Graph signal processing for clustering

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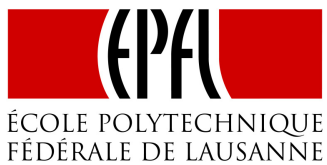
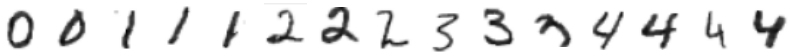


What's clustering ?

Given a series of N objects :



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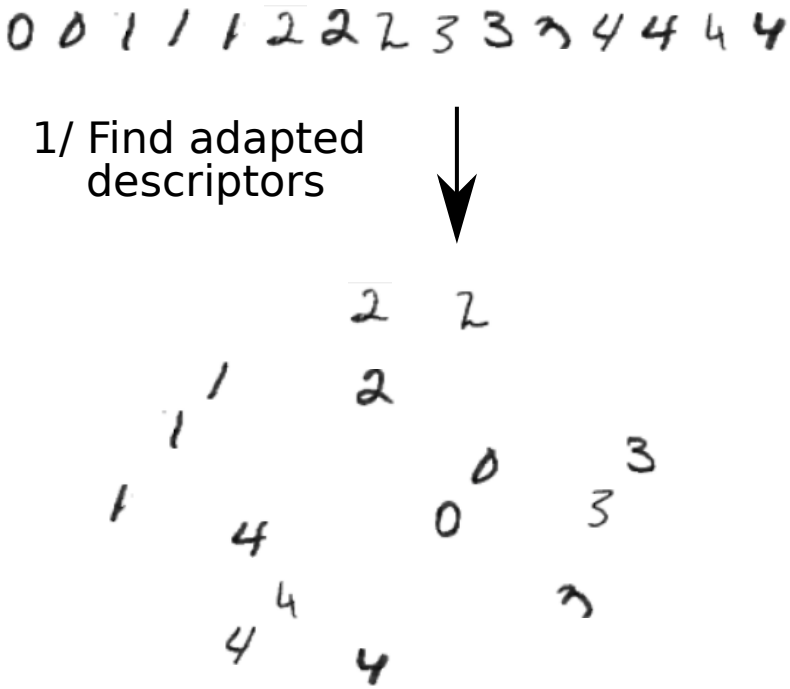

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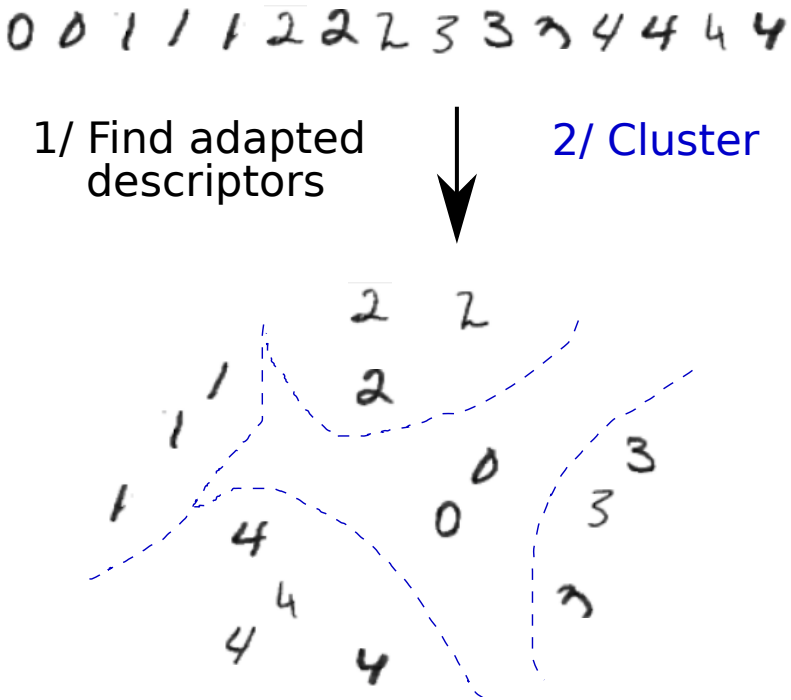

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- graph-based methods.

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- k nearest neighbors : connect each node to its k nearest neighbors.

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Many methods exist [Fortunato '10] :

- Modularity (or other cost-function) optimisation methods [Newman '04]
- Random walk methods [Delvenne '10]
- Methods inspired from statistical physics [Krzakala '12], information theory [Rosvall '07]...
- spectral methods
- ...

