Machine Learning for Graphs and Sequential Data

Graphs - Clustering

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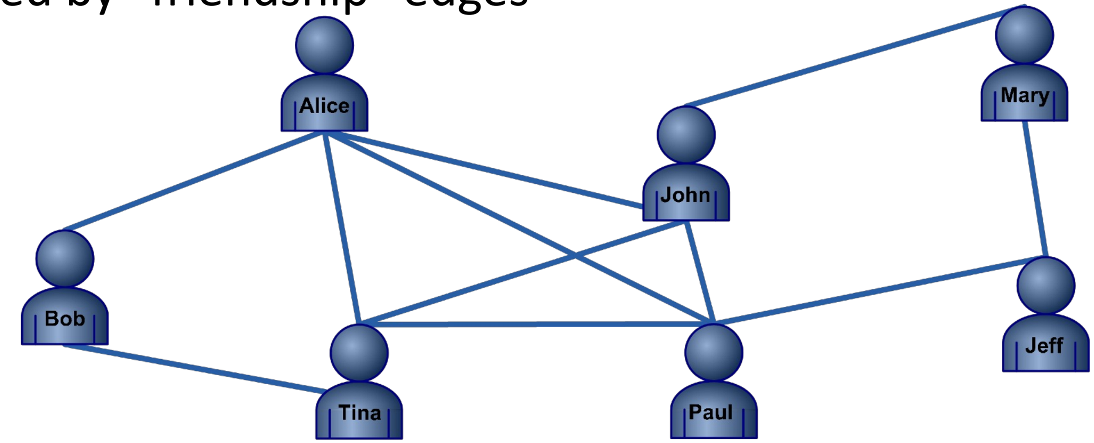
Data Analytics and
Machine Learning

Roadmap

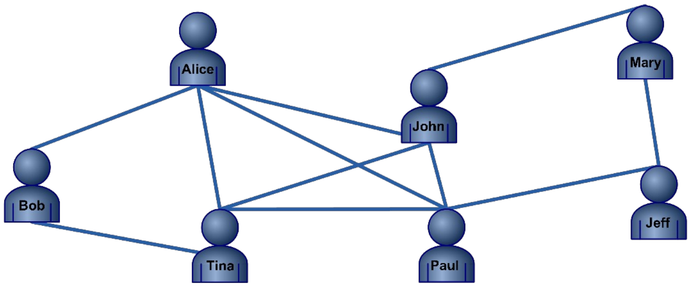
- **Chapter: Graphs**
  1. Graphs & Networks
  2. Generative Models
  3. Ranking
  4. **Clustering**
     - **Introduction**
     - Cuts & Spectral Clustering
     - Probabilistic Approaches
  5. Classification (Semi-Supervised Learning)
  6. Node/Graph Embeddings
  7. Graph Neural Networks (GNNs)

Clustering in Network Data - Introduction

- Input is a graph $G = (V, E)$
- Aim: Find clusters of *vertices* in the graph
- Related to "traditional" clustering (e.g. *k*-Means):
  - In traditional clustering, we cluster objects based on *attribute data*
  - Here, we cluster objects based on *graph data* (information about relationships between the objects)
- Example: Given a social network, find groups of people that are densely connected by "friendship" edges



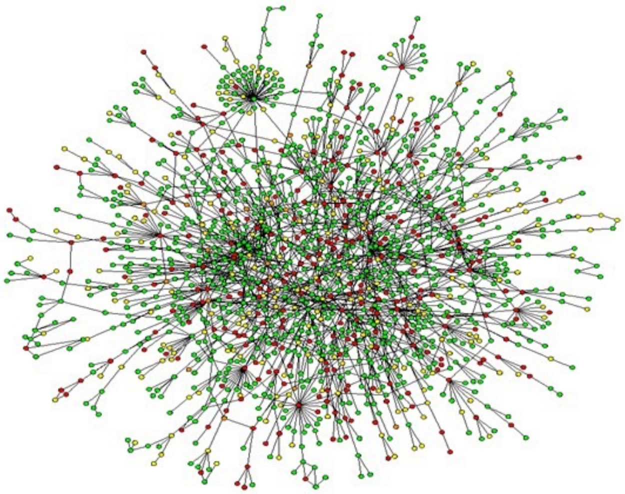
Clustering in Network Data - Introduction



