmin}_{\alpha \in [0,1]} \{\tau_\alpha\}.$$

- From $\max_i \left| \frac{d_i}{\sqrt{d^\top 1_n}} - q_i \right| \xrightarrow{\text{a.s.}} 0$, we obtain **consistent estimator** $\hat{\alpha}_{\text{opt}}$ of α_{opt} .

Simulated Performance Results (2 masses of q_i)

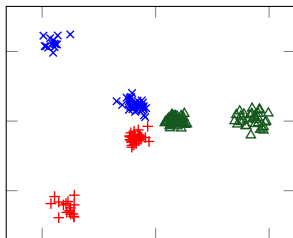


(Modularity)

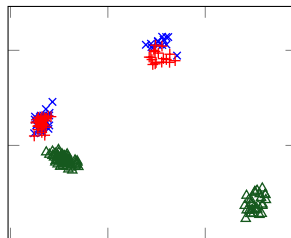


(Bethe Hessian)

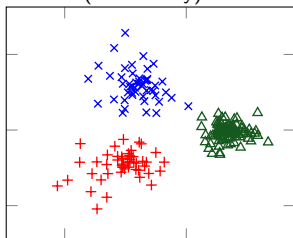
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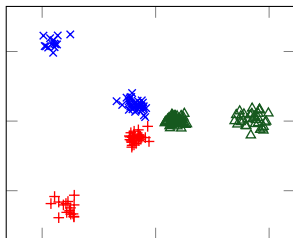
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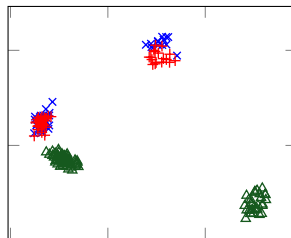
(Algo with $\alpha = 1$)

Figure: Two dominant eigenvectors (x-y axes) for $n = 2000$, $K = 3$, $\mu = \frac{3}{4}\delta_{q_1} + \frac{1}{4}\delta_{q_2}$, $q_1 = 0.1$, $q_2 = 0.5$, $c_1 = c_2 = \frac{1}{4}$, $c_3 = \frac{1}{2}$, $M = 100I_3$.

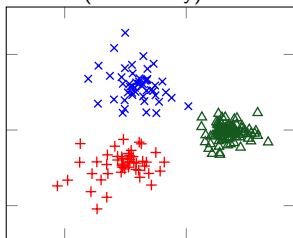
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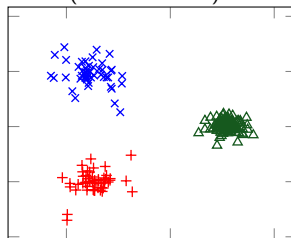
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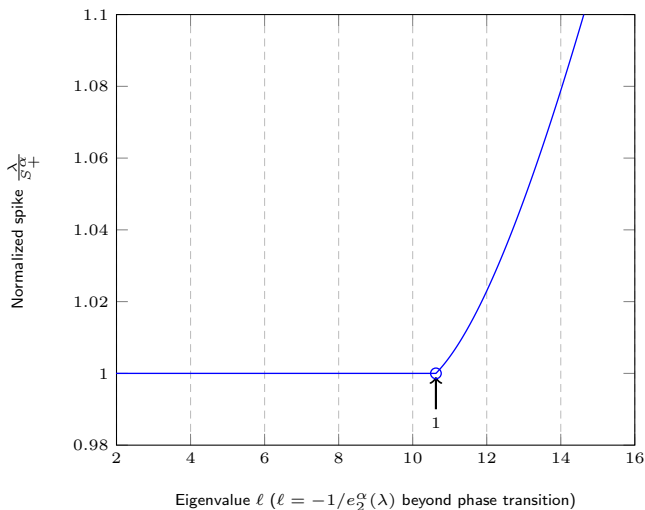


Figure: Largest eigenvalue λ of L_{α} as a function of the largest eigenvalue ℓ of $(\mathcal{D}(c) - cc^{\top})M$, for $\mu = \frac{3}{4}\delta_{q_1} + \frac{1}{4}\delta_{q_2}$ with $q_1 = 0.1$ and $q_2 = 0.5$, for $\alpha \in \{0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1, \alpha_{\text{opt}}\}$ (indicated below the graph). Here, $\alpha_{\text{opt}} = 0.07$. Circles indicate phase transition. Beyond phase transition, $\ell = -1/e_2^{\alpha}(\lambda)$.

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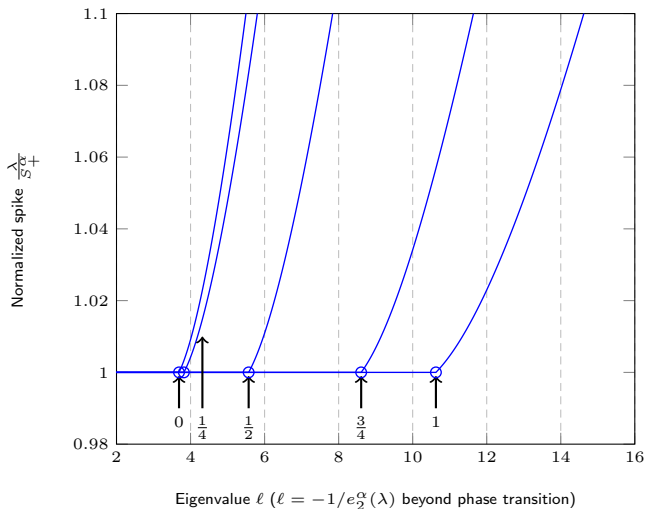


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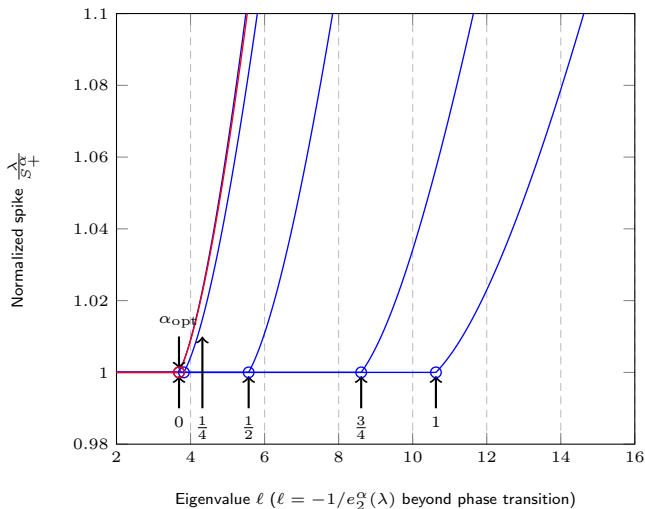


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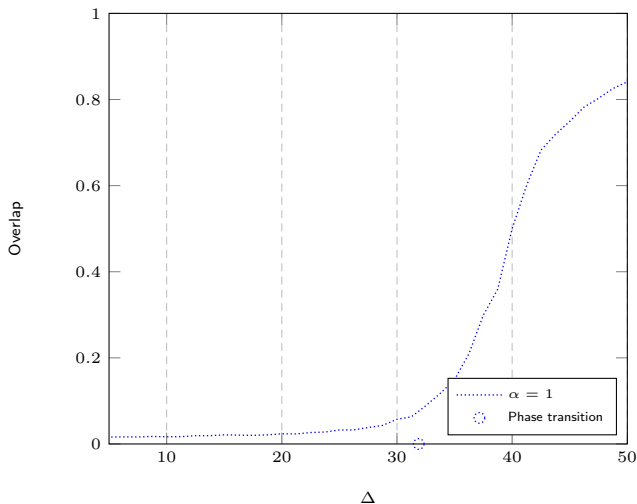


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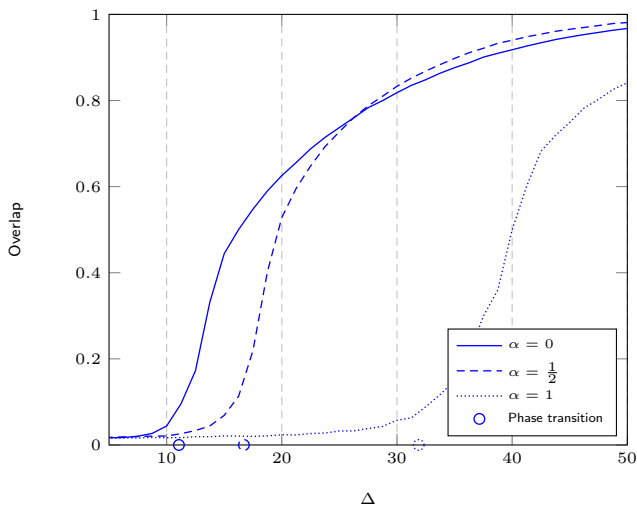


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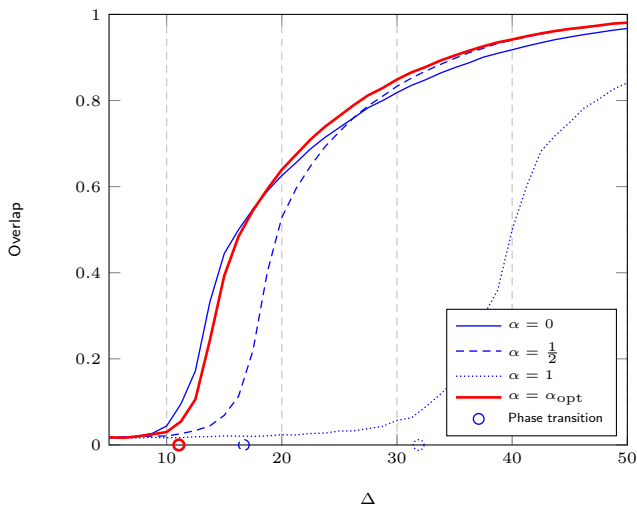


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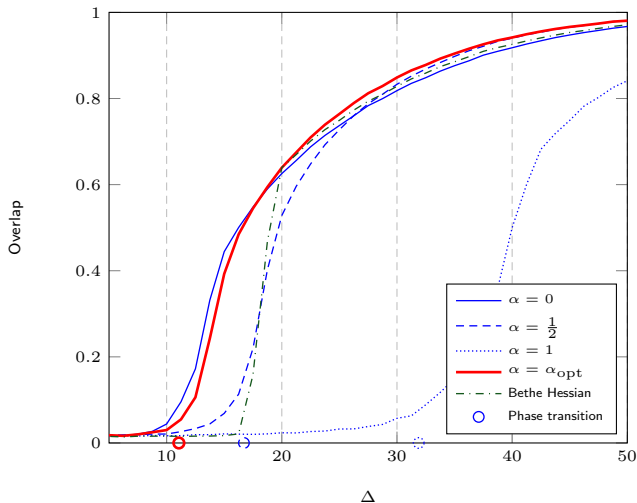


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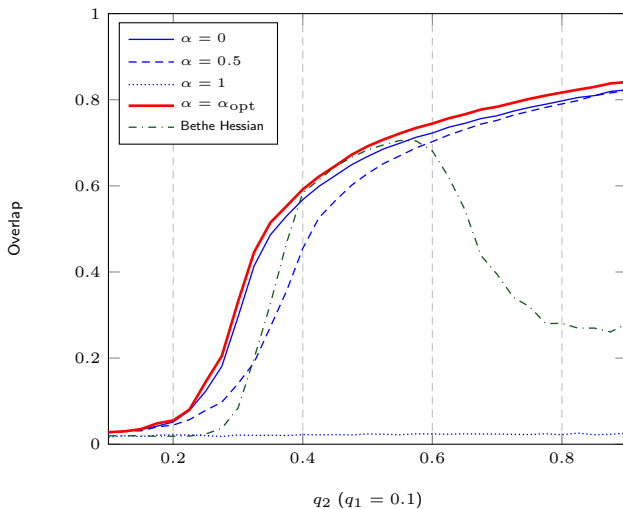


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- ▶ conjectured Gaussian fluctuations of eigenvector entries
- ▶ for $q_i = q_0$ (homogeneous case), same variance for all entries in same class
- ▶ in non-homogeneous case, we can compute “average variance per class”
⇒ Heuristic asymptotic performance upper-bound using EM.