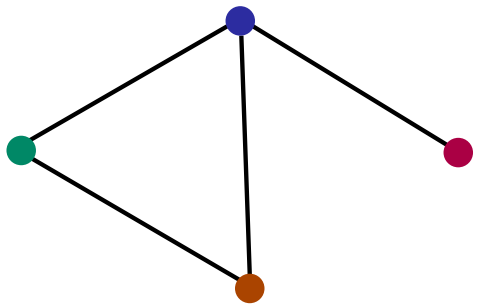
Three useful matrices

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 :

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



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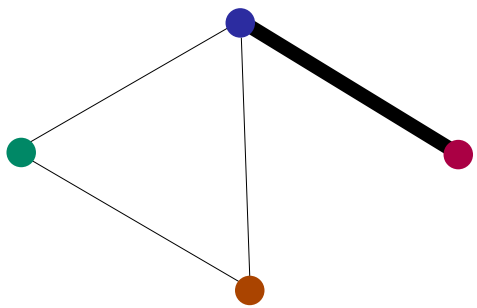

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The classical spectral clustering algorithm [Von Luxburg '06] :

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

1. Compute :

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

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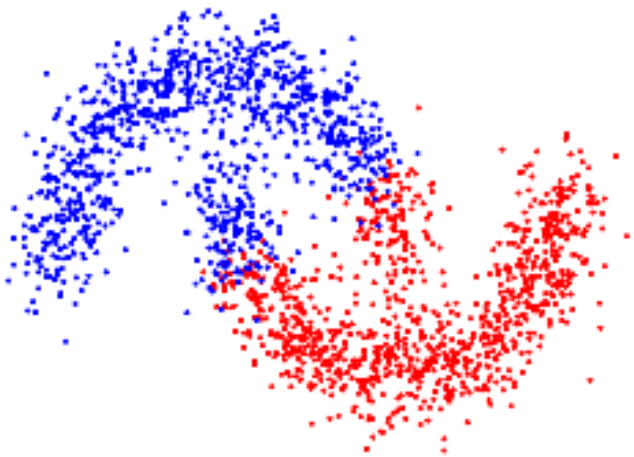
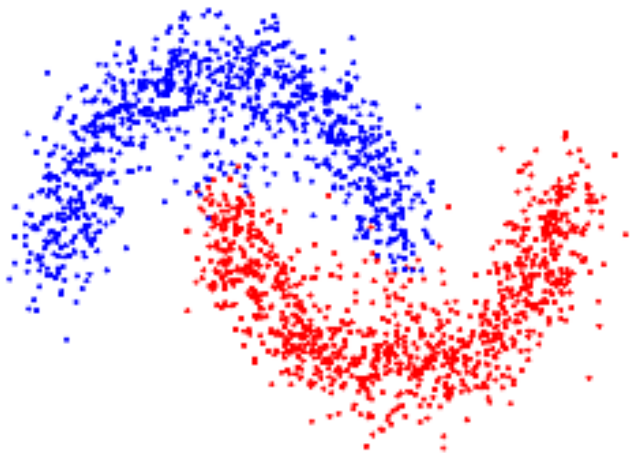
2. Consider each node i as a point in $\mathbb{R}^k$:
$$\boldsymbol{f}_i = \mathrm{U}_k^\top \boldsymbol{\delta}_i.$$
3. Run k-means with the Euclidean distance : $D_{ij} = ||\boldsymbol{f}_i - \boldsymbol{f}_j||$ and obtain k clusters.

What's the point of using a graph ?

N points in $d = 2$ dimensions.
Result with k-means (k=2) :



After creating a graph from the N points' interdistances, and running the spectral clustering algorithm (with k=2) :



Computation bottlenecks of the spectral clustering algorithm

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

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Our goal :

Circumvent both !

What's graph signal processing ?

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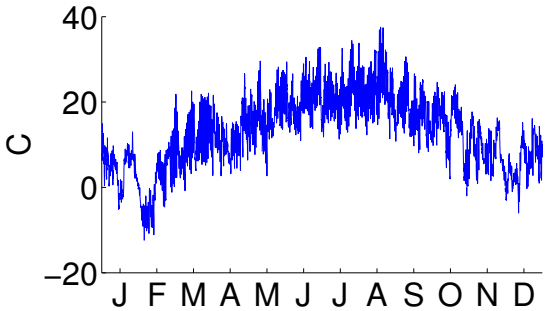

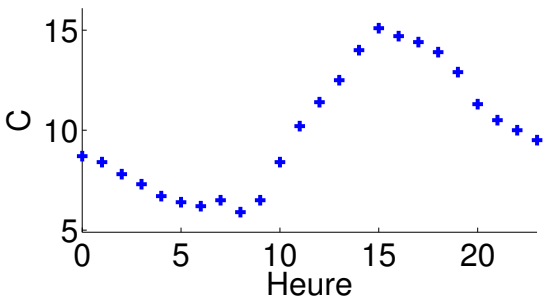

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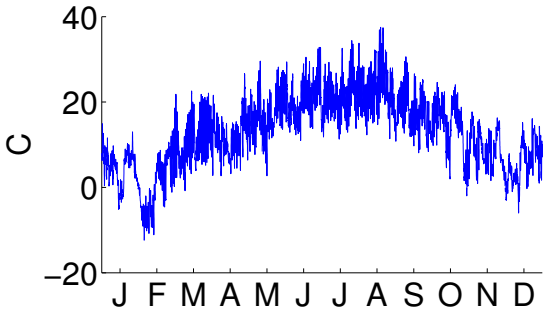