Many different applications:

- Friendship graph: find circles of friends
- Protein-/Gene-Interaction Network: find groups of highly interacting proteins/genes

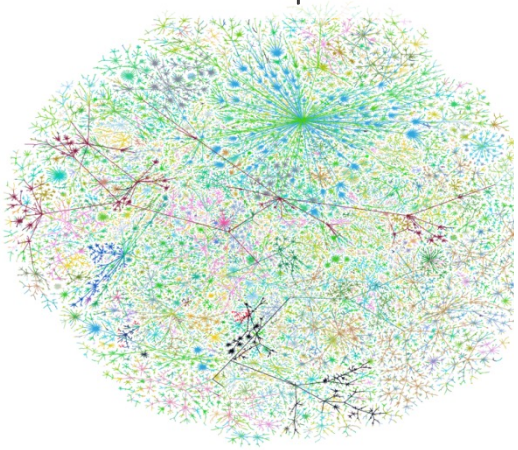
Yeast protein interaction network



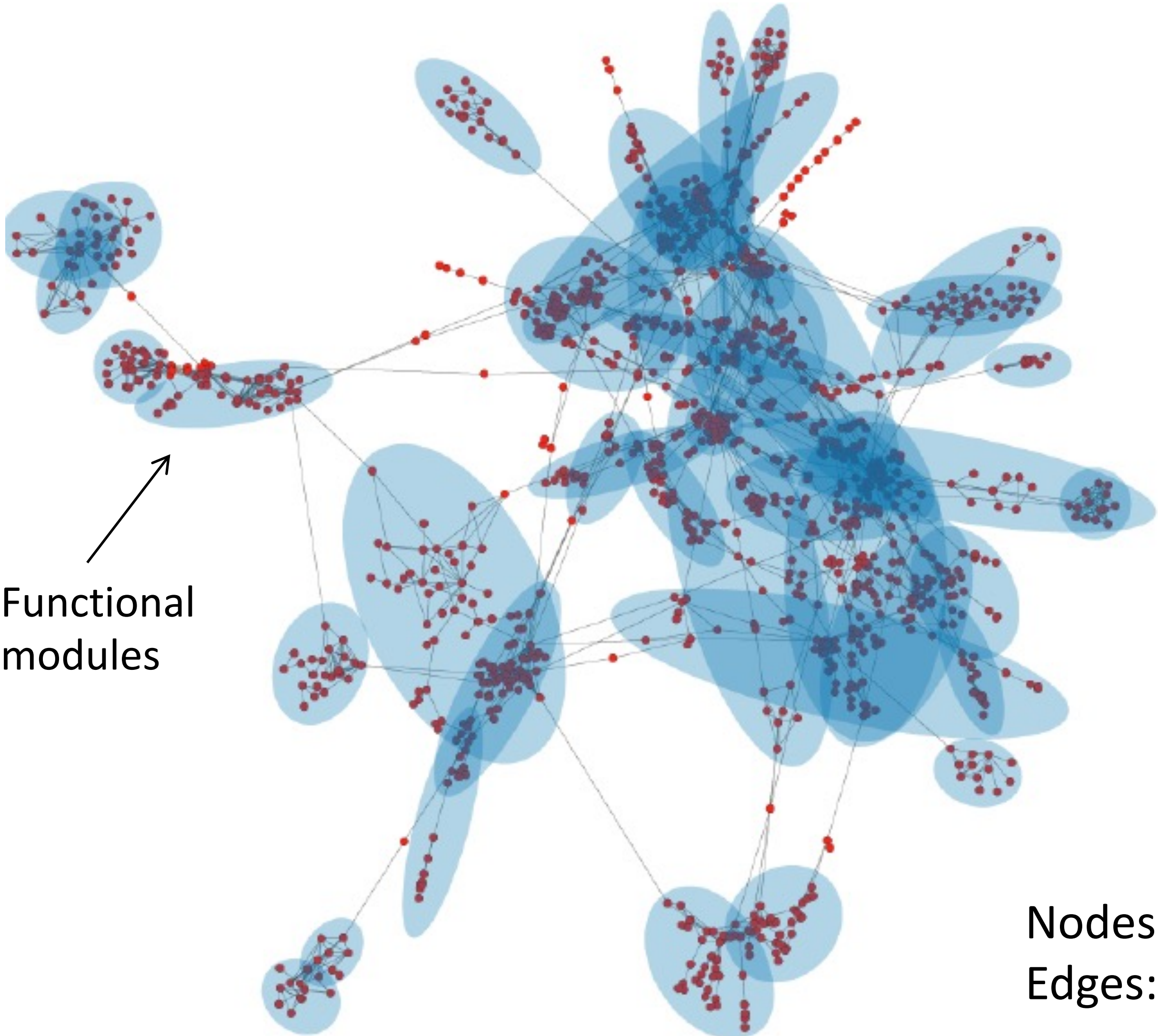
- Internet graph: Find groups of websites

