

Projet RMT4GRAPH

Evaluation à mi-parcours

Romain COUILLET

(en collaboration avec Hafiz Tiomoko Ali)

CentraleSupélec (Paris, France)

9 septembre 2016



CentraleSupélec

Project Status

Machine Learning: Community Detection on Graphs

Machine Learning: Kernel Spectral Clustering

Future Investigations

Project Status

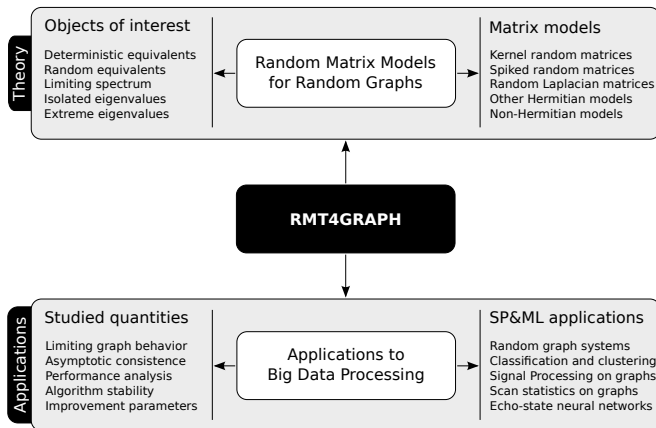
Machine Learning: Community Detection on Graphs

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Future Investigations

Project definition and objectives

“develop a framework of big data processing analysis (notably graph-based methods) relying on random matrix tools”



Work Packages and Timeline

- ▶ **WP1. Random Matrix Models for Random Graphs.**
 - ▶ Task 1.1. Kernel random matrix models.
 - ▶ Task 1.2. Hermitian models and spikes.
 - ▶ **Task 1.3. Random matrices with non-linear or recursive entries**
(formerly "Task 1.3. Non-hermitian random matrix models")

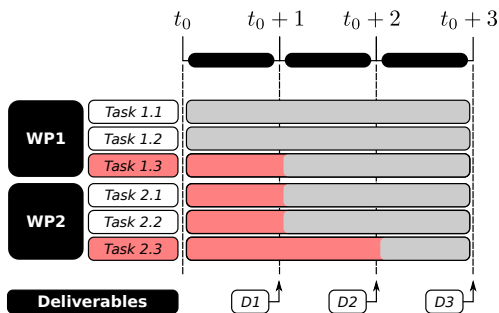
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- ▶ **WP2. Applications to Big Data Processing.**
 - ▶ Task 2.1. Applications to machine learning.
 - ▶ Task 2.2. Signal processing on graphs
 - ▶ **Task 2.3. Neural networks**
(formerly restricted to "Task 2.3. Echo-state neural networks")

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Taskforce and Actions

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 - ▶ Hafiz Tiomoko Ali (PhD student, RMT4GRAPH grant, 2015-2018): community detection, neural networks.
 - ▶ Xiaoyi Mai (PhD student, DIGICOSME grant, 2016-2019): semi-supervised learning.
 - ▶ Zhenyu Liao (intern, ERC-MORE grant, 2016): support vector machines.
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Actions and Publications.

- ▶ **Publications:** 3 journal articles, 7 conference articles
- ▶ **Dissemination:**
 - ▶ Organization of the summer school “Large Random Matrices and High Dimensional Statistical Signal Processing”, Telecom ParisTech, June 7-8, 2016.
 - ▶ SSP'16 Special Session “Random matrices in signal processing and machine learning”
 - ▶ Distinguished keynote speaker at EUSIPCO 2016
 - ▶ Special Issue on Random Matrices in “Revue du Traitement du Signal”
 - ▶ Several invited talks and contributions to local events

