Opinions and conflict in social networks: models, computational problems and algorithms

Lecture 2: Mathematical background

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course overview

- lecture 1: introduction
  - polarization in social media; methods for detecting polarization
- lecture 2: mathematical background
  - submodular maximization; spectral graph theory
- lecture 3: methods for mitigating polarization
  - maximizing diversity, balancing information exposure
- lecture 4: signed networks; theory and applications
- lecture 5: opinion dynamics in social networks

why study these topics?

- spectral graph theory:
  - provides tools to reveal structure in graphs
  - e.g., used for community detection, a fundamental concept in social-network analysis
  - many other applications
  - mathematically interesting
- submodular maximization:
  - common type of optimization problem
  - many ML problems are modeled as submodular maximization

studying material

- spectral graph theory: von Luxburg. A tutorial on spectral clustering
- submodular maximization: several online tutorials, e.g., Krause and Guestrin 2009, Bilmes 2014, or Hassani and Karbasi 2020

spectral graph theory

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 $\mathbf{A}$, i.e., $\mathbf{A} \in \mathbb{R}^{n \times n}$

- $\lambda \in \mathbb{C}$ is an eigenvalue of $\mathbf{A}$ if there exists $\mathbf{x} \in \mathbb{C}^n$, $\mathbf{x} \neq \mathbf{0}$ such that

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

  such a vector $\mathbf{x}$ is called eigenvector of $\mathbf{A}$ corresponding to eigenvalue λ

- alternatively,

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

  it follows that $\mathbf{A}$ has n eigenvalues (possibly complex and possibly with multiplicity > 1)

background: eigenvalues and eigenvectors

- consider a real and symmetric $n \times n$ matrix $\mathbf{A}$

  (e.g., the adjacency matrix of an undirected graph)

  then

  – eigenvalues are real and eigenvectors are orthogonal

- $\mathbf{A}$ is positive semi-definite if $\mathbf{x}^T \mathbf{A}\, \mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$

- a symmetric positive semi-definite real matrix has real and non negative eigenvalues

background: variational characterization of eigenvalues

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

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

- the eigenvalues satisfy the following minimax principles w.r.t. Rayleigh quotient

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

- 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
- consider $G = (V, E)$ an undirected and d-regular graph
  - regular graph is used w.l.o.g. for simplicity of expositions
- question : which matrix to consider ?
  - the adjacency matrix $\mathbf{A}$ of the graph
  - some matrix $\mathbf{B}$ so that $\mathbf{x}^T \mathbf{B}\, \mathbf{x}$ is related to a structural property of the graph
- let $\mathbf{A}$ be the adjacency matrix of G; define the *Laplacian matrix* of G as

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

spectral graph analysis

- for the Laplacian matrix $\mathbf{L} = \mathbf{I} - \frac{1}{d}\mathbf{A}$, we can show that (proof left as exercise)

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

here, x_u is the coordinate of the vector $\mathbf{x}$ that corresponds to vertex $u \in V$

spectral graph analysis

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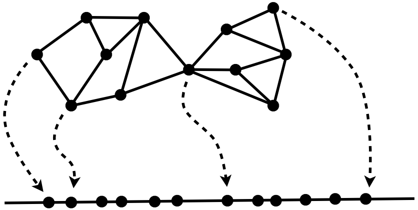
here, x_u is the coordinate of the vector $\mathbf{x}$ that corresponds to vertex $u \in V$

- vector $\mathbf{x}$ is seen as a 1-dimensional embedding
  - i.e., mapping the vertices of the graph onto the real line



the smallest eigenvalue

apply the eigenvalue characterization theorem for $\mathbf{L}$

- what is λ_1 ?

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

- 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 $\mathbf{L}$

- what is λ_2 ?

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

- 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 ?

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

- consider a boolean version of this problem
  - restrict mapping to $\{-1, +1\}$
  - mapping of vertices to $\{-1, +1\}$ corresponds to a graph cut S

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

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

the largest eigenvalue

- consider the graph cut S defined by the mapping of vertices to $\{-1,+1\}$, then :

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

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

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

the largest eigenvalue

- on the other hand

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

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

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

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

summary so far

- eigenvalues and structural properties of G :
  - $\lambda_2 = 0$ if and only if G is disconnected
  - $\lambda_k = 0$ if and only if G has at least k connected components
  - $\lambda_n = 2$ if and only if 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

we can rewrite the expression for λ_2 as

$$\lambda_2 = \min_{\substack{\mathbf{x}\neq\mathbf{0} \\ \mathbf{x}^T\mathbf{x}_1=0}} \frac{\sum_{(u,v)\in E}(x_u - x_v)^2}{d\sum_{u\in V} x_u^2} = \min_{\substack{\mathbf{x}\neq\mathbf{0} \\ \mathbf{x}^T\mathbf{x}_1=0}} \frac{\frac{1}{d}\sum_{(u,v)\in E}(x_u - x_v)^2}{\frac{1}{2n}\sum_{(u,v)\in V^2}(x_u - x_v)^2}$$

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

why?

