Graph Spectra

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IITP-HSE

Overview

1. General introduction

    - Example applications
    - Matrices associated with a graph: A, L, $\mathcal{L}$, P
    - Laplacians, significance
    - Graph spectra
    - Cospectral graphs and graph reconstruction

2. Spectrum of the normalized Laplacian $\mathcal{L}$

    - Patterns of spectral plots (theory & simulations)

3. Spectrum-based distances and kernels

    - Disclaimer: questions rather than answers

General introduction

For a survey and references, see *Cvetcović D. Applications of Graph Spectra: An Introduction to the Literature*

Example applications

1. **Physics**:

   - membrane vibration problem (approximative solving of partial differential equations)
   - thermodynamic properties of a system of molecules adsorbed on the surface of a crystal

2. **Chemistry:**

   - i.e., theory of unsaturated conjugated hydrocarbons (electrons on the molecular graphs)

3. **Computer science**:

   - expanders (-> communication networks, error-correcting codes, optimizing memory space, computing functions, sorting algorithms, etc.)
   - modelling virus propagation in computer networks, Web search engines, etc.

4. **Biology, Geography, Social Sciences**

Notations

Adjacency matrix **A**, unweighted edges:

$$A_G(i,j) = \begin{cases} 1 & \text{if } (i,j) \in E \\ 0 & \text{otherwise.} \end{cases}$$

Adjacency matrix **A**, weighted edges:

$$A_G(a,b) = \begin{cases} w(a,b) & \text{if } (a,b) \in E \\ 0 & \text{otherwise.} \end{cases}$$

Matrix **D**:

$$D_G(a,b) = \begin{cases} \boldsymbol{d}(a) & \text{if } a = b \\ 0 & \text{otherwise.} \end{cases}$$

where d(a) for unweighted:

$$\boldsymbol{d}(a) = |\{b : (a,b) \in E\}|$$

weighted:

$$\boldsymbol{d}(a) = \sum_{b:(a,b)\in E} w(a,b).$$

Matrices

1. Adjacency matrix: A

2. Laplacian: $L = D - A$

   (for unweighted graphs also $L = B^T B$ (B is the incidence matrix)

3. Normalized Laplacian: $\mathcal{L} = D^{-1/2} L D^{-1/2}$

4. Transition probability: $P = D^{-1}A = = D^{-1/2} (I - \mathcal{L}) D^{1/2}$

5. Signless Laplacian $|L| = D + A$ (will be rarely mentioned today)

Note: both for graphs with **weighted** and **unweighted** edges

Sidenote on Laplacians

Definition of (continuous) Laplace operator:

$$\Delta F(M_0) = \lim_{r \to 0} \frac{2k}{r^2} \left\{ \frac{1}{\sigma(S_r)} \int_{S_r} F(M) d\sigma - F(M_0) \right\}$$

Definition of discrete Laplace operator:

$$L(u, v) = \begin{cases} d_v - w(v, v) & \text{if } u = v, \\ -w(u, v) & \text{if } u \text{ and } v \text{ are adjacent,} \\ 0 & \text{otherwise.} \end{cases}$$

or

$$Lf(x) = \sum_{\substack{y \\ x \sim y}} (f(x) - f(y)) w(x, y).$$

(where $f : V \to \mathbb{R}$)

Physical significance

Diffusion (heat) equation, continuous case:

$$u'_t = \alpha \, \Delta u$$

Diffusion equation, discrete case:

$$u'_t = \alpha \, L u$$

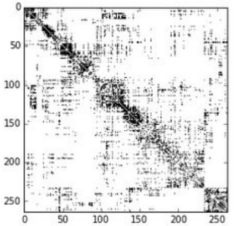
$$u'_t = \alpha \, \mathcal{L} u$$

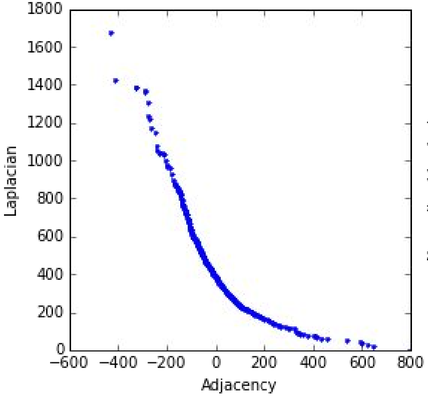
Eigenvalues: $u(t) = C_k V_k e^{\alpha \lambda_k t}$

