Aalto University
School of Science

CS-E4600 – Algorithmic methods of data mining

Slide set 12 : Spectral graph analysis

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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)
- 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 $\lambda_1, \ldots, \lambda_n$ of A can be ordered

$$\lambda_1 \leq \ldots \leq \lambda_n$$

- theorem [variational characterization of eigenvalues]

$$\begin{aligned} \lambda_n &= \max_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \\ \lambda_1 &= \min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \\ \lambda_2 &= \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \quad \text{and “so on” for the other eigenvalues} \end{aligned}$$

- very useful way to think about eigenvalues

background: eigenvalues and eigenvectors

- the inverse holds, i.e.,

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

  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

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

  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 ?
  - 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

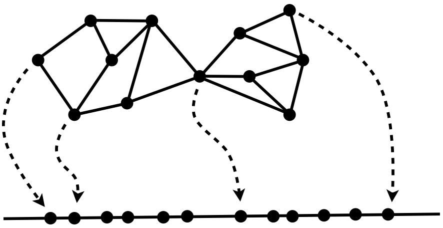
$$L = I - \frac{1}{d} A \qquad \text{or} \qquad L_{ij} = \begin{cases} 1 & \text{if } i = j \\ -1/d & \text{if } (i,j) \in E, i \neq j \\ 0 & \text{if } (i,j) \notin E, i \neq j \end{cases}$$

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 ?

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

  (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 ?

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

- 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 orthogocal to $\mathbb{S}_k$

the largest eigenvalue

- what about λ_n?

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

- 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

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

  ($E(S, T)$ 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

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

- 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?

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

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

the second eigenvalue

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

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

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

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

uniform sparsest cut

- it can be shown that

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

uniform sparsest cut

- it can be shown that

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- 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 $\mathbf{x}$ 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:

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

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

Cheeger's inequality

- Cheeger's inequality:

$$\frac{\lambda_2}{2} \le \frac{\mathrm{usc}(G)}{2} \le \phi(G) \le \sqrt{2\lambda_2}$$

$\Rightarrow$ 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

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

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

Cheeger's inequality

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

- the rightmost inequality is the "difficult one"
- proof sketch (three steps):

1. consider a vector $\mathbf{y} \geq \mathbf{0}$

– we can find a set $S \subseteq \{v \in V \mid y_v > 0\}$ such that

$$\phi(S) \leq \frac{\sum_{(u,v)\in E} |y_u - y_v|}{d \sum_{u \in V} |y_u|} \qquad \text{(no squares)}$$

– pick random $t \in [0, \max_v y_v]$ and define $S = \{v \mid y_v \geq t\}$

– then $\phi(S) \leq$ r.h.s on expectation

– thus, there is some t that the property holds

Cheeger's inequality

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

- proof sketch (three steps):

2. given a vector $\mathbf{x}$ we can find another vector $\mathbf{y}$ such that

$$\frac{\sum_{(u,v)\in E} |y_u - y_v|}{d \sum_{u \in V} |y_u|} \leq \sqrt{2 \frac{\sum_{(u,v)\in E} |x_u - x_v|^2}{d \sum_{u\in V} |x_u|^2}}$$

and $\quad |\{v \mid y_v > 0\}| \leq \frac{n}{2}$

– proof of this claim is constructive; uses Cauchy-Schwarz

3. take $\mathbf{x}$ to be the eigenvector of λ_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)

random walks

random walks

- consider random walk on the graph G by following edges
- from vertex i move to vertex j with prob. $1/d_i$ if $(i,j) \in E$
- $\mathbf{p}_i^{(t)}$ probability of being at vertex i at time t
- process is described by equation $\mathbf{p}^{(t+1)} = \mathbf{p}^{(t)} P$, where $P = D^{-1} A$ is row-stochastic
- process converges to stationary distribution $\pi = \pi P$ (under certain irreducibility conditions)
- for undirected and connected graphs

$$\pi_i = \frac{d_i}{2m} \quad \text{(stationary distribution} \sim \text{degree)}$$

random walks — useful concepts

- hitting time $H(i, j)$: expected number of steps before visiting vertex j, starting from i
- commute time $\kappa(i, j)$: expected number of steps before visiting j and i again, starting at i : $\kappa(i, j) = H(i, j) + H(j, i)$
- cover time: expected number of steps to reach every node
- mixing time $\tau(\epsilon)$: a measure of how fast the random walk approaches its stationary distribution

