Accelerated Spectral Clustering Using Graph Filtering of Random Signals

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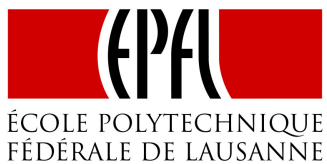
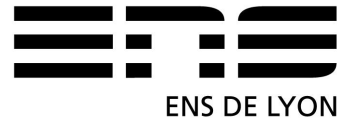
(2) Physics Laboratory, Ens de Lyon, CNRS, France
(3) Signal Processing Laboratory 2, EPFL, Switzerland





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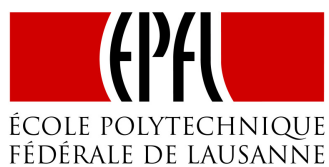
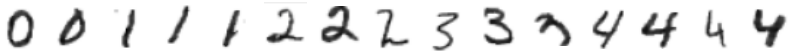
"*Compressive spectral embedding : sidestepping the SVD*", NIPS '15
D. Ramasamy and **U. Madhow**, UC Santa Barbara



What's clustering ?

Given a series of N objects :



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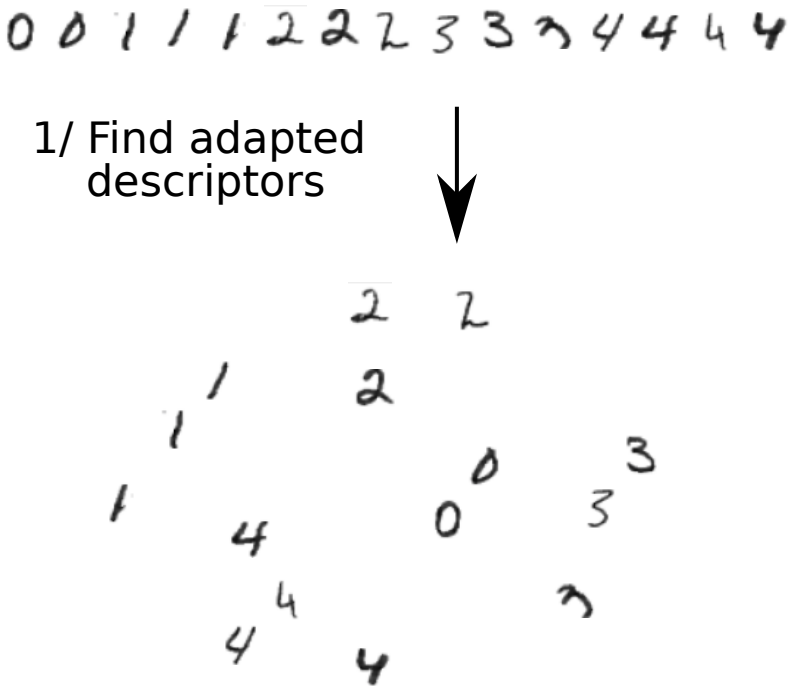

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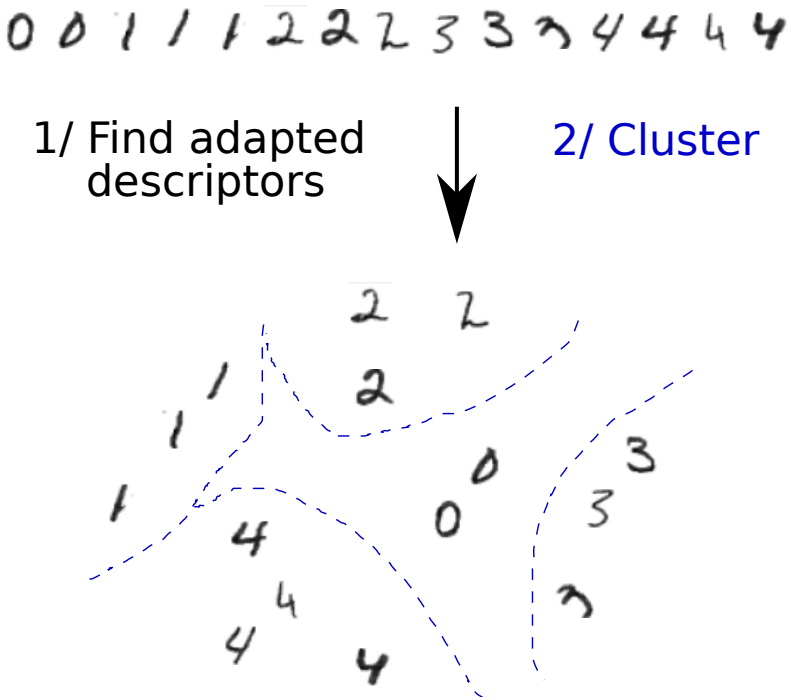