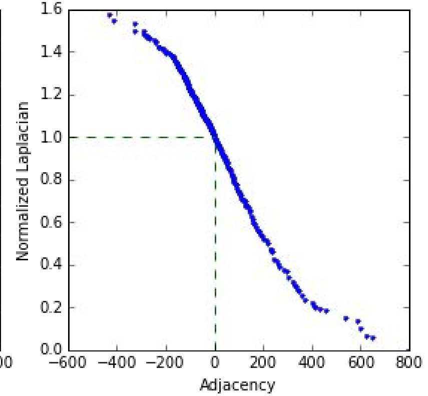
Eigenvalues

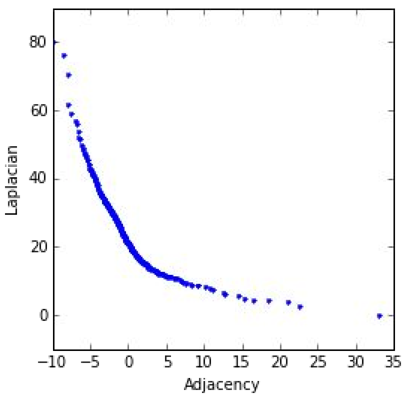
1. A (adjacency matrix) $\alpha_0 \alpha_1 \geqslant \ldots \geqslant \alpha_{n-1}$
2. L = D - A (Laplacian) $\lambda_0 \leqslant \lambda_1 \leqslant \ldots \leqslant \lambda_{n-1}$
3. $\mathcal{L} = D^{-1/2} L D^{-1/2}$ $\nu_0 \leqslant \nu_1 \leqslant \ldots \leqslant \nu_{n-1}$
4. $P = D^{-1}A = D^{-1/2} (I - \mathcal{L}) D^{1/2}$ $\omega_0 \geqslant \omega_1 \geqslant \ldots \geqslant \omega_{n-1},$ $\omega_i = 1 - \nu_i$

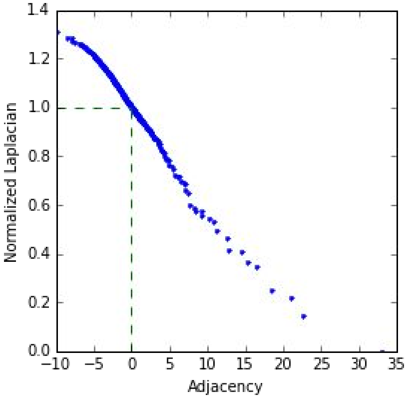
Eigenvalues: illustration



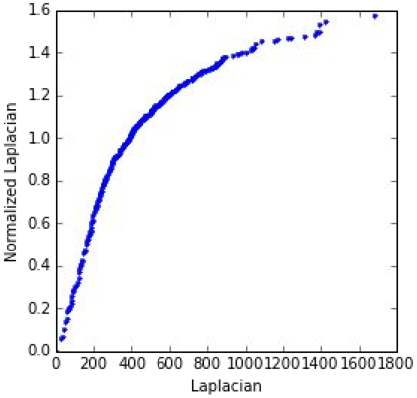




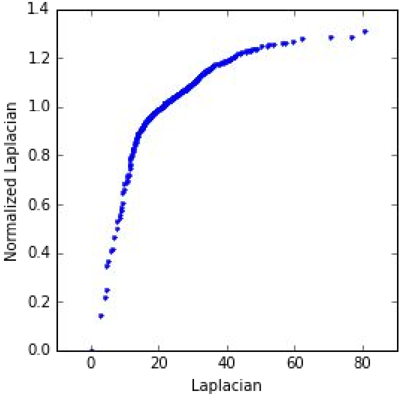




Weighted matrix



Unweighted matrix



Eigenvalues: more on L

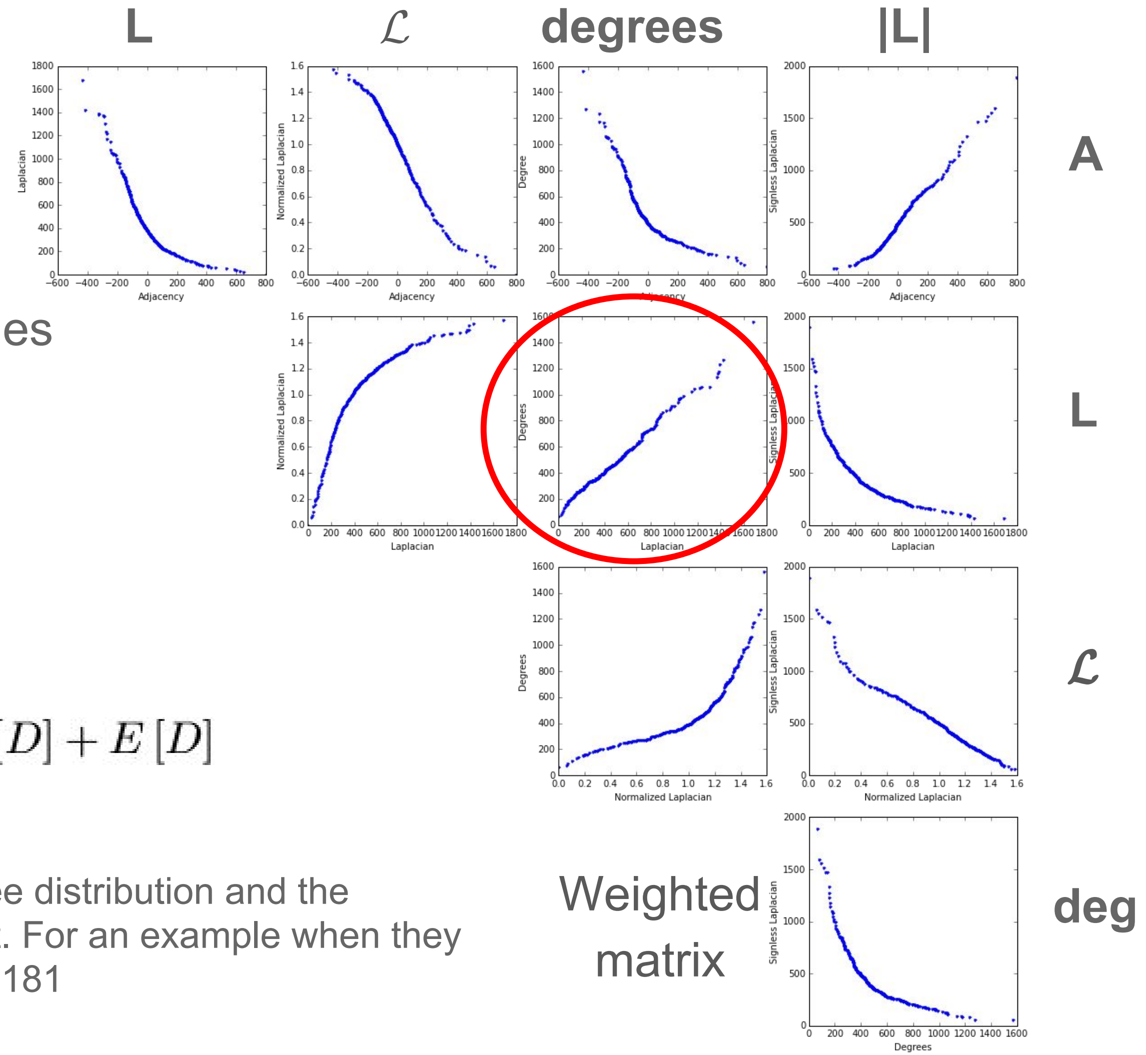
Moments of Laplacian eigenvalues can be expressed via degrees:

$$\mathrm{trace}(Q) = \mathrm{trace}(\Delta) = \sum_{j=1}^{N} d_j$$

$$\sum_{k=1}^{N} \mu_k = 2L$$

$$E[\mu] = E[D]$$

$$\mathrm{Var}[\mu] = \mathrm{Var}[D] + E[D]$$



Still, a general statement is that the degree distribution and the Laplacian distribution are usually different. For an example when they are alike, see a book by Van Mieghem, p.181

Cospectral graphs

Cospectral with respect to what matrix?

Fig. 3. Two graphs cospectral w.r.t. $|L|$, but not w.r.t. L.

Fig. 4. Two graphs cospectral w.r.t. A and L, but not w.r.t. $|L|$.

Fractions of non-DS graphs

n	# graphs	A	L	$\|L\|$
2	2	0	0	0
3	4	0	0	0
4	11	0	0	0.182
5	34	0.059	0	0.118
6	156	0.064	0.026	0.103
7	1044	0.105	0.125	0.098
8	12346	0.139	0.143	0.097
9	274668	0.186	0.155	0.069
10	12005168	0.213	0.118	0.053
11	1018997864	0.211	0.090	0.038

Figures and Table from van Dam E.R. & Haemers W.H. (2003) Which graphs are determined by their spectrum? Linear Algebra and its Applications, 373, 241-272

Spectrum-based graph reconstruction

(Evolutionary reconstruction of networks, Mads Ipsen and Alexander S. Mikhailov)

Evolutionary algorithm *(based on spectrum of unnormalized Laplacian)*:

Mutation: chose node at random, delete all connections and generate new random node degree and node connections.

Algorithm: compute spectral distance* **d’** between new graph and target and spectral distance **d** between old graph and target:

if d’-d<0, accept mutation

if d’-d>0, accept mutation with a certain probability (that depends on the value d’-d)

(to avoid that the evolution gets trapped in a local minimum)

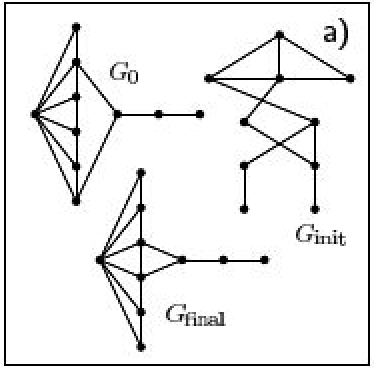
*spectral denstity, spectral distance:

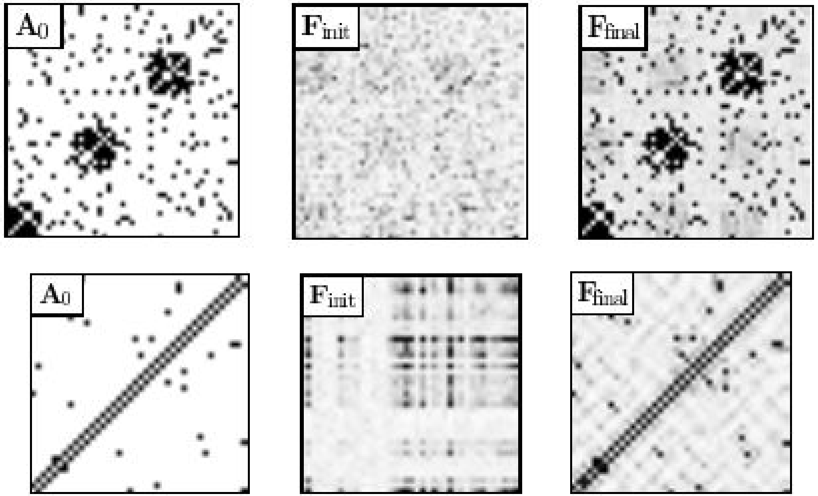
$$\rho(\omega) = C \sum_{k=1}^{N-1} \frac{\gamma}{(\omega - \omega_k)^2 + \gamma^2}$$

$$\epsilon = \sqrt{\int_0^\infty [\rho(\omega) - \rho_0(\omega)]^2 d\omega}.$$

Spectrum-based graph reconstruction

- Random network (N=10)
- Clustered network (N=50, 3 clusters)
- Small world (N=40)





$$\mathbf{F}_{\text{init}} = \mathbf{F}(\mathbf{A}_0, \mathbf{A}_{\text{init}}), \text{ and } \mathbf{F}_{\text{final}} = \mathbf{F}(\mathbf{A}_0, \mathbf{A}_{\text{final}})$$

(Evolutionary reconstruction of networks, Mads Ipsen and Alexander S. Mikhailov)

Spectrum of the normalized Laplacian $\mathcal{L}$

Normalized Laplacian vs. other matrices

Spectra of different matrices might be usefull in their own way:

1. A, ex: $|\alpha_0|+\dots|\alpha_{n-1}|$= graph energy

   $\frac{1}{6}(\alpha_0^3+\dots\alpha_{n-1}^3)$= # triangles in a graph

2. L = D - A , note that for a regular graph with degree d: $\lambda_j = d - \alpha_{N-1-j}$

3. $\mathcal{L} = D^{-1/2} L D^{-1/2}$, information about graph structure, spectral gap (see below)

4. $P = D^{-1}A = D^{-1/2}(I - \mathcal{L}) D^{1/2}$, random walks,spectral gap (also, $\omega_i = 1 - \nu_i$ the spectral gap of a stochastic matrix P also equals the second smallest eigenvalue of normalized Laplacian)

Eigenvalues of $\mathcal{L}$

- $\lambda_i \in [0,2]$, $\lambda_{n-1} = 2$ (largest eigenvalue) iff graph bipartite
- 0 always eigenvalue, eigenvector (1,...1)
- #0 eigenvalues = #connected components
- G=union of disconnected subgraphs $\Rightarrow$ spectrum=union of spectra

  from now on let us consider only connected graphs
- λ_1(second smallest eigenvalue), called **spectral gap**, shows how "connected" a graph is:

  If λ_1 is small, then there exists a cut disconnecting the graph that cuts very few edges. If λ_1 is large, then every cut disconnecting the graph cuts a large number of edges.