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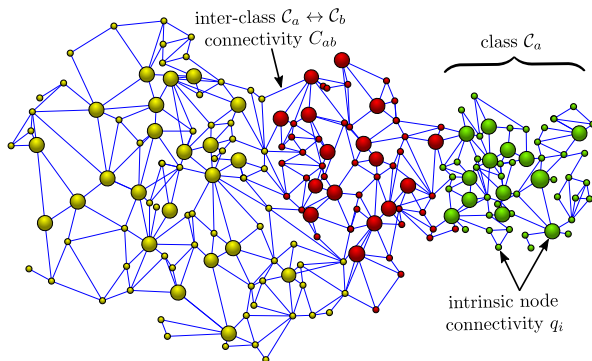
- ▶ “intrinsic” average connectivity $q_1, \dots, q_n \sim \mu$ i.i.d.
- ▶ k classes $\mathcal{C}_1, \dots, \mathcal{C}_k$ independent of $\{q_i\}$ of (large) sizes n_1, \dots, n_k , with preferential attachment C_{ab} between \mathcal{C}_a and \mathcal{C}_b

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- ▶ induces edge probability for node $i \in \mathcal{C}_a, j \in \mathcal{C}_b$,

$$P(i \sim j) = q_i q_j C_{ab}.$$



System Setting

Objective:

Understand and improve performance of **spectral community detection** methods:

- ▶ based on **adjacency** A or **modularity** $A - \frac{dd^T}{2m}$ matrices (adapted to **dense nets**)

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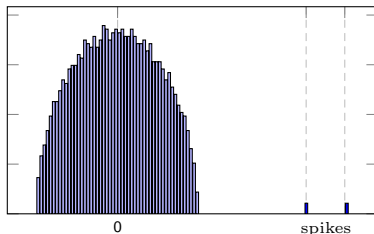
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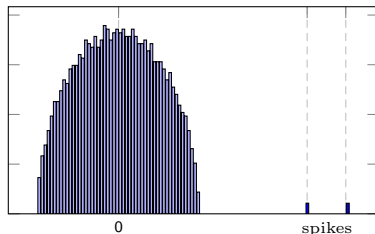


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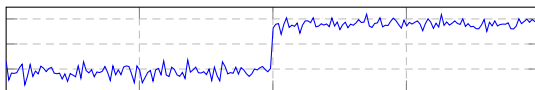
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⇓ **Eigenvectors** ⇓



System Setting

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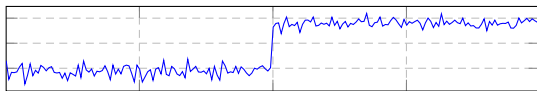


Eigenv. 2



System Setting

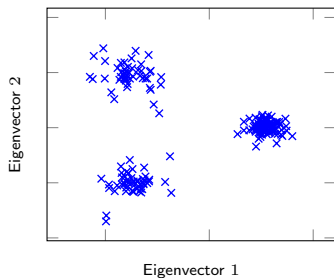
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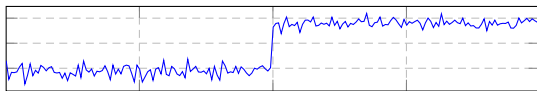


↓ *p*-dimensional representation ↓



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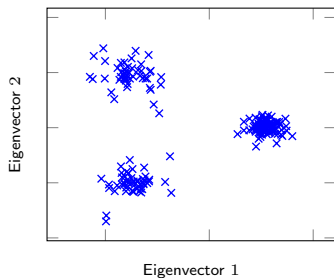
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EM or k-means clustering.

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.**

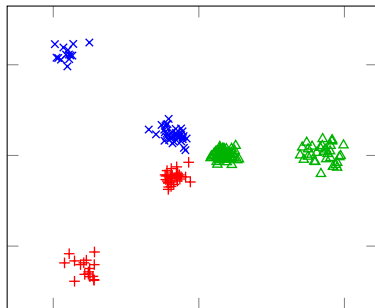
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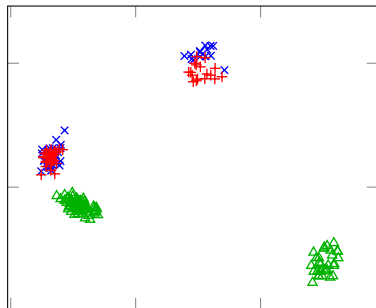
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(Modularity)



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Regularized Modularity Approach

Connectivity Model: $P(i \sim j) = q_i q_j C_{ab}$ for $i \in C_a, j \in C_b$.

