



Aalto University
School of Science

CS-E4600 – Algorithmic methods of data mining

Slide set 12 : Spectral graph analysis

Aristides Gionis

Aalto University

fall 2018

spectral graph theory

reading material

- “*Spectral graph theory*”
book chapter by Dan Spielman
section 16.1 – 16.8
- additional suggested reading
“*A tutorial on spectral clustering*”
by Ulrike von Luxburg
(about spectral clustering in general, not just graphs)

spectral graph theory

objective :

- view the adjacency (or related) matrix of a graph with a linear algebra lens
- identify connections between spectral properties of such a matrix and structural properties of the graph
 - connectivity
 - bipartiteness
 - cuts
 - ...
- spectral properties = eigenvalues and eigenvectors
- in other words, what does the eigenvalues and eigenvectors of the adjacency (or related) matrix tell us about the graph?

background: eigenvalues and eigenvectors

- consider a real $n \times n$ matrix A , i.e., $A \in \mathbb{R}^{n \times n}$
- $\lambda \in \mathbb{C}$ is an **eigenvalue** of A

if there exists $\mathbf{x} \in \mathbb{C}^n$, $\mathbf{x} \neq \mathbf{0}$

such that

$$A\mathbf{x} = \lambda\mathbf{x}$$

- such a vector \mathbf{x} is called **eigenvector** of λ
- alternatively,

$$(A - \lambda I)\mathbf{x} = \mathbf{0} \quad \text{or} \quad \det(A - \lambda I) = 0$$

- it follows that A has n eigenvalues
(possibly complex and possibly with multiplicity > 1)

background: eigenvalues and eigenvectors

- consider a real and symmetric $n \times n$ matrix A
(e.g., the adjacency matrix of an undirected graph)

background: eigenvalues and eigenvectors

- consider a real and symmetric $n \times n$ matrix A
(e.g., the adjacency matrix of an undirected graph)
- then
 - all eigenvalues of A are real
 - eigenvectors of different eigenvalues are orthogonal
i.e., if \mathbf{x}_1 an eigenvector of λ_1
and \mathbf{x}_2 an eigenvector of λ_2
then $\lambda_1 \neq \lambda_2$ implies $\mathbf{x}_1 \perp \mathbf{x}_2$ (or $\mathbf{x}_1^T \mathbf{x}_2 = 0$)

background: eigenvalues and eigenvectors

- consider a real and symmetric $n \times n$ matrix A
(e.g., the adjacency matrix of an undirected graph)
- then
 - all eigenvalues of A are real
 - eigenvectors of different eigenvalues are orthogonal
i.e., if \mathbf{x}_1 an eigenvector of λ_1
and \mathbf{x}_2 an eigenvector of λ_2
then $\lambda_1 \neq \lambda_2$ implies $\mathbf{x}_1 \perp \mathbf{x}_2$ (or $\mathbf{x}_1^T \mathbf{x}_2 = 0$)
- A is positive semi-definite if $\mathbf{x}^T A \mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$
- a symmetric positive semi-definite real matrix has real and non negative eigenvalues

background: eigenvalues and eigenvectors

- consider a real and symmetric $n \times n$ matrix A
- the eigenvalues $\lambda_1, \dots, \lambda_n$ of A can be ordered

$$\lambda_1 \leq \dots \leq \lambda_n$$

- theorem [variational characterization of eigenvalues]

$$\lambda_n = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}}$$

$$\lambda_1 = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}}$$

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \quad \text{and "so on" for the other eigenvalues}$$

- very useful way to think about eigenvalues

background: eigenvalues and eigenvectors

- the inverse holds, i.e.,

$$\lambda_1 = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{ij} A_{ij} x_i x_j}{\sum_i x_i^2}$$

and if \mathbf{x} is an “optimal vector”, then \mathbf{x} is eigenvector of λ_1
(optimal vector: $\arg \min$ of the expression above)

background: eigenvalues and eigenvectors

- the inverse holds, i.e.,

$$\lambda_1 = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{ij} A_{ij} x_i x_j}{\sum_i x_i^2}$$

and if \mathbf{x} is an “optimal vector”, then \mathbf{x} is eigenvector of λ_1
(optimal vector: **arg min** of the expression above)