$$\tau(\epsilon) = \min\{t \mid d(t) \leq \epsilon\}$$

where

$$d(t) = \max_i ||\mathbf{p}^t(i, \cdot) - \pi|| = \max_i \left\{ \sum_j |\mathbf{p}^t(i, j) - \pi_j| \right\}$$

random walks vs. spectral analysis

- consider the normalized laplacian $L = I - D^{-1/2} A D^{-1/2}$

$$
\begin{aligned}
L\,\mathbf{u} &= \lambda\,\mathbf{u} \\
(I - D^{-1/2} A D^{-1/2})\,\mathbf{u} &= \lambda\,\mathbf{u} \\
(D - A)\,\mathbf{u} &= \lambda\,D\,\mathbf{u} \\
D\,\mathbf{u} &= A\,\mathbf{u} + \lambda\,D\,\mathbf{u} \\
(1 - \lambda)\,\mathbf{u} &= D^{-1} A\,\mathbf{u} \\
\mu\,\mathbf{u} &= P\,\mathbf{u}
\end{aligned}
$$

- $(\lambda, \mathbf{u})$ is an eigenvalue–eigenvector pair for L if and only if $(1 - \lambda, \mathbf{u})$ is an eigenvalue–eigenvector pair for P
- the eigenvector with smallest eigenvalue for L is the eigenvector with largest eigenvalue for P

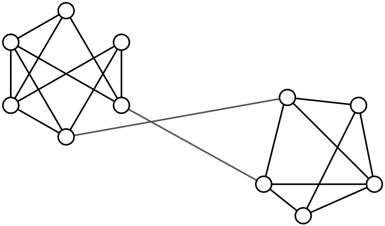
random walks vs. spectral analysis

- stochastic matrix P, describing the random walk
- eigenvalues: $-1 < \mu_n \leq \ldots \leq \mu_2 < \mu_1 = 1$
- spectral gap: $\gamma_* = 1 - \mu_2 = \lambda_2$
- relaxation time: $\tau_* = \frac{1}{\gamma_*}$
- theorem: for an aperiodic, irreducible, and reversible random walk, and any ϵ

$$(\tau_* - 1)\log\left(\frac{1}{2\epsilon}\right) \leq \tau(\epsilon) \leq \tau_* \log\left(\frac{1}{2\epsilon\sqrt{\pi_{\min}}}\right)$$

random walks vs. spectral analysis

- intuition: fast mixing related to graph being an expander



small spectral gap $\Leftrightarrow$ large mixing time $\Leftrightarrow$ bottlenecks $\Leftrightarrow$

$\Leftrightarrow$ clusters $\Leftrightarrow$ low conductance $\Leftrightarrow$ small λ_2

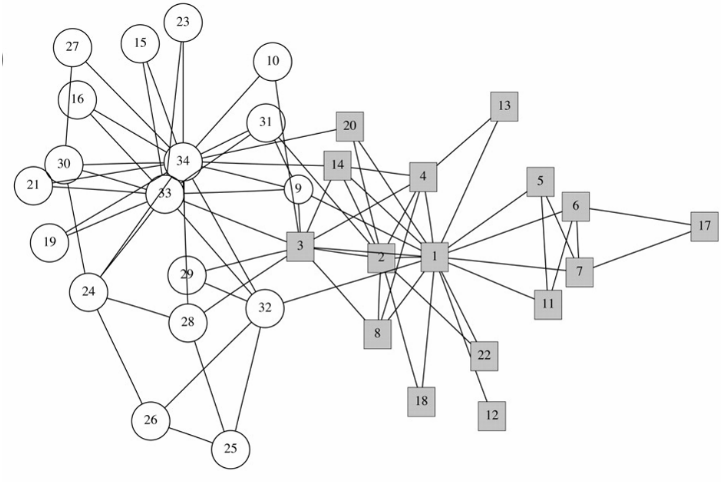
graph partitioning

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 $\mathbf{x}_2$ (Fielder 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 $\phi(S)$

