Spectral clustering and random matrices

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Lyon

Clustering

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Goal : cluster observations $x_1, \ldots, x_n$ with maximum similarity intra classes and minimum similarity inter classes

$$x_1 \quad , \ldots , \quad x_n \quad \Longrightarrow \mathcal{C}_1 = \{x_3, x_{18}, \ldots\}, \ldots, \mathcal{C}_k = \{x_1, x_{20}, \ldots\}$$

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Examples : k-means, EM, hierarchical clustering

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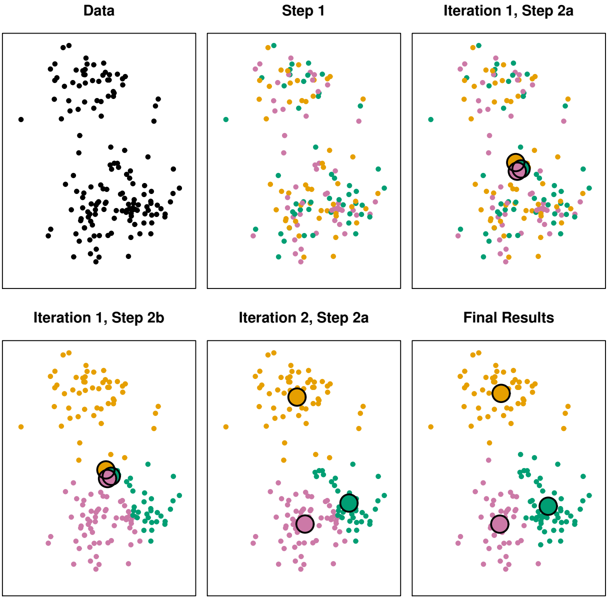

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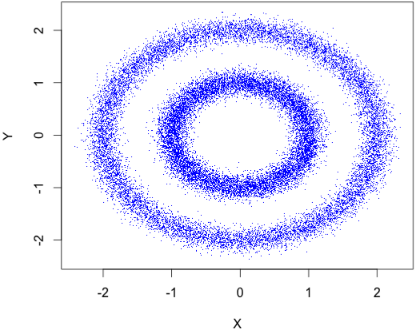

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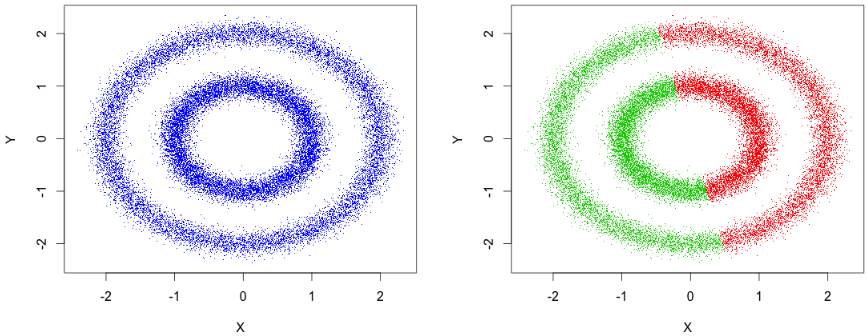

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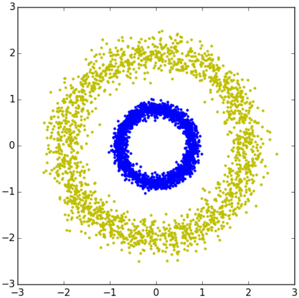

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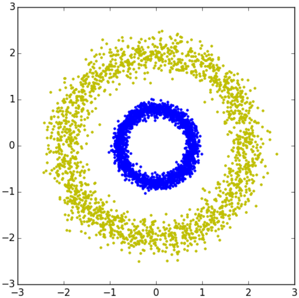