- similarly

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{ij} A_{ij} x_i x_j}{\sum_i x_i^2}$$

and if \mathbf{x} is an “optimal vector”, then \mathbf{x} is eigenvector of λ_2
(optimal vector: **arg min** of the expression above)

spectral graph analysis

- apply the eigenvalue characterization for graphs
- **question** : which matrix to consider ?

spectral graph analysis

- apply the eigenvalue characterization for graphs
- question : which matrix to consider ?
 - the adjacency matrix A of the graph

spectral graph analysis

- apply the eigenvalue characterization for graphs
- question : which matrix to consider ?
 - the adjacency matrix A of the graph
 - some matrix B so that $\mathbf{x}^T B \mathbf{x}$ is related to a structural property of the graph

spectral graph analysis

- apply the eigenvalue characterization for graphs
- question : which matrix to consider ?
 - the adjacency matrix A of the graph
 - some matrix B so that $\mathbf{x}^T B \mathbf{x}$ is related to a structural property of the graph
- consider $G = (V, E)$ an undirected and d -regular graph (regular graph is used wlog for simplicity of expositions)
- let A be the adjacency matrix of G :
- define the *laplacian matrix* of G as

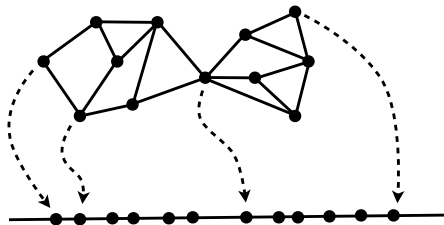
$$L = I - \frac{1}{d} A \quad \text{or} \quad L_{ij} = \begin{cases} 1 & \text{if } i = j \\ -1/d & \text{if } (i, j) \in E, i \neq j \\ 0 & \text{if } (i, j) \notin E, i \neq j \end{cases}$$

spectral graph analysis

- for the laplacian matrix $L = I - \frac{1}{d} A$ it is

$$\mathbf{x}^T L \mathbf{x} = \frac{1}{d} \sum_{(u,v) \in E} |x_u - x_v|^2$$

- here, x_u is the coordinate of the eigenvector \mathbf{x} that corresponds to vertex $u \in V$
- eigenvector \mathbf{x} is seen as a **one-dimensional embedding**
- i.e., mapping the vertices of the graph onto the real line



spectral graph analysis

high-level remark

- many graph problems can be modeled as mapping of vertices to a discrete space

e.g., a cut is a mapping of vertices to $\{0, 1\}$

- we aim to find a spectral formulation so that an eigenvector \mathbf{x} is a **relaxation** of the discrete graph problem
i.e., optimizes the same objective but without the integrality constraint

the smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_1 ?

the smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_1 ?

$$\lambda_1 = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

(show this!)

the smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_1 ?

$$\lambda_1 = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

(show this!)

- observe that $\lambda_1 \geq 0$

the smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_1 ?

$$\lambda_1 = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

(show this!)

- observe that $\lambda_1 \geq 0$
- can it be $\lambda_1 = 0$?

the smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_1 ?

$$\lambda_1 = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

(show this!)

- observe that $\lambda_1 \geq 0$
- can it be $\lambda_1 = 0$?
- **yes** : take \mathbf{x} to be the constant vector

the second smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_2 ?

the second smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_2 ?

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

the second smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_2 ?

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

- can it be $\lambda_2 = 0$?

the second smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_2 ?

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

- can it be $\lambda_2 = 0$?
- $\lambda_2 = 0$ if and only if the graph is **disconnected**

the second smallest eigenvalue

apply the eigenvalue characterization theorem for L

- what is λ_2 ?

