GRAPH LAPLACEANS AND THEIR APPLICATIONS

- *Graph Laplaceans, definitions and basic properties*
- *Graph partitioning –*
- *Introduction to clustering*
- *Graph Embeddings, vertex embeddings . The problem*
- *Use of Graph Laplaceans, Laplacean Eigenmaps*
- *Use of similarity graphs: Locally Linear Embeddings*
- *Explicit dimension reduction method: PCA, LLP, ...*

Graph Laplaceans - Definition

➤ "Laplace-type" matrices associated with general undirected graphs – useful in many applications

➤ Given a graph $G = (V, E)$ define

- A matrix W of weights w_{ij} for each edge
- Assume $w_{ij} \geq 0,$, $w_{ii} = 0$, and $w_{ij} = w_{ji} \; \forall(i, j)$
- The diagonal matrix $D = diag(d_i)$ with $d_i = \sum_{j \neq i} w_{ij}$

➤ Corresponding *graph Laplacean* of G is: $L = D - W$

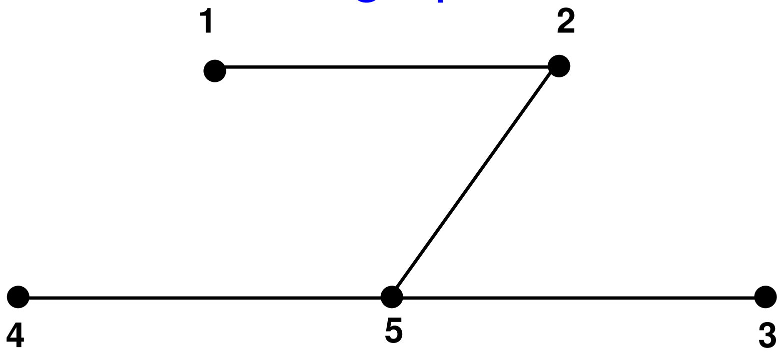
➤ Gershgorin's theorem $\rightarrow$ L is positive semidefinite.

- Simplest case:

$$w_{ij} = \begin{cases} 1 & \text{if } (i,j) \in E \& i \neq j \\ 0 & \text{else} \end{cases} \qquad D = \text{diag}\left[d_i = \sum_{j \neq i} w_{ij} \right]$$

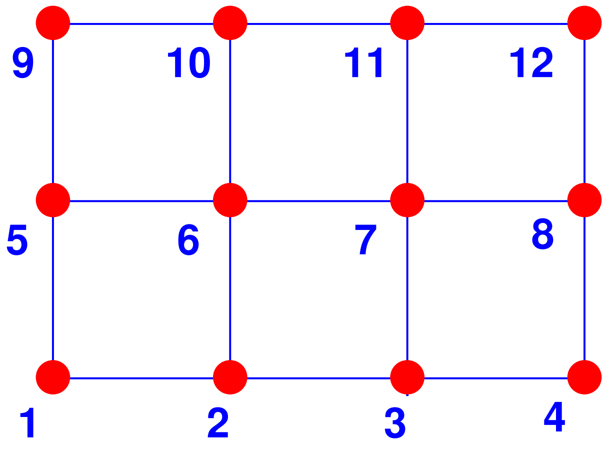
Example:

Consider the graph



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

✍1 Define the graph Laplacean for the graph associated with the simple mesh shown next. [use the simple weights of 0 or 1]. What is the difference with the discretization of the Laplace operator for case when mesh is the same as this graph?



Proposition:

(i) L is symmetric semi-positive definite.

(ii) L is singular with $\mathbb{1}$ as a null vector.