Theoretical Performance Results (uniform distribution for q_i)

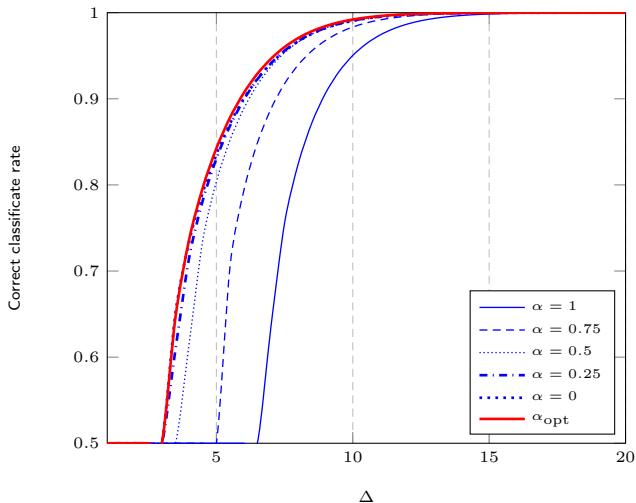


Figure: Theoretical probability of correct recovery for $n = 2000$, $K = 2$, $c_1 = 0.6$, $c_2 = 0.4$, μ uniformly distributed in $[0.2, 0.8]$, $M = \Delta I_2$, for $\Delta \in [0, 20]$.

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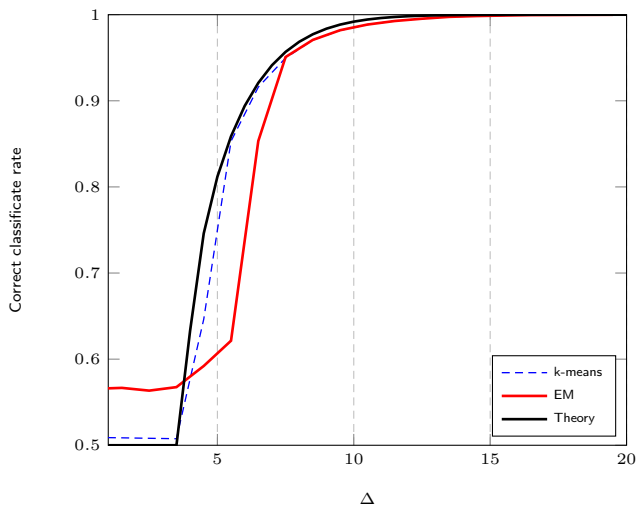


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- ▶ Simulations on small networks in fact give ridiculous arbitrary results.
- ▶ When is sparse sparse and dense dense?
 - ▶ in theory, $d_i = O(\log(n))$ is dense...
 - ▶ in practice, assuming dense regime, eigenvalues smear beyond support edges in critical scenarios.

Spectral Clustering Methods and Random Matrices

Community Detection on Graphs

Kernel Spectral Clustering

Kernel Spectral Clustering: Subspace Clustering

Semi-supervised Learning

Support Vector Machines

Neural Networks: Extreme Learning Machines

Random Matrices and Robust Estimation

Perspectives

Problem Statement

- ▶ Dataset $x_1, \dots, x_n \in \mathbb{R}^p$
- ▶ Objective: “cluster” data in k similarity classes $\mathcal{S}_1, \dots, \mathcal{S}_k$.

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for some similarity kernel $\kappa(x, y) \geq 0$ (large if x similar to y).

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where $\mathcal{M} \subset \mathbb{R}^{n \times k} \cap \left\{ M; M_{ij} \in \{0, |\mathcal{S}_j|^{-\frac{1}{2}}\} \right\}$ (in particular, $M^T M = I_k$) and

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- ▶ But **integer problem!** Usually NP-complete.

Towards kernel spectral clustering

- ▶ Kernel spectral clustering: **discrete-to-continuous relaxations** of such metrics

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- ▶ Refinements:

- ▶ working on K , $D - K$, $I_n - D^{-1}K$, $I_n - D^{-\frac{1}{2}}KD^{-\frac{1}{2}}$, etc.
- ▶ several steps algorithms: Ng–Jordan–Weiss, Shi–Malik, etc.

Kernel Spectral Clustering

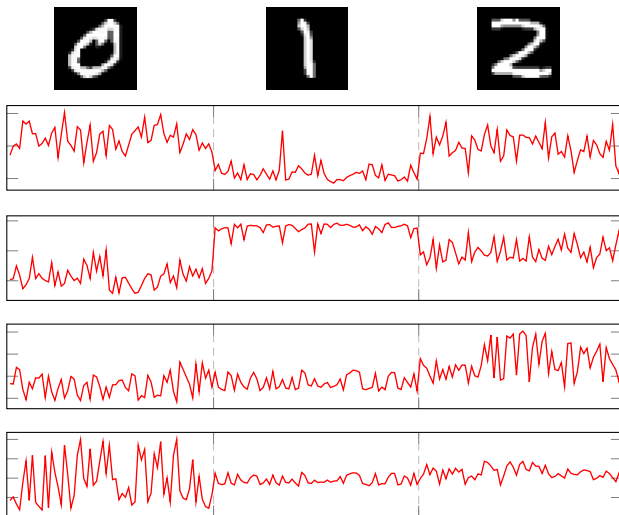


Figure: Leading four eigenvectors of $D^{-1/2} K D^{-1/2}$ for MNIST data.

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- ▶ Algorithms derived from ad-hoc procedures (e.g., relaxation).
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Methodology:

- ▶ Use statistical assumptions (Gaussian mixture)
- ▶ Benefit from doubly-infinite independence and **random matrix tools**

Model and Assumptions

Gaussian mixture model:

- ▶ $x_1, \dots, x_n \in \mathbb{R}^p$,
- ▶ k classes $\mathcal{C}_1, \dots, \mathcal{C}_k$,
- ▶ $x_1, \dots, x_{n_1} \in \mathcal{C}_1, \dots, x_{n-n_k+1}, \dots, x_n \in \mathcal{C}_k$,
- ▶ $\mathcal{C}_a = \{x \mid x \sim \mathcal{N}(\mu_a, C_a)\}$.

Then, for $x_i \in \mathcal{C}_a$, with $w_i \sim N(0, C_a)$,

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[Convergence Rate] As $n \rightarrow \infty$,

1. **Data scaling:** $\frac{p}{n} \rightarrow c_0 \in (0, \infty)$,
2. **Class scaling:** $\frac{n_a}{n} \rightarrow c_a \in (0, 1)$,
3. **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

$$\|\mu_a^\circ\| = O(1)$$

4. **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

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

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 .

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- ▶ We study the normalized recentered Laplacian:

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

with $d = K1_n$, $D = \text{diag}(d)$.

Difficulty: L is a very intractable random matrix

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 - ▶ **concentration:** $K_{ij} \rightarrow \text{constant}$ as $n, p \rightarrow \infty$ (for all $i \neq j$)
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 - ▶ eigenvector projections on canonical class-basis

Random Matrix Equivalent

Results on K :

- **Key Remark:** Under our assumptions, uniformly on $i, j \in \{1, \dots, n\}$,

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- large dimensional approximation for K :

$$K = \underbrace{f(\tau)1_n 1_n^T}_{O_{\|\cdot\|}(n)} + \underbrace{\sqrt{n}A_1}_{\text{low rank, } O_{\|\cdot\|}(\sqrt{n})} + \underbrace{A_2}_{\text{informative terms, } O_{\|\cdot\|}(1)}$$

Random Matrix Equivalent

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- ▶ **Key Remark:** Under our assumptions, uniformly on $i, j \in \{1, \dots, n\}$,

$$\frac{1}{p} \|x_i - x_j\|^2 \xrightarrow{\text{a.s.}} \tau$$

for some **common limit** τ .

- ▶ large dimensional approximation for K :

$$K = \underbrace{f(\tau)1_n 1_n^T}_{O_{\|\cdot\|}(n)} + \underbrace{\sqrt{n}A_1}_{\text{low rank, } O_{\|\cdot\|}(\sqrt{n})} + \underbrace{A_2}_{\text{informative terms, } O_{\|\cdot\|}(1)}$$

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⇒ Naturally leads to study:

- ▶ Projected normalized Laplacian (or “modularity”-type Laplacian):

$$L' = nD^{-\frac{1}{2}}KD^{-\frac{1}{2}} - n \frac{D^{\frac{1}{2}}1_n 1_n^\top D^{\frac{1}{2}}}{1_n^\top D 1_n} = nD^{-\frac{1}{2}} \left(K - \frac{dd^\top}{1^\top d} \right) D^{-\frac{1}{2}}.$$

- ▶ Dominant (normalized) eigenvector $\frac{D^{\frac{1}{2}}1_n}{\sqrt{1_n^\top D 1_n}}$.

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Theorem (Random Matrix Equivalent)

As $n, p \rightarrow \infty$, in operator norm, $\|L' - \hat{L}'\| \xrightarrow{\text{a.s.}} 0$, where

$$\hat{L}' = -2 \frac{f'(\tau)}{f(\tau)} \left[\frac{1}{p} P W^\top W P + U B U^\top \right] + \alpha(\tau) I_n$$

and $\tau = \frac{2}{p} \text{tr} C^\circ$, $W = [w_1, \dots, w_n] \in \mathbb{R}^{p \times n}$ ($x_i = \mu_a + w_i$), $P = I_n - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^\top$,

$$U = \left[\frac{1}{\sqrt{p}} J, \Phi, \psi \right] \in \mathbb{R}^{n \times (2k+4)}$$

$$B = \begin{bmatrix} B_{11} & I_k - \mathbf{1}_k c^\top & \left(\frac{5f'(\tau)}{8f(\tau)} - \frac{f''(\tau)}{2f'(\tau)} \right) t \\ I_k - c \mathbf{1}_k^\top & 0_{k \times k} & 0_{k \times 1} \\ \left(\frac{5f'(\tau)}{8f(\tau)} - \frac{f''(\tau)}{2f'(\tau)} \right) t^\top & 0_{1 \times k} & \frac{5f'(\tau)}{8f(\tau)} - \frac{f''(\tau)}{2f'(\tau)} \end{bmatrix} \in \mathbb{R}^{(2k+4) \times (2k+4)}$$

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Important Notations:

$\frac{1}{\sqrt{p}} J = [j_1, \dots, j_k] \in \mathbb{R}^{n \times k}$, j_a canonical vector of class \mathcal{C}_a .

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Further analysis:

- ▶ Determine separability condition for eigenvalues
- ▶ Evaluate eigenvalue positions when separable
- ▶ Evaluate eigenvector projection to canonical basis j_1, \dots, j_k
- ▶ Evaluate fluctuation of eigenvectors.

Isolated eigenvalues: Gaussian inputs

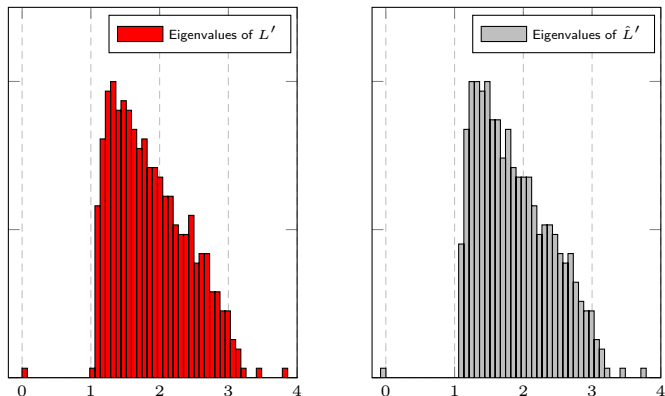


Figure: Eigenvalues of L' and \hat{L}' , $k = 3$, $p = 2048$, $n = 512$, $c_1 = c_2 = 1/4$, $c_3 = 1/2$, $[\mu_a]_j = 4\delta_{aj}$, $C_a = (1 + 2(a - 1)/\sqrt{p})I_p$, $f(x) = \exp(-x/2)$.