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

- can it be $\lambda_2 = 0$?
- $\lambda_2 = 0$ if and only if the graph is **disconnected**

map the vertices of each connected component to a different constant

the k -th smallest eigenvalue

- alternative characterization for λ_k

$$\lambda_k = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x} \in \mathbb{S}_{k-1}^\perp}} \max \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

- $\lambda_k = 0$ if and only if the graph has at least k connected components

where

\mathbb{S}_k : space spanned by k independent vectors

\mathbb{S}_k^\perp : space orthogonal to \mathbb{S}_k

the largest eigenvalue

- what about λ_n ?

$$\lambda_n = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

the largest eigenvalue

- what about λ_n ?

$$\lambda_n = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T L \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

- consider a **boolean** version of this problem
- restrict mapping to $\{-1, +1\}$

$$\lambda_n \geq \max_{\mathbf{x} \in \{-1, +1\}^n} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2}$$

‘ \geq ’ because $\mathbf{x} \in \{-1, +1\}^n$ is more restricted case

the largest eigenvalue

- mapping of vertices to $\{-1, +1\}$ corresponds to a cut S
then

$$\begin{aligned}\lambda_n &\geq \max_{\mathbf{x} \in \{-1, +1\}^n} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2} \\&= \max_{S \subseteq V} \frac{4 E(S, V \setminus S)}{d n} \\&= \max_{S \subseteq V} \frac{4 E(S, V \setminus S)}{2 |E|} \\&= \frac{2 \text{maxcut}(G)}{|E|}\end{aligned}$$

$(E(S, T))$ is the number of edges between $S, T \subseteq V$

- it follows that if G is bipartite then $\lambda_n \geq 2$

the largest eigenvalue

- mapping of vertices to $\{-1, +1\}$ corresponds to a cut S
then

$$\begin{aligned}\lambda_n &\geq \max_{\mathbf{x} \in \{-1, +1\}^n} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2} \\&= \max_{S \subseteq V} \frac{4 E(S, V \setminus S)}{d n} \\&= \max_{S \subseteq V} \frac{4 E(S, V \setminus S)}{2 |E|} \\&= \frac{2 \text{maxcut}(G)}{|E|}\end{aligned}$$

($E(S, T)$ is the number of edges between $S, T \subseteq V$)

- it follows that if G is bipartite then $\lambda_n \geq 2$
(because if G is bipartite, there exists S that cuts all edges)

the largest eigenvalue

- on the other hand

$$\begin{aligned}\lambda_n &= \max_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2} \\&= \max_{\mathbf{x} \neq \mathbf{0}} \frac{2d \sum_{u \in V} x_u^2 - \sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2} \\&= 2 - \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2}\end{aligned}$$

the largest eigenvalue

- on the other hand

$$\begin{aligned}\lambda_n &= \max_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2} \\&= \max_{\mathbf{x} \neq \mathbf{0}} \frac{2d \sum_{u \in V} x_u^2 - \sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2} \\&= 2 - \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2}\end{aligned}$$

- first note that $\lambda_n \leq 2$

the largest eigenvalue

- on the other hand

$$\begin{aligned}\lambda_n &= \max_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2} \\&= \max_{\mathbf{x} \neq \mathbf{0}} \frac{2d \sum_{u \in V} x_u^2 - \sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2} \\&= 2 - \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2}\end{aligned}$$

- first note that $\lambda_n \leq 2$
- $\lambda_n = 2$ iff there is \mathbf{x} s.t. $x_u = -x_v$ for all $(u, v) \in E$

the largest eigenvalue

- on the other hand

$$\begin{aligned}\lambda_n &= \max_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} |x_u - x_v|^2}{d \sum_{u \in V} x_u^2} \\&= \max_{\mathbf{x} \neq \mathbf{0}} \frac{2d \sum_{u \in V} x_u^2 - \sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2} \\&= 2 - \min_{\mathbf{x} \neq \mathbf{0}} \frac{\sum_{(u,v) \in E} (x_u + x_v)^2}{d \sum_{u \in V} x_u^2}\end{aligned}$$

- first note that $\lambda_n \leq 2$
- $\lambda_n = 2$ iff there is \mathbf{x} s.t. $x_u = -x_v$ for all $(u, v) \in E$
- $\lambda_n = 2$ iff G has a bipartite connected component

summary so far

eigenvalues and structural properties of G :

- $\lambda_2 = 0$ iff G is disconnected
- $\lambda_k = 0$ iff G has at least k connected components
- $\lambda_n = 2$ iff G has a bipartite connected component

robustness

- how robust are these results ?

- for instance, what if $\lambda_2 = \epsilon$?

is the graph G almost disconnected ?

i.e., does it have small cuts ?