(iii) If G is connected, then $\mathbf{Null}(L) = \mathbf{span}\{\mathbb{1}\}$

(iv) If G has $k > 1$ connected components $G_1, G_2, \cdots, G_k$, then the nullity of L is k and $\mathbf{Null}(L)$ is spanned by the vectors $z^{(j)}$, $j = 1, \cdots, k$ defined by:

$$(z^{(j)})_i = \begin{cases} 1 & \text{if } i \in G_j \\ 0 & \text{if not.} \end{cases}$$

Proof: (i) and (ii) seen earlier and are trivial. (iii) Clearly $u = \mathbb{1}$ is a null vector for L. The vector $D^{-1/2}u$ is an eigenvector for the matrix $D^{-1/2}LD^{-1/2} = I - D^{-1/2}WD^{-1/2}$ associated with the smallest eigenvalue. It is also an eigenvector for $D^{-1/2}WD^{-1/2}$ associated with the largest eigenvalue. By the Perron Frobenius theorem this is a simple eigenvalue... (iv) Can be proved from the fact that L can be written as a direct sum of the Laplacian matrices for $G_1, \cdots, G_k$. ■

A few properties of graph Laplaceans

Define: oriented incidence matrix H: (1)First orient the edges $i \sim j$ into $i \to j$ or $j \to i$. (2) Rows of H indexed by vertices of G. Columns indexed by edges. (3) For each (i, j) in E, define the corresponding column in H as $\sqrt{w(i,j)}(e_i - e_j)$.

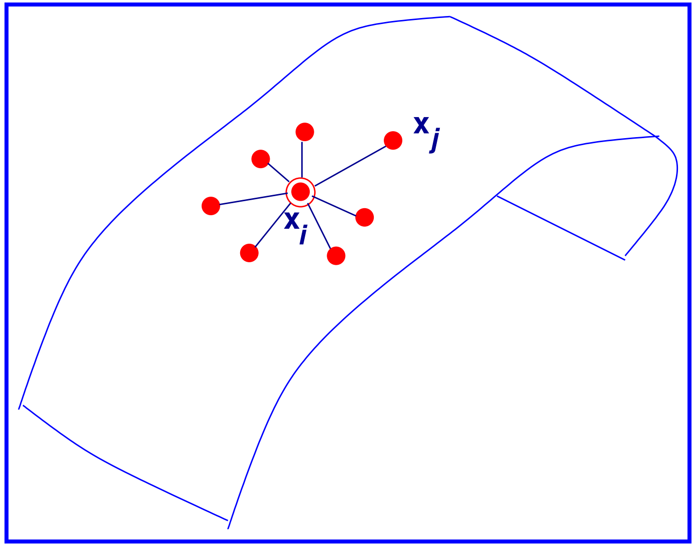
Example: In previous example (4 p. back) orient $i \to j$ so that $j > i$ [lower triangular matrix representation]. Then matrix H is:

$$H = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & -1 & -1 & -1 \end{bmatrix}$$

Property 1 $\boxed{L = HH^T}$

✍2 Re-prove part (iv) of previous proposition by using this property.

A few properties of graph Laplaceans



Strong relation between $x^T L x$ and local distances between entries of x

➤ Let L = any matrix s.t. $L = D - W$, with $D = diag(d_i)$ and

$$w_{ij} \geq 0, \qquad d_i = \sum_{j \neq i} w_{ij}$$

Property 2: for any $x \in \mathbb{R}^n$:

$$x^\top L x = \frac{1}{2} \sum_{i,j} w_{ij} |x_i - x_j|^2$$

Property 3: (generalization) for any $Y \in \mathbb{R}^{d\times n}$:

$$\text{Tr}\,[YLY^\top] = \frac{1}{2}\sum_{i,j} w_{ij}\|y_i - y_j\|^2$$

➤ Note: y_j = j-th colunm of Y. Usually $d < n$. Each column can represent a data sample.

Property 4: For the particular $L = I - \frac{1}{n}\mathbb{1}\,\mathbb{1}^\top$

$$XLX^\top = \bar{X}\bar{X}^\top == n \times \text{Covariance matrix}$$

Property 5: L is singular and admits the null vector

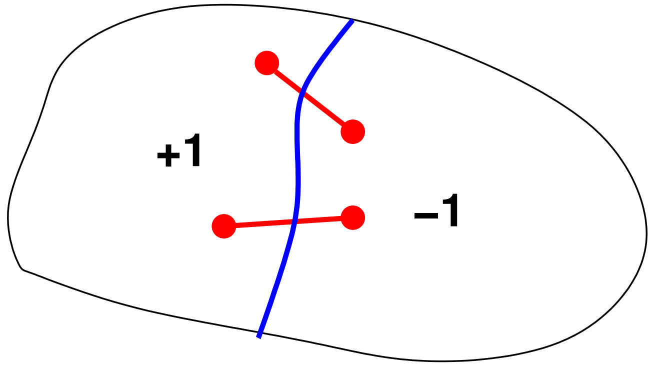
$\mathbb{1}$ =`ones(n,1)`

Property 6: (Graph partitioning) Consider situation when $w_{ij} \in \{0, 1\}$. If x is a vector of signs (± 1) then