After step 1, one has :

- N vectors in d dimensions (descriptor dimension) :

$$\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_N \in \mathbb{R}^d$$

- and their *distance matrix* $\boldsymbol{\Delta} \in \mathbb{R}^{N \times N}$.

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Goal of clustering : assign a label $c(i) = 1, \cdots, k$ to each object i in order to organize / simplify / analyze the data.

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Goal of clustering : assign a label $c(i) = 1, \cdots, k$ to each object i in order to organize / simplify / analyze the data.

There exists two different general types of methods :

- methods directly based on the $\boldsymbol{x}_i$ and/or $\boldsymbol{\Delta}$ like k-means or hierarchical clustering.
- graph-based methods.

Graph construction from the distance matrix Δ

Create a graph $\mathcal{G} = (V, E)$:

- each node in V is one of the N objects
- each pair of nodes (i, j) is connected if the associated distance $\Delta(i, j)$ is small enough.

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For example, two connectivity possibilities :

- Gaussian kernel :
  1. all pairs of nodes are connected with links of weights $\exp(-\Delta(i, j)/\sigma)$
  2. remove all links of weight inferior to ϵ
- k nearest neighbors : connect each node to its k nearest neighbors.

The problem now states :

Given the graph $\mathcal{G}$ representing the similarity between the N objects, find a partition of all nodes in k clusters.

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Many methods exist [Fortunato '10] :

- Modularity (or other cost-function) optimisation methods [Newman '06]
- Random walk methods [Schaub '12]
- Methods inspired from statistical physics [Krzakala '13], information theory [Rosvall '08]...
- spectral methods
- ...

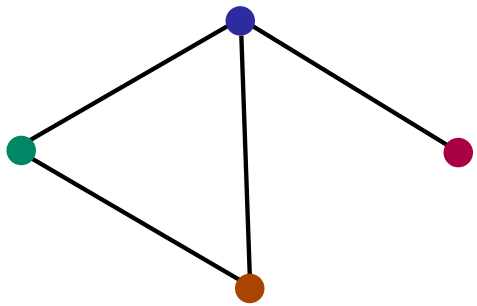
Three useful matrices

The adjacency matrix :

$$W = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

The degree matrix :

$$S = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$



The Laplacian matrix :

$$L = S - W = \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 2 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}$$

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$$W = \begin{bmatrix} 0 & \mathbf{.5} & \mathbf{.5} & 0 \\ \mathbf{.5} & 0 & \mathbf{.5} & \mathbf{4} \\ \mathbf{.5} & \mathbf{.5} & 0 & 0 \\ 0 & \mathbf{4} & 0 & 0 \end{bmatrix}$$

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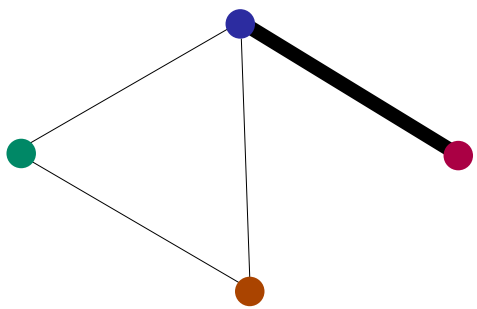

