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CR16: Signal Processing and Networks Data analysis and processing for networks

# Part 1 - Data, signal and image processing on graphs using spectral theory

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## Overview of the lecture

- General objective: revisit classical data analysis techniques (most used in signal and image processing) in the context of discrete structures such as networks and signals defined on graphs.
- The things we will discuss:
  - Introduce you to the emerging field of graph signal & image processing
  - Basic of spectral analysis of graphs, and on the graph Laplacian
  - Harmonic analysis on graphs: wavelets
  - Examples: denoising on graphs; communities;...
- Organization:
  - 1. This introduction with several examples
  - 2. Spectral analysis of the Laplacian; properties
  - 3. Spectral graph Fourier transform, operators and wavelets
  - 4. Laplacian pyramid, graph downsampling; applications

## Introduction: on signals and graphs

- **My own bias**: I work in the SISYPHE (Signal, Systems and Physics) group in statistical signal processing, located in the Physics Laboratory of ENS de Lyon
- I have worked also on Internet traffic analysis, and on studies of complex systems
- Strong bias: nonstationary and/or multiscale approaches
- Hence, I will talk about

### data analysis and processing for network

• Examples of topics that we study:

Technological networks (Internet, mobile phones, sensor networks,...)

Social networks; Transportation networks (Vélo'v) Biosignals: Human brain networks; genomic data; ECG

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Introduction

## Introduction: on signals and graphs

Why data analysis and processing is useful for networks?

- Many examples of data having both labels or values ("signals") and relational properties (graphs)
- Non-trivial estimation issues (e.g., non repeated measures; variables with large distributions (or power-laws); ...) → advanced statistical approaches
- large networks

 $\rightarrow$  multiscale approaches

dynamical networks

 $\rightarrow$  nonstationary methods



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## Examples of networks from our digital world



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## Examples of graph signals





**USA** Temperature



Color Point Cloud



### fcMRI Brain Network



Image Database

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### Typical problems [P. Vandergheynst, EPFL, 2013]

#### Compression / Visualization



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# Recovery of signals on graphs [P. Vandergheynst, EPFL, 2013]

• Denoising of a signal with Tikhonov regularization

$$\arg\min_{f} ||f - y||_2^2 + \gamma f^\top L f$$



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## Writing Tikhonov denoising as a Graph filter [P. Vandergheynst, EPFL, 2013]

It is easy to solve this regularization problem in the spectral domain

$$\arg\min_{f} \frac{\tau}{2} ||f - y||_{2}^{2} + f^{\top} L f \Rightarrow L f_{*} + \frac{\tau}{2} (f_{*} - y) = 0$$

Move to the spectral domain of the Laplacian

$$\widehat{Lf}_{*}(i) + \frac{\tau}{2}(\widehat{f}_{*}(i) - \widehat{y}(i)) = 0, \quad \forall i \in \{0, 1, ..., N-1\}$$

• Solution:

$$\hat{f}_*(i) = \frac{\tau}{\tau + 2\lambda_i} \hat{y}(i)$$

• This is a 1st-order "low pass" filtering

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### Recovery of signals on graphs [P. Vandergheynst, EPFL, 2013]

Limit of Tikhonov regularization

$$\arg\min_{f} ||f - y||_2^2 + \gamma f^\top L f$$



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## Recovery of signals on graphs [P. Vandergheynst, EPFL, 2013]

### • Denoising of a signal with Wavelet regularization

$$\arg\min_{a} ||W^{\top}a - y||_{2}^{2} + \gamma ||a||_{1}$$



Wavelets will be described later on in the lectures... Stay tuned.