  upper bound: $\lambda_1 \leq \dfrac{n}{n-1}$, with equality iff complete graph

Eigenvalues of $\mathcal{L}$

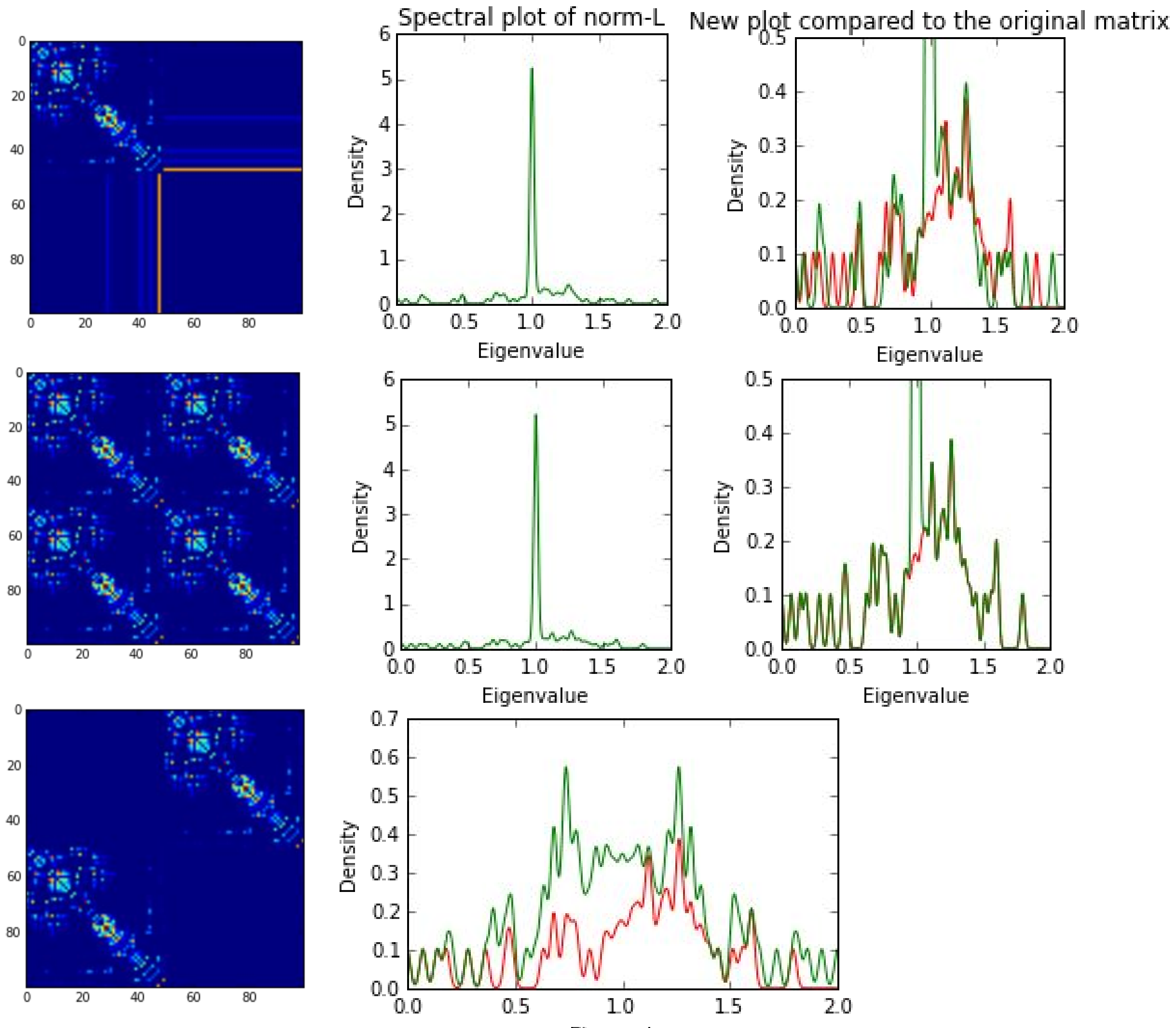
High multiplicity of 1:

- one node is copied many times
- every node is doubled

Symmetric distribution:

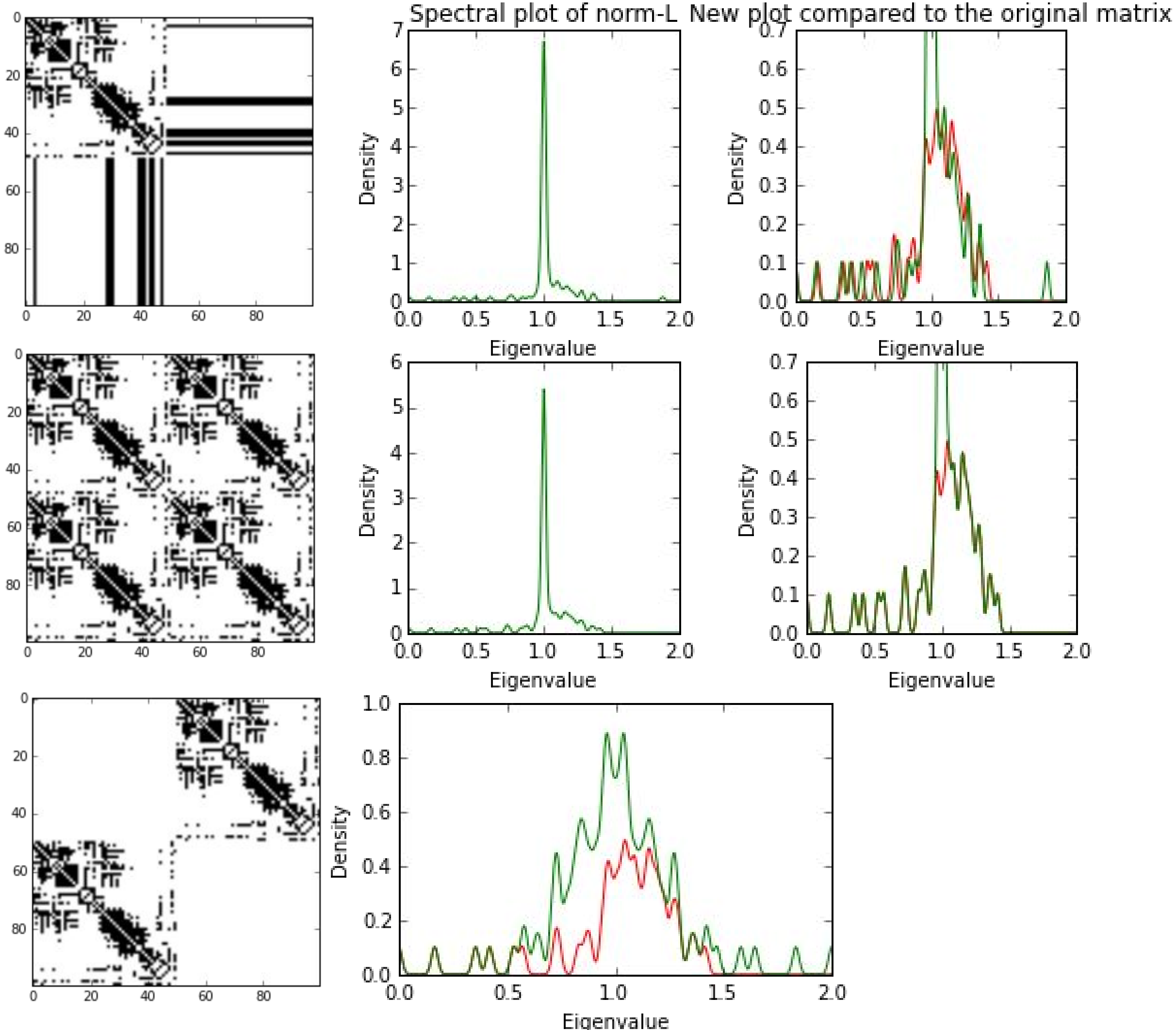
- bipartite graph

See also: Anirban Banerjee, Jürgen Jost (2008) On the spectrum of the normalized graph Laplacian



Eigenvalues of $\mathcal{L}$

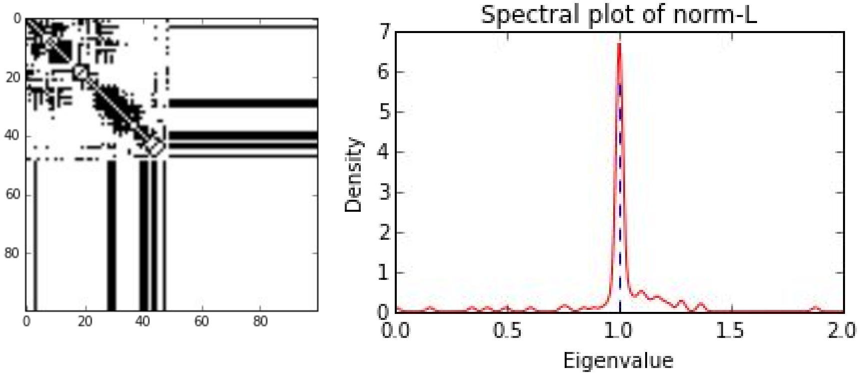
Same story for binarized matrices:

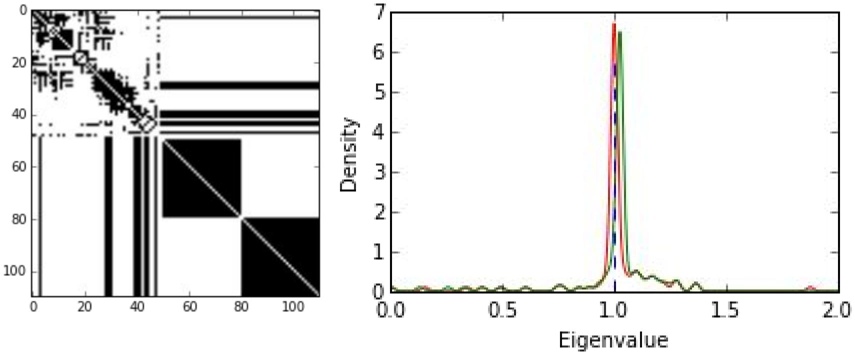


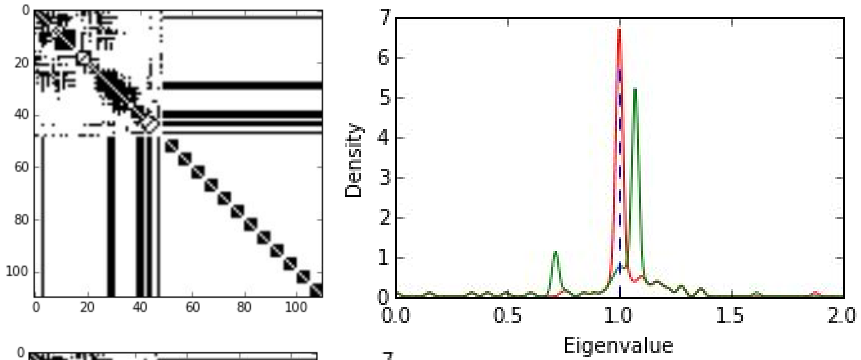
See also: Anirban Banerjee, Jürgen Jost (2008) On the spectrum of the normalized graph Laplacian