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The classical spectral clustering algorithm [Von Luxburg '06] :

Given the N-node graph $\mathcal{G}$ of laplacian matrix L :

1. Compute L's first k eigenvectors :

$$\mathrm{U}_k = (\boldsymbol{u}_1 | \boldsymbol{u}_2 | \cdots | \boldsymbol{u}_k) .$$

2. Consider each node i as a point in $\mathbb{R}^k$:

$$\boldsymbol{f}_i = \mathrm{U}_k^\top \boldsymbol{\delta}_i .$$

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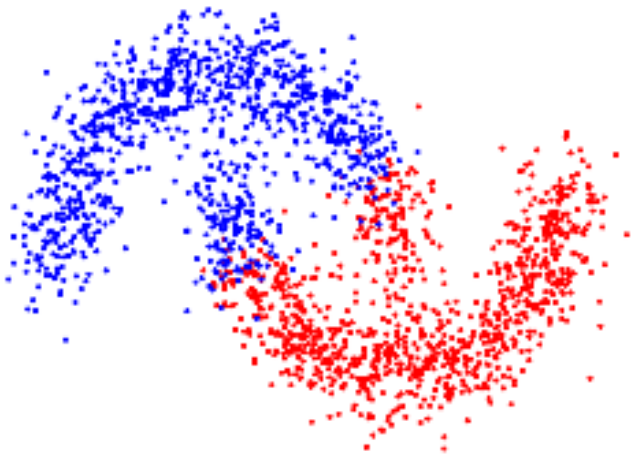
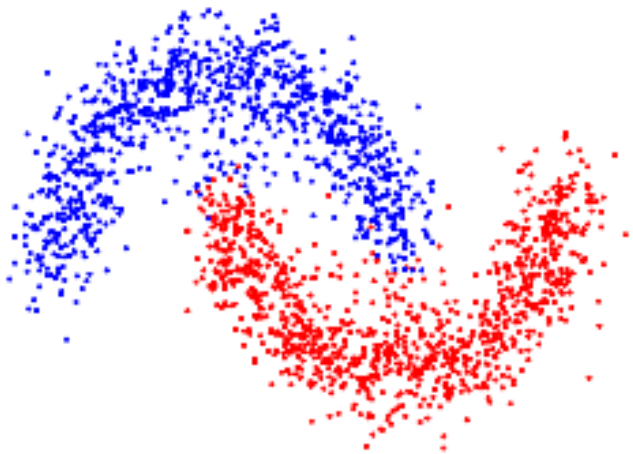
Definition : Let us call D_{ij} the *spectral clustering distance*.

What's the point of using a graph ?

N points in $d = 2$ dims. Result with k-means (k=2) on $\mathbf{\Delta}$:



After creating a graph, partial daigonalisation of L and running k-means (k=2) on $\boldsymbol{D}$:



Overview

Problem : When N and/or k become too large, there are two main bottlenecks in the algorithm :

1. The partial eigendecomposition of the (sparse) Laplacian with restarted Arnoldi method [$O(k^3 + Nk^2 + N\#Ek)$] [Chen '11a]
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Scheme of existing lines of work :

1. approximate U_k : $\tilde{\mathrm{U}}_k$ via power methods [$O(pk\#E)$] [Lin '10, Boutsidis '15] or Nystrom-type methods [$O(n^3 + nN)$] [Fowlkes '04, Wang '09, Chen '11b, . . .].
2. compute approximate feature vectors $\tilde{\boldsymbol{f}}_i = \tilde{\mathrm{U}}_k^\top \boldsymbol{\delta}_i \simeq \boldsymbol{f}_i$.
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Contribution : directly estimate D_{ij} without approximating U_k in $O(m\#E \log N)$.