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# Generalized translations

[Shuman, Ricaud, Vandergheynst, 2014]

Classical translation:

$$(\mathcal{T}_{ au}g)(t)=g(t- au)=\sum_{\mathbb{R}}\hat{g}(\xi)e^{-i2\pi au\xi}e^{-i2\pi t\xi}d\xi$$

• Graph translations by fundamental analogy:

$$(T_n f)(a) = \sum_{i=0}^{N-1} \hat{f}(i)\chi_i^*(n)\chi_i(a)$$

· Example on the Minnesota road networks





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## Empirical mode decomposition on graphs

 Objective: decompose a graph signal in various "elementary" modes in a data-driven and non stationary approach



[N. Tremblay, P. Flandrin, P. Borgnat, 2014]

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# Fourier transform of signals

### "Signal processing 101"

The Fourier transform is of paramount importance: Given a times series  $x_n$ , n = 1, 2, ..., N, let its Discrete Fourier Transform (DFT) be

$$\forall k \in \mathbb{Z} \quad \hat{x}_k = \sum_{n=0}^{N-1} x_n e^{-i2\pi k n/N}$$

### Why?

- Inversion:  $x_n = \frac{1}{N} \sum_{k=0}^{N-1} \hat{x}_k e^{-i2\pi kn/N}$
- Best domain to define Filtering (operator is diagonal)
- Definition of the **Spectral analysis** (FT of the autocorrelation)
- Alternate representation domains of signals are useful: Fourier domain, DCT, time-frequency representations,
- <sup>p. 14</sup> wavelets, chirplets,...

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# Spectral analysis of networks

### Spectral theory for network

This is the study of graphs through the **spectral analysis** (eigenvalues, eigenvectors) of matrices **related to the graph**: the adjacency matrix, the Laplacian matrices,....

### Notations

$$\mathcal{G} = (V, E, w)$$

$$N = |V|$$

$$A$$

$$d$$

$$D$$

$$f$$

a weighted graph number of nodes adjacency matrix vector of strengths matrix of strengths signal (vector) defined on V

$$egin{aligned} & A_{ij} = w_{ij} \ d_i = \sum_{j \in V} w_{ij} \ D = diag(d) \end{aligned}$$

Relating the Laplacian of graphs to Signal Processing

### Laplacian matrix

L or $\mathscr{L}$	laplacian matrix	L = D - A
$(\lambda_i)$	L's eigenvalues	$0 = \lambda_0 < \lambda_1 \le \lambda_2 \le \dots \le \lambda_{N-1}$
$(\chi_i)$	L's eigenvectors	$L \chi_i = \lambda_i \chi_i$

### A simple example: the straight line

For this regular line graph, *L* is the 1-D classical laplacian operator (i.e. double derivative operator):

its eigenvectors are the Fourier vectors, and its eigenvalues the associated (squared) frequencies

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A fundamental analogy [Shuman et al., *IEEE SP Mag*, 2013]

# Objective: Definition of a Fourier Transform adapted to graph signals

f: signal defined on V  $\leftrightarrow \hat{f}$ : Fourier transform of f

### Fundamental analogy

On *any* graph, the eigenvectors  $\chi_i$  of the Laplacian matrix *L* will be considered as the Fourier vectors, and its eigenvalues  $\lambda_i$  the associated (squared) frequencies.

- Works exactly for all regular graphs (+ Beltrami-Laplace)
- Conduct to natural generalizations of signal processing

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# The graph Fourier transform

•  $\hat{f}$  is obtained from *f*'s decomposition on the eigenvectors  $\chi_i$ :

$$\hat{f} = \begin{pmatrix} <\chi_0, f > \\ <\chi_1, f > \\ <\chi_2, f > \\ \dots \\ <\chi_{N-1}, f > \end{pmatrix}$$

Define 
$$\boldsymbol{\chi} = (\chi_0 | \chi_1 | ... | \chi_{N-1}) : \widehat{\boldsymbol{f}} = \boldsymbol{\chi}^\top \boldsymbol{f}$$

- Reciprocally, the inverse Fourier transform reads:  $|f = \chi \hat{f}|$

 The Parseval theorem is valid:  $\forall (q,h) < q, h > = < \hat{q}, \hat{h} >$ 

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Fourier modes: examples in 1D and in graphs