- or, what if $\lambda_n = 2 - \epsilon$?

does it have a component that is “close” to bipartite ?

the second eigenvalue

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{(u,v) \in E} (x_u - x_v)^2}{d \sum_{u \in V} x_u^2} = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{d}{n} \sum_{(u,v) \in V^2} (x_u - x_v)^2}$$

where V^2 is the set of **ordered** pairs of vertices

why?

$$\sum_{(u,v) \in V^2} (x_u - x_v)^2 = 2n \sum_v x_v^2 - 2 \sum_{u,v} x_u x_v = n \sum_v x_v^2 - 2 \left(\sum_u x_u \right)^2$$

$$\text{and } \sum_u x_u = 0 \text{ since } \mathbf{x}^T \mathbf{x}_1 = 0$$

the second eigenvalue

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{d}{n} \sum_{(u,v) \in V^2} (x_u - x_v)^2} = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{n \mathbb{E}_{(u,v) \in E} [(x_u - x_v)^2]}{d \mathbb{E}_{(u,v) \in V^2} [(x_u - x_v)^2]}$$

consider again **discrete version** of the problem, $x_u \in \{0, 1\}$

$$\min_{\substack{\mathbf{x} \neq \{0,1\}^n \\ \mathbf{x} \text{ non const}}} \frac{n \mathbb{E}_{(u,v) \in E} [(x_u - x_v)^2]}{d \mathbb{E}_{(u,v) \in V^2} [(x_u - x_v)^2]} = \min_{S \subseteq V} \frac{n E(S, \bar{S})}{d |S| |\bar{S}|} = \text{usc}(G)$$

$\text{usc}(G)$: **uniform sparsest cut** of G

uniform sparsest cut

- it can be shown that

$$\lambda_2 \leq \text{usc}(G) \leq \sqrt{8\lambda_2}$$

uniform sparsest cut

- it can be shown that

$$\lambda_2 \leq \text{usc}(G) \leq \sqrt{8\lambda_2}$$

- the first inequality holds by the fact that usc is a relaxation

uniform sparsest cut

- it can be shown that

$$\lambda_2 \leq \text{usc}(G) \leq \sqrt{8\lambda_2}$$

- the first inequality holds by the fact that **usc** is a **relaxation**
- the second inequality is constructive :
- if **x** is an eigenvector of λ_2

then there is some $t \in V$ such that

the cut $(S, V \setminus S) = (\{u \in V \mid x_u \leq x_t\}, \{u \in V \mid x_u > x_t\})$

has cost $\text{usc}(S) \leq \sqrt{8\lambda_2}$

conductance

- **conductance** : another popular measure for cuts
- the conductance of a set $S \subseteq V$ is defined as

$$\phi(S) = \frac{E(S, V \setminus S)}{d|S|}$$

- expresses the probability to “move out” of S by following a random edge from S
- we are interested in sets of small conductance
- the conductance of the graph G is defined as

$$\phi(G) = \min_{\substack{S \subseteq V \\ 0 \leq |S| \leq |V|/2}} \phi(S)$$

Cheeger's inequality

- Cheeger's inequality:

$$\frac{\lambda_2}{2} \leq \frac{\text{usc}(G)}{2} \leq \phi(G) \leq \sqrt{2\lambda_2}$$

\Rightarrow conductance is small if and only if λ_2 is small

Cheeger's inequality

- Cheeger's inequality:

$$\frac{\lambda_2}{2} \leq \frac{\text{usc}(G)}{2} \leq \phi(G) \leq \sqrt{2\lambda_2}$$

\Rightarrow conductance is small if and only if λ_2 is small

- the two leftmost inequalities are “easy” to show
- the first follows by the definition of relaxation
- the second follows by

$$\frac{\text{usc}(S)}{2} = \frac{n}{2d} \frac{E(S, V \setminus S)}{|S||V \setminus S|} \leq \frac{E(S, V \setminus S)}{d|S|} = \phi(S)$$

since $|V \setminus S| \geq n/2$

generalization to non-regular graphs

- $G = (V, E)$ is **undirected** and **non-regular**
- let d_u be the degree of vertex u
- define D to be a **diagonal** matrix whose u -th diagonal element is d_u
- the **normalized laplacian matrix** of G is defined