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

$$C_{ab} = 1 + \frac{M_{ab}}{\sqrt{n}}$$

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Considered Matrix:

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

$$L_\alpha = (2m)^\alpha \frac{1}{\sqrt{n}} D^{-\alpha} \left[A - \frac{dd^T}{2m} \right] D^{-\alpha}.$$

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

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

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

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

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

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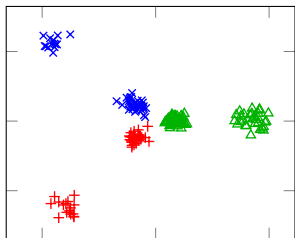
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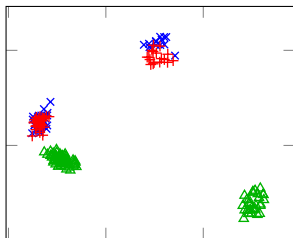
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- ▶ \tilde{L}_α is a well-known spiked random matrix
- ▶ it is “easy” to study and leads to a full analysis of the spectral clustering performance!
- ▶ it helps us correct and optimize classical spectral clustering into a powerful new algorithm.

Performance Results (2 masses of q_i)

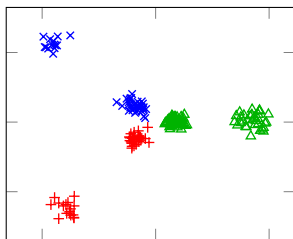


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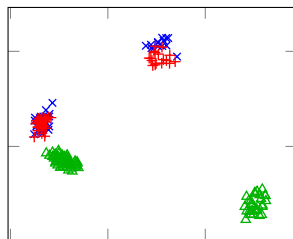


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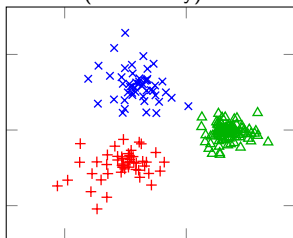
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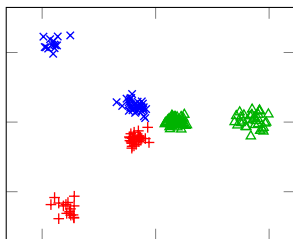
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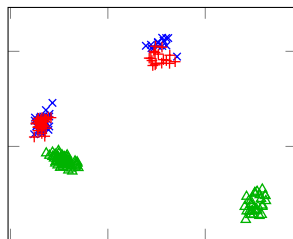
(Algo with $\alpha = 1$)

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

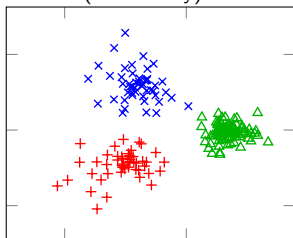
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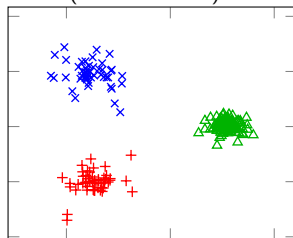
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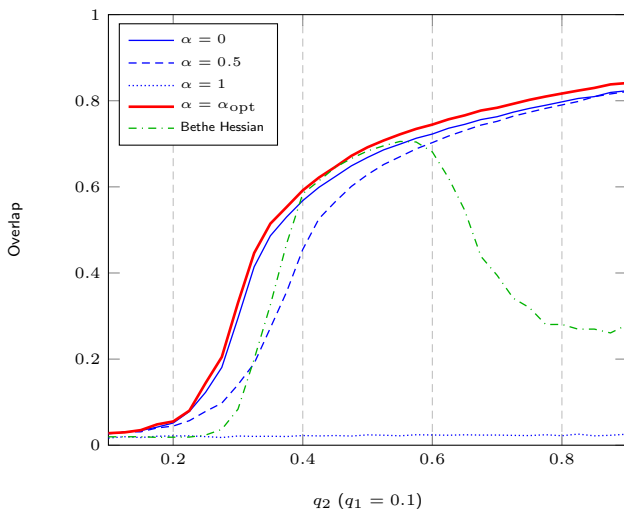


Figure: Overlap performance for $n = 3000$, $K = 3$, $\mu = \frac{3}{4}\delta_{q_1} + \frac{1}{4}\delta_{q_2}$ with $q_1 = 0.1$ and $q_2 \in [0.1, 0.9]$, $M = 10(2I_3 - 1_3 1_3^T)$, $c_i = \frac{1}{3}$.