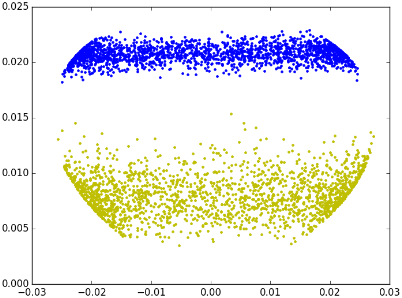

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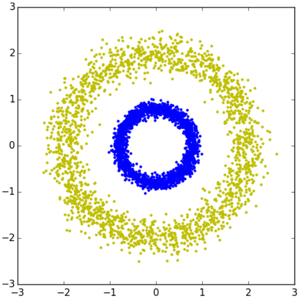

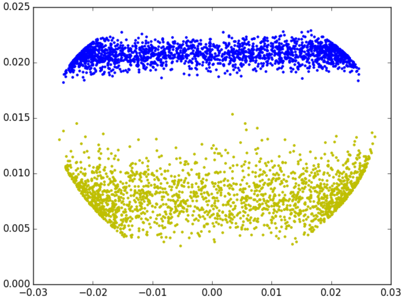

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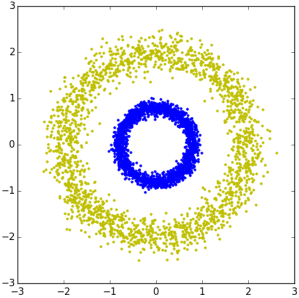

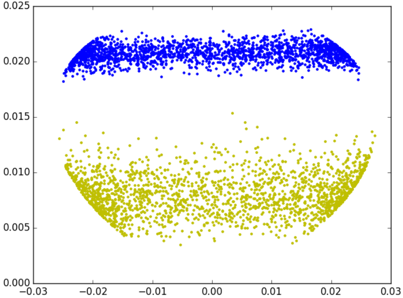

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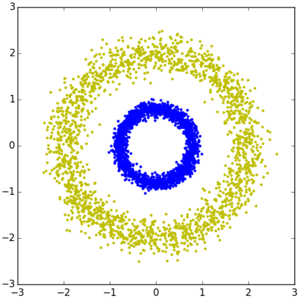

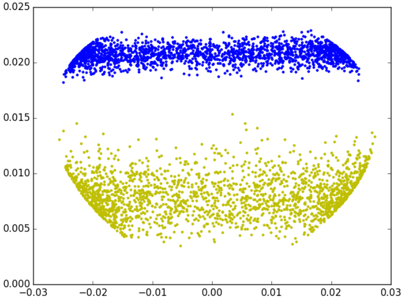

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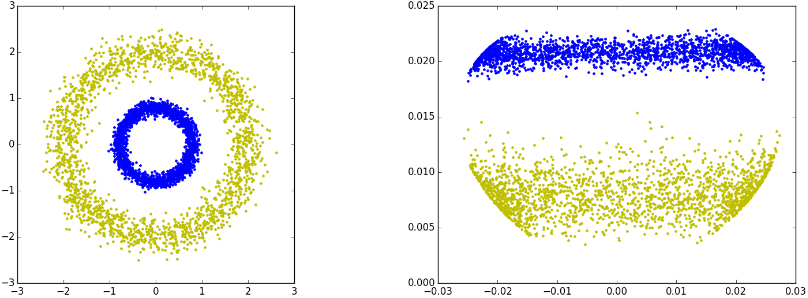

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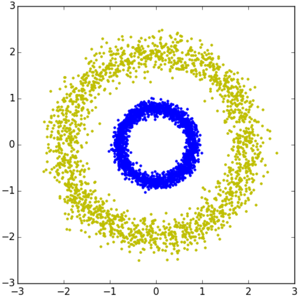