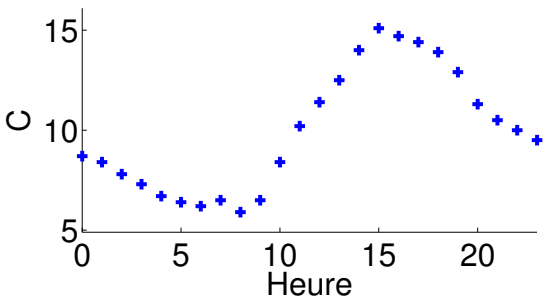

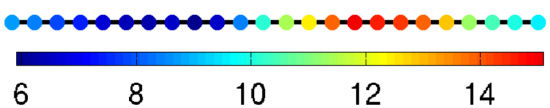

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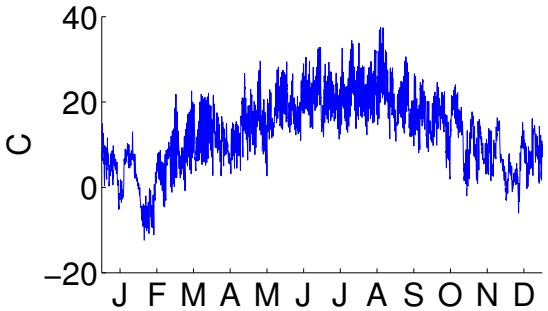

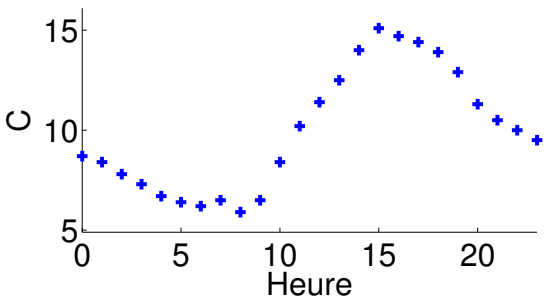

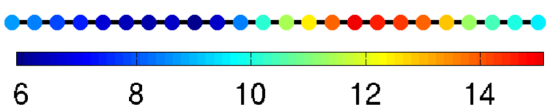

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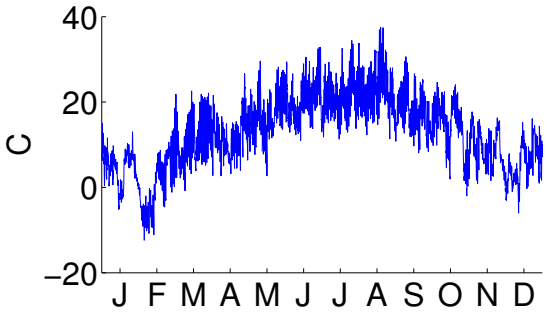

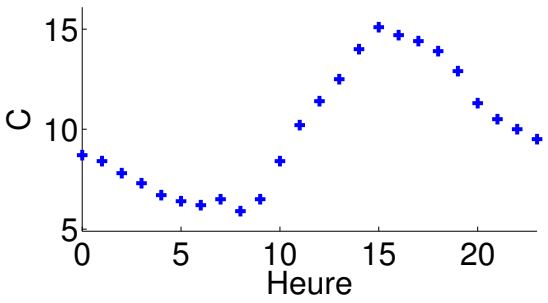

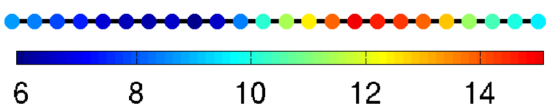

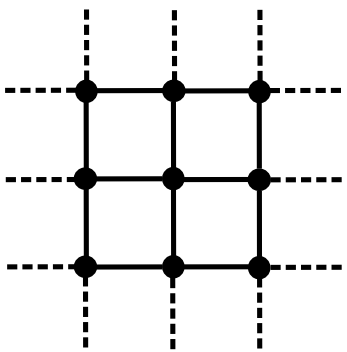

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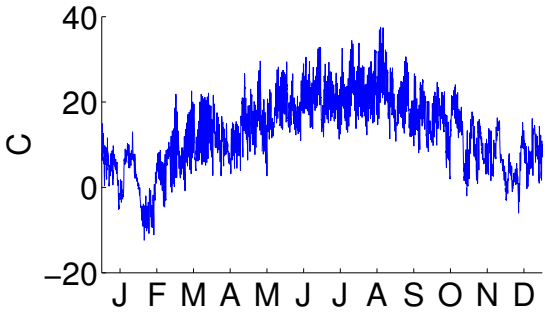