  with similar topics

Internet snapshot



Example: Protein-Protein Interactions

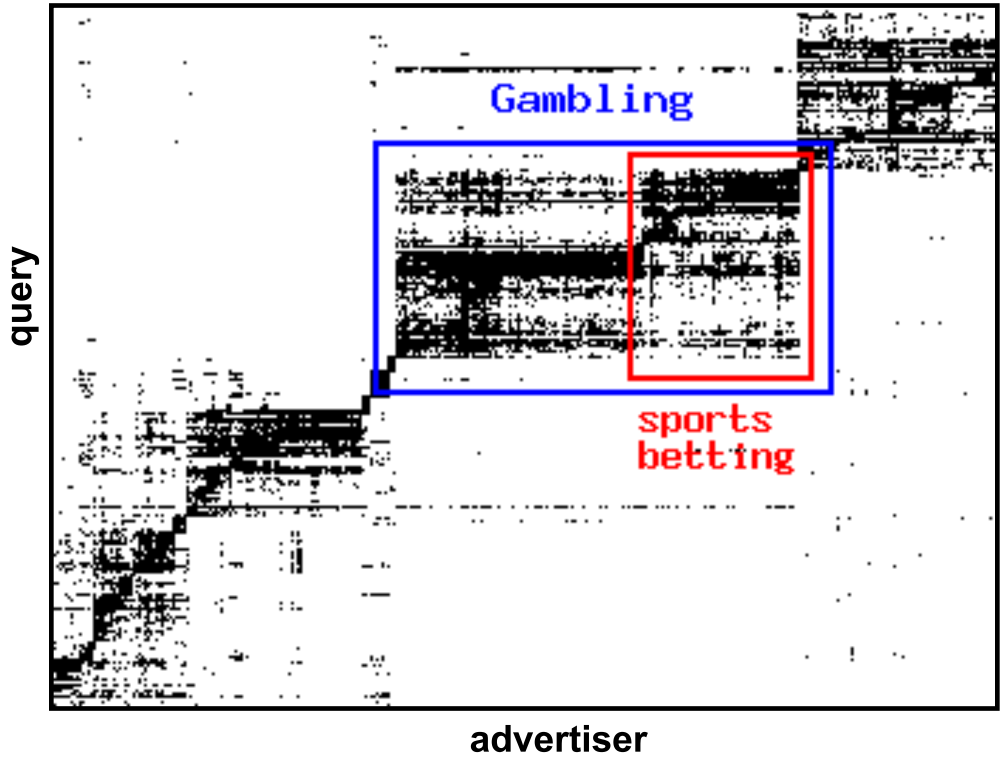


Functional modules

Nodes: Proteins