Theoretical Findings versus MNIST

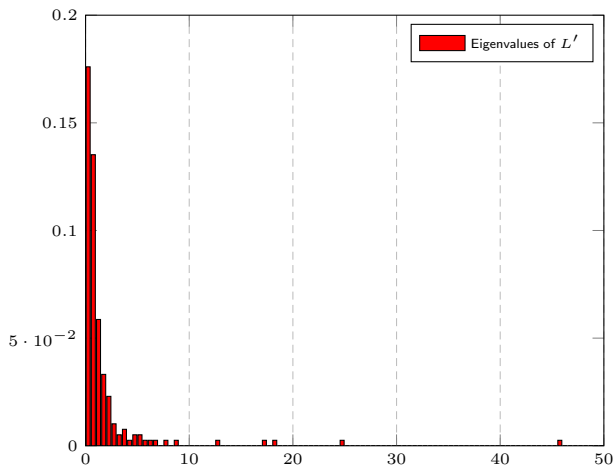


Figure: Eigenvalues of L' (red) and (equivalent Gaussian model) \hat{L}' (white), MNIST data, $p = 784$, $n = 192$.

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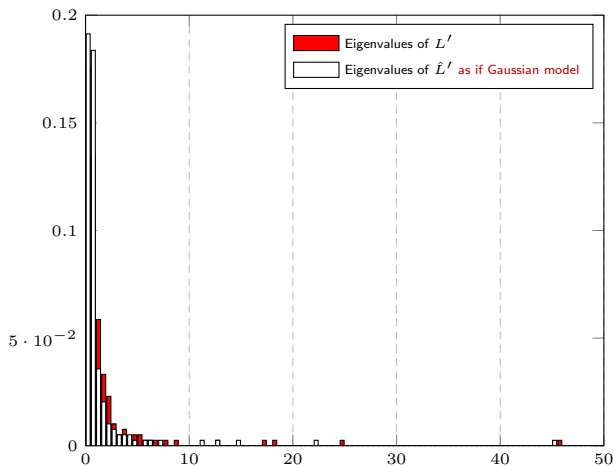


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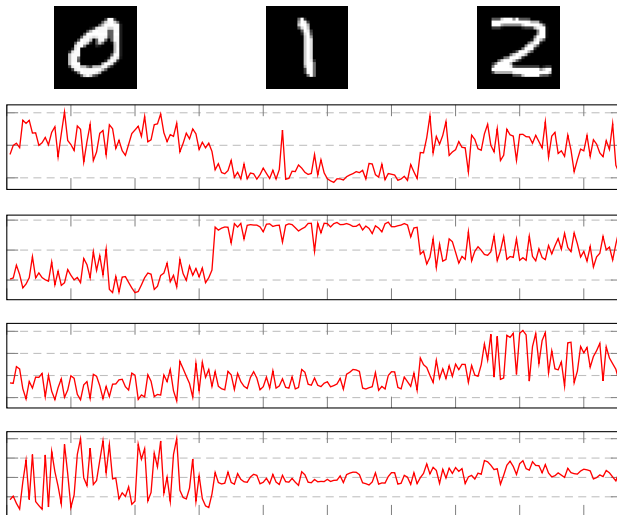


Figure: Leading four eigenvectors of $D^{-\frac{1}{2}} K D^{-\frac{1}{2}}$ for MNIST data (red) and theoretical findings (blue).

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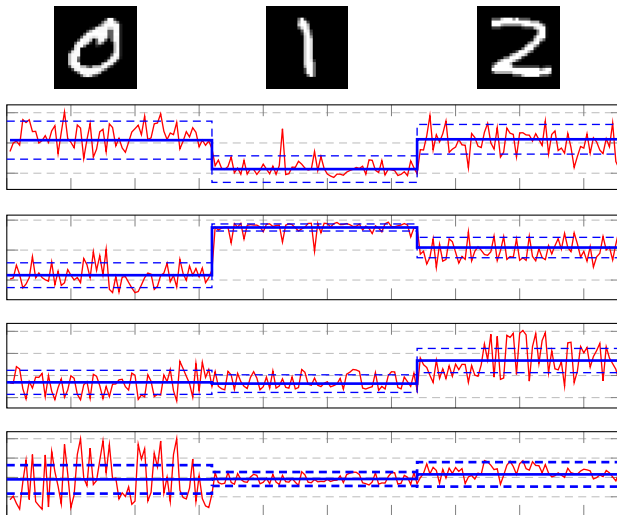


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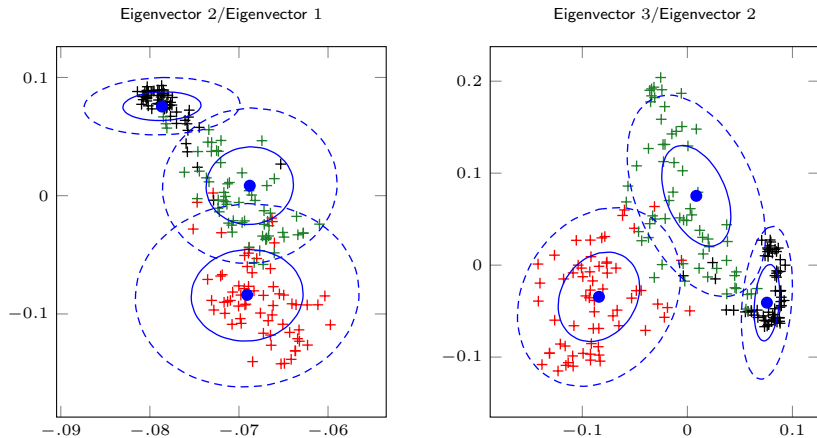


Figure: 2D representation of eigenvectors of L , for the MNIST dataset. Theoretical means and 1- and 2-standard deviations in **blue**. Class 1 in **red**, Class 2 in **black**, Class 3 in **green**.

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- ▶ Invalid for heavy-tailed distributions (where $\|x_i\| = \|\sqrt{\tau_i} z_i\|$ needs not converge).
- ▶ **Suprising fit between theory and practice:** are images like Gaussian vectors?
 - ▶ kernels extract primarily first order properties (means, covariances)
 - ▶ without image processing (rotations, scale invariance), good enough features.

Last word: the suprising case $f'(\tau) = 0...$

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- Means M disappears \Rightarrow Impossible classification from means.

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When $f'(\tau) \rightarrow 0$,

- ▶ Means M disappears \Rightarrow Impossible classification from means.
- ▶ **More importantly:** $P W W^T P$ disappears
 \Rightarrow Asymptotic **deterministic** matrix equivalent!
 \Rightarrow **Perfect asymptotic clustering in theory!**

Spectral Clustering Methods and Random Matrices

Community Detection on Graphs

Kernel Spectral Clustering

Kernel Spectral Clustering: Subspace Clustering

Semi-supervised Learning

Support Vector Machines

Neural Networks: Extreme Learning Machines

Random Matrices and Robust Estimation

Perspectives

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

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- ▶ Performance of $L = nD^{-\frac{1}{2}}KD^{-\frac{1}{2}} - n\frac{D^{\frac{1}{2}}1_n1_n^TD^{\frac{1}{2}}}{1_n^TD1_n}$, 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 $n, p \rightarrow \infty$.

Model and Reminders

Assumption 1 [Classes]. Vectors $x_1, \dots, x_n \in \mathbb{R}^p$ 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).

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

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Theorem (Corollary of Previous Section)

Let f smooth with $f'(2) \neq 0$. Then, under Assumptions 1–2a,

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

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

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

has sufficiently large eigenvalues.

The case $f'(2) = 0$

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

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

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

$$\mathcal{L} \equiv \sqrt{p} \frac{f(2)}{2f''(2)} \left[\textcolor{red}{L} - \frac{f(0) - f(2)}{f(2)} P \right], \quad P = I_n - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^\top.$$

Then, under Assumptions 1–2b,

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

where $\Phi_{ij} = \delta_{i \neq j} \sqrt{p} [(x_i^\top x_j)^2 - E[(x_i^\top x_j)^2]]$.

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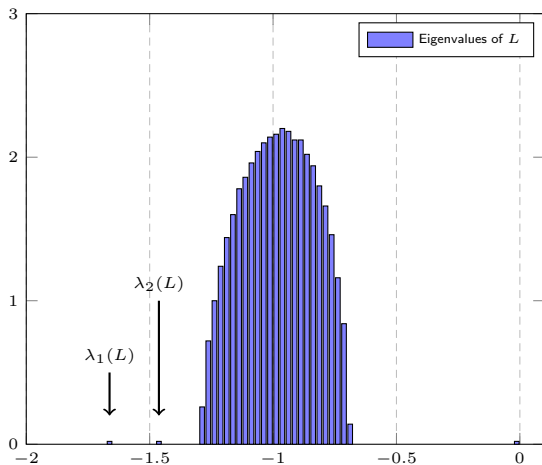
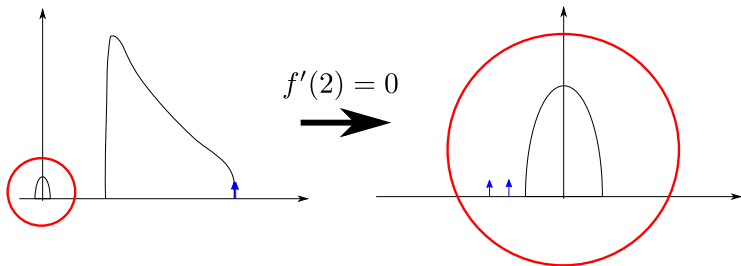


Figure: Eigenvalues of L , $p = 1000$, $n = 2000$, $k = 3$, $c_1 = c_2 = 1/4$, $c_3 = 1/2$,
 $C_i \propto I_p + (p/8)^{-\frac{5}{4}} W_i W_i^T$, $W_i \in \mathbb{R}^{p \times (p/8)}$ of i.i.d. $\mathcal{N}(0, 1)$ entries, $f(t) = \exp(-(t - 2)^2)$.

\Rightarrow No longer a Marcenko–Pastur like bulk, but rather a semi-circle bulk!