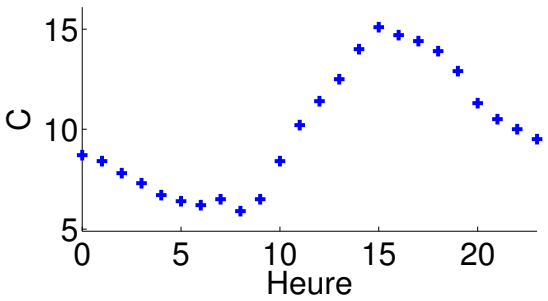

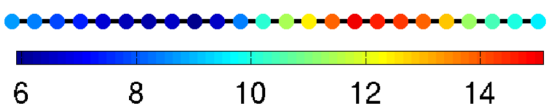

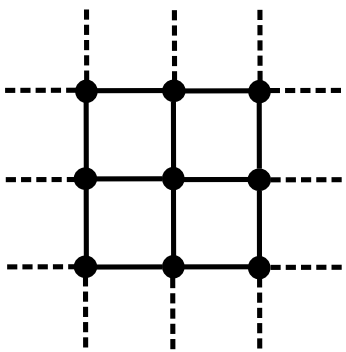

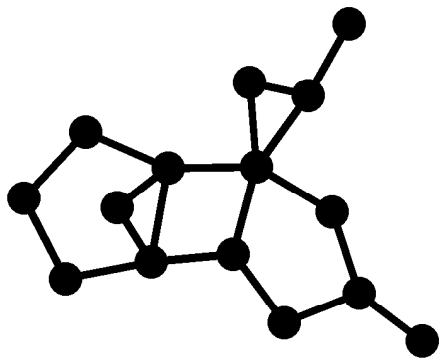

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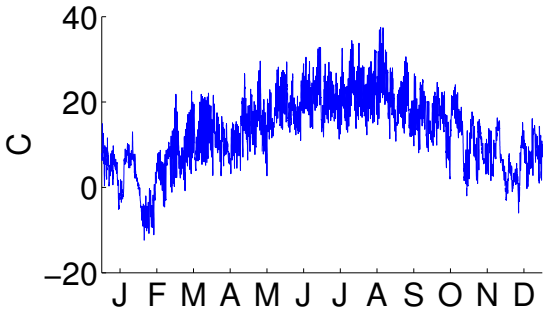
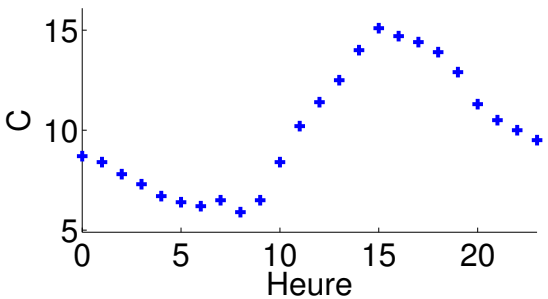
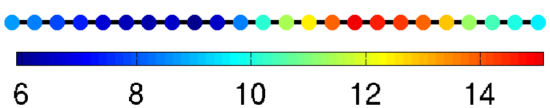
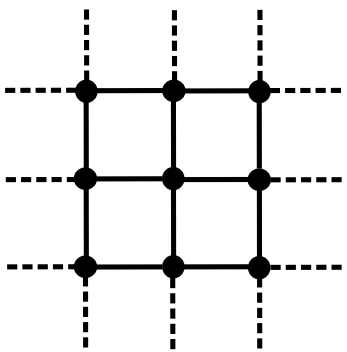
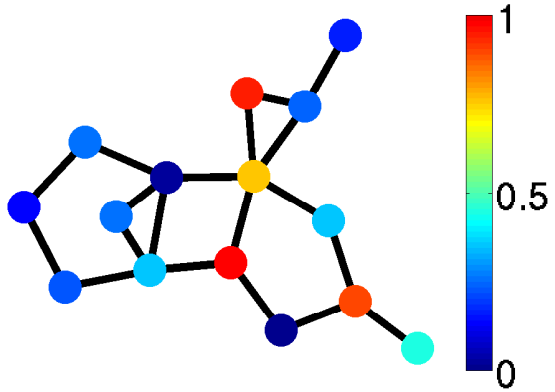
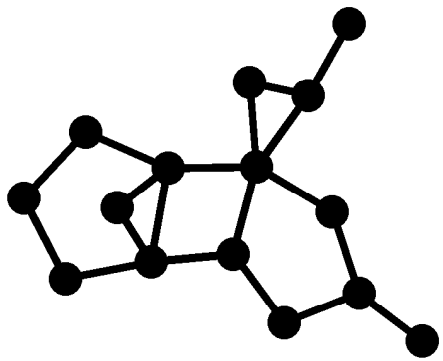








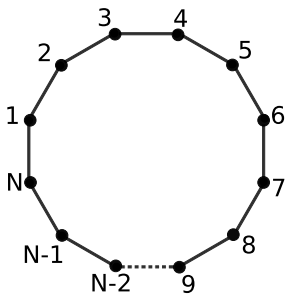




What's the graph Fourier matrix ?