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

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

the second eigenvalue

we can further rewrite the expression for λ_2 as follows:

note that we change the argument over which we take min

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\frac{1}{d} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{2n} \sum_{(u,v) \in V^2} (x_u - x_v)^2} = \min_{\mathbf{x} \text{ non const}} \frac{\frac{2}{d} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{n} \sum_{(u,v) \in V^2} (x_u - x_v)^2}$$

why?

because for any $\mathbf{y}$ that is not a constant vector,

and having $\mathbf{y}^T \mathbf{x}_1 = \sum_u y_u = s \neq 0$,

the vector $\mathbf{x} = \mathbf{y} - s/n$ achieves the same value

and it satisfies $\mathbf{x}^T \mathbf{x}_1 = \sum_u x_u = 0$ and $\mathbf{x} \neq \mathbf{0}$

the second eigenvalue

we can further rewrite the expression for λ_2 as follows:

note that we change the argument over which we take min

$$\lambda_2 = \min_{\substack{\mathbf{x} \neq \mathbf{0} \\ \mathbf{x}^T \mathbf{x}_1 = 0}} \frac{\frac{1}{d} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{2n} \sum_{(u,v) \in V^2} (x_u - x_v)^2} = \min_{\mathbf{x} \text{ non const}} \frac{\frac{2}{d} \sum_{(u,v) \in E} (x_u - x_v)^2}{\frac{1}{n} \sum_{(u,v) \in V^2} (x_u - x_v)^2}$$

why?

so, for any non-constant $\mathbf{y}$ that minimizes the r.h.s. ratio

there is an $\mathbf{x}$ (with $\mathbf{x}^T \mathbf{x}_1 = 0$ and $\mathbf{x} \neq \mathbf{0}$) that minimizes the l.h.s. ratio

(notice that since $\mathbf{x}$ subtracts the constant s/n from $\mathbf{y}$ the ratios are the same,

as the constant s/n cancels out inside the differences)

the second eigenvalue

we can now write

$$\lambda_2 = \min_{\mathbf{x} \text{ non const}} \frac{\frac{2}{nd} \sum_{(u,v)\in E} (x_u - x_v)^2}{\frac{1}{n^2} \sum_{(u,v)\in V^2} (x_u - x_v)^2} = \min_{\mathbf{x} \text{ non const}} \frac{\mathbb{E}_{(u,v)\in E}[(x_u - x_v)^2]}{\mathbb{E}_{(u,v)\in V^2}[(x_u - x_v)^2]}$$

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

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

where $usc(G)$ is the uniform sparsest cut of G defined as

$$usc(G) = \min_{S\subseteq V} \frac{n}{d} \frac{E(S, \overline{S})}{|S|\,|\overline{S}|}$$

uniform sparsest cut

- it can be shown that

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

- the first inequality holds because λ_2 is a relaxation to usc
- 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 $usc(S) \leq \sqrt{8\lambda_2}$

conductance

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

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

- it 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:
$$\frac{\lambda_2}{2} \leq \frac{usc(G)}{2} \leq \phi(G) \leq \sqrt{2\lambda_2}$$

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

  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 $\mathbf{D}$ to be a diagonal matrix whose u-th diagonal element is d_u
- the *normalized Laplacian matrix* of G is defined

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

or

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

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

- eigenvalues and structural properties of G :
  - $\lambda_2 = 0$ if and only if G is disconnected
  - $\lambda_k = 0$ if and only if G has at least k connected components
  - $\lambda_n = 2$ if and only if G has a bipartite connected component
  - small λ_2 if and only if G is "almost" disconnected (small conductance)