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

or

$$L_{uv} = \begin{cases} 1 & \text{if } u = v \\ -1/\sqrt{d_u d_v} & \text{if } (u, v) \in E, u \neq v \\ 0 & \text{if } (u, v) \notin E, u \neq v \end{cases}$$

generalization to non-regular graphs

- with the *normalized laplacian*

the eigenvalue expressions become (e.g., λ_2)

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \langle \mathbf{x}, \mathbf{x}_1 \rangle_D = 0}} \frac{\sum_{(u,v) \in E} (x_u - x_v)^2}{\sum_{u \in V} d_u x_u^2}$$

where we use weighted inner product

$$\langle \mathbf{x}, \mathbf{y} \rangle_D = \sum_{u \in V} d_u x_u y_u$$

summary so far

eigenvalues and structural properties of G :

- $\lambda_2 = 0$ iff G is disconnected
- $\lambda_k = 0$ iff G has at least k connected components
- $\lambda_n = 2$ iff G has a bipartite connected component
- small λ_2 iff G is “almost” disconnected (small conductance)

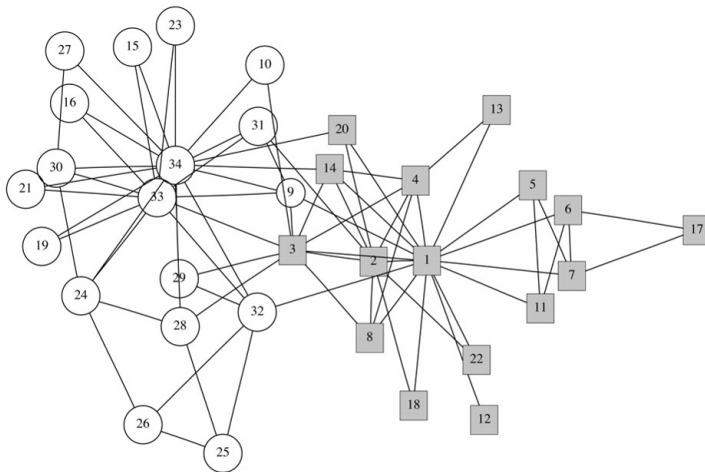
graph partitioning

graph partitioning and community detection

motivation

- knowledge discovery
 - partition the web into sets of related pages (web graph)
 - find groups of scientists who collaborate with each other (co-authorship graph)
 - find groups of related queries submitted in a search engine (query graph)
- performance
 - partition the nodes of a large social network into different machines so that, to a large extent, friends are in the same machine (social networks)

graph partitioning



(Zachary's karate-club network, figure from [\[Newman and Girvan, 2004\]](#))

basic spectral-partition algorithm

1. form **normalized Laplacian** $L' = I - D^{-1/2} A D^{-1/2}$
2. compute eigenvector \mathbf{x}_2 (Fiedler vector)
3. order vertices according their coefficient value on \mathbf{x}_2
4. consider only **sweeping cuts**: splits that respect the order
5. take the sweeping cut S that minimizes $\phi(S)$

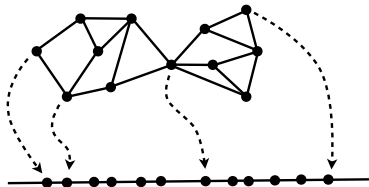
theorem: the basic spectral-partition algorithm finds a cut S such that $\phi(S) \leq 2\sqrt{\phi(G)}$

proof: by Cheeger inequality

$$\phi(S) \leq \sqrt{2 \cdot \lambda_2} \leq \sqrt{2 \cdot 2 \cdot \phi(G)}$$

spectral partitioning rules

1. **conductance**: find the partition that minimizes $\phi(G)$
2. **bisection**: split in two equal parts
3. **sign**: separate positive and negative values
4. **gap**: separate according to the largest gap