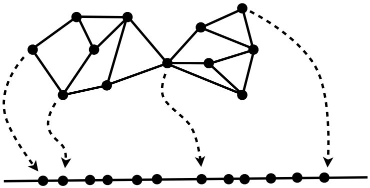
theorem: the basic spectral-partition algorithm finds a cut S such that $\phi(S) \leq 2\sqrt{\phi(G)}$

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

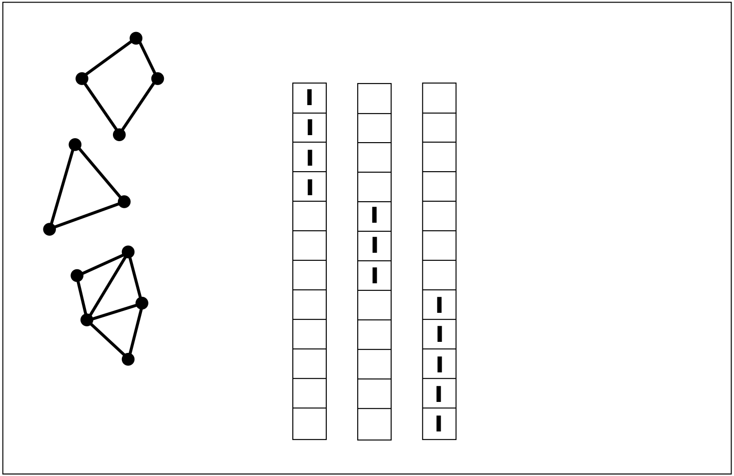
1. utilize more eigenvectors than just the Fielder vector
   use k eigenvectors