discussion

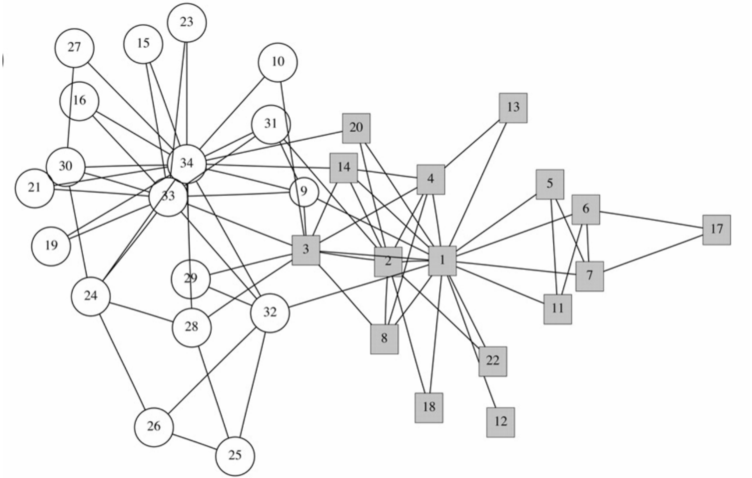
- deep connections between spectral properties of appropriately-defined matrices and structural properties of a graph
- spectral analysis provides a means to embed the graph nodes into low-dimensional Euclidean spaces
- spectral embeddings can be used to solve a number of different learning problems on graphs
- many other state-of-the-art embeddings are known, going beyond spectral analysis

graph partitioning and community detection

motivation

- knowledge discovery
  - partition the web into sets of related pages (web graph)
  - find communities of friends in a social network (social graph)
  - find groups of related proteins (protein-protein interaction network)
- 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]

community detection via conductance minimization

- recall conductance
  - the conductance of a set $S \subseteq V$ is defined as

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

  - the conductance of the graph G is defined as

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

  it expresses the probability to "move out" of S by following a random edge from S
  - a set S with small conductance value is a good community
- but there are exponentially many candidate sets S;
  - so, we need efficient and accurate methods
- basic definition works for partitioning the graph in two sets
  - for finding k communities we need to extend the definition

Cheeger's inequality

- Cheeger's inequality:

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

$$\Rightarrow \quad \text{conductance is small if and only if } \lambda_2 \text{ is small}$$

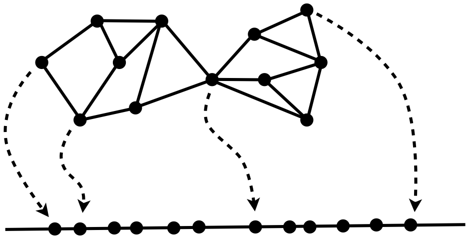
- right hand side inequality involves finding a cut based on the second smallest eigenvector

second smallest eigenvector $\mathbf{x}_2$

- $\mathbf{x}_2$ is also known as Fielder vector
- $\mathbf{x}_2$ is given by

$$\mathbf{x}_2 = \arg \min_{\substack{\|\mathbf{x}\|=1 \\ \mathbf{x}^T\mathbf{x}_1=0}} \sum_{(u,v)\in E} (x_u - x_v)^2$$

- can be seen as 1-dimensional embedding that minimizes the above “potential function”



basic spectral-partition algorithm

partition nodes in two sets S and $V \setminus S$; measure of quality is conductance $\phi(S)$

1. form normalized Laplacian $\mathbf{L}' = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\,\mathbf{D}^{-1/2}$
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 the conductance measure $\phi(S)$

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

proof: by Cheeger inequality, we know that the cut S induced by $\mathbf{x}_2$ satisfies $\phi(S) \leq \sqrt{2\,\lambda_2}$

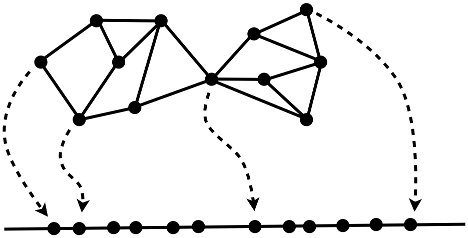
by Cheeger inequality again, we know that $\lambda_2 \leq 2\,\phi(G)$, thus