Filtering random graph signals for clustering

What's graph signal filtering ? [Shuman '13]

$$\boxed{L = S - W = U \Lambda U^\top}$$

- U is the Fourier basis of the graph
- the Fourier transform of a signal f reads : $\boxed{\hat{f} = U^\top f}$
- $\Lambda = \mathrm{Diag}(\lambda_1, \lambda_2, \cdots, \lambda_N)$ the spectrum

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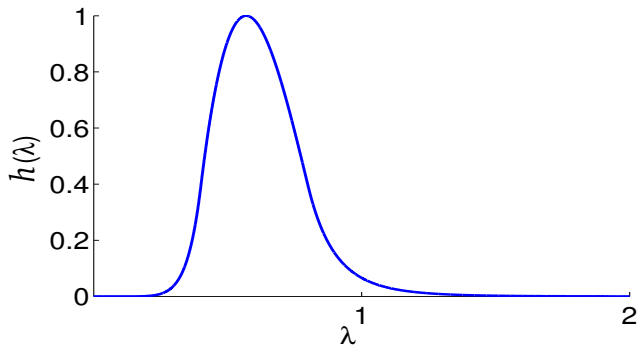
Given a filter function h defined in the Fourier space.



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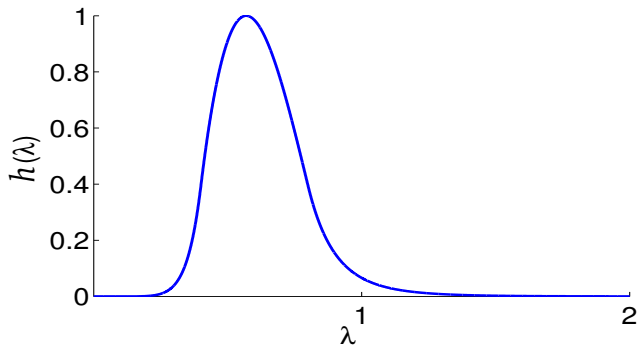


In the node space, the signal f filtered by h reads :

$$\boxed{f^h = \mathrm{U}\, h(\Lambda)\, \mathrm{U}^\top\, f = \mathrm{H}f}$$

So where's the link with clustering ?

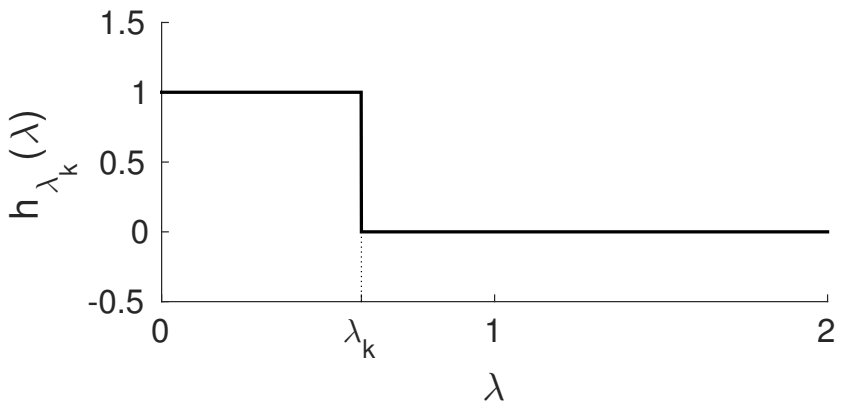
Remember : the classical spectral clustering algorithm

Given the N-node graph $\mathcal{G}$ of adjacency matrix W :

1. Compute L's first k eigenvectors : $\mathrm{U}_k = (\boldsymbol{u}_1|\boldsymbol{u}_2|\cdots|\boldsymbol{u}_k)$.
2. Consider each node i as a point in $\mathbb{R}^k$: $\boldsymbol{f}_i = \mathrm{U}_k^\top \boldsymbol{\delta}_i$.
3. Run k-means with $D_{ij} = ||\boldsymbol{f}_i - \boldsymbol{f}_j||$ and obtain k clusters.