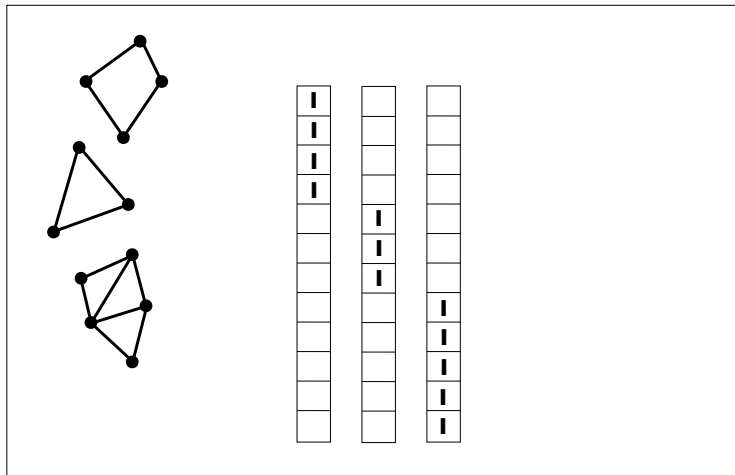
other common spectral-partitioning algorithms

1. utilize more eigenvectors than just the Fiedler vector
use k eigenvectors
2. different versions of the Laplacian matrix

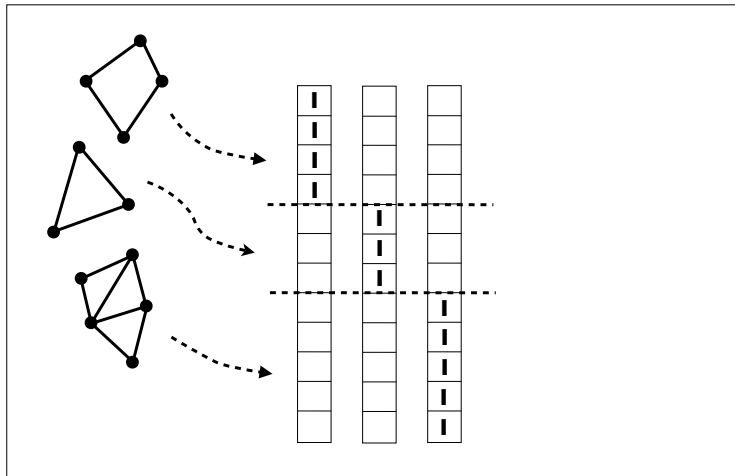
using k eigenvectors

- **ideal scenario:** the graph consists of k disconnected components (perfect clusters)
- **then:** eigenvalue 0 of the Laplacian has **multiplicity** k
the **eigenspace** of eigenvalue 0 is spanned by indicator vectors of the graph components