$$\phi(S) \leq \sqrt{2\,\lambda_2} \leq \sqrt{4\,\phi(G)} \leq 2\sqrt{\phi(G)}$$

spectral partitioning criteria

a number of different partitioning criteria can be used

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



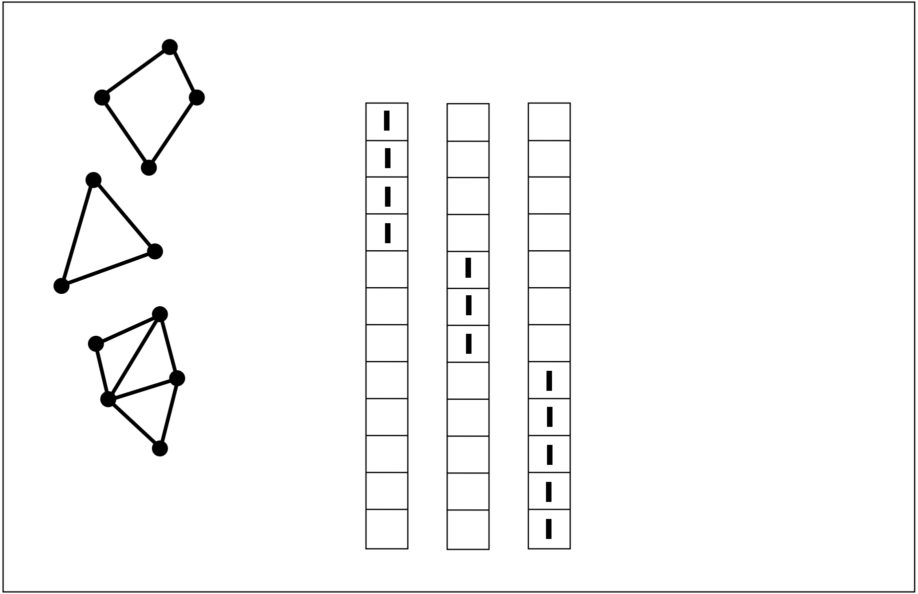
practical spectral-partitioning algorithms

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

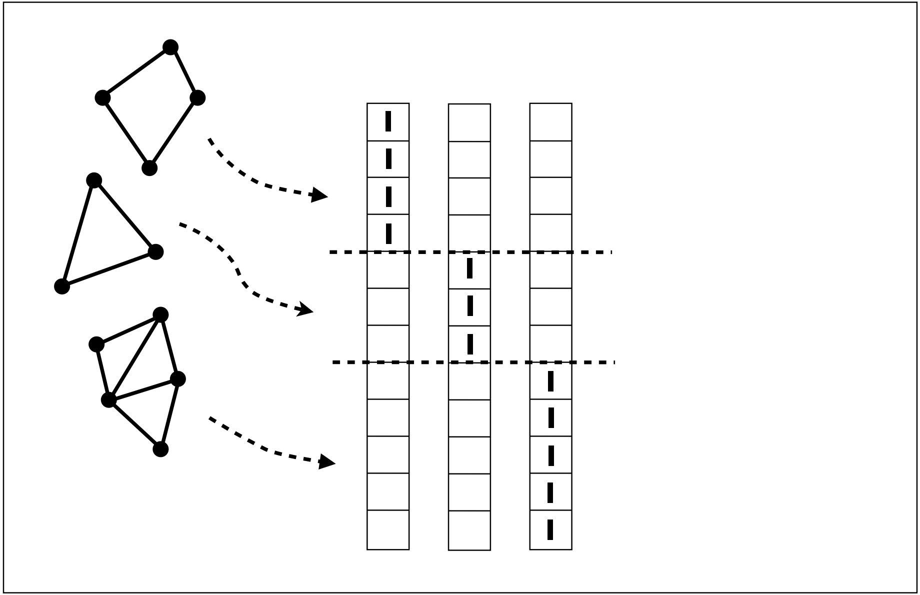
using k eigenvectors

- ideal scenario: the graph consists of k disconnected components (perfect clusters)
- in this case, the multiplicity of the eigenvalue 0 of the graph Laplacian is k
  - the eigenspace of eigenvalue 0 is spanned by indicator vectors of the graph components