Edges: Physical interactions

Example: Micro-Markets in Sponsored Search

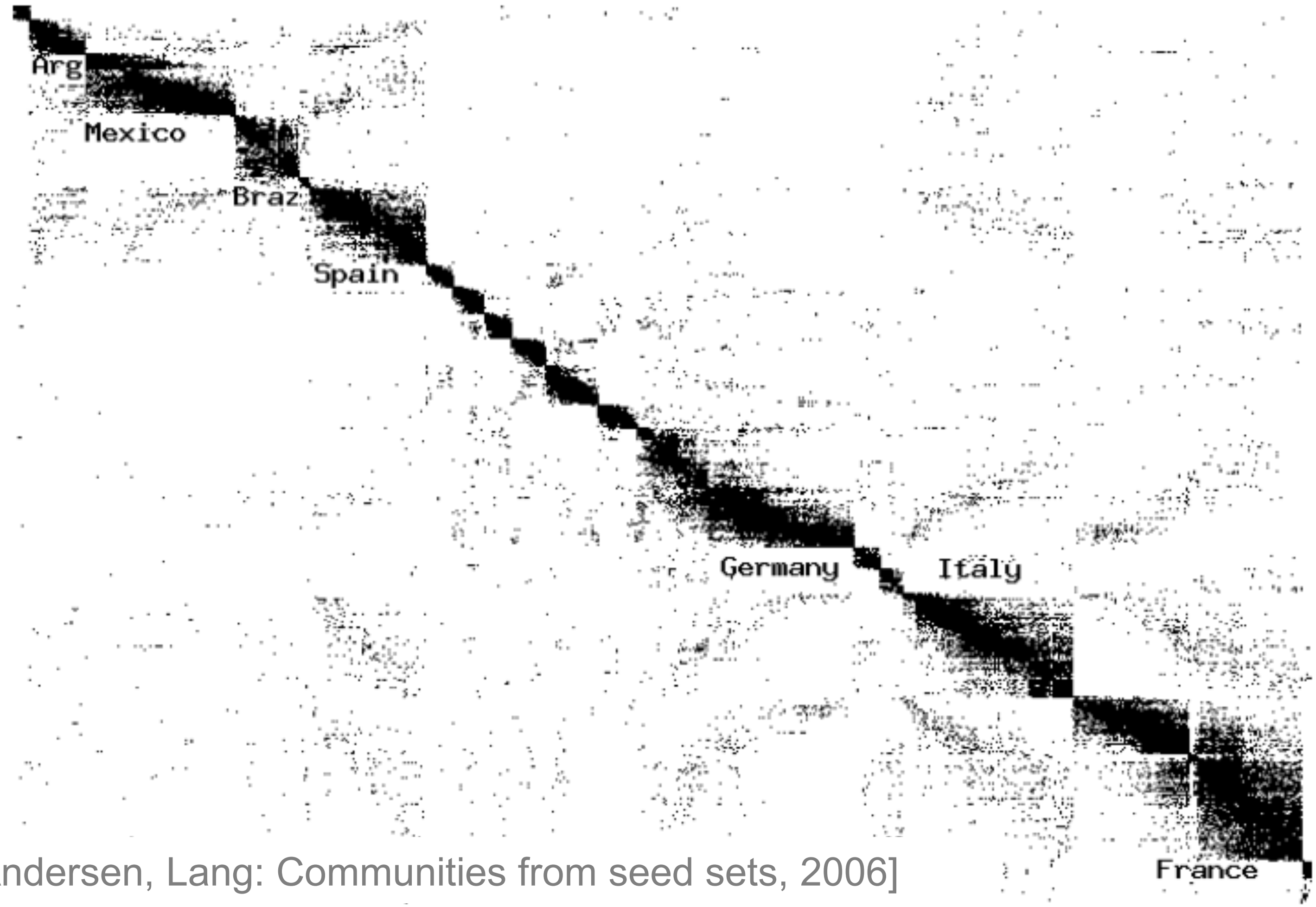
- Find micro-markets by partitioning the query-to-advertiser graph:



[Andersen, Lang: Communities from seed sets, 2006]

Example: Movies and Actors

- Clusters in Movies-to-Actors graph:



[Andersen, Lang: Communities from seed sets, 2006]

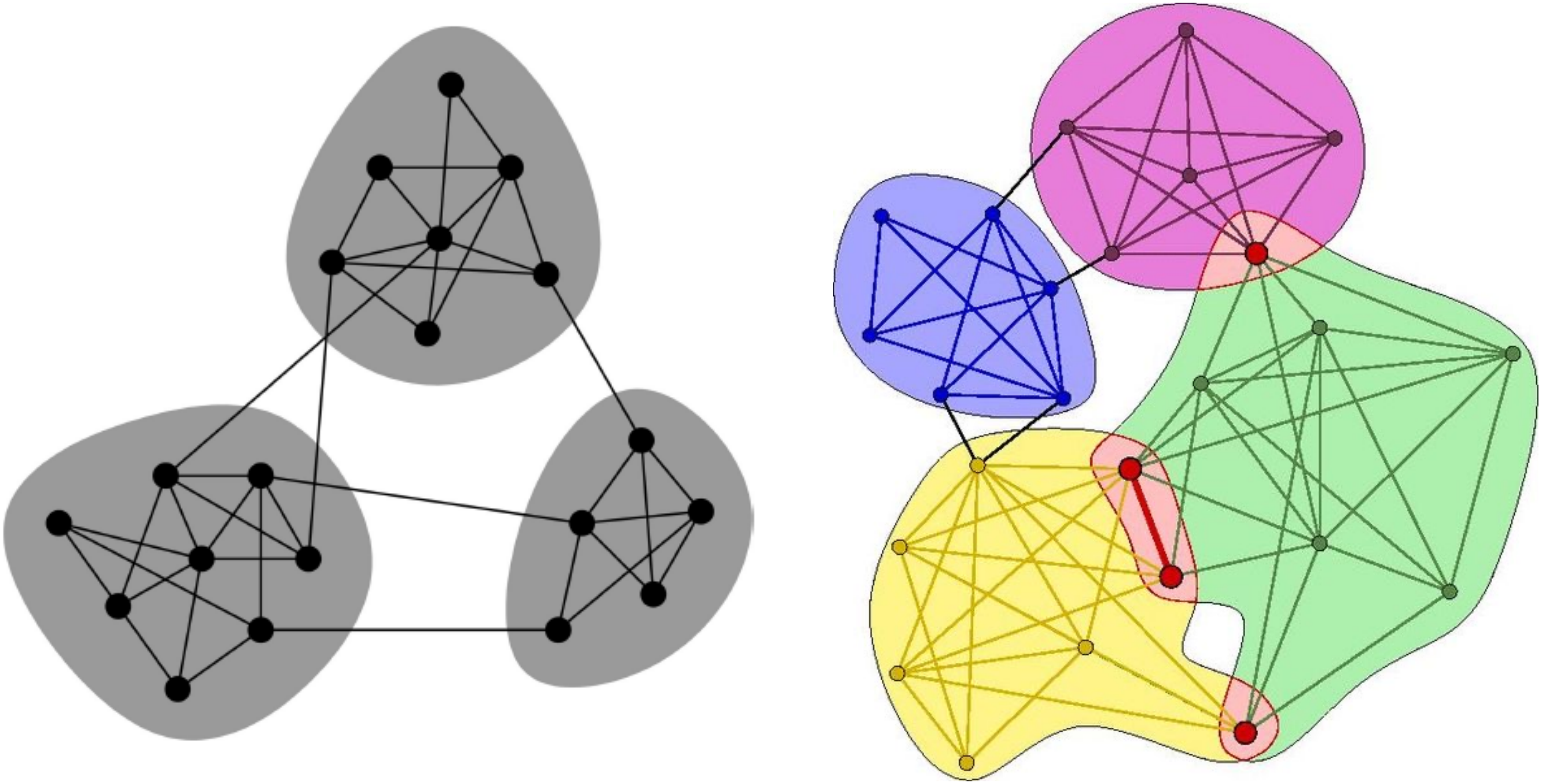
Clustering in Network Data - Introduction