[Hammond '11]

THE "CLASSICAL" GRAPH :



$$L_{cl} = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ -1 & 0 & 0 & \cdots & -1 & 2 \end{bmatrix}$$

All classical Fourier modes are the eigenvectors of L_{cl}

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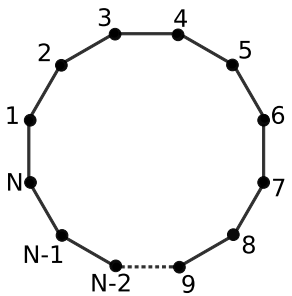
The "classical" graph :



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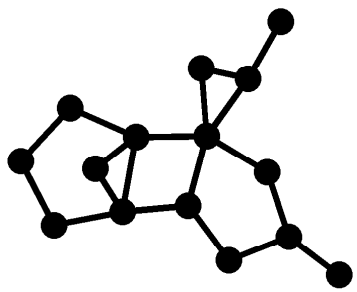


L

By analogy, any graph's Fourier modes are the eigenvectors of its Laplacian matrix L.

The graph Fourier matrix

$$\boxed{L = S - W}$$

Its eigenvectors :

$$U = (\boldsymbol{u}_1 | \boldsymbol{u}_2 | \cdots | \boldsymbol{u}_N)$$

form the graph Fourier orthonormal basis.

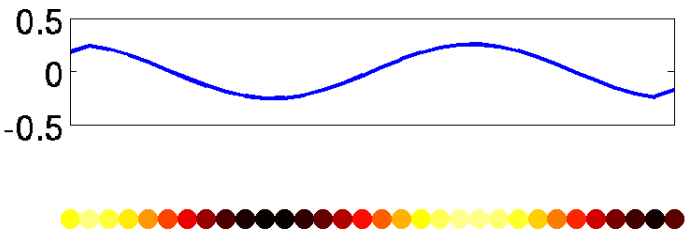
Its eigenvalues :

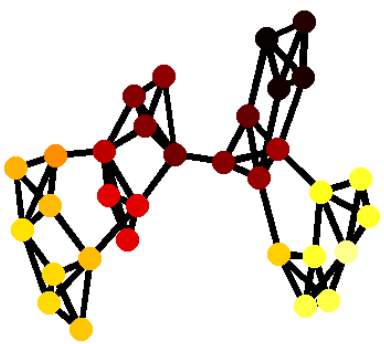
$$0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$$

represent the graph frequencies. λ_i is the squared frequency associated to the Fourier mode $\boldsymbol{u}_i$.

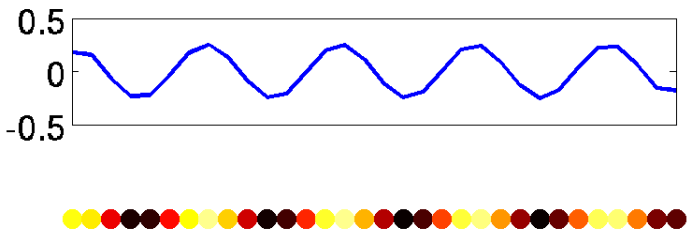
Illustration

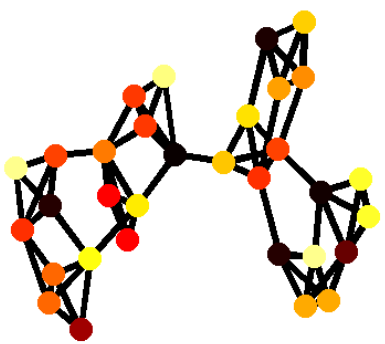
Low frequency :





High frequency :





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- Inversely, the inverse Fourier transform reads :

$$\boxed{f = \mathrm{U}\,\hat{f}}$$

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- given $f \in \mathbb{R}^N$ a signal on a graph of size N.
- $\hat{f}$ is obtained by decomposing f on the eigenvectors $\boldsymbol{u}_i$:

$$\hat{f} = \begin{pmatrix} < \boldsymbol{u}_1, f > \\ < \boldsymbol{u}_2, f > \\ < \boldsymbol{u}_3, f > \\ \dots \\ < \boldsymbol{u}_N, f > \end{pmatrix}, \text{ i.e. } \boxed{\hat{f} = \mathrm{U}^\top f}$$