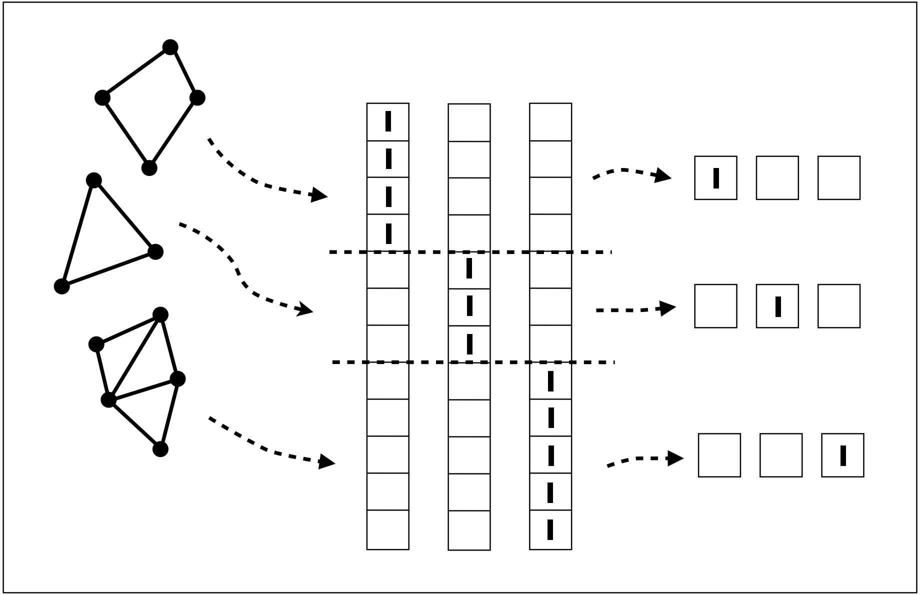
using k eigenvectors



using k eigenvectors



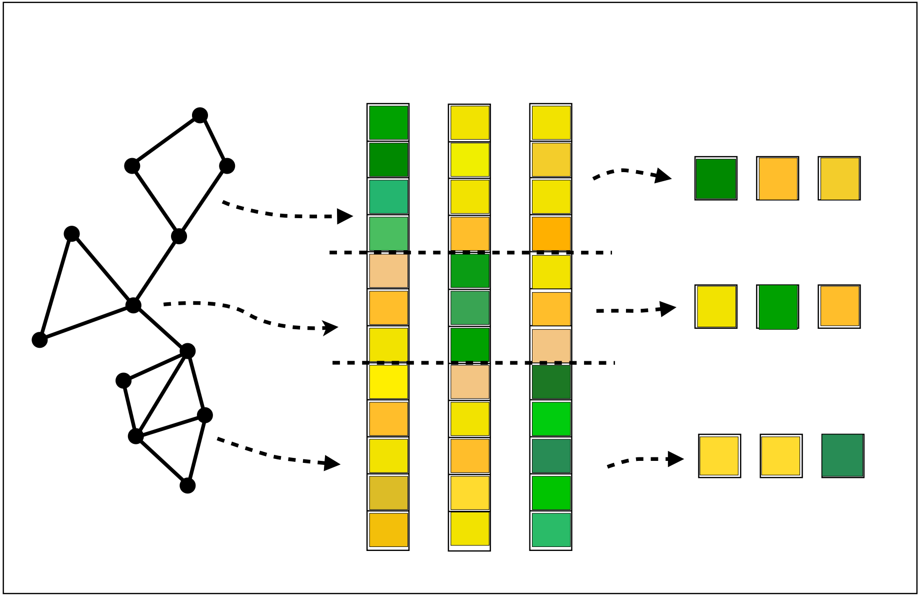
using k eigenvectors



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 : $\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\,\mathbf{D}^{-1/2}$
- unnormalized Laplacian : $\mathbf{L}_u = \mathbf{D} - \mathbf{A}$
- normalized “random-walk” Laplacian : $\mathbf{L}_{\mathrm{rw}} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{A}$

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 :

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

- $(\lambda, \mathbf{u})$ is an eigenvalue/vector of $\mathbf{L}_{\mathrm{rw}}$ if and only if $(\lambda, \mathbf{D}^{1/2}\,\mathbf{u})$ is an eigenvalue/vector of $\mathbf{L}$

- $(\lambda, \mathbf{u})$ is an eigenvalue/vector of $\mathbf{L}_{\mathrm{rw}}$ if and only if $(\lambda, \mathbf{u})$ is a solution to the generalized eigen-problem $\mathbf{L}_u\,\mathbf{u} = \lambda\,\mathbf{D}\,\mathbf{u}$

algorithm 1: unnormalized spectral clustering

input : graph adjacency matrix $\mathbf{A}$, number k

1. form diagonal matrix $\mathbf{D}$
2. form unnormalized Laplacian $\mathbf{L} = \mathbf{D} - \mathbf{A}$
3. compute the first k eigenvectors $u_1, \ldots, u_k$ of $\mathbf{L}$
4. form matrix $\mathbf{U} \in \mathbb{R}^{n \times k}$ with columns $u_1, \ldots, u_k$
5. consider the i-th row of $\mathbf{U}$ 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 $\mathbf{A}$, number k

1. form diagonal matrix $\mathbf{D}$
2. form unnormalized Laplacian $\mathbf{L} = \mathbf{D} - \mathbf{A}$
3. compute the first k eigenvectors $u_1, \ldots, u_k$ of the generalized eigen-problem $\mathbf{L}\,\mathbf{u} = \lambda\,\mathbf{D}\,\mathbf{u}$