2. different versions of the Laplacian matrix

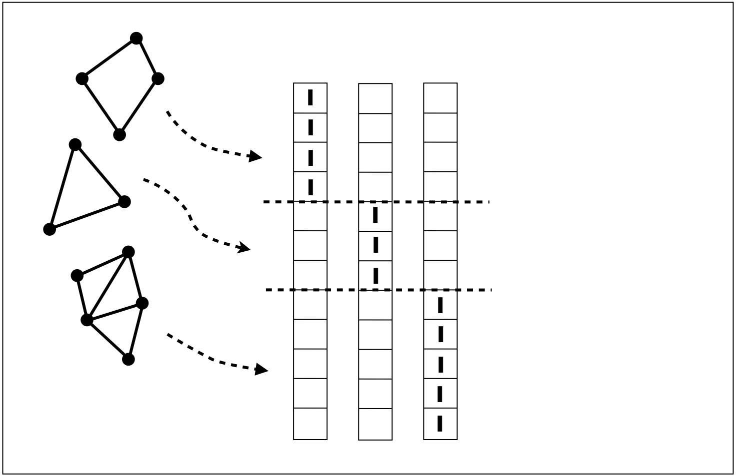
using k eigenvectors

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

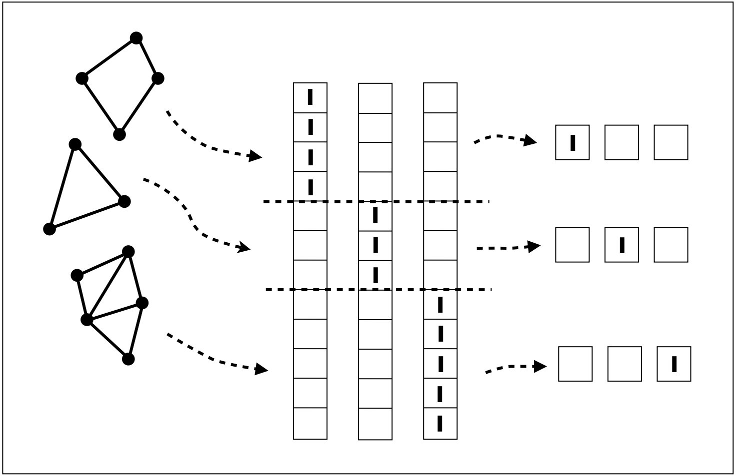
using k eigenvectors



using k eigenvectors



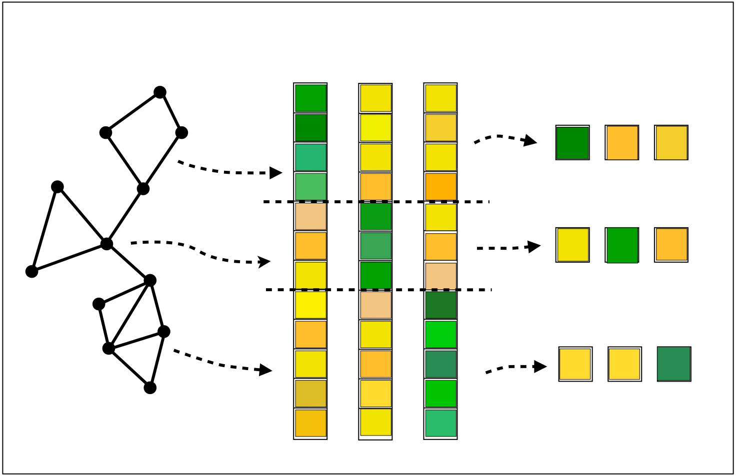
using *k* eigenvectors



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: $L = I - D^{-1/2} A\, D^{-1/2}$
- unormalized laplacian: $L_u = D - A$
- normalized "random-walk" laplacian: $L_{\mathrm{rw}} = I - D^{-1} A$

all laplacian matrices are related

- unormalized 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:

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

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

algorithm 1: unormalized spectral clustering

input graph adjacency matrix A, number k

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

   e.g., with k-means clustering

output clusters $A_1, \ldots, A_k$ 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 unormalized Laplacian $L = D - A$
3. compute the first k eigenvectors $u_1, \ldots, u_k$ 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 $u_1, \ldots, u_k$
5. consider the i-th row of U as point $y_i \in \mathbb{R}^k, i = 1, \ldots, n$,
6. cluster the points $\{y_i\}_{i=1,\ldots,n}$ into clusters $C_1, \ldots, C_k$

   e.g., with k-means clustering

output clusters $A_1, \ldots, A_k$ 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 $u_1, \ldots, u_k$ of L'
4. form matrix $U \in \mathbb{R}^{n \times k}$ with columns $u_1, \ldots, u_k$
5. normalize U so that rows have norm 1
6. consider the i-th row of U as point $y_i \in \mathbb{R}^k, i = 1, \ldots, n$,
7. cluster the points $\{y_i\}_{i=1,\ldots,n}$ into clusters $C_1, \ldots, C_k$

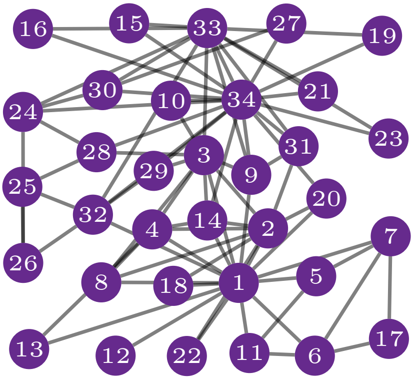
   e.g., with k-means clustering

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

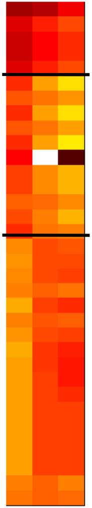
notes on the spectral algorithms

- 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

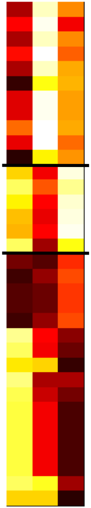
Zachary’s karate-club network



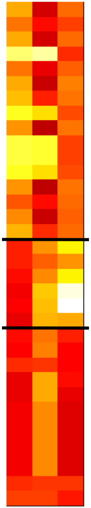
Zachary's karate-club network



unormalized
Laplacian

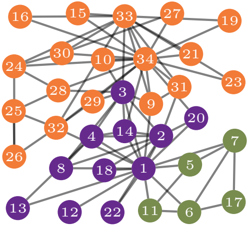


normalized
symmetric
Laplacian

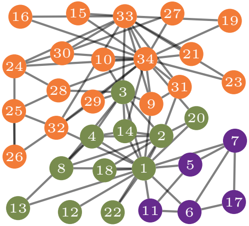


normalized
random walk
Laplacian

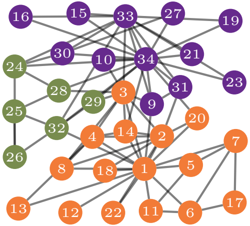
Zachary's karate-club network



unormalized
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 $\mathrm{vol}(S)$ 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

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