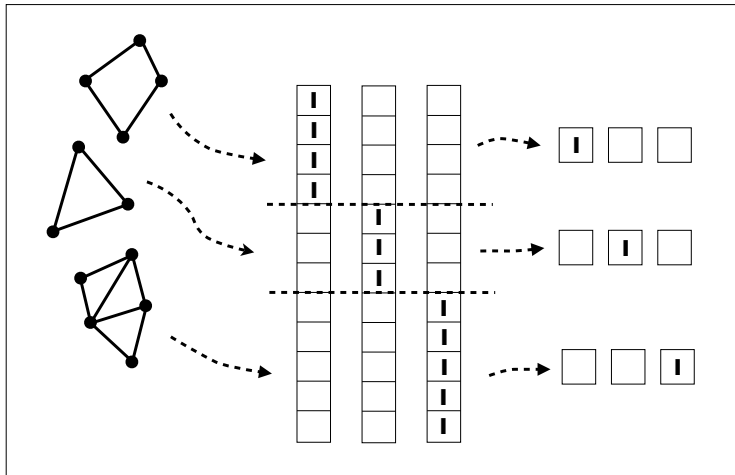
using k eigenvectors



using k eigenvectors



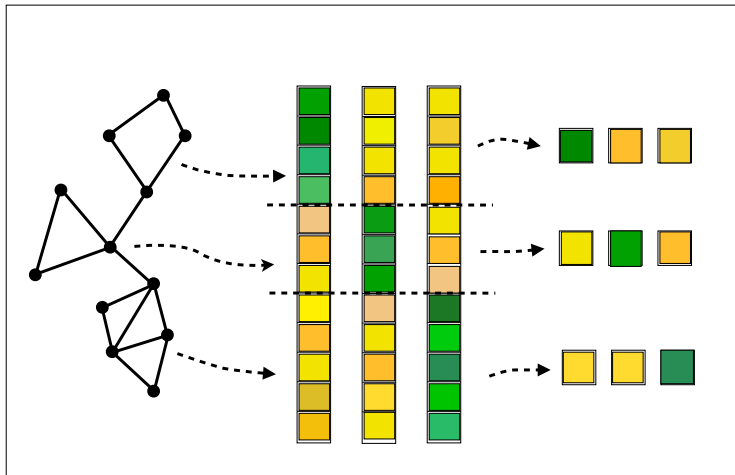
using k eigenvectors



using k eigenvectors

- **robustness under perturbations**: if the graph has less well-separated components the previous structure holds approximately
- **clustering of Euclidean points** can be used to separate the components

using k eigenvectors



laplacian matrices

- normalized laplacian: $L = I - D^{-1/2} A D^{-1/2}$
- unnormalized laplacian: $L_u = D - A$
- normalized “random-walk” laplacian: $L_{rw} = I - D^{-1} A$

all laplacian matrices are related

- **unnormalized Laplacian:** $\lambda_2 = \min_{\substack{\|\mathbf{x}\|=1 \\ \mathbf{x}^T \mathbf{u}_1=0}} \sum_{(i,j) \in E} (x_i - x_j)^2$
- **normalized Laplacian:**

$$\lambda_2 = \min_{\substack{\|\mathbf{x}\|=1 \\ \mathbf{x}^T \mathbf{u}_1=0}} \sum_{(i,j) \in E} \left(\frac{x_i}{\sqrt{d_i}} - \frac{x_j}{\sqrt{d_j}} \right)^2$$

- (λ, \mathbf{u}) is an eigenvalue/vector of L_{rw} if and only if $(\lambda, D^{1/2} \mathbf{u})$ is an eigenvalue/vector of L
- (λ, \mathbf{u}) is an eigenvalue/vector of L_{rw} if and only if (λ, \mathbf{u}) solve the generalized eigen-problem $L_u \mathbf{u} = \lambda D \mathbf{u}$

algorithm 1: unnormalized spectral clustering

input graph adjacency matrix A , number k

1. form diagonal matrix D
2. form unnormalized Laplacian $L = D - A$
3. compute the first k eigenvectors u_1, \dots, u_k of L
4. form matrix $U \in \mathbb{R}^{n \times k}$ with columns u_1, \dots, u_k
5. consider the i -th row of U as point $y_i \in \mathbb{R}^k, i = 1, \dots, n$,
6. cluster the points $\{y_i\}_{i=1, \dots, n}$ into clusters C_1, \dots, C_k
e.g., with k -means clustering

output clusters A_1, \dots, A_k with $A_i = \{j \mid y_j \in C_i\}$

algorithm 2: normalized spectral clustering

[Shi and Malik, 2000]

input graph adjacency matrix A , number k

1. form diagonal matrix D
2. form unnormalized Laplacian $L = D - A$
3. compute the first k eigenvectors u_1, \dots, u_k of the generalized eigenproblem $L\mathbf{u} = \lambda D\mathbf{u}$ (eigvctrs of L_{rw})
4. form matrix $U \in \mathbb{R}^{n \times k}$ with columns u_1, \dots, u_k
5. consider the i -th row of U as point $y_i \in \mathbb{R}^k, i = 1, \dots, n$,
6. cluster the points $\{y_i\}_{i=1, \dots, n}$ into clusters C_1, \dots, C_k
e.g., with k -means clustering

output clusters A_1, \dots, A_k with $A_i = \{j \mid y_j \in C_i\}$

algorithm 3: normalized spectral clustering

[Ng et al., 2001]