Our goal : Estimate D_{ij} without computing exactly U_k.

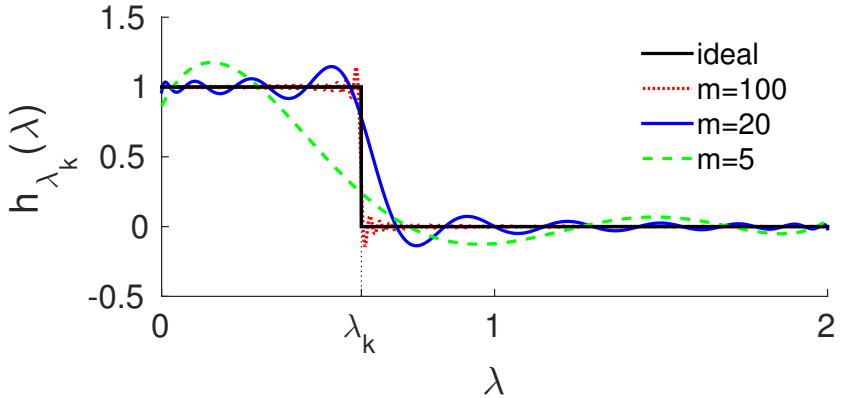
$$
\begin{aligned}
D_{ij} &= \left\| \mathrm{U}_k^\top (\boldsymbol{\delta}_i - \boldsymbol{\delta}_j) \right\| \\
&= \left\| \mathrm{U}_k^\top \boldsymbol{\delta}_{ij} \right\| \\
&= \left\| \mathrm{U}_k \mathrm{U}_k^\top \boldsymbol{\delta}_{ij} \right\| \\
&= \left\| \mathrm{U}\, h_{\lambda_k}(\Lambda)\, \mathrm{U}^\top \boldsymbol{\delta}_{ij} \right\| \\
&= \left\| \mathrm{H}_{\lambda_k} \boldsymbol{\delta}_{ij} \right\| .
\end{aligned}
$$



Fast filtering [Hammond, ACHA '11]

In practice, we use a poly approx of order m of h_{λ_k} :

$$\tilde{h}_{\lambda_k} = \sum_{l=1}^{m} \alpha_l \lambda^l \simeq h_{\lambda_k}.$$



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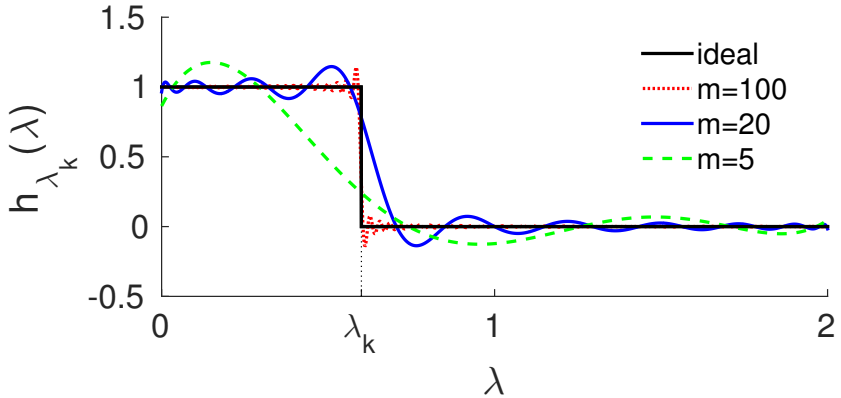

Indeed, in this case, filtering a signal $\boldsymbol{f}$ reads :

$$\mathrm{H}_{\lambda_k}\boldsymbol{f} \simeq \tilde{\mathrm{H}}_{\lambda_k}\boldsymbol{f} = \mathrm{U}\tilde{h}_{\lambda_k}(\Lambda)\mathrm{U}^\top \boldsymbol{f} = \mathrm{U}\sum_{l=1}^{m} \alpha_l \Lambda^l \mathrm{U}^\top \boldsymbol{f} = \sum_{l=1}^{m} \alpha_l \mathrm{L}^l f$$