LOW FREQUENCY:

HIGH FREQUENCY:









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## More Fourier modes





## Alternative fundamental spectral correspondance

With the Normalized Laplacian matrix

 $\mathscr{L} = I - D^{-1/2} A D^{-1/2}$ 

- Related to Ng. et al. normalized spectral clustering
- Good for degree heterogeneities
- Related to random walks
- For community detection
- With the random-walk Laplacian matrix (non symmetrized)

$$L_{rw} = D^{-1}L = I - D^{-1}W$$

- Better related to random walks
- Used by Shi-Malik spectral clustering (and graph cuts)
- Using the Adjacency matrix
  - Wigner semi-circular law
  - Discrete Signal Processing in Graphs (good for undirected graphs) [Sandryhaila, Moura, *IEEE TSP*, 2013]

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## Filtering

### Definition of graph filtering

We define a filter function g in the Fourier space. It is discrete and defined on the eigenvalues  $\lambda_i \rightarrow g(\lambda_i)$ .

$$\hat{f}^{g} = \begin{pmatrix} \hat{f}(0) g(\lambda_{0}) \\ \hat{f}(1) g(\lambda_{1}) \\ \hat{f}(2) g(\lambda_{2}) \\ \dots \\ \hat{f}(N-1) g(\lambda_{N-1}) \end{pmatrix} = \hat{G} \hat{f} \text{ with } \hat{G} = \begin{pmatrix} g(\lambda_{0}) & 0 & 0 & \dots & 0 \\ 0 & g(\lambda_{1}) & 0 & \dots & 0 \\ 0 & 0 & g(\lambda_{2}) & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & g(\lambda_{N-1}) \end{pmatrix}$$

In the node-space, the filtered signal  $f^g$  can be written:  $f^g = \chi \, \hat{\mathbf{G}} \, \chi^{ op} \, f$ 

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### For a graph with multiscale structure

### finest scale (16 com.):



fine scale (8 com.):



coarser scale (4 com.):



coarsest scale (2 com.):



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### Spectral analysis: the $\chi_i$ and $\lambda_i$ of a multiscale toy graph



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### Cuts, clustering and communities The good, the bad and the ugly

- Networks are often inhomogeneous, with important links, hubs, clusters, or communities (modules)
- These are observed in various types of data on networks: social, technological, biological,...
- Importance of cuts: the min-cut max-flow theorem.
   These are two primal-dual linear programs.
   The max value of a flow = the min capacity over all cuts.
- For clusters and communities, see the extensive surveys:

[S. Fortunato, Physic Reports, 2010]

[von Luxburg, Statistics and Computating, 2007]

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End

# Some examples of networks with clusters or communities

Social face-to-face interaction networks





(Lab. physique, ENSL, 2013)

(école primaire, Sociopatterns)



# Some examples of networks with clusters or communities

- Mobile phones (The Belgium case, [Blondel et al., 2008])
- Scientometric (co)-citation (or publication) networks [Jensen et al., 2011]



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### Purpose of community detection?



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## Purpose of community detection?



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## Purpose of community detection?

1) Gives us a sketch of the network:



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### Purpose of community detection?

### 1) Gives us a sketch of the network:



2) Gives us intuition about its components:



## Methods to find clusters or communities

- I will not pretend to make a full survey... Some important steps are:
- Cut algorithms (classical problem in computer science)
- Spectral clustering (seen as relaxed cut problem)
- Modularity optimization (there arrive the physicists) [Newman, Girvan, 2004]
- Greedy modulatity optimization a la Louvain (computer science strikes back)
   [Blondel et al., 2008]
- Ideas from information compression (and random walks) [Rosvall, Bergstrom, 2008]