$$x^\top L x = 4 \times (\text{'number of edge cuts'})$$

edge-cut = pair (i, j) with $x_i \neq x_j$

- Consequence: Can be used to partition graphs



- Would like to minimize (Lx, x) subject to $x \in \{-1, 1\}^n$ and $e^T x = 0$ [balanced sets]

- WIl solve a relaxed form of this problem

✍3 What if we replace x by a vector of ones (representing one partition) and zeros (representing the other)?

✍4 Let x be any vector and $y = x + \alpha \mathbb{1}$ and L a graph Laplacean. Compare (Lx, x) with (Ly, y).

➤ Consider any symmetric (real) matrix A with eigenvalues $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$ and eigenvectors $u_1, \cdots, u_n$

➤ Recall that:
(Min reached for $x = u_1$)

$$\min_{x \in \mathbb{R}^n} \frac{(Ax, x)}{(x, x)} = \lambda_1$$

➤ In addition:
(Min reached for $x = u_2$)

$$\min_{x \perp u_1} \frac{(Ax, x)}{(x, x)} = \lambda_2$$

➤ For a graph Laplacean $u_1 = \mathbb{1}$ = vector of all ones and

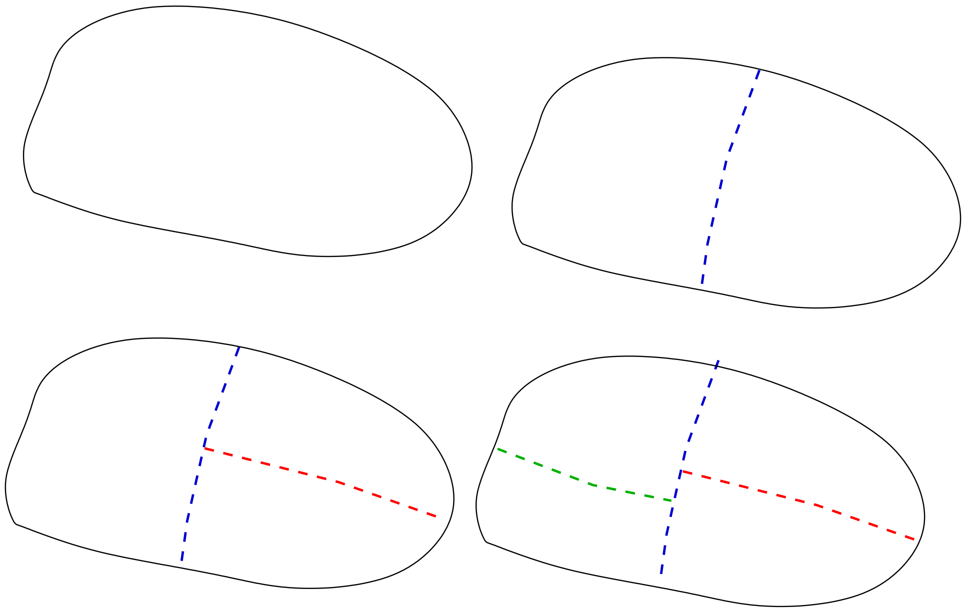
➤ ...vector u_2 is called the Fiedler vector. It solves a relaxed form of the problem -

$$\min_{x\in\{-1,1\}^n;\ \mathbb{1}^T x=0} \frac{(Lx,x)}{(x,x)} \quad \rightarrow \quad \min_{x\in\mathbb{R}^n;\ \mathbb{1}^T x=0} \frac{(Lx,x)}{(x,x)}$$

- Define $v = u_2$ then $lab = sign(v - med(v))$

Recursive Spectral Bisection

1. Form graph Laplacean
2. Partition graph in 2 based on Fielder vector
3. Partition largest subgraph in two recursively ...
4. ... Until the desired number of partitions is reached