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Future Investigations

Kernel Spectral Clustering

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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$$\text{(RatioCut)} \quad \operatorname{argmin}_{\mathcal{S}_1 \cup \dots \cup \mathcal{S}_k = \{1, \dots, n\}} \sum_{i=1}^k \sum_{\substack{j \in \mathcal{S}_i \\ j \notin \mathcal{S}_i}} \frac{\kappa(x_j, x_{\bar{j}})}{|\mathcal{S}_i|}$$

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

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$$\text{(RatioCut)} \quad \operatorname{argmin}_{M \in \mathcal{M}} \operatorname{tr} M^T (D - K) M$$

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

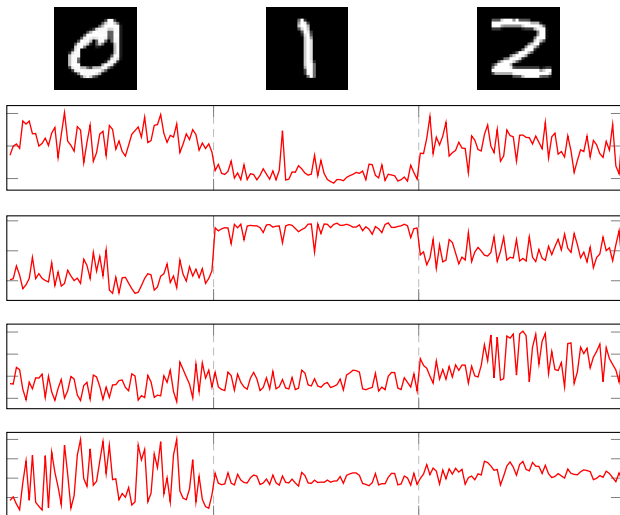


Figure: Leading four eigenvectors of $D^{-\frac{1}{2}}KD^{-\frac{1}{2}}$ for MNIST data.

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Methodology:

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

Gaussian mixture model:

- ▶ $x_1, \dots, x_n \in \mathbb{R}^P$,
- ▶ k classes $\mathcal{C}_1, \dots, \mathcal{C}_k$,
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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 Laplacian:

$$L = nD^{-\frac{1}{2}}KD^{-\frac{1}{2}}$$

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

Difficulty: L is a very intractable random matrix

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Theoretical Findings versus MNIST

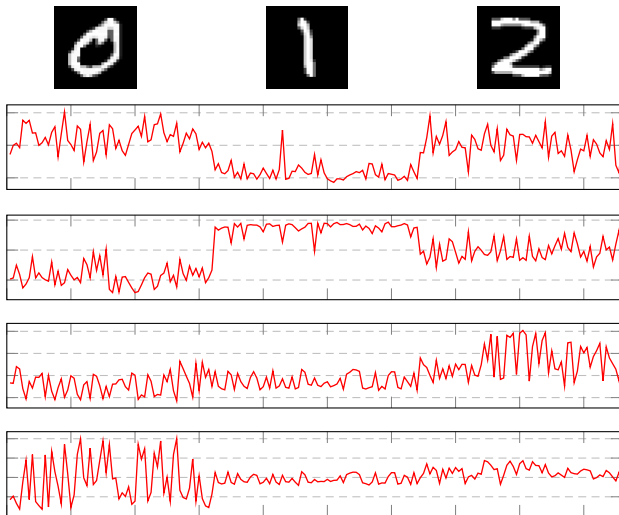


Figure: Leading four eigenvectors of $D^{-\frac{1}{2}} K D^{-\frac{1}{2}}$ for MNIST data (red), versus Gaussian equivalent model (black), and theoretical findings (blue).