## From graph cuts to spectral clustering

- Graph cuts in 2 (or bisection): find the partition in two groups of nodes that minimize the cut size (i.e., the number of links cut)
- Exhaustive search can be computationally challenging
- Also, the cut has to be normalized correctly to find groups of relevant sizes
- One usual metric: the Ratio-Cut between sets / and J of nodes

$$R(I,J) = \sum_{i \in I, j \in J} A_{ij}$$

and

$$\mathsf{RatioC}(A,\bar{A}) = \frac{1}{2} \frac{R(A,\bar{A})}{|A|}.$$

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## Spectral clustering for min-cut

- Spectral interpretation: compute the cut as function of the adjacency matrix *A*
- We have  $R = \frac{1}{2} \sum_{i,j \text{ in }\neq \text{ groups}} A_{ij}$ . This is equal to the cut size between the two groups
- Let us note s<sub>i</sub> = ±1 the assignment of node *i* to group labelled +1 or −1

• 
$$R = \frac{1}{2} \sum_{i,j} A_{ij} (1 - s_i s_j) = \frac{1}{4} \sum_{i,j} L_{ij} s_i s_j = \frac{1}{4} \mathbf{s}^\top L \mathbf{s}$$

• Hence, the problem reads as:

$$\min_{\mathbf{s}} \mathbf{s}^{\top} L \mathbf{s}$$

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## Spectral clustering for min-cut

• Let us assume the spectral decomposition of the Laplacian (to be seen later on):

$$L_{ij} = \sum_{k=1}^{N-1} \lambda_k(\chi_k)_i(\chi_k)_j$$

- The optimal assignment vector (that minimizes *R*) would be s<sub>i</sub> = (χ<sub>1</sub>)<sub>i</sub>... if there were no constraints on the s<sub>i</sub>'s... Note: χ<sub>1</sub> is known as the the Fiedler vector.
- However,  $s_i = +1$  or -1...
- Approximated solution:  $s_i = sign((\chi_1)_i)$ .
- The estimated groups are still close to χ<sub>1</sub>.

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# Spectral clustering for min-RatioCut

- Normalization by the size of the sets:  $\min_{A \subset V} \text{RatioC}(A, \overline{A})$
- The same problem written in a relaxed form introducing:

$$\mathbf{f}(i) = +\sqrt{rac{|ar{A}|}{|m{A}|}} ext{ if } i \in m{A} ext{ and } \mathbf{f}(i) = -\sqrt{rac{|m{A}|}{|ar{A}|}} ext{ if } i \in ar{m{A}}$$

Then,  $||\mathbf{f}|| = \sqrt{|V|}$  and  $\mathbf{f}^{\top}\mathbf{1} = \mathbf{0}$ .

Finally, one has

$$\mathbf{f}^{\top} L \mathbf{f} = |V| \cdot \operatorname{RatioC}(A, \overline{A}).$$

• Hence, problem with relaxed constraints:

$$\min_{\mathbf{f}} \mathbf{f}^{\top} \mathbf{L} \mathbf{f}$$
such that  $\mathbf{f}^{\top} \mathbf{1} = 0$ ,  $||\mathbf{f}||_2 = \sqrt{|\mathbf{V}|}$ 

- This allows also for *Spectral clustering of data* represented by networks
- cf. [von Luxburg, Statistics and Computating, 2007]

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## Spectral clustering

• Example of spectral bisection on an irregular mesh



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## Spectral clustering

 Example of spectral bisection on data irregularly spread in a space



- · It's good, very good in fact for clustering
- · However, not really good for natural modules / communities

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## Quality of a partition: the Modularity

- Problems with spectral clustering:
  - 1) No assessment of the quality of the partitions
  - 2) No reference to comparison to some null hypothesis (or "mean field") situation
- Improvement: the modularity

[Newman, 2003]

$$Q = \frac{1}{2m} \sum_{ij} \left[ A_{ij} - \frac{d_i d_j}{2m} \right] \delta(c_i, c_j)$$

where  $2m = \sum_i d_i$ .