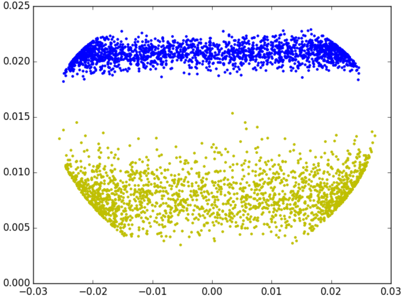

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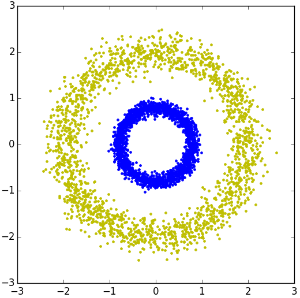

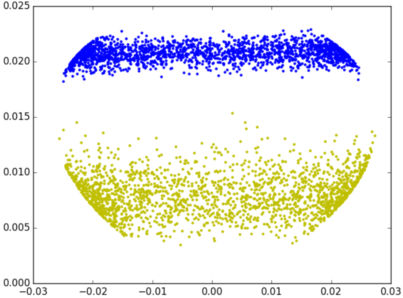

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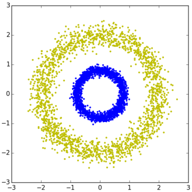

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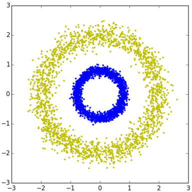

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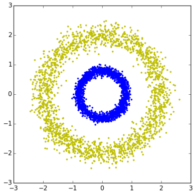

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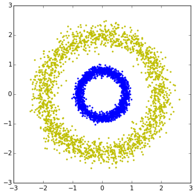

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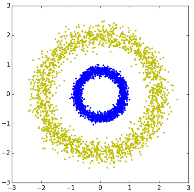

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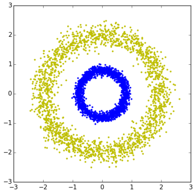

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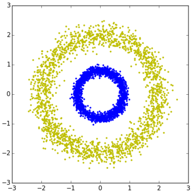

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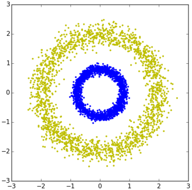

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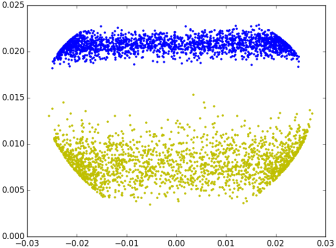

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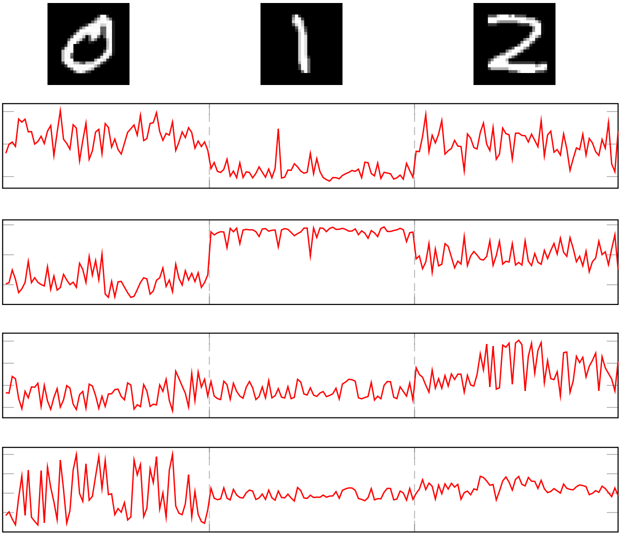
Spectral clustering of $x_1, \ldots, x_n$ in k classes (2) :

L : symmetric Laplacian matrix. Replace observations $x_1, \ldots, x_n$ by the rows of the matrix of the largest eigenvectors of L and apply k-means on these (new) observations.