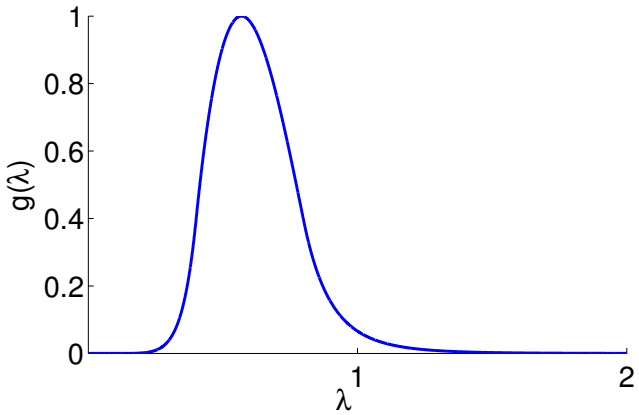
- Inversely, the inverse Fourier transform reads :

$$\boxed{f = \mathrm{U}\,\hat{f}}$$

- The Parseval theorem stays valid : $\forall (g, h) \; < g, h > = < \hat{g}, \hat{h} >$

Filtering

Given a filter function g defined in the Fourier space.



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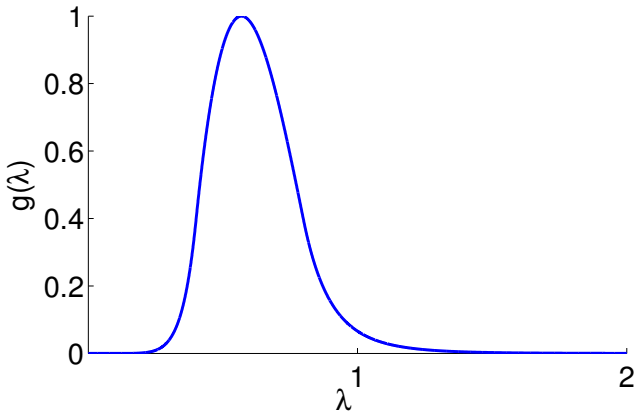

In the Fourier space, the signal filtered by g reads :

$$\hat{f}^g = \begin{pmatrix} \hat{f}(1)\, g(\lambda_1) \\ \hat{f}(2)\, g(\lambda_2) \\ \hat{f}(3)\, g(\lambda_3) \\ \dots \\ \hat{f}(N)\, g(\lambda_N) \end{pmatrix} = \hat{\mathrm{G}}\, \hat{f} \text{ with } \hat{\mathrm{G}} = \begin{pmatrix} g(\lambda_1) & 0 & 0 & \dots & 0 \\ 0 & g(\lambda_2) & 0 & \dots & 0 \\ 0 & 0 & g(\lambda_3) & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & g(\lambda_N) \end{pmatrix}$$

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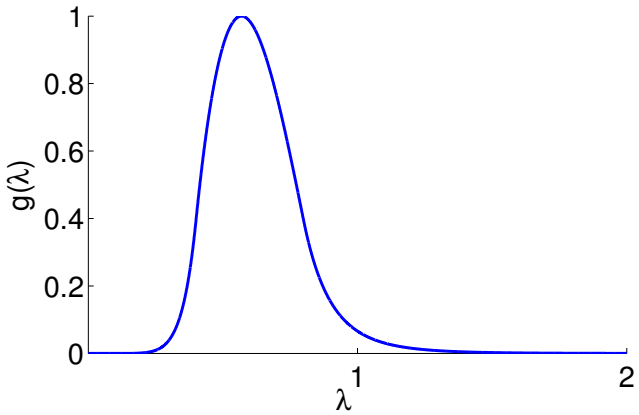

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In the node space, the filtered signal f^g reads therefore :

$$\boxed{f^g = \mathrm{U}\, \hat{\mathrm{G}}\, \mathrm{U}^\top f = \mathrm{G} f}$$

So where's the link ?

Remember : the classical spectral clustering algorithm

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

1. Compute :
$$\mathrm{U}_k = (\boldsymbol{u}_1|\boldsymbol{u}_2|\cdots|\boldsymbol{u}_k)$$
the first k eigenvectors of $\mathrm{L} = \mathrm{S} - \mathrm{W}$.
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 the Euclidean distance : $D_{ij} = ||\boldsymbol{f}_i - \boldsymbol{f}_j||$ and obtain k clusters.