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Theorem (Semi-circle law for Φ)

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

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

with μ the semi-circle distribution

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

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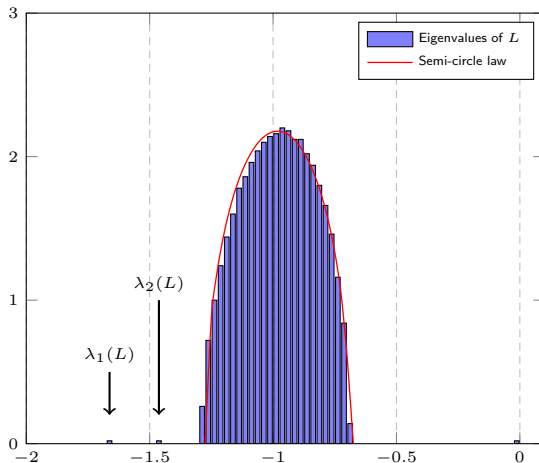


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Denote now

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

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Theorem (Isolated Eigenvalues)

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

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

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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 $j_a = [0_{n_1}^\top, \dots, 1_{n_a}^\top, \dots, 0_{n_k}^\top]^\top$, $(w_i^a)^\top j_a = 0$, $\text{supp}(w_i^a) = \text{supp}(j_a)$, $\|w_i^a\| = 1$.
Then, under Assumptions 1-2b,

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

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

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

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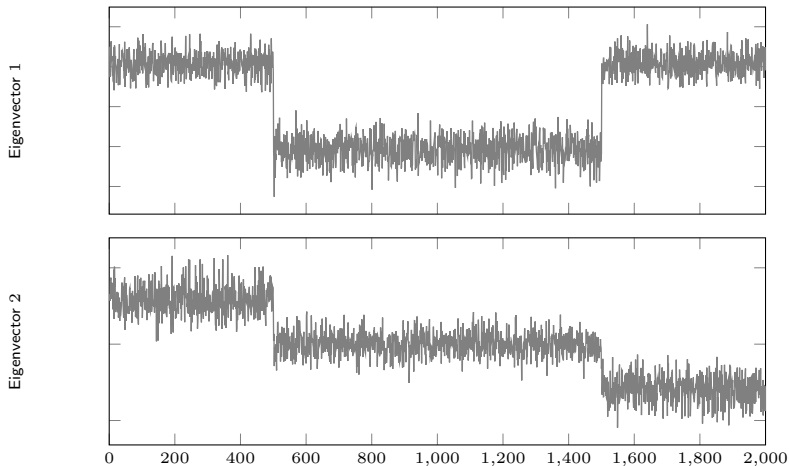


Figure: Leading two eigenvectors of \mathcal{L} (or equivalently of L) versus deterministic approximations of $\alpha_i^a \pm \sigma_i^a$.

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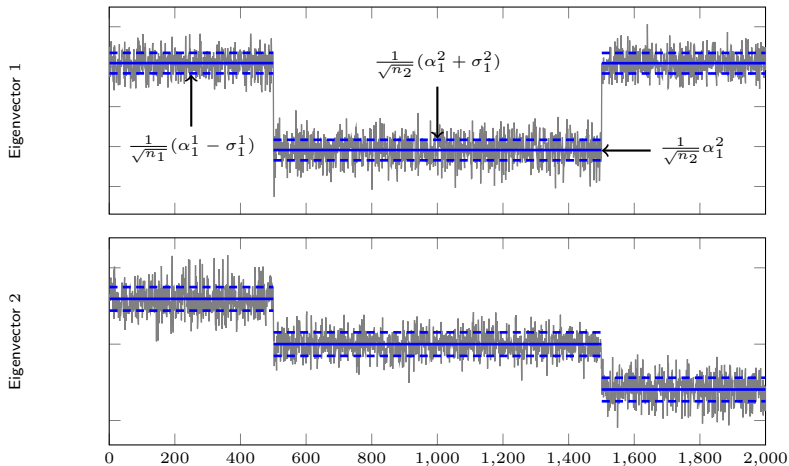


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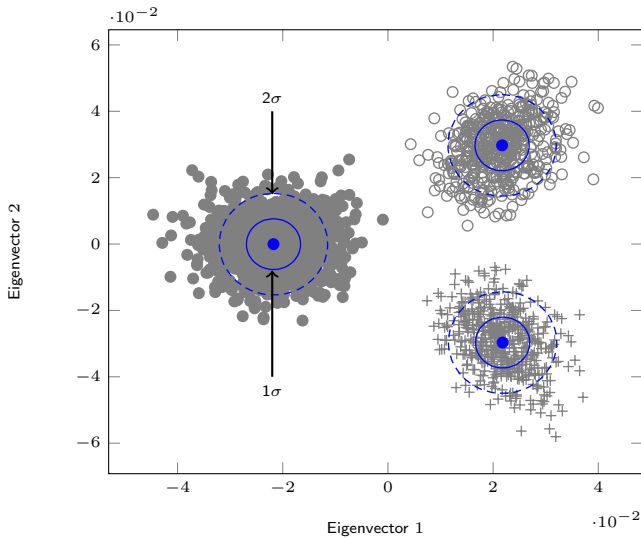


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Spectral Clustering Methods and Random Matrices

Community Detection on Graphs

Kernel Spectral Clustering

Kernel Spectral Clustering: Subspace Clustering

Semi-supervised Learning

Support Vector Machines

Neural Networks: Extreme Learning Machines

Random Matrices and Robust Estimation

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Context: Similar to clustering:

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$$F = \operatorname{argmin}_{F \in \mathbb{R}^{n \times k}} \sum_{a=1}^k \sum_{i,j} K_{ij} (F_{ia} d_i^{\alpha-1} - F_{ja} d_j^{\alpha-1})^2$$

such that $F_{ia} = \delta_{\{x_i \in \mathcal{C}_a\}}$, for all labelled x_i .

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- ▶ **Solution:** denoting $F^{(u)} \in \mathbb{R}^{n_u \times k}$, $F^{(l)} \in \mathbb{R}^{n_l \times k}$ the restriction to 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

$$K = \begin{bmatrix} K_{(l,l)} & K_{(l,u)} \\ K_{(u,l)} & K_{(u,u)} \end{bmatrix}$$
$$D = \begin{bmatrix} D_{(l)} & 0 \\ 0 & D_{(u)} \end{bmatrix} = \operatorname{diag} \{K1_n\}.$$

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⇒ From which classification probability is retrieved.

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⇒ From which classification probability is retrieved.
- Understanding the impact of α
⇒ Finding optimal α choice online?

MNIST Data Example

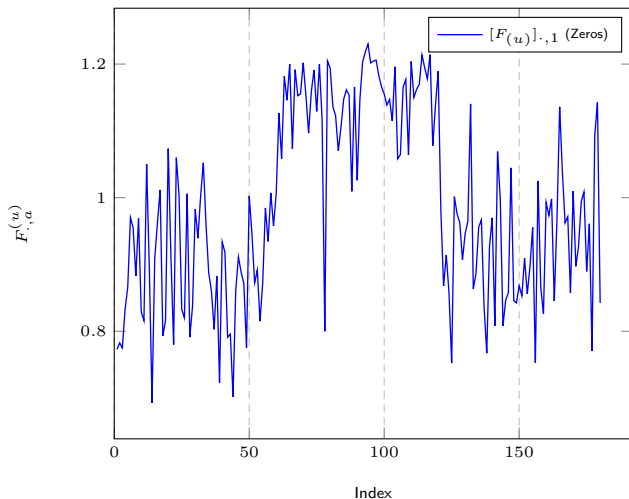


Figure: Vectors $[F^{(u)}]_{.,a}$, $a = 1, 2, 3$, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

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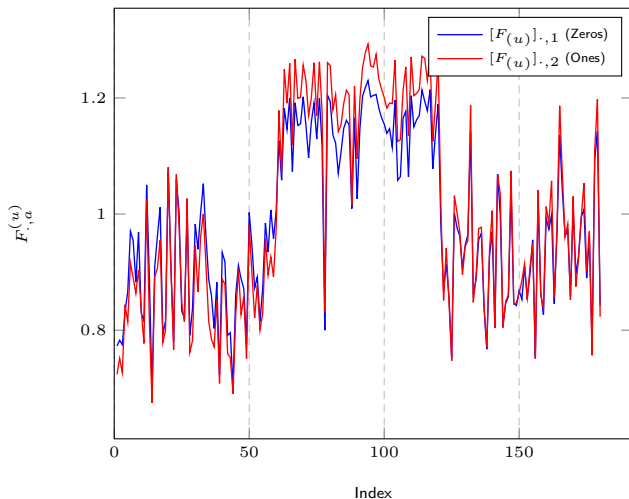


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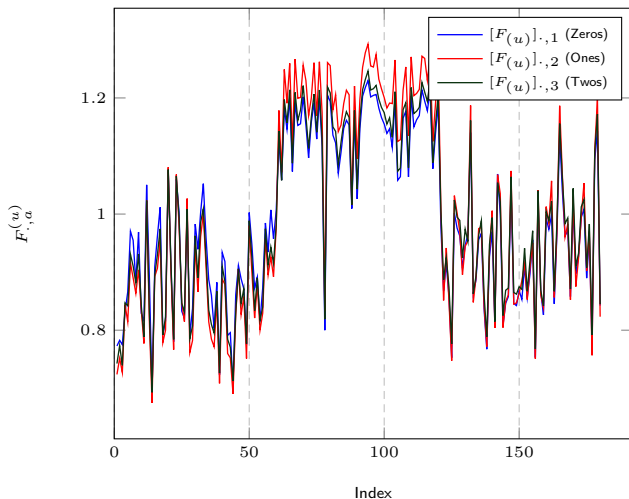


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We need to understand why...

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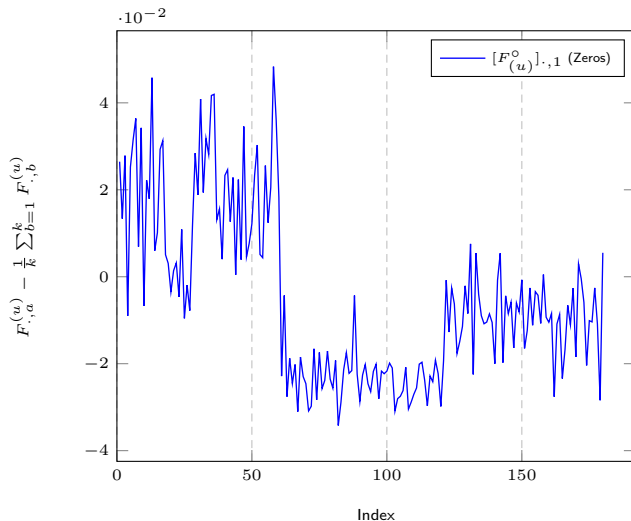


Figure: Centered Vectors $[F^{(u)\circ}_{(u)}]_{\cdot,a} = [F^{(u)}_{(u)} - \frac{1}{k} F^{(u)}_{(u)} \mathbf{1}_k \mathbf{1}_k^T]_{\cdot,a}$, $a = 1, 2, 3$, for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

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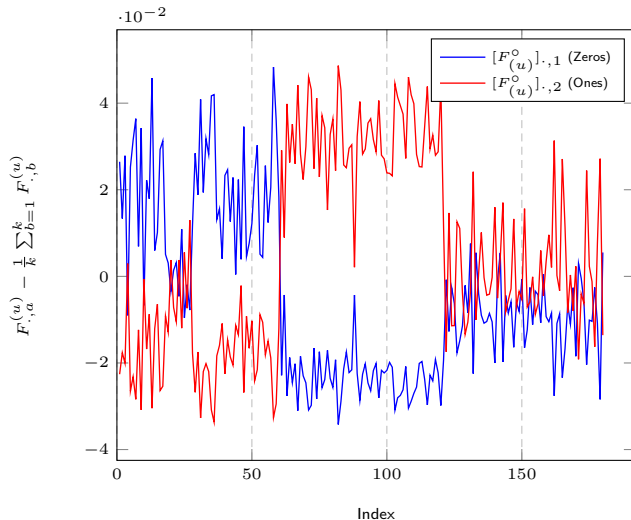


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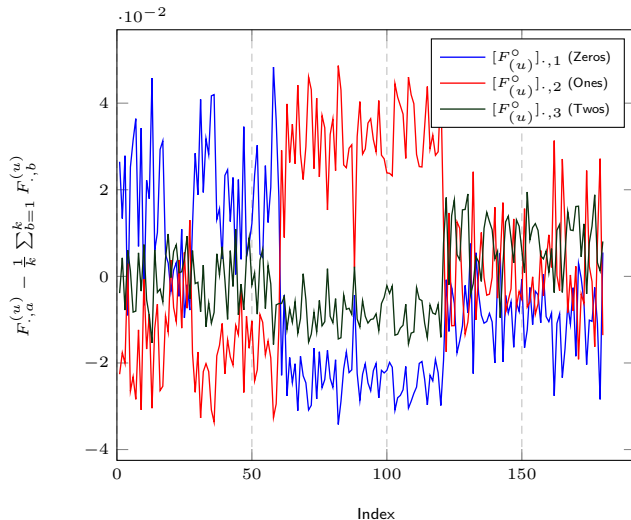


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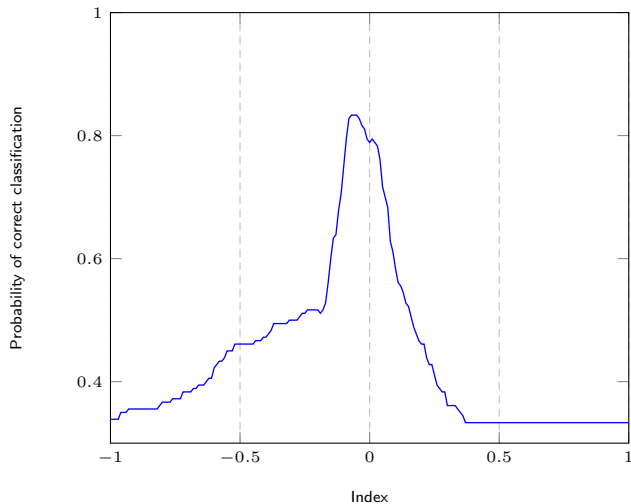


Figure: Performance as a function of α , for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

Theoretical Findings

Method: We assume $n_l/n \rightarrow c_l \in (0, 1)$ (“numerous” labelled data setting)

- ▶ Recall that we aim at characterizing

$$F^{(u)} = \left(I_{n_u} - D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1} \right)^{-1} D_{(u)}^{-\alpha} K_{(u,l)} D_{(l)}^{\alpha-1} F^{(l)}$$

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and similarly for $K_{(u,l)}$, $D_{(l)}$.