• *Q* is between -1 and +1 (in fact, lower than  $1 - 1/n_c$  if  $n_c$  groups)

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# Quality of a partition: the Modularity

• Interpretation:  $\frac{d_i d_j}{2m}$  is, for a null model as a Bernoulli random graph (with prob. 2m/N/(N-1) of existence of each edge), the fraction of edges expected between nodes *i* and *j*.

(Note: in fact, it's best seen as a Chung-Lu model (2002))

• Re-written in term of groups, it gives

$$Q = \sum_{c=1}^{n_c} \left[ \frac{l_c}{m} - \left( \frac{d_c}{2m} \right)^2 \right]$$

where  $l_c$  is the number of edges in group c and  $d_c$  is the sum of degrees of nodes in group c.

- Consequence: the larger *Q* is, the most pronounced the communities are
- Algebraic form: modularity matrix B = A/2m dd<sup>⊤</sup>/(2m)<sup>2</sup> and Q = Tr(c<sup>⊤</sup>Bc) for a partition matrix c (size n<sub>c</sub> × N) of the nodes.

# Community detection with modularity

- By optimization of Q
- For instance: by simulated annealing, by spectral approaches,...
- Works well, better than spectral clustering.



 Better algorithm: the greedy (ascending) Louvain approach (ok for millions of nodes !)
 [Blondel et al., 2008]

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### Multiscale community structure in a graph

Classical community detection algorithms do not have this "scale-vision" of a graph. Modularity optimisation finds:



Where the modularity function reads:  $Q = \frac{1}{2N} \sum_{ij} \left[ A_{ij} - \frac{d_i d_j}{2N} \right] \delta(c_i, c_j)$ 

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# Multiscale community structure in a graph



Q=0.74 :







Q=0.50:



All representations are correct but modularity optimisation favours one.

• Added to that: limit in resolution for modularity [Fortunato, Barthelemy, 2007]

## Integrate a scale into modularity

- [Arenas et al., 2008] Remplace A by A + rI in Q. Self-loops.
- [Reichardt and Bornholdt, 2006]

$$m{Q}_{\gamma} = rac{1}{2m}\sum_{ij}\left[m{A}_{ij} - \gammarac{m{d}_im{d}_j}{2m}
ight]\delta(m{c}_i,m{c}_j)$$

- Equivalent for regular graph if  $\gamma = 1 + \frac{r}{\overline{d}}$ .
- "Corrected Arenas modularity": use  $A_{ij} + r \frac{d_i}{\bar{d}} \delta_{ij}$ ; equivalent to Reichardt and Bornholdt [Lambiotte, 2010]

## Some works on multiscale communities

- Lambiotte, "Multiscale modularity in complex networks" [*WiOpt*, 2010]
- Schaub, Delvenne et al., "Markov dynamics as a zooming lens for multiscale community detection: non clique-like communities and the field-of-view limit" [*PloS One*, 2012]
- Arenas et al., "Analysis of the structure of complex networks at different resolution levels" [*New Journal of Physics*, 2008]
- Reichardt and Bornholdt, "Statistical Mechanics of Community Detection" [*Physical Review E*, 2006]
- Mucha et al., "Community Structure in Time-Dependent, Multiscale, and Multiplex Networks" [*Science*, 2010]
- Tremblay, Borgnat, "Graph Wavelets for Multiscale Community Mining" [*IEEE TSP*, 2014]

More on that later in the next part of the lecture

# Spectral clustering

- More general spectral clustering: Use all (or some) of the eigenvectors χ<sub>i</sub> of L
- Then, use a classical *K*-means on the first *K* non-null eigenvectors of *L* (each node *a* has the (χ<sub>k</sub>)<sub>a</sub> avec features)
- If large heterogeneity of degrees: the normalized Laplacian gives better results