   # i.e., eigenvectors of $\mathbf{L}_{\mathrm{rw}}$
4. form matrix $\mathbf{U} \in \mathbb{R}^{n \times k}$ with columns $u_1, \ldots, u_k$
5. consider the i-th row of $\mathbf{U}$ 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 $\mathbf{A}$, number k

1. form diagonal matrix $\mathbf{D}$
2. form normalized Laplacian $\mathbf{L}' = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\,\mathbf{D}^{-1/2}$
3. compute the first k eigenvectors $u_1, \ldots, u_k$ of $\mathbf{L}'$
4. form matrix $\mathbf{U} \in \mathbb{R}^{n \times k}$ with columns $u_1, \ldots, u_k$
5. normalize $\mathbf{U}$ so that rows have norm 1
6. consider the i-th row of $\mathbf{U}$ 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

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 $vol(S)$ 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

submodular maximization

submodular set functions

- consider a ground set U
- a function $f : 2^U \to \mathbb{R}$ is submodular if

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$$

  for all $A, B \subseteq U$

- equivalently ("diminishing returns")

$$f(A \cup \{x\}) - f(A) \geq f(B \cup \{x\}) - f(B)$$

  for all $A \subseteq B \subseteq U$ and $x \in U \setminus B$

submodular set functions

may or not satisfy the following properties

- non-negative : $f(A) \geq 0$ for all $A \subseteq U$
- monotone : $f(A) \leq f(B)$ for all $A \subseteq B \subseteq U$
- symmetric : $f(A) = f(U \setminus A)$ for all $A \subseteq U$

example: coverage in set systems

- $S_1, \ldots, S_n$ subsets of U
- function $f : 2^{\{1,\ldots,n\}} \to \mathbb{R}_+$
- coverage :

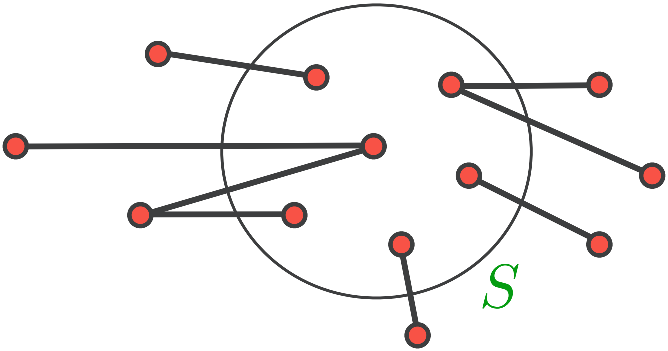
$$f(A) = |\cup_{i \in A} S_i|$$

- weighted coverage :

$$w : U \to \mathbb{R}_+ \quad \text{and} \quad f(A) = \sum_{x \in \cup_{i \in A} S_i} w(x)$$

example: cut in graphs

- consider undirected graph $G = (V, E)$
- cut function $f : 2^V \to R_+$ defined as $f(S) = |E(S, V \setminus S)|$



in the previous examples

- coverage in set systems

  $\Rightarrow$ monotone and non-negative

- cut functions in undirected graphs and hypergraphs

  $\Rightarrow$ symmetric and non-negative

- cut functions in directed graphs

  $\Rightarrow$ non-negative

the maximization problem

- given submodular function $f : 2^U \to \mathbb{R}$

  find $S \subseteq X$ to maximize $f(S)$

  subject to constraints

- value-oracle model
- generalizes many interesting problems **NP**-hard problems
- minimization problem is polynomial (e.g., min-cut)

monotone functions

- $f(U)$ trivial maximizer

- more interesting to maximize under cardinality constraints
- find $S \subseteq U$ subject to $|S| \leq k$ that maximizes $f(S)$

- MAX k-COVER is a special case
- greedy gives $(1 - 1/e)$ approximation [Nemhauser et al., 1978]
- no better approximation unless **P**=**NP**

the greedy algorithm

1. $S \leftarrow \emptyset$
2. while $|S| < k$
3. $\quad i \leftarrow \arg\max_j f(S \cup \{j\})$
4. $\quad S \leftarrow S \cup \{i\}$
5. return S

analysis of the greedy

let $S_j = \{e_1, \ldots, e_j\}$ be first j elements picked by the greedy

$$
\begin{aligned}
f(S^*) &\leq f(S_{i-1}) + \sum_{e \in S^* \setminus S_{i-1}} f_{S_{i-1}}(e) && \text{(monotonicity and submodularity)} \\
&\leq f(S_{i-1}) + \sum_{e \in S^* \setminus S_{i-1}} f(S_i) - f(S_{i-1}) && \text{(greediness)} \\
&\leq f(S_{i-1}) + k(f(S_i) - f(S_{i-1})) && (|S^*| \leq k)
\end{aligned}
$$