input graph adjacency matrix A , number k

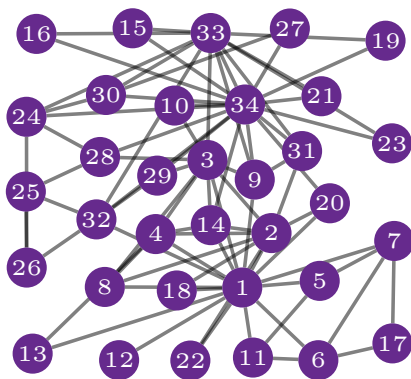
1. form diagonal matrix D
2. form normalized Laplacian $L' = I - D^{-1/2} A D^{-1/2}$
3. compute the first k eigenvectors u_1, \dots, u_k of L'
4. form matrix $U \in \mathbb{R}^{n \times k}$ with columns u_1, \dots, u_k
5. normalize U so that rows have norm 1
6. consider the i -th row of U as point $y_i \in \mathbb{R}^k, i = 1, \dots, n$,
7. cluster the points $\{y_i\}_{i=1, \dots, n}$ into clusters C_1, \dots, C_k
e.g., with k -means clustering

output clusters A_1, \dots, A_k with $A_i = \{j \mid y_j \in C_i\}$

notes on the spectral algorithms

- quite similar except for using different Laplacians
- can be used to cluster any type of data, not just graphs
form **all-pairs similarity matrix** and use as adjacency matrix
- computation of the first eigenvectors of sparse matrices
can be done efficiently using the Lanczos method

Zachary's karate-club network



Zachary's karate-club network



unnormalized
Laplacian

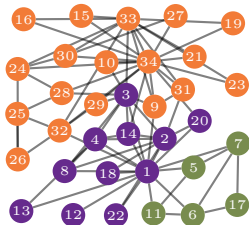


normalized
symmetric
Laplacian

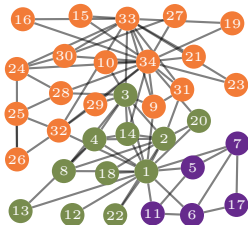


normalized
random walk
Laplacian

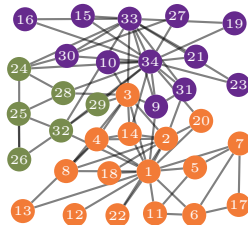
Zachary's karate-club network



unnormalized
Laplacian



normalized
symmetric
Laplacian



normalized
random walk
Laplacian

which Laplacian to use?

[von Luxburg, 2007]

- when graph vertices have about the same degree all laplacians are about the same
- for skewed degree distributions normalized laplacians tend to perform better
- normalized laplacians are associated with conductance, which is a good objective
(conductance involves $\text{vol}(S)$ rather than $|S|$ and captures better the community structure)

summary

- spectral analysis reveals structural properties of a graph
- used for graph partitioning, but also for other problems
- well-studied area, many results and techniques
- for graph partitioning and community detection many other methods are available

acknowledgements



Luca Trevisan

references



Agarwal, G. and Kempe, D. (2008).

Modularity-maximizing graph communities via mathematical programming.

The European Physical Journal B, 66(3).



Ailon, N., Charikar, M., and Newman, A. (2008).

Aggregating inconsistent information: ranking and clustering.

Journal of the ACM (JACM), 55(5).



Brandes, U., Delling, D., Gaertler, M., Görke, R., Höfer, M., Nikoloski, Z., and Wagner, D. (2006).

Maximizing modularity is hard.

Technical report, DELIS – Dynamically Evolving, Large-Scale Information Systems.



Clauset, A., Newman, M., and Moore, C. (2004).

Finding community structure in very large networks.

arXiv.org.

references (cont.)



Karypis, G. and Kumar, V. (1998).

A fast and high quality multilevel scheme for partitioning irregular graphs.

SIAM J. Sci. Comput., 20(1):359–392.



Newman, M. (2004).

Fast algorithm for detecting community structure in networks.

Physical review E, 69(6).



Newman, M. E. J. and Girvan, M. (2004).

Finding and evaluating community structure in networks.

Physical Review E, 69(2).



Ng, A., Jordan, M., and Weiss, Y. (2001).

On spectral clustering: Analysis and an algorithm.

NIPS.



Shi, J. and Malik, J. (2000).

Normalized cuts and image segmentation.

IEEE transactions on Pattern Analysis and Machine Intelligence, 22(8).

references (cont.)



Smyth, P. and White, S. (2005).

A spectral clustering approach to finding communities in graphs.

SDM.



von Luxburg, U. (2007).

A Tutorial on Spectral Clustering.

arXiv.org.