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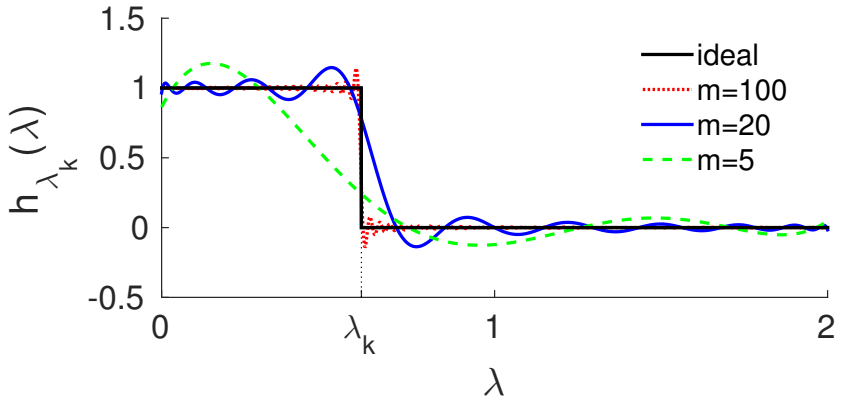

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- Does not require to compute U_k : no partial diagonalisation.
- Only involves matrix-vector multiplications [costs $O(m\#E)$].

Main idea

The spectral distance reads : $\boxed{D_{ij} = \|\mathrm{H}_{\lambda_k}\boldsymbol{\delta}_{ij}\| = \lim_{m\to\infty}\left\|\tilde{\mathrm{H}}_{\lambda_k}\boldsymbol{\delta}_{ij}\right\|}$

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Let $\mathrm{R} = (\boldsymbol{r}_1|\boldsymbol{r}_2|\cdots|\boldsymbol{r}_\eta) \in \mathbb{R}^{N\times\eta}$ be a random Gaussian matrix, i.e. a collection of η random graph signals, with 0 mean and var. $1/\eta$.

$$\boxed{\text{We define } \tilde{\boldsymbol{f}}_i = (\tilde{\mathrm{H}}_{\lambda_k}\mathrm{R})^\top\boldsymbol{\delta}_i \in \mathbb{R}^\eta \text{ and } \tilde{D}_{ij} = \left\|\tilde{\boldsymbol{f}}_i - \tilde{\boldsymbol{f}}_j\right\|}$$

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Norm conservation theorem (case of infinite m)

Let $\epsilon > 0$, if $\eta > \eta_0 \sim \frac{\log N}{\epsilon^2}$, then, with proba $> 1 - 1/N$, we have :

$$\forall (i,j) \in [1,N]^2 \qquad (1-\epsilon)D_{ij} \leq \tilde{D}_{ij} \leq (1+\epsilon)D_{ij}.$$

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Consequence : to estimate D_{ij} with no partial diagonalisation of L, fast filter only $\eta \sim \log N$ random signals !

How to quickly estimate λ_k, the sole unknown of the fast filtering operation ?

Goal : given a SDP L, estimate its k-th eigenvalue as fast as possible.

We use eigencount techniques [Napoli '13] (also based on polynomial filtering of random vectors !) :

- given the interval $[0, b]$, get an approximation of the number of enclosed eigenvalues.
- And find λ_k by dichotomy on b.

Accelerated spectral algorithm

Given the N-node graph $\mathcal{G}$ of adjacency matrix W :

Inputs : k, polynomial order m, # random signals $\eta \sim \log N$.