it follows

$$f(S_i) - f(S^*) \geq \frac{k-1}{k}(f(S_{i-1}) - f(S^*))$$

which by induction implies

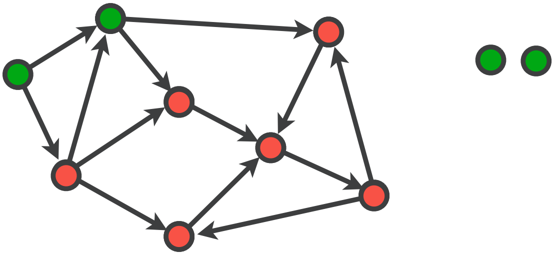
$$f(S_i) \geq \left(1 - (1 - 1/k)^i\right) f(S^*)$$

and so

$$f(S_{greedy}) = f(S_k) \geq \left(1 - (1 - 1/k)^k\right) f(S^*) \geq \left(1 - \frac{1}{e}\right) f(S^*)$$

widely applicable in data mining

- example : maximize the spread of influence in social networks [Kempe et al., 2003]
- assume that an action is spread in a social network
- assume a spreading model such as independent cascade
- find a set of k initial seeds to maximize the spread
- spreading model is randomized, so we want to maximize expected spread



non-monotone functions

- unconstrainted version becomes interesting
- find $S \subseteq X$ to maximize $f(S)$

- a particularly interesting case is the MAX-CUT problem
- what do we know about the approximation of MAX-CUT?
- picking a random set of vertices gives $1/2$ ($1/4$ for MAX-DICUT)
- SDP relaxation technique gives 0.878 (0.796 for MAX-DICUT)

  (major breakthrough) [Goemans and Williamson, 1995]
- 0.53 by spectral approach [Trevisan, 2012]

unconstrainted problem

[Feige et al., 2011]

- first constant-factor approximations for non-negative submodular functions
- $1/2$ approximation for symmetric functions
- $2/5 = 0.4$ approximation for the non-negative functions
- lower bound: better than $1/2$ approximation requires exponential number of value queries

unconstrainted problem

[Feige et al., 2011]

- pick a random set

  $1/4$ for non-negative function (on expectation)

  $1/2$ for symmetric function (on expectation)

- local search
  - initialize S to best singleton
  - $S =$ local optimum (add or delete elements)
  - return the best of S and $U \setminus S$

  $1/3$ approximation for non-negative function

  $1/2$ for non-negative symmetric function

random set analysis

- for $A \subseteq U$, $A(p)$ is a random set where each element of A is selected with prob p
- algorithm returns $R = U(1/2)$
- lemma I

$$E[f(A(p))] \geq (1-p)\, f(\emptyset) + p\, f(A)$$

  can proven by induction on the size of A and using submodularity
- lemma II

$$\begin{aligned} E[f(A(p) \cup B(q))] \quad \geq \quad & (1-p)(1-q)\, f(\emptyset) + \\ & p(1-q)\, f(A) + \\ & (1-p)q\, f(B) + \\ & pq\, f(A \cup B) \end{aligned}$$

  to prove use lemma I

random set analysis

- algorithm returns

$$R = U(1/2) = S^*(1/2) \cup \overline{S^*}(1/2)$$

- by applying lemma II

$$\begin{aligned} E[f(R)] &= E[f(S^*(1/2) \cup \overline{S^*}(1/2))] \\ &= \frac{1}{4}f(\emptyset) + \frac{1}{4}f(S^*) + \frac{1}{4}f(\overline{S^*}) + \frac{1}{4}f(U) \end{aligned}$$

- gives $1/4$ for non-negative and $1/2$ for symmetric function

unconstrained problem

[Feige et al., 2011]

- local search
  - initialize S to best singleton
  - $S =$ local optimum (add or delete elements)
  - return the best of S and $U \setminus S$

$1/3$ approximation for non-negative function

$1/2$ for non-negative symmetric function

analysis of local search

- lemma III: if S is a local optimum then $f(S) \geq f(T)$ for all $S \subseteq T$ and $T \subseteq S$
- proof

  take $S \subseteq T$ and consider $S = X_0 \subseteq \ldots \subseteq X_\ell = T$

  by submodularity and local optimality

$$0 \geq f(S \cup \{x_i\}) - f(S) \geq f(X_i) - f(X_{i-1})$$

  summing up gives $0 \geq f(X_\ell) - (X_0)$ or $f(S) \geq (T)$
- corollary

  for optimum S^* and local optimum S it is $f(S) \geq f(S \cup S^*)$ and $f(S) \geq f(S \cap S^*)$

analysis of local search (cont)