- So that

$$\left(I_{n_u} - D_{(u)}^{-\alpha} K_{(u,u)} D_{(u)}^{\alpha-1} \right)^{-1} = \left(I_{n_u} - \frac{1_{n_u} 1_{n_u}^T}{n} + O_{\|\cdot\|}(n^{-\frac{1}{2}}) \right)^{-1}$$

which can be **easily Taylor expanded!**

Results:

- In the first order,

$$F_{\cdot,a}^{(u)} = C \frac{n_{l,a}}{n} \left[v + \alpha \frac{t_a \mathbf{1}_{n_u}}{\sqrt{n}} \right] + \underbrace{O(n^{-1})}_{\text{Information is here!}}$$

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- ▶ Relevant information hidden in smaller order terms!

Main Results

As a consequence of the remarks above, we take

$$\alpha = \frac{\beta}{\sqrt{p}}$$

and define

$$\hat{F}_{i,a}^{(u)} = \frac{np}{\textcolor{red}{n}_{l,a}} F_{ia}^{(u)}.$$

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Theorem

For $x_i \in \mathcal{C}_b$ unlabelled, we have

$$\hat{F}_{i,\cdot} - G_b \rightarrow 0, \quad G_b \sim \mathcal{N}(m_b, \Sigma_b)$$

where $m_b \in \mathbb{R}^k$, $\Sigma_b \in \mathbb{R}^{k \times k}$ given by

$$(m_b)_a = -\frac{2f'(\tau)}{f(\tau)} \tilde{M}_{ab} + \frac{f''(\tau)}{f(\tau)} \tilde{t}_a \tilde{t}_b + \frac{2f''(\tau)}{f(\tau)} \tilde{T}_{ab} - \frac{f'(\tau)^2}{f(\tau)^2} t_a t_b + \beta \frac{n}{n_l} \frac{f'(\tau)}{f(\tau)} t_a + B_b$$

$$(\Sigma_b)_{a_1 a_2} = \frac{2tr C_b^2}{p} \left(\frac{f'(\tau)^2}{f(\tau)^2} + \frac{f''(\tau)}{f(\tau)} \right)^2 t_{a_1} t_{a_2} + \frac{4f'(\tau)^2}{f(\tau)^2} \left([M^\top C_b M]_{a_1 a_2} + \frac{\delta_{a_1}^2 p}{n_{l,a_1}} T_{ba_1} \right)$$

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 $a \neq b$,

$$P(\hat{F}_{i,a} > \hat{F}_{i,b} \mid x_i \in \mathcal{C}_b) - Q\left(\frac{(m_b)_b - (m_b)_a}{\sqrt{[1, -1]\Sigma_b[1, -1]^T}}\right) \rightarrow 0.$$

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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

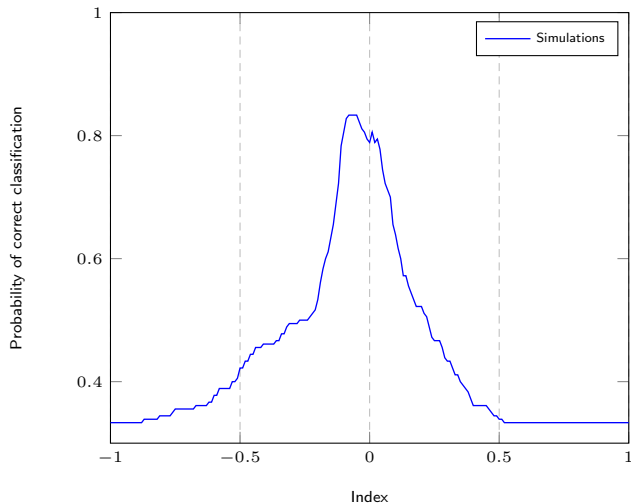


Figure: Performance as a function of α , for 3-class MNIST data (zeros, ones, twos), $n = 192$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

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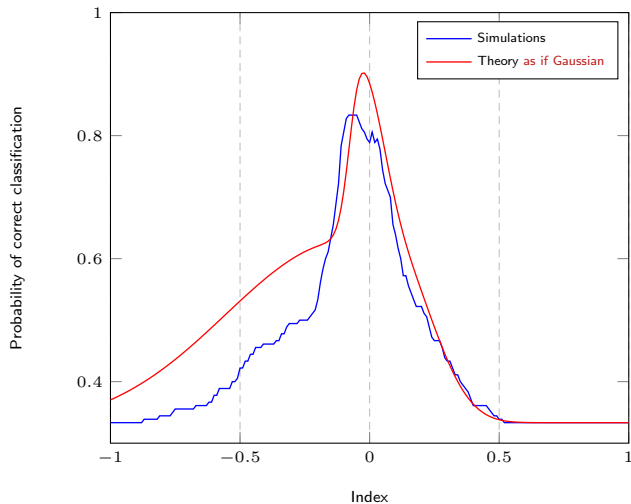


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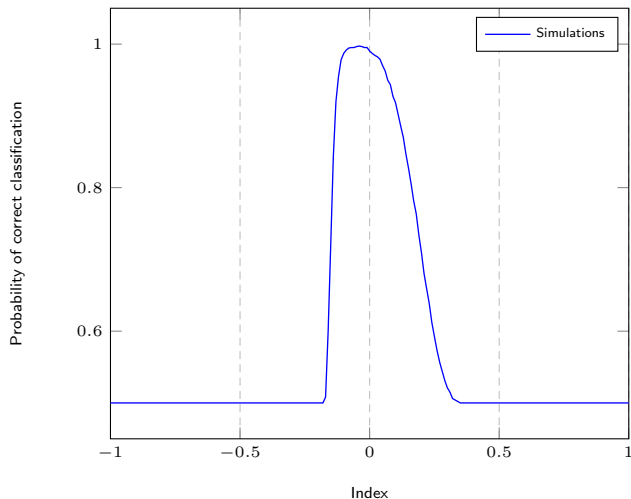


Figure: Performance as a function of α , for 2-class MNIST data (zeros, ones), $n = 1568$, $p = 784$, $n_l/n = 1/16$, Gaussian kernel.

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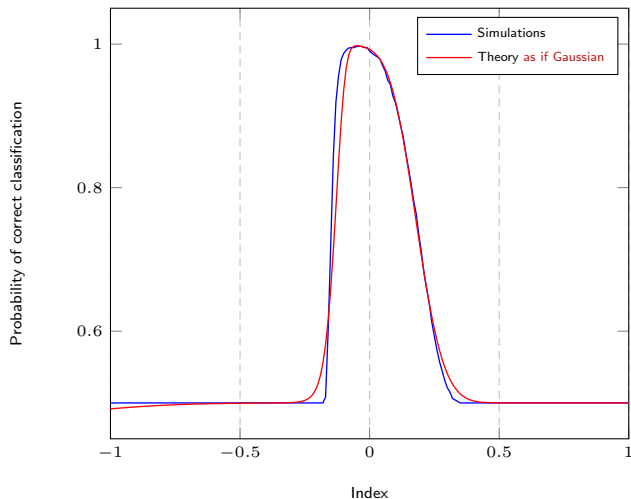


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$$(w, b) = \operatorname{argmin}_{w \in \mathbb{R}^{q-1}} \|w\|^2 + \frac{1}{n} \sum_{i=1}^n c(x_i; w, b)$$

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- ▶ **Classical SVM:**

$$c(x_i; w, b) = \mathbb{1}_{\{y_i(w^\top \phi(x_i) + b) \geq 1\}}$$

with $y_i = \pm 1$ depending on class.

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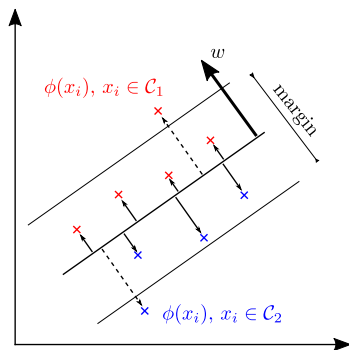
- ▶ **LS SVM:**

$$c(x_i; w, b) = \gamma e_i^2 \equiv \gamma (y_i - w^\top \phi(x_i) - b)^2.$$

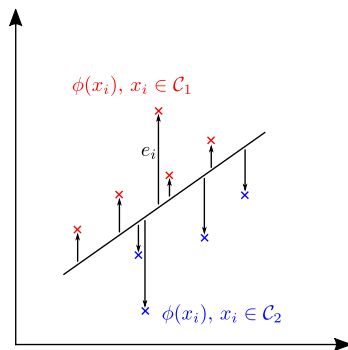
⇒ **Explicit solution** (but not sparse!).

Problem Statement

Classical SVM



LS SVM



For new datum x , decision based on (sign of)

$$g(x) = \alpha^\top K(\cdot, x) + b$$

where $\alpha \in \mathbb{R}^n$ and b given by

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As before, $x_i \sim \mathcal{N}(\mu_a, C_a)$, $a = 1, \dots, k$, with identical growth conditions, here for $k = 2$.

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► asymptotic Gaussian behavior of $G(x)$:

Theorem

For $x \in \mathcal{C}_b$, $G(x) - G_b \rightarrow 0$, $G_b \sim \mathcal{N}(m_b, \sigma_b)$, where

$$m_b = \begin{cases} -2c_2 \cdot c_1 c_2 \gamma \mathcal{D}, & b = 1 \\ +2c_1 \cdot c_1 c_2 \gamma \mathcal{D}, & b = 2 \end{cases}$$

$$\mathcal{D} = -2f'(\tau) \|\mu_2 - \mu_1\|^2 + \frac{f''(\tau)}{p} (\text{tr}(C_2 - C_1))^2 + \frac{2f''(\tau)}{p} \text{tr}((C_2 - C_1)^2)$$

$$\sigma_b = 8\gamma^2 c_1^2 c_2^2 \left[\frac{(f''(\tau))^2}{p^2} (\text{tr}(C_2 - C_1))^2 \text{tr} C_b^2 + 2(f'(\tau))^2 (\mu_2 - \mu_1)^\top C_b (\mu_2 - \mu_1) \right. \\ \left. + \frac{2(f'(\tau))^2}{n} \left(\frac{\text{tr} C_1 C_b}{c_1} + \frac{\text{tr} C_2 C_b}{c_2} \right) \right]$$

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- ▶ Need to choose $f'(\tau) < 0$ and $f''(\tau) > 0$ (not the case for clustering or SSL!)