1. Estimate λ_k, the k-th eigenvalue of L.
2. Generate η random graph signals in matrix $\mathrm{R} \in \mathbb{R}^{N \times \eta}$.
3. Filter them with $\tilde{\mathrm{H}}_{\lambda_k}$ and treat each node i as a point in $\mathbb{R}^{\eta}$:

$$\tilde{\boldsymbol{f}}_i^{\top} = \boldsymbol{\delta}_i^{\top} \tilde{\mathrm{H}}_{\lambda_k} \mathrm{R}.$$

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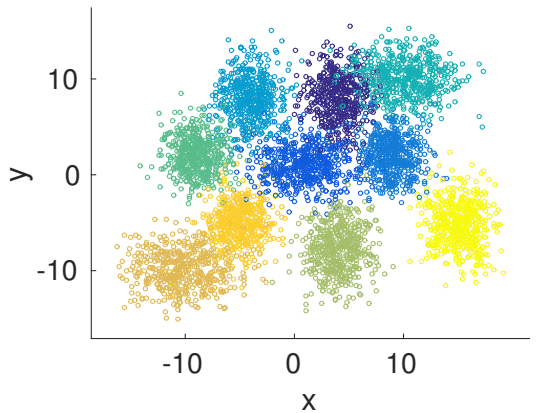
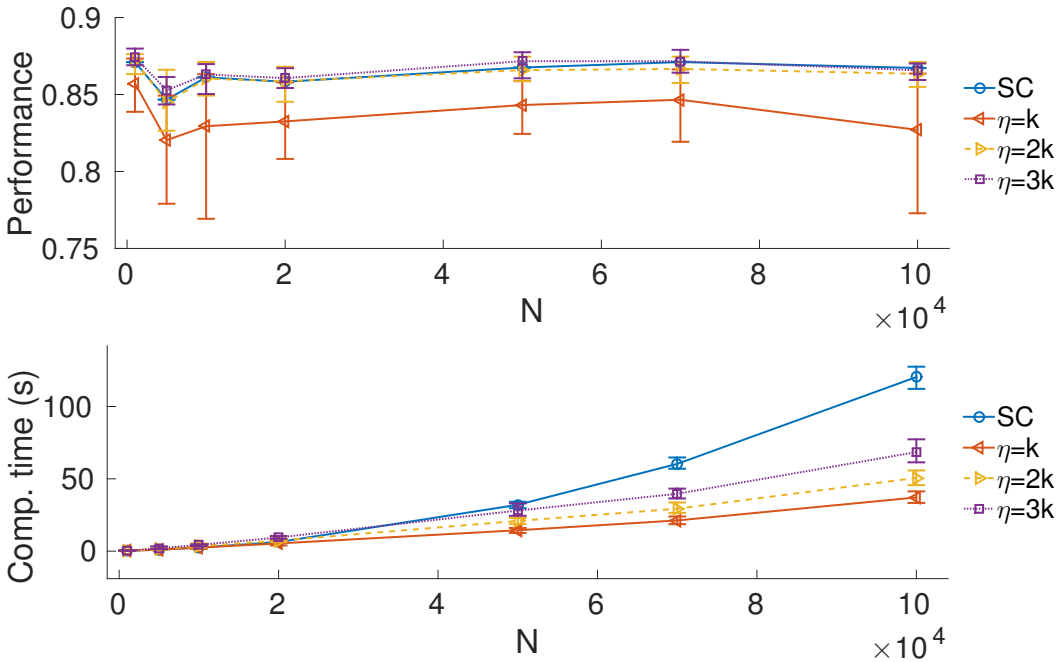
Computing the features (steps 1 to 3) costs $O(m\#E \log N) \simeq O(mN \log N)$.