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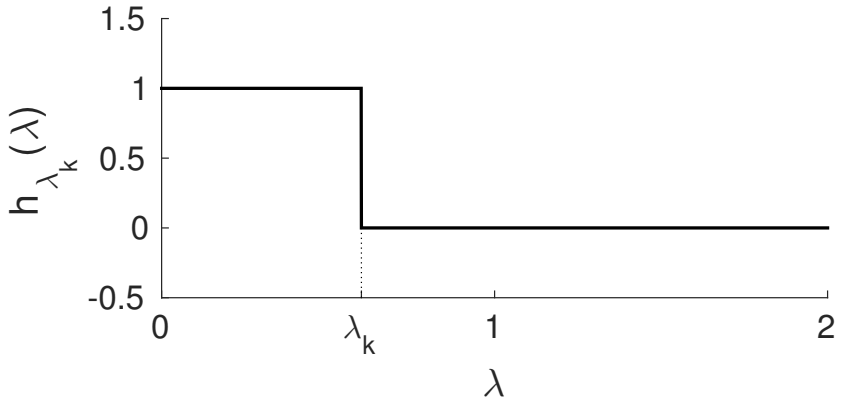
Let's work on the first bottleneck : estimate D_{ij} without partially diagonalizing the Laplacian matrix.

Ideal low-pass filtering

1st step : assume we know U_k and λ_k

Given h_{λ_k} an ideal LP, $H_{\lambda_k} = U\hat{H}_{\lambda_k}U^\top = U_k U_k^\top$ is its filter matrix.



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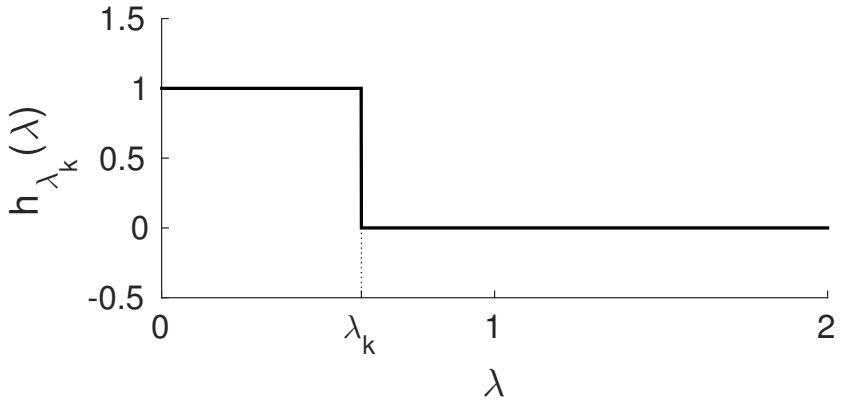

Let $R = (\boldsymbol{r}_1|\boldsymbol{r}_2|\cdots|\boldsymbol{r}_\eta) \in \mathbb{R}^{N\times\eta}$ be a random Gaussian matrix.
We define $\tilde{\boldsymbol{f}}_i = (H_{\lambda_k}R)^\top \boldsymbol{\delta}_i \in \mathbb{R}^\eta$ and $\tilde{D}_{ij} = ||\tilde{\boldsymbol{f}}_i - \tilde{\boldsymbol{f}}_j||$.

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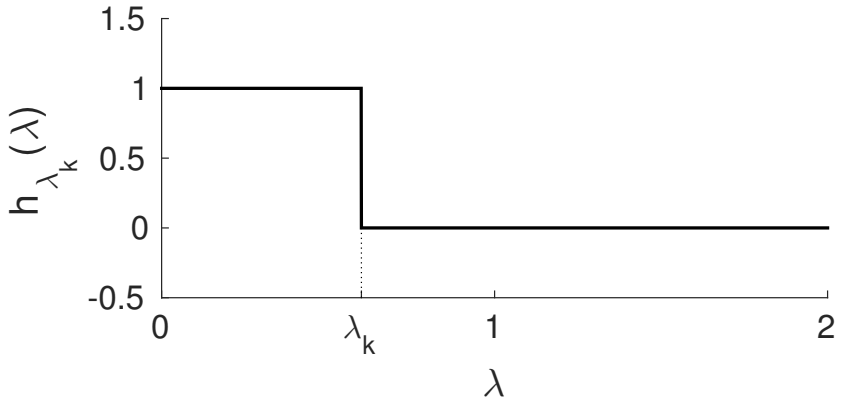

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Norm conservation theorem for ideal filter

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

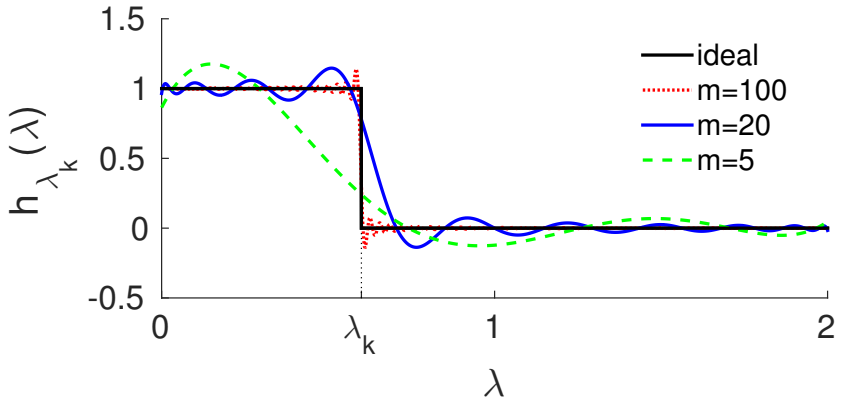
$$\forall (i,j) \in [1,N]^2 \qquad (1-\epsilon)D_{ij} \leq \tilde{D}_{ij} \leq (1+\epsilon)D_{ij}.$$