Theory and simulations of $g(x)$

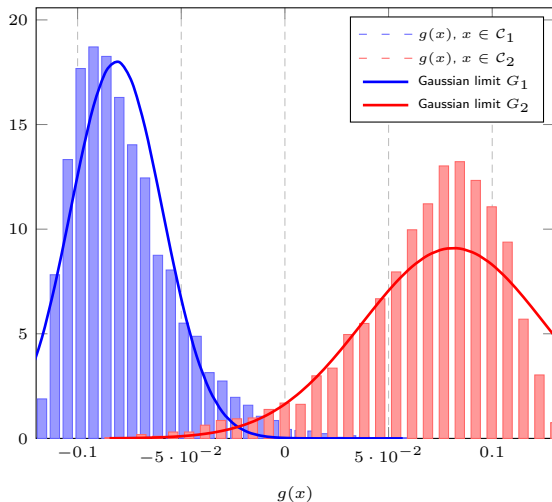


Figure: Values of $g(x)$ for MNIST data (1's and 7's), $n = 256$, $p = 784$, standard Gaussian kernel.

Classification performance

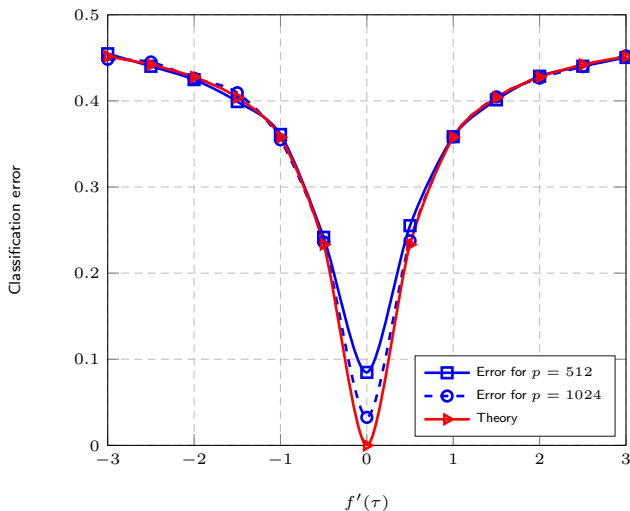


Figure: Performance of LS-SVM, $c_0 = 1/4$, $c_1 = c_2 = 1/2$, $\gamma = 1$, polynomial kernel with $f(\tau) = 4$, $f''(\tau) = 2$, $x \in \mathcal{N}(0, C_a)$, with $C_1 = I_p$, $[C_2]_{i,j} = .4^{|i-j|}$.

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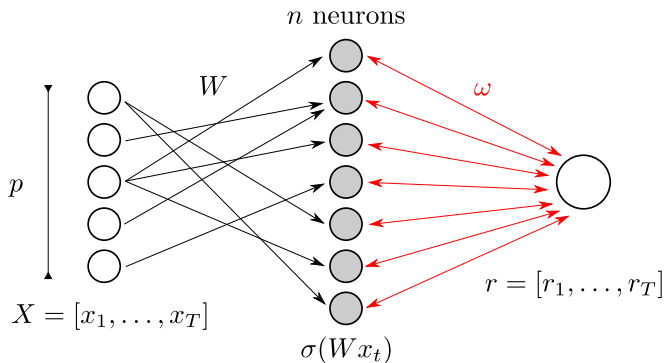
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 - ▶ **Deeper structures**: back-propagation of error.

Extreme Learning Machines

Context: for a learning period T

- ▶ input vectors $x_1, \dots, x_T \in \mathbb{R}^p$, output scalars (or binary values) $r_1, \dots, r_T \in \mathbb{R}$
- ▶ n -neuron layer, randomly connected input $W \in \mathbb{R}^{n \times p}$
- ▶ ridge-regressed output $\omega \in \mathbb{R}^n$
- ▶ non-linear activation function σ .



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- ▶ Then **deterministic approximation** of $\frac{1}{\hat{T}} \sigma(W a)^{\top} \Sigma Q_{\gamma} b$ for deterministic a, b .

Main technical difficulty: $\Sigma = \sigma(WX) \in \mathbb{R}^{n \times T}$ has

- ▶ independent rows
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$$w^\top X A X^\top w \simeq \frac{1}{n} \text{tr} X A X^\top$$

BUT what about:

$$\sigma(w^\top X) A \sigma(X^\top w) \simeq ?$$

Updated trace lemma:

Lemma

For A deterministic and $\sigma(t)$ polynomial, $w \in \mathbb{R}^p$ with i.i.d. entries, $E[w_i] = 0$, $E[w_i^k] = \frac{m_k}{n^{k/2}}$,

$$\frac{1}{T} \sigma(w^\top X) A \sigma(X^\top w) - \frac{1}{T} \text{tr} \Phi_X A \xrightarrow{\text{a.s.}} 0$$

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Technique of proof:

- ▶ Use concentration of vector w
- ▶ transfer concentration by Lipschitz property through mapping $w \mapsto \sigma(w^\top X)$, i.e.,

$$P \left(f \left(\sigma(w^\top X) \right) - E \left[f \left(\sigma(w^\top X) \right) \right] > t \right) \leq c_1 e^{-c_2 n t^2}$$

for all Lipschitz f (and beyond...), with $c_1, c_2 > 0$.

Results:

- Deterministic equivalent: as $n, p, T \rightarrow \infty$ with $\sigma(t)$ smooth, W_{ij} i.i.d. $E[W_{ij}] = 0$, $E[W_{ij}^k] = \frac{m_k}{n^{k/2}}$,

$$Q_\gamma \leftrightarrow \bar{Q}_\gamma$$

where

$$Q_\gamma \left(\frac{1}{T} \Sigma \Sigma^\top + \gamma I_T \right)^{-1}$$
$$\bar{Q}_\gamma = \left(\frac{n}{T} \frac{1}{1 + \delta} \Phi_{\mathbf{X}} + \gamma I_T \right)^{-1}$$

with δ unique solution to

$$\delta = \frac{1}{T} \text{tr} \Phi_{\mathbf{X}} \left(\frac{n}{T} \frac{1}{1 + \delta} \Phi_{\mathbf{X}} + \gamma I_T \right)^{-1}.$$

Neural Network Performances:

- ▶ Training performance:

$$E_{\gamma}(X, r) \leftrightarrow \gamma^2 \frac{1}{T} r^{\top} \bar{Q}_{\gamma} \left[\frac{\frac{1}{n} \text{tr}(\Psi_X \bar{Q}_{\gamma}^2)}{1 - \frac{1}{n} \text{tr}(\Psi_X \bar{Q}_{\gamma})^2} \Psi_X + I_T \right] \bar{Q}_{\gamma} r.$$

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- ▶ Testing performance:

$$\begin{aligned} \hat{E}_{\gamma}(X, r; \hat{X}, \hat{r}) \leftrightarrow & \frac{1}{\hat{T}} \left\| \hat{r} - \Psi_{X, \hat{X}}^{\top} \bar{Q}_{\gamma} r \right\|^2 + \frac{\frac{1}{n} r^{\top} \bar{Q}_{\gamma} \Psi_X \bar{Q}_{\gamma} r}{1 - \frac{1}{n} \text{tr}(\Psi_X \bar{Q}_{\gamma})^2} \\ & \times \left[\frac{1}{\hat{T}} \text{tr} \Psi_{\hat{X}} - \frac{\gamma}{\hat{T}} \text{tr}(\bar{Q}_{\gamma} \Psi_{X, \hat{X}} \Psi_{\hat{X}, X} \bar{Q}_{\gamma}) - \frac{1}{\hat{T}} \text{tr}(\Psi_{\hat{X}, X} \bar{Q}_{\gamma}) \Psi_{X, \hat{X}} \right]. \end{aligned}$$

where $\Psi_{A,B} = \frac{n}{T} \frac{1}{1+\delta} \Phi_{A,B}$, $\Psi_A = \Psi_{A,A}$, $\Phi_{A,B} = E[\frac{1}{n} \sigma(WA)^{\top} \sigma(WB)]$.

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In the limit where $n/p, n/T \rightarrow \infty$, taking $\gamma = \frac{n}{T} \Gamma$:

$$\begin{aligned} E_{\gamma}(X, r) & \leftrightarrow \frac{1}{T} \Gamma^2 r^{\top} (\Phi_X + \Gamma I_T)^{-2} r \\ \hat{E}_{\gamma}(X, r) & \leftrightarrow \frac{1}{\hat{T}} \left\| \hat{r} - \Phi_{\hat{X}, X} (\Phi_X + \Gamma I_T)^{-1} r \right\|^2. \end{aligned}$$

Special Cases of $\Phi_{A,B}$:

$\sigma(t)$	W_{ij}	$[\Phi_{A,B}]_{ij}$
t	any	$\frac{m_2}{n} a_i^\top b_j$
$At^2 + Bt + C$	any	$A^2 \left[\frac{m_2^2}{n^2} \left(2(a_i^\top b_j)^2 + \ a_i\ ^2 \ b_j\ ^2 \right) + \frac{m_4 - 3m_2^2}{n^2} (a_i^2)^\top (b_j^2) \right]$ $+ B^2 \frac{m_2}{n} a_i^\top b_j + AB \frac{m_3}{n^{3/2}} \left[(a_i^2)^\top b_j + a_i^\top (b_j^2) \right]$ $+ AC \frac{m_2}{n} [\ a_i\ ^2 + \ b_j\ ^2] + C^2$
$\max(t, 0)$	$\mathcal{N}(0, \frac{1}{n})$	$\frac{1}{2\pi n} \ a_i\ \ b_j\ \left(Z_{ij} (-Z_{ij}) + \sqrt{1 - Z_{ij}^2} \right)$
$\text{erf}(t)$	$\mathcal{N}(0, \frac{1}{n})$	$\frac{2}{\pi} \left(\frac{2a_i^\top b_j}{\sqrt{(n+2\ a_i\ ^2)(n+2\ b_j\ ^2)}} \right)$
$1_{\{t>0\}}$	$\mathcal{N}(0, \frac{1}{n})$	$\frac{1}{2} - \frac{1}{2\pi} (Z_{ij})$
$\text{sign}(t)$	$\mathcal{N}(0, \frac{1}{n})$	$1 - \frac{1}{\pi} (Z_{ij})$
$\cos(t)$	$\mathcal{N}(0, \frac{1}{n})$	$\exp \left(-\frac{1}{2} [\ a_i\ ^2 + \ b_j\ ^2] \right) \cosh \left(a_i^\top b_j \right).$

Figure: $\Phi_{A,B}$ for W_{ij} i.i.d. zero mean, k -th order moments $m_k n^{-\frac{k}{2}}$, $Z_{ij} \equiv \frac{a_i^\top b_j}{\|a_i\| \|b_j\|}$, $(a^2) = [a_i^2]_{i=1}^n$.

Test on MNIST data

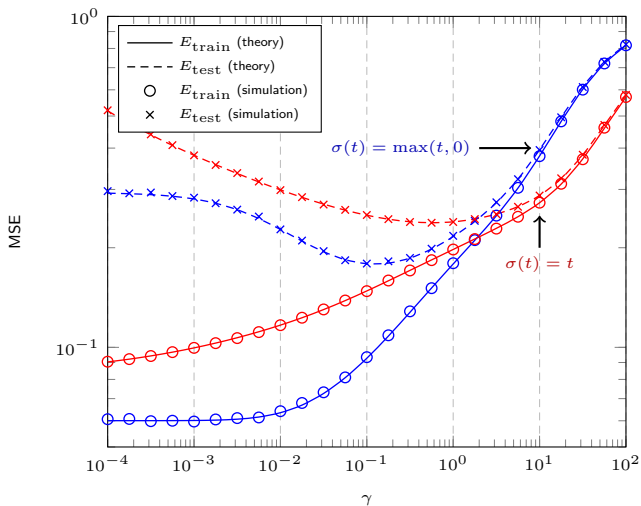


Figure: MSE performance for $\sigma(t) = t$ and $\sigma(t) = \max(t, 0)$, as a function of γ , for 2-class MNIST data (sevens, nines), $n = 512$, $T = 1024$, $p = 784$.