- Basic aims for a good clustering:
  - Vertices in the **same cluster** should be connected by **many edges** (*intra-cluster* edges)
  - Only **few edges** between **different clusters** (*inter-cluster* edges)

- Two main categories of clustering algorithms:
  - **Partitioning approaches**: Each vertex is assigned to *exactly one* cluster
  - **Non-partitioning approaches**: Clusters can overlap, "outliers" that belong to no cluster are possible

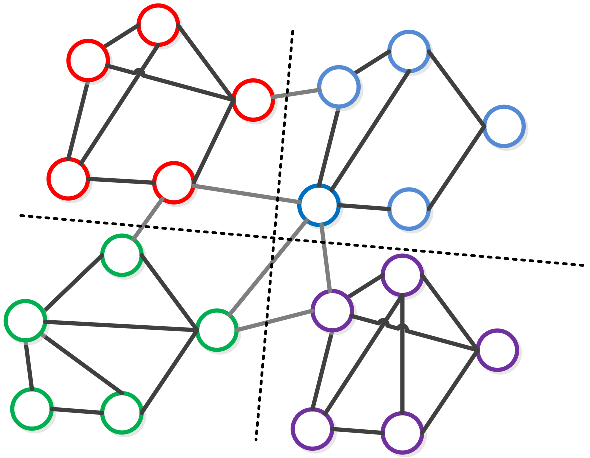
General Categorization

- Non-overlapping vs. overlapping clustering



Partitioning Approaches

- Basic idea: (Constrained) Optimization Problem
- Given a graph *G = (V, E)*, partition vertex set *V* into a set of clusters $\mathcal{C} = \{C_1, \dots, C_k\}$ such that
  - A given objective function $Q(\mathcal{C})$ is optimized
  - Subject to the constraints
    - $C_1 \cup \dots \cup C_k = V$ (Every vertex from *V* belongs to a cluster)
    - $\forall\, 1 \leq i < j \leq k$: $C_i \cap C_j = \emptyset$ (Clusters are disjoint; no overlap)
- Usually NP-hard problem since discrete optimization
  - for k=2 sometimes polynomial time algorithms exist
- Cf. k-Means: Objects are partitioned such that Total Distance is minimized



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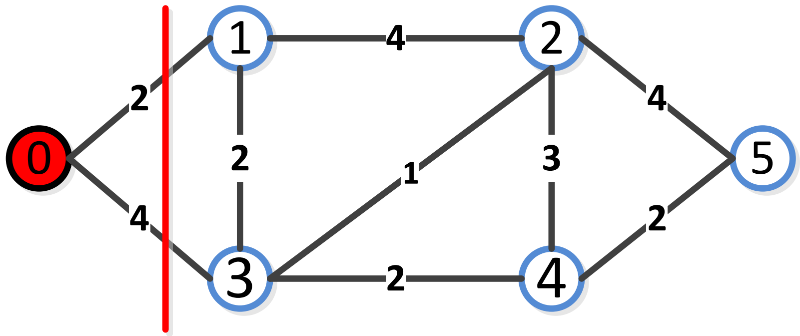
Global Minimum Cut