Non-ideal low-pass filtering

2nd step : assume all we know is λ_k

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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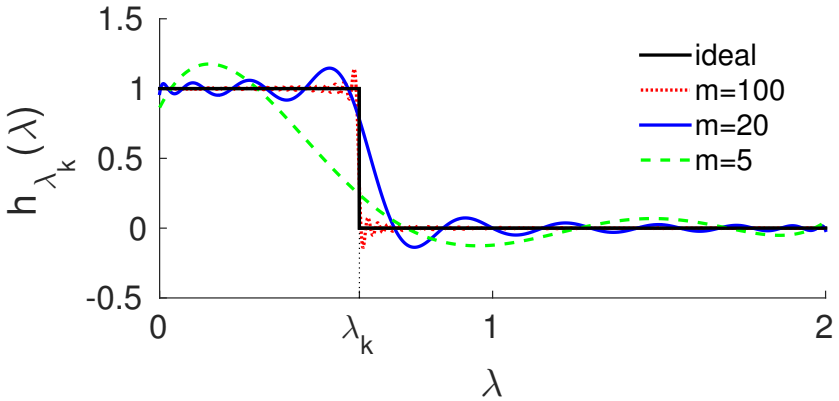

Indeed, in this case, filtering a vector $\boldsymbol{x}$ reads :

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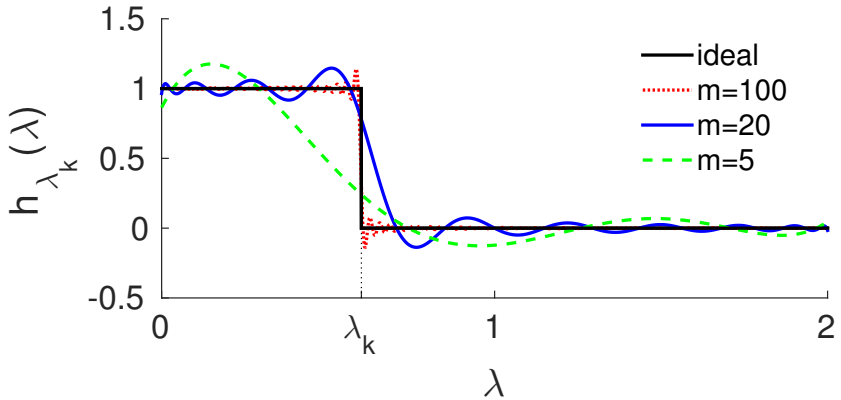

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The theorem stays (more or less) valid with this non-ideal filtering !

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We use eigencount techniques (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.

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Let's work on the second bottleneck : avoid k-means in possibly very large dimension N (step 4).

Fast spectral algorithm ?

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

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4. Sample randomly $\rho \simeq k \log k << N$ nodes out of N :

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

5. Run k-means in this reduced space with the Euclidean distance : $\tilde{D}_{ij}^r = ||\tilde{\boldsymbol{f}}_i^r - \tilde{\boldsymbol{f}}_j^r||$ and obtain k clusters.
6. Interpolate cluster indicator functions $\boldsymbol{c}_l^r$ on the whole graph :

$$\tilde{\boldsymbol{c}}_l = \arg \min_{\boldsymbol{x} \in \mathbb{R}^N} ||\mathrm{M}\boldsymbol{x} - \boldsymbol{c}_l^r||^2 + \mu \boldsymbol{x} \mathrm{L}^{\top} \boldsymbol{x}.$$

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4. interpolate the cluster indicator vectors back to the complete graph.

This work was done in collaboration with :

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Part of this work has been published (or submitted) :

- Circumventing the first bottleneck has been accepted to ICASSP 2016
- Interpolation of k-bandlimited graph signals has been submitted to ACHA in November (an application of which helps us circumvent the second bottleneck).

Perspectives and difficult questions

Two difficult questions (among others) :

1. Given a semi-definite positive matrix, how to estimate as fast as possible its k-th eigenvalue, and only that one ?
2. How to subsample ρ nodes out of N while ensuring that clustering them in k classes is the result one would have obtained by clustering all N nodes ?

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Perspectives

1. How about if nodes are added one by one ?
2. Rational filters instead of polynomial filters ?
3. Approximating other spectral clustering algorithms ?