Toy experiment

Gaussian data around 10 centroids :





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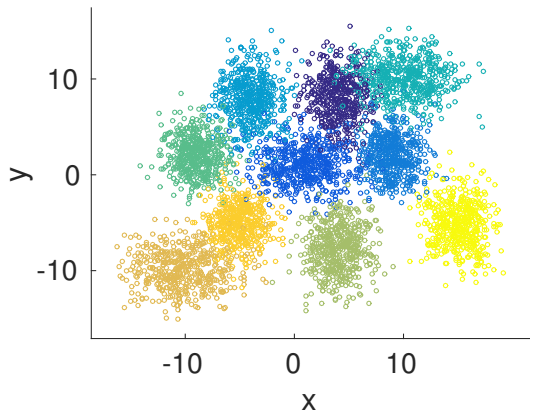

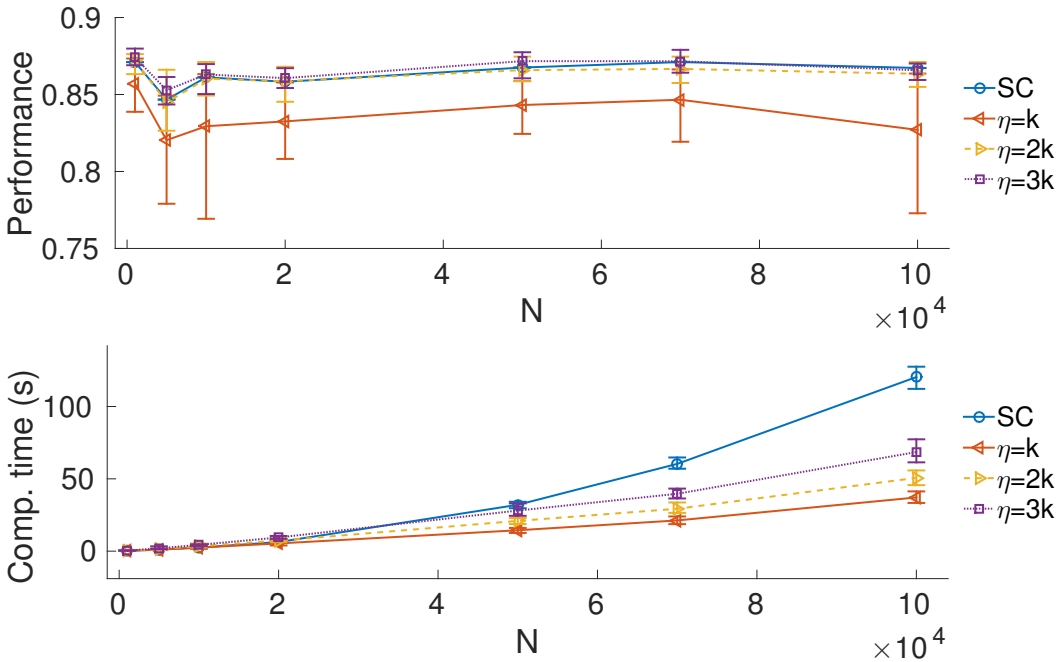

Example : $N = 10^5, k = 10$: filtering only $\eta = 20$ random signals gives same performance... 3x faster.

Main idea of this paper

Low-pass graph fast filtering of random signals : a way to by-pass the Laplacian's diagonalisation for learning tasks.

Ideas surrounding this paper : *compressive* spectral clustering [arXiv : Tremblay '16, Puy '15]

1. **Cluster indicator functions are k-bandlimited signals on the graph** : they can be recovered after appropriate sampling schemes ! 1/ Compute features, 2/ Sample a few nodes, 3/ Run low-dimensional k-means, 4/ Interpolate
2. **Norm conservation theorem for finite polynomial order m**
3. **Generalisation to the use of the normalized Laplacian** (but not the random walk Laplacian yet)

Perspectives and difficult questions

Two difficult questions (among others) :

1. Given a SDP matrix, how to estimate as fast as possible its k-th eigenvalue, and only that one ?
2. How to choose automatically the appropriate polynomial order m ?

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Perspectives

1. Rational filters instead of polynomial filters ? [Shi '15b]
2. How about if nodes are added one by one ?

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