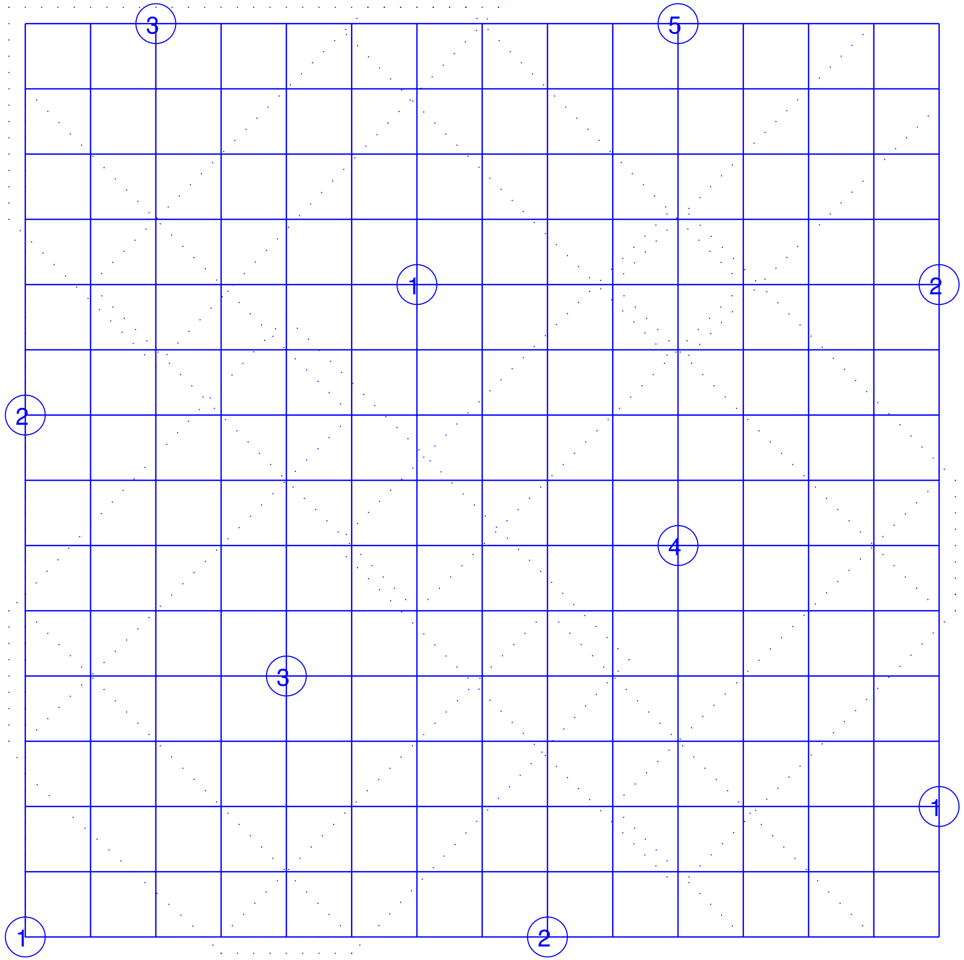
Three approaches to graph partitioning:

1. Spectral methods - Just seen + add Recursive Spectral Bisection.
2. Geometric techniques. Coordinates are required. [Houstis & Rice et al., Miller, Vavasis, Teng et al.]
3. Graph Theory techniques – multilevel,... [use graph, but no coordinates]
   - Currently best known technique is Metis (multi-level algorithm)
   - Simplest idea: Recursive Graph Bisection; Nested dissection (George & Liu, 1980; Liu 1992]
   - Advantages: simplicity – no coordinates required

✍5 Run *testBis_simple* and *testMeshPart* in matlab class site

Example of a graph theory approach

- Level Set Expansion Algorithm
- Given: p nodes 'uniformly' spread in the graph (roughly same distance from one another).
- Method: Perform a level-set traversal (BFS) from each node simultaneously.
- Best described for an example on a 15×15 five – point Finite Difference grid.
- See [Goehring-YS '94, See Cai-YS '95]
- Approach also known under the name 'bubble' algorithm and implemented in some packages [Party, DibaP]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