: Four leading eigenvectors of L for (partial) MNIST data ($n = 192$, $p = 784$, $k = 3$)

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   - $\|\mu_a\| \ll \sqrt{p}$ et $|\operatorname{Tr} C_a - \operatorname{Tr} C_b| \gg \sqrt{p} \implies k$-means on $\|x_i\|$ is efficient

Model and Assumptions

Gaussian mixture model :

- $x_1, \ldots, x_n \in \mathbb{R}^p$ independent
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Convergence rate : We have $n, p \gg 1$ and :

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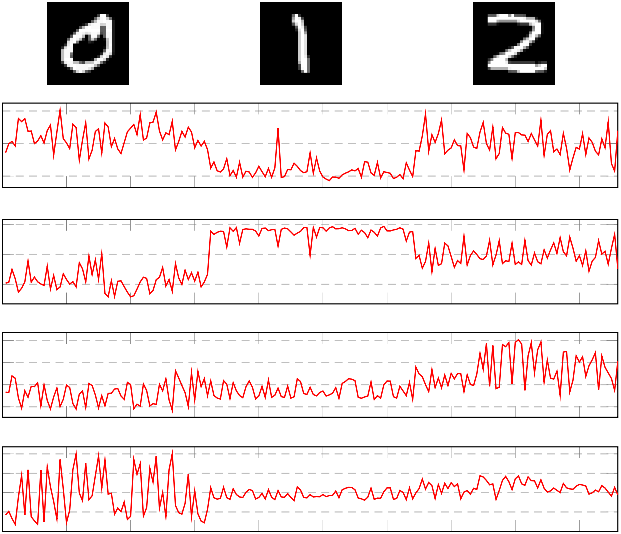
for $\vec{W}$ another leading eigenvector

Class-wise eigenvector means and fluctuations



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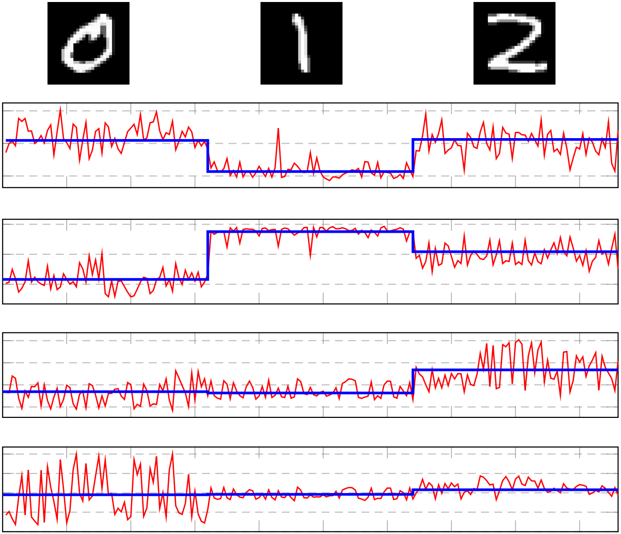

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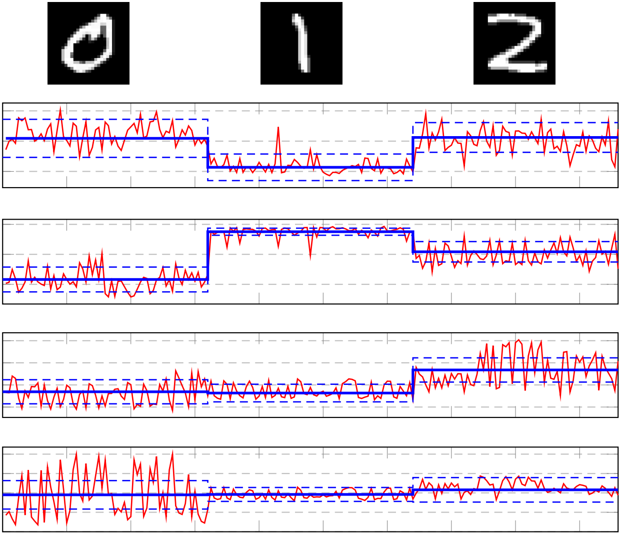