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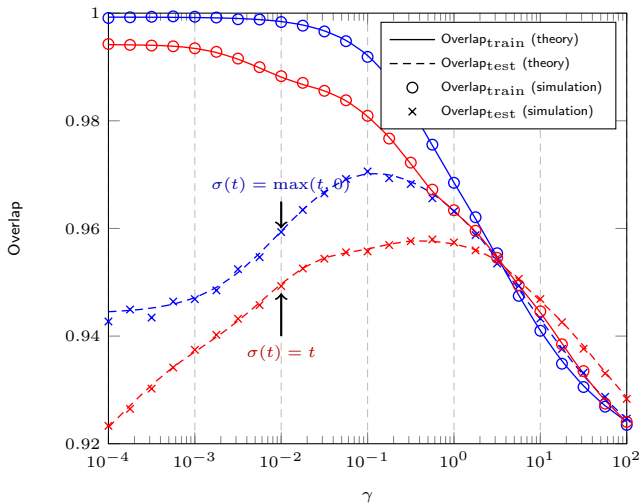


Figure: Overlap performance for $\sigma(t) = t$ and $\sigma(t) = \max(t, 0)$, as a function of γ , for 2-class MNIST data (sevens, nines), $n = 512$, $T = 1024$, $p = 784$.

Interpretations and Improvements:

- ▶ General formulas for Φ_X , $\Phi_{X,\hat{x}}$
- ▶ On-line optimization of γ , $\sigma(\cdot)$, n ?

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Generalizations:

- ▶ Multi-layer ELM?
- ▶ Optimize layers vs. number of neurons?
- ▶ Backpropagation error analysis?
- ▶ Connection to auto-encoders?
- ▶ Introduction of non-linearity to more involved structures (ESN, deep nets?).

Spectral Clustering Methods and Random Matrices

Community Detection on Graphs

Kernel Spectral Clustering

Kernel Spectral Clustering: Subspace Clustering

Semi-supervised Learning

Support Vector Machines

Neural Networks: Extreme Learning Machines

Random Matrices and Robust Estimation

Perspectives

Baseline scenario: $x_1, \dots, x_n \in \mathbb{C}^N$ (or \mathbb{R}^N) i.i.d. with $E[x_1] = 0$, $E[x_1 x_1^*] = C_N$:

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

$$\hat{C}_N = \frac{1}{n} \sum_{i=1}^n x_i x_i^*.$$

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- **[Pascal'13; Chen'11]** If $N > n$, x_1 elliptical or with outliers, shrinkage extensions

$$\hat{C}_N(\rho) = (1 - \rho) \frac{1}{n} \sum_{i=1}^n \frac{x_i x_i^*}{\frac{1}{N} x_i^* \hat{C}_N^{-1}(\rho) x_i} + \rho I_N$$

$$\check{C}_N(\rho) = \frac{\check{B}_N(\rho)}{\frac{1}{N} \text{tr } \check{B}_N(\rho)}, \quad \check{B}_N(\rho) = (1 - \rho) \frac{1}{n} \sum_{i=1}^n \frac{x_i x_i^*}{\frac{1}{N} x_i^* \check{C}_N^{-1}(\rho) x_i} + \rho I_N$$

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- ▶ Application interest:
 - ▶ comparison between SCM and robust estimators
 - ▶ performance of robust/non-robust estimation methods
 - ▶ improvement thereof (by proper parametrization)

Definition (Maronna's Estimator)

For $x_1, \dots, x_n \in \mathbb{C}^N$ with $n > N$, \hat{C}_N is the solution (upon existence and uniqueness) of

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where $u : [0, \infty) \rightarrow (0, \infty)$ is

- ▶ non-increasing
- ▶ such that $\phi(x) \triangleq xu(x)$ increasing of supremum ϕ_∞ with

$$1 < \phi_\infty < c^{-1}, \quad c \in (0, 1).$$

The Results in a Nutshell

For various models of the x_i 's,

- First order convergence:

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

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- ▶ Applications:

- ▶ improved robust covariance matrix estimation
- ▶ improved robust tests / estimators
- ▶ specific examples in **statistics** at large, **array processing**, statistical **finance**, etc.

(Elliptical) scenario

Theorem (Large dimensional behavior, elliptical case)

For $x_i = \sqrt{\tau_i} w_i$, τ_i impulsive (random or not), w_i unitarily invariant, $\|w_i\| = N$,

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Corollaries

- **Spectral measure:** $\mu_{\hat{C}_N} - \mu_{\hat{S}_N} \xrightarrow{\mathcal{L}} 0$ a.s. ($\mu_N^X \triangleq \frac{1}{n} \sum_{i=1}^n \delta_{\lambda_i(X)}$)

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- ▶ **Norm boundedness:** $\limsup_N \|\hat{C}_N\| < \infty$

→ Bounded spectrum (unlike SCM!)

Large dimensional behavior

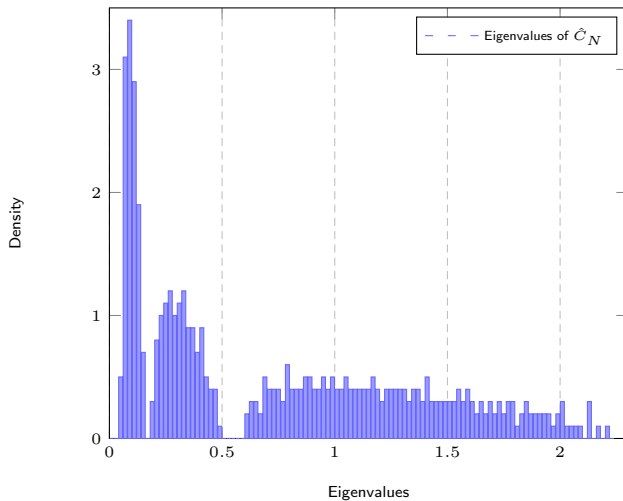


Figure: $n = 2500$, $N = 500$, $C_N = \text{diag}(I_{125}, 3I_{125}, 10I_{250})$, $\tau_i \sim \Gamma(.5, 2)$ i.i.d.

Large dimensional behavior

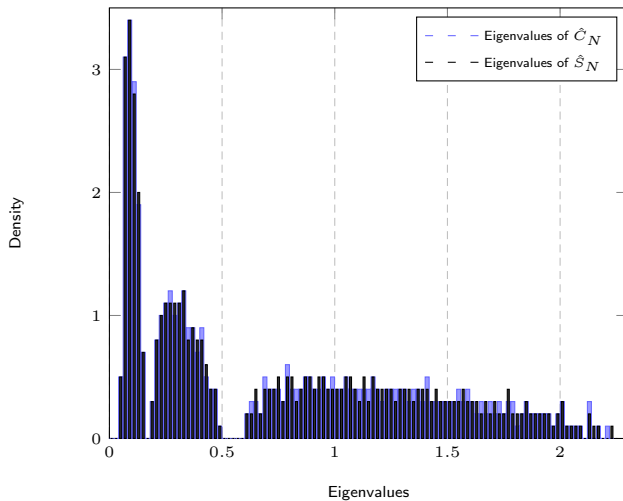


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Large dimensional behavior

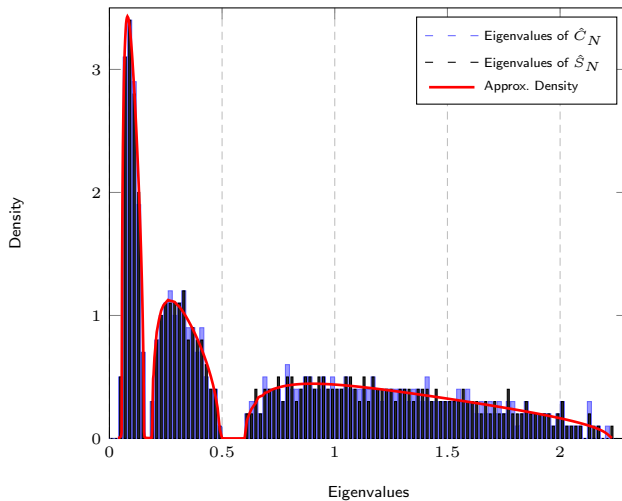


Figure: $n = 2500$, $N = 500$, $C_N = \text{diag}(I_{125}, 3I_{125}, 10I_{250})$, $\tau_i \sim \Gamma(.5, 2)$ i.i.d.

Definition (v and ψ)

Letting $g(x) = x(1 - c\phi(x))^{-1}$ (on \mathbb{R}_+),

$$v(x) \triangleq (u \circ g^{-1})(x) \quad \text{non-increasing}$$

$$\psi(x) \triangleq xv(x) \quad \text{increasing and bounded by } \psi_\infty.$$

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Lemma (Rewriting \hat{C}_N)

It holds (with $C_N = I_N$) that

$$\hat{C}_N \triangleq \frac{1}{n} \sum_{i=1}^n \tau_i v(\tau_i d_i) w_i w_i^*$$

with $(d_1, \dots, d_n) \in \mathbb{R}_+^n$ a.s. unique solution to

$$d_i = \frac{1}{N} w_i^* \hat{C}_{(i)}^{-1} w_i = \frac{1}{N} w_i^* \left(\frac{1}{n} \sum_{j \neq i} \tau_j v(\tau_j d_j) w_j w_j^* \right)^{-1} w_i, \quad i = 1, \dots, n.$$

Remark (Quadratic Form close to Trace)

Random matrix insight: $(\frac{1}{n} \sum_{j \neq i} \tau_j v(\tau_j d_j) w_j w_j^*)^{-1}$ “almost independent” of w_i , so

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for some deterministic sequence $(\gamma_N)_{N=1}^{\infty}$, irrespective of i .

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for some deterministic sequence $(\gamma_N)_{N=1}^\infty$, irrespective of i .

Lemma (Key Lemma)

Letting $e_i \triangleq \frac{v(\tau_i d_i)}{v(\tau_i \gamma_N)}$ with γ_N unique solution to

$$1 = \frac{1}{n} \sum_{k=1}^n \frac{\psi(\tau_k \gamma_N)}{1 + c\psi(\tau_k \gamma_N)}$$

we have

$$\max_{1 \leq i \leq n} |e_i - 1| \xrightarrow{\text{a.s.}} 0.$$

Proof of the Key Lemma: $\max_i |e_i - 1| \xrightarrow{\text{a.s.}} 0$, $e_i = \frac{v(\tau_i d_i)}{v(\tau_i \gamma_N)}$

Property (Quadratic form and γ_N)

$$\max_{1 \leq i \leq n} \left| \frac{1}{N} w_i^* \left(\frac{1}{n} \sum_{j \neq i} \tau_j v(\tau_j \gamma_N) w_j w_j^* \right)^{-1} w_i - \gamma_N \right| \xrightarrow{\text{a.s.}} 0.$$

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Proof of the Property

- Uniformity easy (moments of all orders for $[w_i]_j$).
- By a “quadratic form similar to trace” approach, we get

$$\max_{1 \leq i \leq n} \left| \frac{1}{N} w_i^* \left(\frac{1}{n} \sum_{j \neq i} \tau_j v(\tau_j \gamma_N) w_j w_j^* \right)^{-1} w_i - m(0) \right| \xrightarrow{\text{a.s.}} 0$$

with $m(0)$ unique positive solution to **[MarPas'67; BaiSil'95]**

$$m(0) = \frac{1}{n} \sum_{i=1}^n \frac{\tau_i v(\tau_i \gamma_N)}{1 + c \tau_i v(\tau_i \gamma_N) m(0)}.$$

- γ_N precisely solves this equation, thus $m(0) = \gamma_N$.