- it is

$$f(S) \geq f(S \cup S^*) \quad \text{and} \quad f(S) \geq f(S \cap S^*)$$

- by submodularity and non-negativity

$$f(S \cup S^*) + f(U \setminus S) \geq f(S^* \setminus S) + f(U) \geq f(S^* \setminus S)$$

$$f(S \cap S^*) + f(S^* \setminus S) \geq f(S^*) + f(\emptyset) \geq f(S^*)$$

- combining we get

$$2f(S) + f(U \setminus S) \geq f(S^*)$$

- and so

$$\max\{f(S), f(U \setminus S)\} \geq \frac{1}{3} f(S^*)$$

unconstrainted problem

[Buchbinder et al., 2015]

- tight $1/2$ approximation for general non-negative submodular function
- randomized algorithm, approximation $1/2$
- deterministic algorithm, approximation $1/3$

deterministic algorithm

[Buchbinder et al., 2015]

Algorithm 1: DeterministicUSM$(f, \mathcal{N})$

$X_0 \leftarrow \emptyset$, $Y_0 \leftarrow \mathcal{N}$.
for i = 1 *to* n **do**
    $a_i \leftarrow f(X_{i-1} \cup \{u_i\}) - f(X_{i-1})$.
    $b_i \leftarrow f(Y_{i-1} \setminus \{u_i\}) - f(Y_{i-1})$.
    if $a_i \geq b_i$ **then** $X_i \leftarrow X_{i-1} \cup \{u_i\}$, $Y_i \leftarrow Y_{i-1}$.
    else $X_i \leftarrow X_{i-1}$, $Y_i \leftarrow Y_{i-1} \setminus \{u_i\}$.
return X_n (or equivalently Y_n).

randomized algorithm

[Buchbinder et al., 2015]

Algorithm 2: RandomizedUSM$(f, \mathcal{N})$

$X_0 \leftarrow \emptyset$, $Y_0 \leftarrow \mathcal{N}$.
for i = 1 *to* n **do**
  $a_i \leftarrow f(X_{i-1} \cup \{u_i\}) - f(X_{i-1})$.
  $b_i \leftarrow f(Y_{i-1} \setminus \{u_i\}) - f(Y_{i-1})$.
  $a'_i \leftarrow \max\{a_i, 0\}$, $b'_i \leftarrow \max\{b_i, 0\}$.
  with probability $a'_i/(a'_i + b'_i)^*$ **do**: $X_i \leftarrow X_{i-1} \cup \{u_i\}$, $Y_i \leftarrow Y_{i-1}$.
  else (with the compliment probability $b'_i/(a'_i + b'_i)$) **do**: $X_i \leftarrow X_{i-1}$, $Y_i \leftarrow Y_{i-1} \setminus \{u_i\}$.
return X_n (or equivalently Y_n).

* If $a'_i = b'_i = 0$, we assume $a'_i/(a'_i + b'_i) = 1$.

max-sum diversification

[Borodin et al., 2012]

- U is a ground set
- $d : U \times U \rightarrow \mathbb{R}$ is a metric distance function on U
- $f : 2^U \rightarrow \mathbb{R}$ is a submodular function

- we want to find $S \subseteq U$ such that
  $\phi(S) = f(S) + \lambda \sum_{u,v \in S} d(u, v)$ is maximized and
  $|S| \leq k$

max-sum diversification

[Borodin et al., 2012]

- consider $S \subseteq U$ and $x \in U \setminus S$
- define the following types of marginal gain

  $d_x(S) = \sum_{v \in S} d(x, v)$

  $f_x(S) = f(S \cup \{x\}) - f(S)$

  $\phi_x(S) = \frac{1}{2} f_x(S) + \lambda d_x(S)$

- greedy algorithm on marginal gain $\phi_x(S)$ gives factor 2 approximation

max-sum diversification – the greedy

[Borodin et al., 2012]

1. $S \leftarrow \emptyset$
2. while $|S| < k$
3. $\quad i \leftarrow \arg\max_{\{j \in U \setminus S\}} \phi_j(S)$
4. $\quad S \leftarrow S \cup \{i\}$
5. return S

conclusions

- maximization of submodular functions
- monotone, constraints, symmetric, ...
- recent developments in theory community
- simple algorithms
- neat analysis
- many applications in machine learning

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