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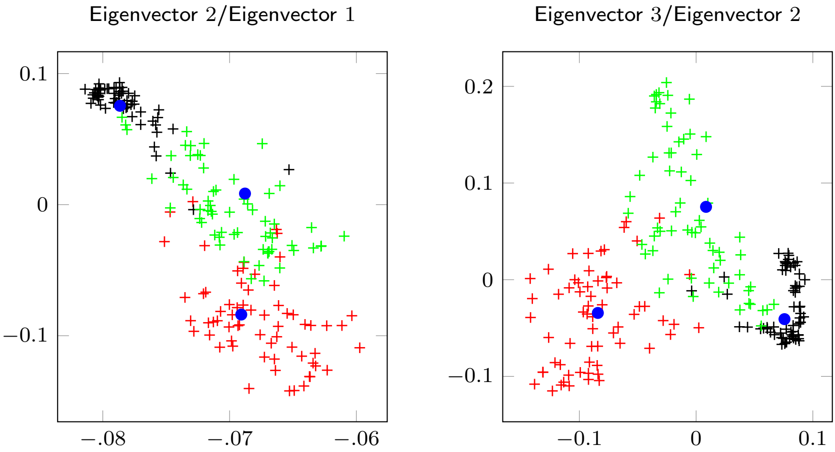

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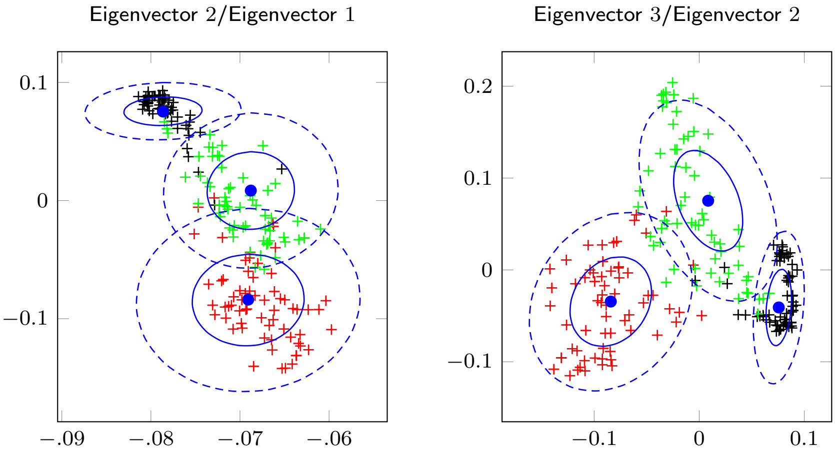

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- **next (and main) step :** study the projected normalized Laplacian :

$$L' = nD^{-\frac{1}{2}} K D^{-\frac{1}{2}} - n \frac{D^{\frac{1}{2}} 1_n 1_n^\mathsf{T} D^{\frac{1}{2}}}{1_n^\mathsf{T} D 1_n}.$$

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Theorem (Random Matrix Equivalent)

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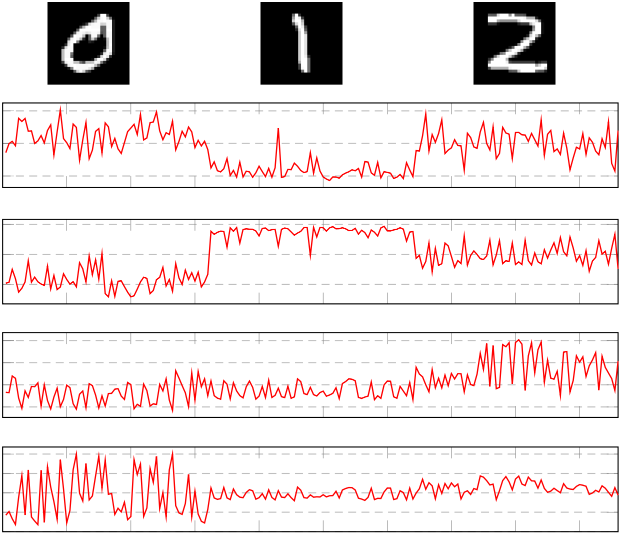
Equivalence between L and $\hat{L}$: eigenvectors