Proof of the Key Lemma: $\max_i |e_i - 1| \xrightarrow{\text{a.s.}} 0$, $e_i = \frac{v(\tau_i d_i)}{v(\tau_i \gamma_N)}$

Substitution Trick (case $\tau_i \in [a, b] \subset (0, \infty)$)

Up to relabelling $e_1 \leq \dots \leq e_n$, use

$$\begin{aligned} v(\tau_n \gamma_N) \mathbf{e}_n &= v(\tau_n d_n) = v \left(\tau_n \frac{1}{N} w_n^* \left(\frac{1}{n} \sum_{i < n} \tau_i \underbrace{v(\tau_i d_i)}_{=v(\tau_i \gamma_N) \mathbf{e}_i} w_i w_i^* \right)^{-1} w_n \right) \\ &\leq v \left(\tau_n \mathbf{e}_n^{-1} \frac{1}{N} w_n^* \left(\frac{1}{n} \sum_{i < n} \tau_i v(\tau_i \gamma_N) w_i w_i^* \right)^{-1} w_n \right) \\ &\leq v \left(\tau_n \mathbf{e}_n^{-1} (\gamma_N - \varepsilon_n) \right) \text{ a.s., } \varepsilon_n \rightarrow 0 \text{ (slow).} \end{aligned}$$

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Use properties of ψ to get

$$\psi(\tau_n \gamma_N) \leq \psi(\tau_n \mathbf{e}_n^{-1} \gamma_N) \left(1 - \varepsilon_n \gamma_N^{-1}\right)^{-1}$$

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Conclusion: If $e_n > 1 + \ell$ i.o., as $\tau_n \in [a, b]$, on subsequence $\begin{cases} \tau_n \rightarrow \tau_0 > 0 \\ \gamma_N \rightarrow \gamma_0 > 0 \end{cases}$,

$$\psi(\tau_0 \gamma_0) \leq \psi\left(\frac{\tau_0 \gamma_0}{1 + \ell}\right), \text{ a contradiction.}$$

Theorem (Outlier Rejection)

Observation set

$$X = [x_1, \dots, x_{(1-\varepsilon_n)n}, a_1, \dots, a_{\varepsilon_n n}]$$

where $x_i \sim \mathcal{CN}(0, C_N)$ and $a_1, \dots, a_{\varepsilon_n n} \in \mathbb{C}^N$ *deterministic* outliers. Then,

$$\|\hat{C}_N - \hat{S}_N\| \xrightarrow{\text{a.s.}} 0$$

where

$$\hat{S}_N \triangleq v(\gamma_N) \frac{1}{n} \sum_{i=1}^{(1-\varepsilon_n)n} x_i x_i^* + \frac{1}{n} \sum_{i=1}^{\varepsilon_n n} v(\alpha_{i,n}) a_i a_i^*$$

with γ_N and $\alpha_{1,n}, \dots, \alpha_{\varepsilon_n n, n}$ unique positive solutions to

$$\gamma_N = \frac{1}{N} \text{tr} C_N \left(\frac{(1-\varepsilon)v(\gamma_N)}{1 + cv(\gamma_N)\gamma_N} C_N + \frac{1}{n} \sum_{i=1}^{\varepsilon_n n} v(\alpha_{i,n}) a_i a_i^* \right)^{-1}$$

$$\alpha_{i,n} = \frac{1}{N} a_i^* \left(\frac{(1-\varepsilon)v(\gamma_N)}{1 + cv(\gamma_N)\gamma_N} C_N + \frac{1}{n} \sum_{j \neq i}^{\varepsilon_n n} v(\alpha_{j,n}) a_j a_j^* \right)^{-1} a_i, \quad i = 1, \dots, \varepsilon_n n.$$

- For $\varepsilon_n n = 1$,

$$\hat{S}_N = v \left(\frac{\phi^{-1}(1)}{1-c} \right) \frac{1}{n} \sum_{i=1}^{n-1} x_i x_i^* + \left(v \left(\frac{\phi^{-1}(1)}{1-c} \frac{1}{N} a_1^* C_N^{-1} a_1 \right) + o(1) \right) a_1 a_1^*$$

Outlier rejection relies on $\frac{1}{N} a_1^* C_N^{-1} a_1 \leq 1$.

Outlier Data

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- For $a_i \sim \mathcal{CN}(0, D_N)$, $\varepsilon_n \rightarrow \varepsilon \geq 0$,

$$\begin{aligned} \hat{S}_N &= v(\gamma_n) \frac{1}{n} \sum_{i=1}^{(1-\varepsilon_n)n} x_i x_i^* + v(\alpha_n) \frac{1}{n} \sum_{i=1}^{\varepsilon_n n} a_i a_i^* \\ \gamma_n &= \frac{1}{N} \text{tr} C_N \left(\frac{(1-\varepsilon)v(\gamma_n)}{1+cv(\gamma_n)\gamma_n} C_N + \frac{\varepsilon v(\alpha_n)}{1+cv(\alpha_n)\alpha_n} D_N \right)^{-1} \\ \alpha_n &= \frac{1}{N} \text{tr} D_N \left(\frac{(1-\varepsilon)v(\gamma_n)}{1+cv(\gamma_n)\gamma_n} C_N + \frac{\varepsilon v(\alpha_n)}{1+cv(\alpha_n)\alpha_n} D_N \right)^{-1}. \end{aligned}$$

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For $\varepsilon_n \rightarrow 0$,

$$\hat{S}_N = v \left(\frac{\phi^{-1}(1)}{1-c} \right) \frac{1}{n} \sum_{i=1}^{(1-\varepsilon_n)n} x_i x_i^* + \frac{1}{n} \sum_{i=1}^{\varepsilon_n n} v \left(\frac{\phi^{-1}(1)}{1-c} \frac{1}{N} \text{tr} D_N C_N^{-1} \right) a_i a_i^*$$

Outlier rejection relies on $\frac{1}{N} \text{tr} D_N C_N^{-1} \leq 1$.

Outlier Data

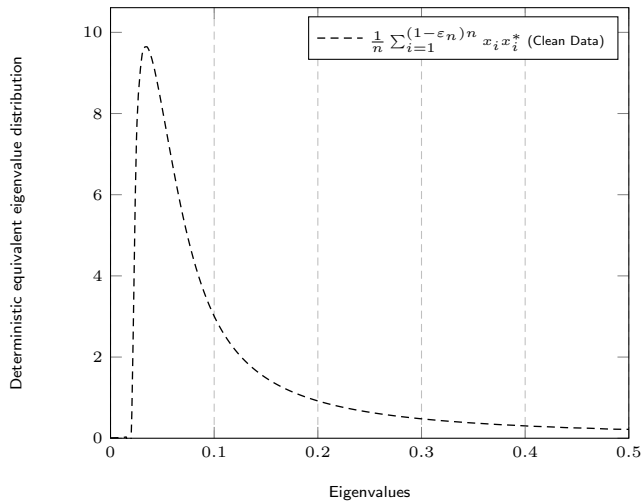


Figure: Limiting eigenvalue distributions. $[C_N]_{ij} = .9^{|i-j|}$, $D_N = I_N$, $\varepsilon = .05$.

Outlier Data

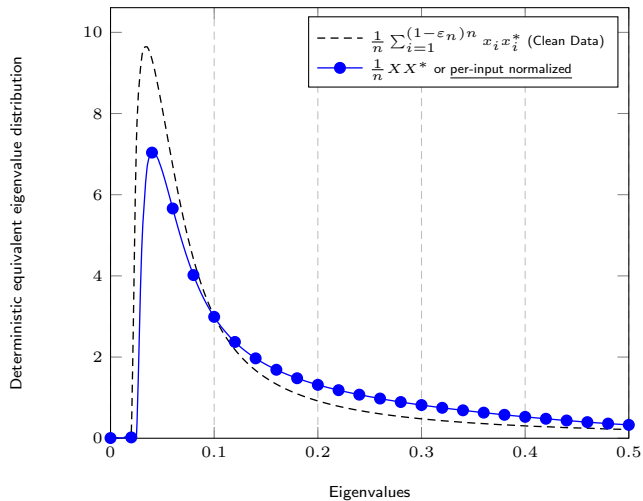


Figure: Limiting eigenvalue distributions. $[C_N]_{ij} = .9^{|i-j|}$, $D_N = I_N$, $\varepsilon = .05$.

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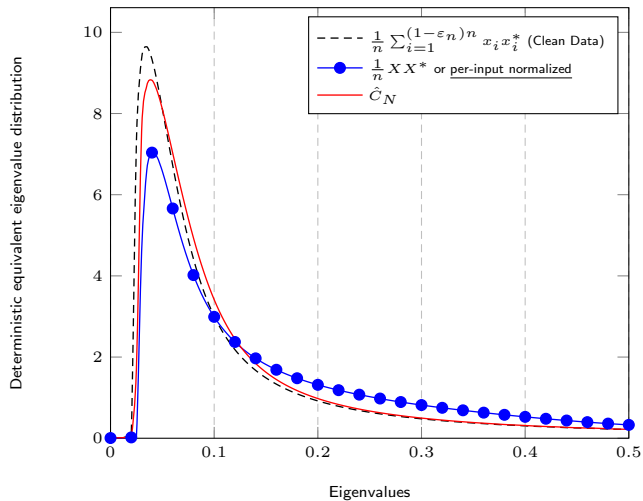


Figure: Limiting eigenvalue distributions. $[C_N]_{ij} = .9^{|i-j|}$, $D_N = I_N$, $\varepsilon = .05$.

Spectral Clustering Methods and Random Matrices

Community Detection on Graphs

Kernel Spectral Clustering

Kernel Spectral Clustering: Subspace Clustering

Semi-supervised Learning

Support Vector Machines

Neural Networks: Extreme Learning Machines

Random Matrices and Robust Estimation

Perspectives

Summary of Results and Perspectives I

Robust statistics.

- ✓ Tyler, Maronna (and regularized) estimators
- ✓ Elliptical data setting, deterministic outlier setting
- ✓ Central limit theorem extensions
- 💡 Joint mean and covariance robust estimation
- 💡 Study of robust regression (preliminary works exist already using strikingly different approaches)

Applications.

- ✓ Statistical finance (portfolio estimation)
- ✓ Localisation in array processing (robust GMUSIC)
- ✓ Detectors in space time array processing

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Summary of Results and Perspectives III



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Summary of Results and Perspectives I

Kernel methods.

- ✓ Subspace spectral clustering
- ✓ Subspace spectral clustering for $f'(\tau) = 0$
- ✎ Spectral clustering with outer product kernel $f(x^T y)$
- ✓ Semi-supervised learning, kernel approaches.
- ✓ Least square support vector machines (LS-SVM).
- ✎ Support vector machines (SVM).

Applications.

- ✓ Massive MIMO user clustering

References.



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Summary of Results and Perspectives II



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Community detection.

- ✓ Complete study of eigenvector contents in adjacency/modularity methods.
- 💡 Study of Bethe Hessian approach for the DCSBM model.
- 💡 Analysis of non-necessarily spectral approaches (wavelet approaches).

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Summary of Results and Perspectives I

Neural Networks.

- ✓ Non-linear extreme learning machines (ELM)
- ✎ Multi-layer ELM
- 💡 Backpropagation in ELM
- ✎ Random convolutional networks for image processing
- ✓ Linear echo-state networks (ESN)
- 💡 Non-linear ESN
- 💡 Connecting kernel methods to neural networks

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Sparse PCA

- ✓ Spike random matrix sparse PCA
- ✎ Sparse kernel PCA

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Signal processing on graphs, distributed optimization, etc.

- 💡 Turning signal processing on graph methods random.
- 💡 Random matrix analysis of diffusion networks performance.

Thank you.