Theoretical Findings versus MNIST

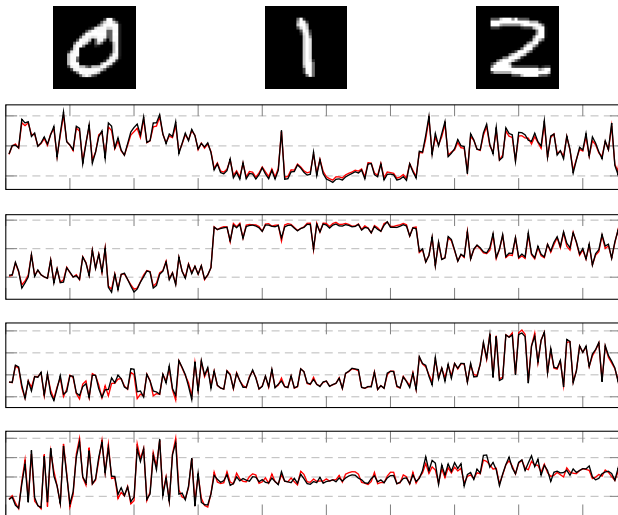


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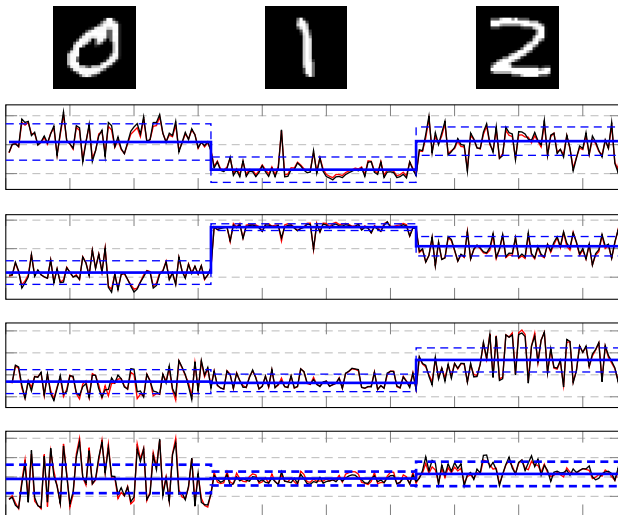


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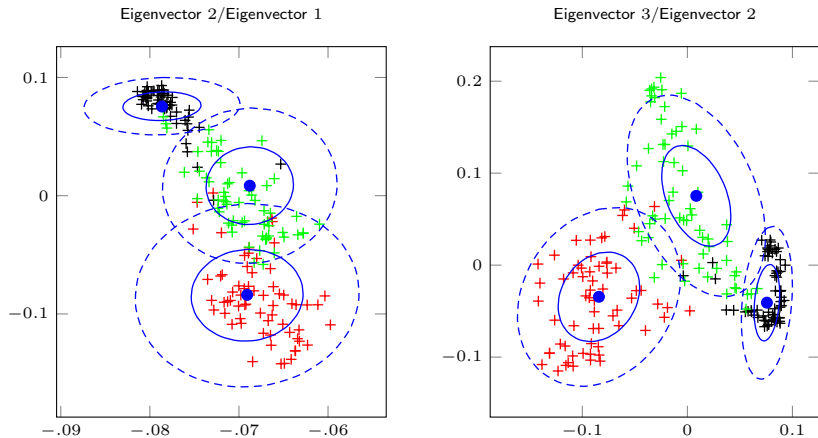


Figure: 2D representation of eigenvectors of L , for the MNIST dataset. Theoretical means and 1- and 2-standard deviations in **blue**. Class 1 in **red**, Class 2 in **black**, Class 3 in **green**.

Project Status

Machine Learning: Community Detection on Graphs

Machine Learning: Kernel Spectral Clustering

Future Investigations

Objectives:

▶ Kernel methods.

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▶ Signal processing on graphs, further graph inference, etc.

- 💡 Making graph methods random.

Thank you.