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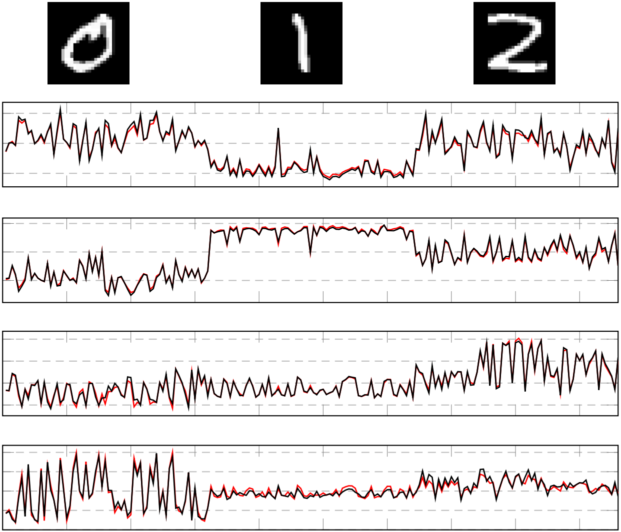

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$$\text{Spectral Projection of } \hat{L}' \text{ on } I \;=\; \frac{1}{2\mathrm{i}\pi}\oint_{\gamma_I}(z - \hat{L})^{-1}\mathrm{d}z$$

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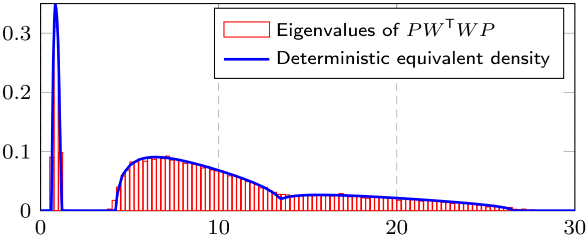
Eigenvalue distribution of $PW^{\mathsf{T}}WP$



: Eigenvalues of $PW^{\mathsf{T}}WP$ (across $1\,000$ realizations) versus deterministic equivalent density, $n = 32$, $p = 256$, $k = 3$.

Deterministic equivalent computed throught its Stieltjes transform :

$$S(z) \;=\; \frac{p}{n}\sum_{a=1}^{k}\frac{n_a}{n}g_a(z)$$

and the formula

$$\mathrm{density}(x) = \lim_{\eta\downarrow 0}\frac{1}{\pi}\Im(S(x+\mathrm{i}\eta))$$

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$\hookrightarrow$ key-tool : the $r \times r$ matrix $U^\mathsf{T}(z - PW^\mathsf{T}WP)^{-1}BU$

Step 2 : isolated eigenvalues of $\hat{L}'$

As

$$(z - PW^{\mathsf{T}}WP)^{-1} = -\frac{p}{n}\operatorname{diag}\left\{g_a(z)1_{n_a}\right\}_{a=1}^{k} + o(1)$$

for $(g_a(z))_{a=1,\ldots,k} \in \mathbb{C}^k$ solution of fixed point equation

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Theorem

There is a (complicated but human) function $F(z)$ such that (up to some technical hypotheses) the isolated eigenvalues of $\hat{L}'$ are the roots of

$$F(z) = 0.$$

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$$\alpha_a(\vec{V}) := \frac{1}{\#\mathcal{C}_a} \left\langle \vec{V}, 1_{\mathcal{C}_a} \right\rangle$$