### Normalized Laplacian matrix

$\mathscr{L}$	Laplacian matrix	$\mathscr{L} = I - D^{-1/2} A D^{-1/2}$
$(\lambda_i)$	$\mathscr{L}$ 's eigenvalues	$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \leq \lambda_{N-1}$
$(\chi_i)$	$\mathscr{L}$ 's eigenvectors	$\mathscr{L}\chi_i=\lambda_i\chi_i$

• Choice of K by eigengaps  $|\lambda_{k+1} - \lambda_k|$ 

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### Graph embedding, Laplacian maps

• Spectral clustering := embedding + K-means

 $\forall a \in V : a \rightarrow (\chi_1(a), \chi_2(a), ..., \chi_k(a)) \in \mathbb{R}^k$ 

 Objective of embedding: embed vertices in low dimensional space, so as to discover geometry

$$x_i \in \mathbb{R}^d \to y_i \in \mathbb{R}^k$$
 with  $k < d$ 



# Graph embedding, Laplacian maps

- A good embedding preserves locality in the embedding space, so that nearby points are mapped nearby. It preserves smoothness.
- For that, minimize the variations of the embedding:

$$\sum_{i,j} A_{ij} (y_i - y_j)^2$$

Laplacian eigenmaps:

argmin 
$$\mathbf{y}^{\top} L \mathbf{y}$$
  
such that  $\mathbf{y}^{\top} A \mathbf{y} = 1$   
and  $\mathbf{y}^{\top} L \mathbf{1} = 0$ 

Alternative formulation:

$$L\mathbf{y} = \lambda A\mathbf{y}$$

(generalized eigenproblem)

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## Graph embedding, Laplacian maps

### Some examples







[Belkin, Niyogi, 2003]

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## A recommander system

### [Vandergheynst et al., EPFL, 2014]

• Assume data in the form *M*[movie, user] = movie rating



- One observes only a subset of *M*. How to complete it?
- Hypotheses:
  - Users structured as communities,

and users in community rate similarly

- Movies are clustered in genres,

and similar movies are rated similarly by users

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# A recommander system

[Vandergheynst et al., EPFL, 2014]

- Let us write  $A_{\Omega}(M)$  the observed part of the matrix M
- Matrix completion problem:

$$\min_{X} \operatorname{rank}(X) \ s.t. \ A_{\Omega}(X) = A_{\Omega}(M).$$

- Problem relaxed with the nuclear norm:
   ||X||<sub>\*</sub> = Tr((XX<sup>T</sup>)<sup>1/2</sup>) = ∑<sub>k</sub> σ<sub>k</sub>
   (where the σ<sub>k</sub> are the singular values of X = UΣV<sup>T</sup>)
- Tolerance to noise: change A<sub>Ω</sub>(X) = A<sub>Ω</sub>(M) into a penalty term ||A<sub>Ω</sub> ∘ (A − M)||
- Completion by smoothness on the two graphs (users and movies), as quantified by a term

$$\gamma XLX^{\top} = \gamma \sum_{j,j'} Aij ||x_j - x_{j'}||^2.$$

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## A recommander system

[Vandergheynst et al., EPFL, 2014]

Hence an optimization problem to solve

 $\min_{X} \gamma_n ||X||_* + ||A_{\Omega} \circ (A - M)|| + \gamma_r X L_r X^\top + \gamma_c X L_c X^\top$ 

- Solution by advanced optimization tools for convex non-smooth functions.
- Here, the ADMM approach (Alternating Direction Method of Multipliers) works well (see other parts of the lectures)



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# A small pause

- This was an invitation to "The emerging field of signal processing on graphs: Extending high-dimensional data analysis to networks and other irregular domains" See [Shuman, Narang, Frossard, Ortega, Vandergheynst, *IEEE SP Mag*, 2013]
- Next on our program:
  - Spectral analysis of the Laplacian; some properties
  - Spectral graph Fourier transform, operators and wavelets (hence a notion of scales)
  - Laplacian pyramid, graph downsampling Applications http://perso.ens-lyon.fr/pierre.borgnat

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