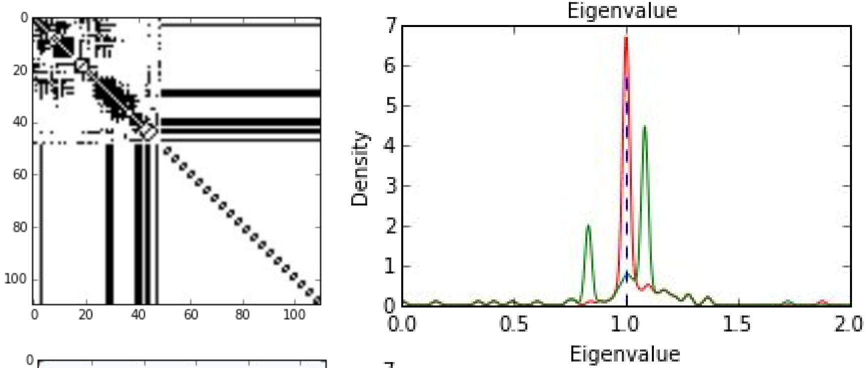
Eigenvalues of $\mathcal{L}$

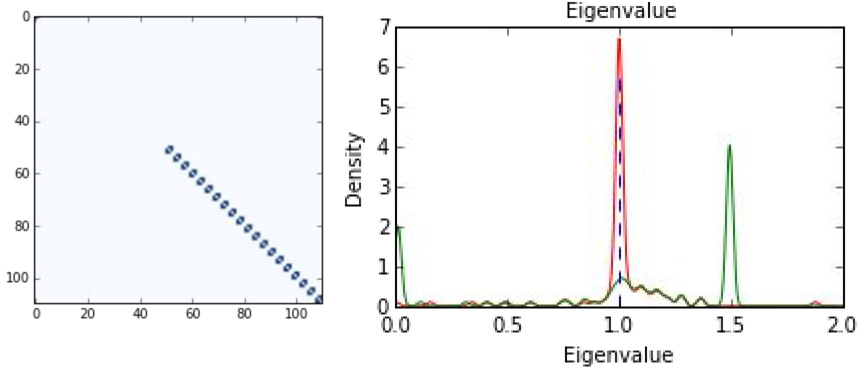
Multiplicity of arbitrary values:



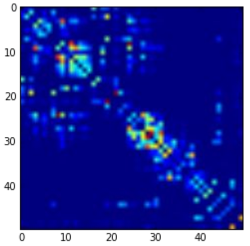








Eigenvectors



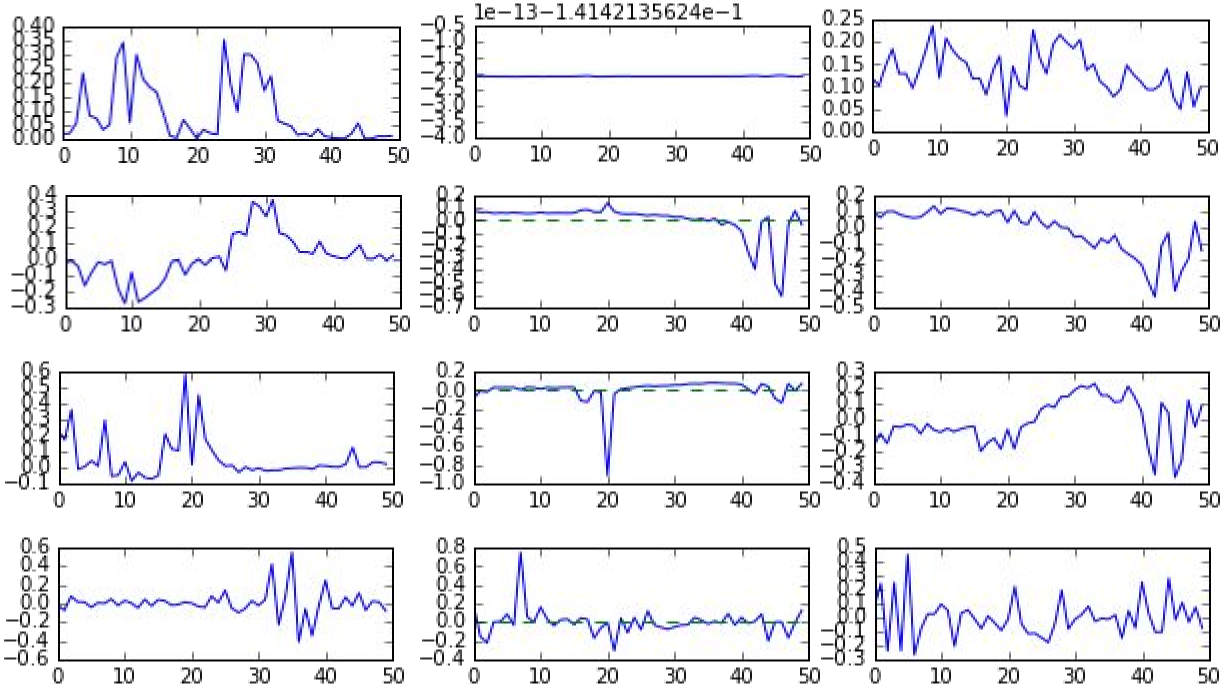
A **L** **$\mathcal{L}$**

1st important

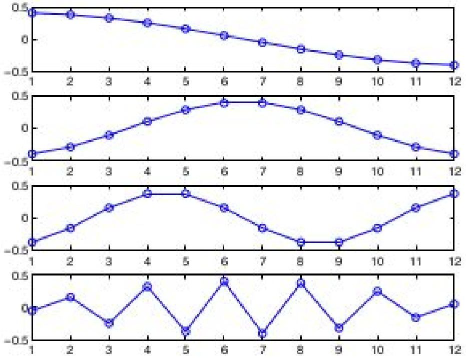
2d important

3d important

30th important



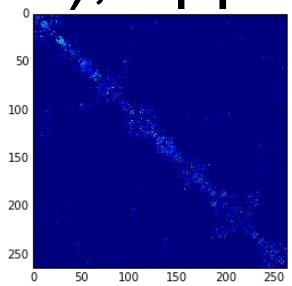
L for Path of 12 nodes

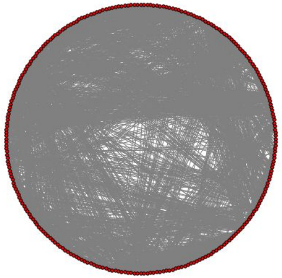


From: Spielman D. Spectral graph theory

Eigenvectors (of A and $\mathcal{L}$), applications

- **L: nice drawing**

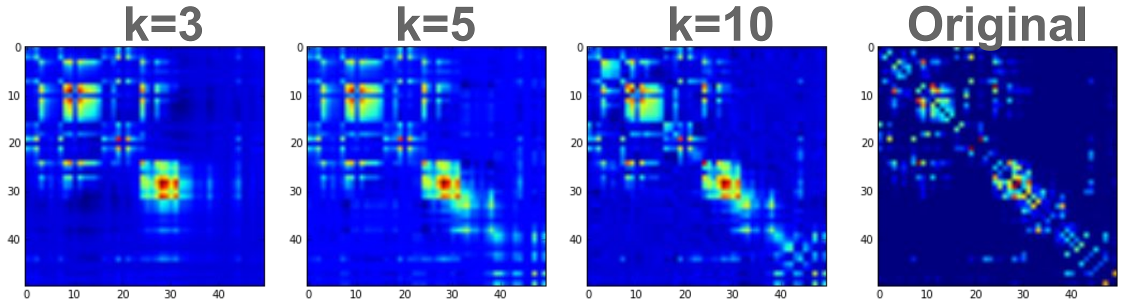




- **A: Low-rank approximation**

$$A = \sum_i \alpha_i \boldsymbol{v}_i \boldsymbol{v}_i^T$$

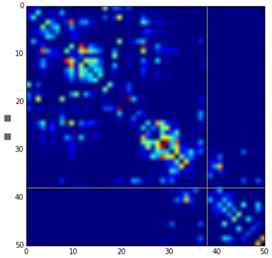
Take k largest eigenvalues - the best approximation of A by a k-rank matrix



- **L: Spectral clustering**

  Compute eigenvector e_1 for second-largest eigenvalue λ_1 of $\mathcal{L}$
  Partitioning may be done in different ways, ex:
  Compute median m of the components of e_1
  Two clusters, depending on whether component < or > than m

Example:



Coefficients of the characteristic polynomial

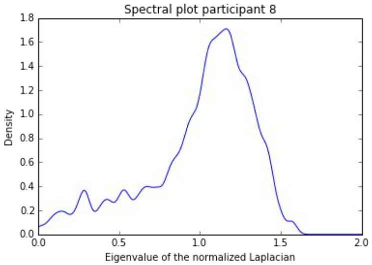
- Not today!

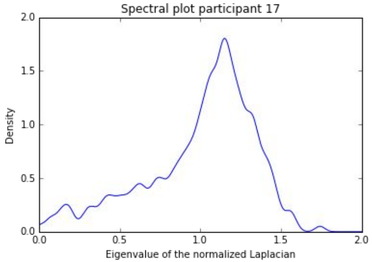
- But there are some facts there too, e.g.

Theorem 12 (Matrix Tree Theorem) *In a graph G with N nodes, the coefficient $(-1)^{N-m} c_{N-m}(Q)$ of the characteristic polynomial of the Laplacian Q equals the number of all spanning trees with m links in all subgraphs of G that are obtained after deleting $N-m$ nodes in all possible ways.*

Spectrum-based distances and kernels

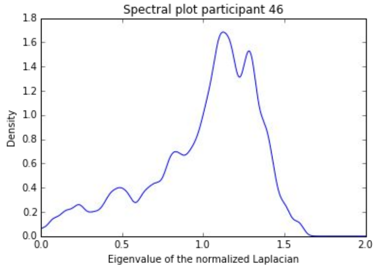
Suggestions?





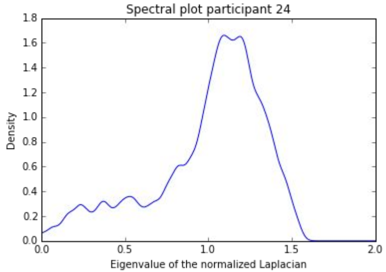
1. Spectral-based metrics

- Algebraic connectivity
- Eigenvector centrality
- Graph energy
- Effective graph resistance (the difficulty of transport in a graph)



2. Spectra

- Vectors of sorted eigenvalues
- Distances (Euclidean, Manhattan) - how to convert to kernels? exp(- distance)?



3. Eigenvalue distributions

- Distances between densities (i.e., K-L) - yet again, how to convert to kernels?
- or just features describing relevant properties of distributions (i.e., multiplicity, symmetry)

4. Other ideas? (i.e., projection of one matrix to the vector space of the other)

Thank you!

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