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$\hookrightarrow$ one needs, for $\Pi = \vec{V}\vec{V}^\mathsf{T}$ and $\Pi' = \vec{W}\vec{W}^\mathsf{T}$, the numbers

$$p^{-1} J^\mathsf{T} \Pi J \qquad ; \qquad p^{-1} J^\mathsf{T} \Pi \operatorname{diag}(1_{\mathcal{C}_a}) \Pi' J \qquad (1 \leq a \leq k)$$

for $J = [1_{\mathcal{C}_1} \cdots 1_{\mathcal{C}_k}] \in \mathbb{R}^{n \times k}$.

Step 3 : isolated eigenvectors of $\hat{L}'$

- Cauchy Formula :

$$\text{Spectral Projection of } \hat{L}' \text{ on } I \; = \; -\frac{1}{2\mathrm{i}\pi}\oint_{\gamma_I}(\hat{L}' - z)^{-1}\mathrm{d}z$$

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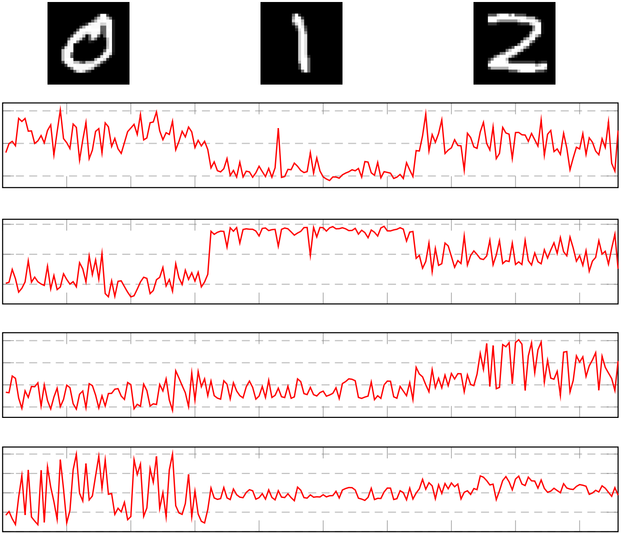
Theorem

The deterministic equivalents of the $k\times k$ matrices

$$p^{-1}J^\mathsf{T}\Pi J \qquad ; \qquad p^{-1}J^\mathsf{T}\Pi\,\mathrm{diag}(1_{\mathcal{C}_a})\Pi' J \qquad (1\le a\le k)$$

can be computed thanks to the parameters and the solutions of the fixed point equations $g_a(z)$, $a=1,\ldots,k$.

Class-wise eigenvector means and fluctuations



: MNIST data : four leading eigenvectors of L (**red**) and theoretical findings (**blue**).

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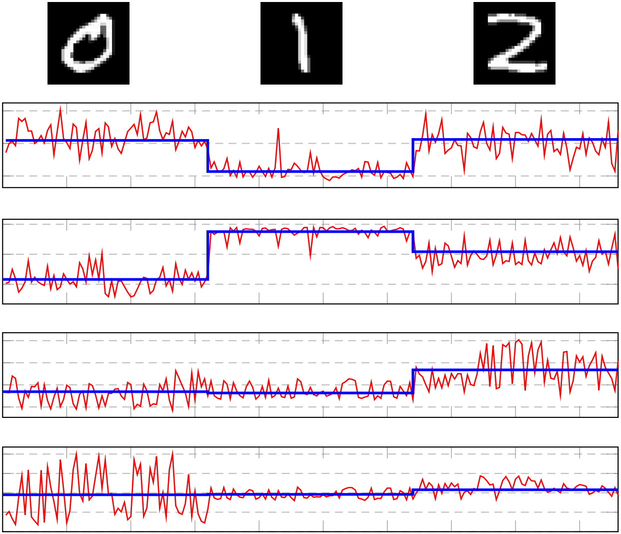

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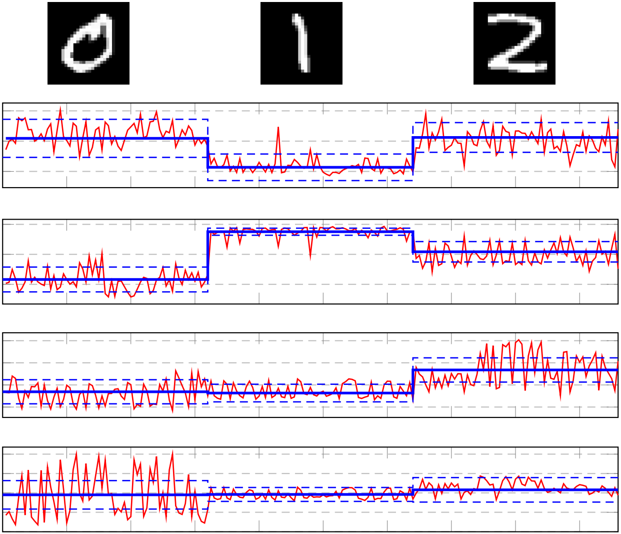

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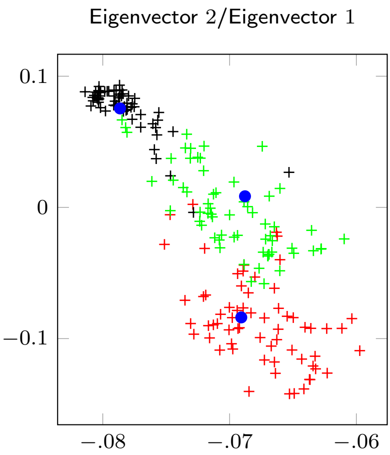
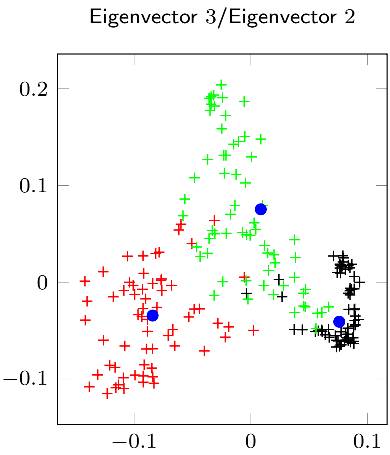
Class-wise means, fluctuations and cross correlations





: 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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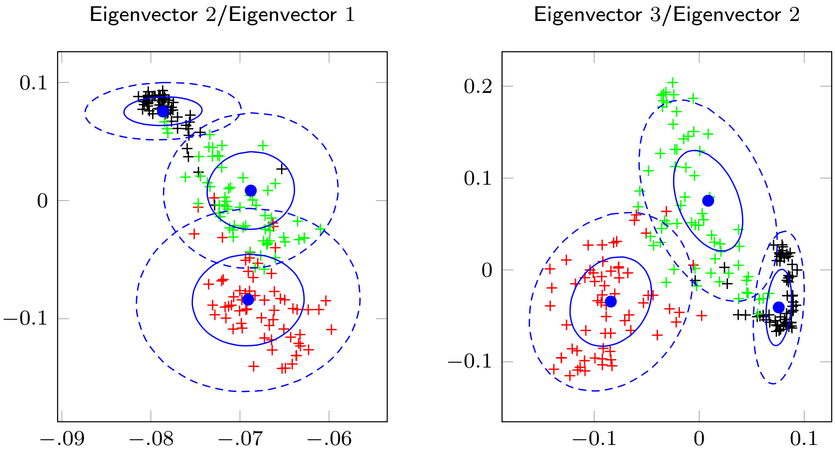

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Perspectives :

- (joint) class-wise eigenvector fluctuations
- implications to spectral clustering performance
- algorithm comparison
- ideally, (data-driven) algorithm improvement.