- First idea: minimize the number of edges/weights between the clusters
  - small value of the cut
- Task: Partition V into two sets C_1 and C_2, such that the sum of the inter-cluster edge weights $\text{cut}(C_1, C_2) = \sum_{v_1 \in C_1, v_2 \in C_2} w(v_1, v_2)$ is minimized
  - here: undirected edges, i.e. $w(a, b) = w(b, a)$



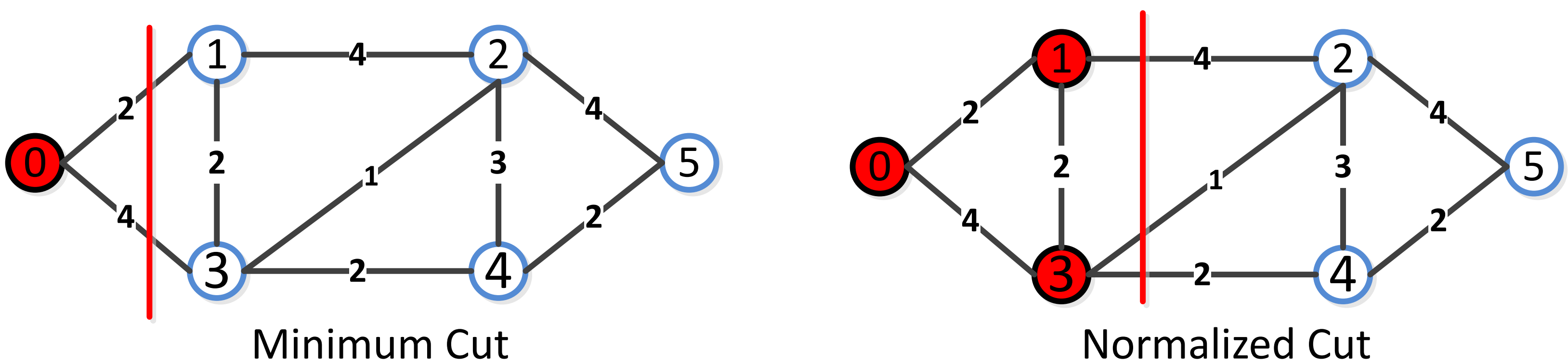
- Note: Computing an s-t-cut (i.e. where a source s and sink t are given) can be done in polynomial time via the algorithm of Ford and Fulkerson
  - Graph Clustering: no source/sink is given; any partitioning is possible, "global" minimum cut

Normalized Cut Criteria

- Drawbacks of Minimum Cut:
  - Tends to cut small vertex sets from the rest of the graph
  - Considers only inter-cluster edges, no intra-cluster edges
- Therefore, normalized cut criteria were introduced:
  - Ratio Cut: Minimize $\frac{cut(C_1,C_2)}{|C_1|} + \frac{cut(C_2,C_1)}{|C_2|}$
  - Normalized Cut: Minimize $\frac{cut(C_1,C_2)}{\mathrm{vol}(C_1)} + \frac{cut(C_2,C_1)}{\mathrm{vol}(C_2)}$

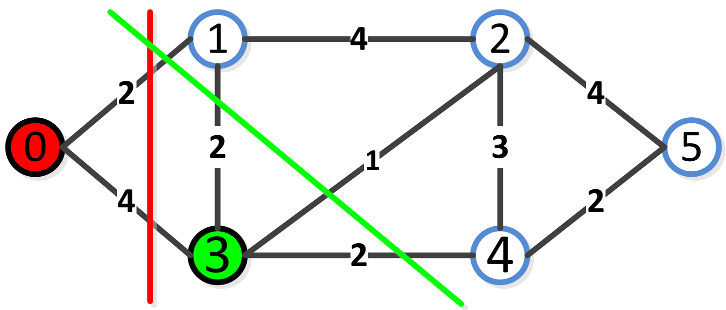
volume of a set of nodes

$$\mathrm{vol}(\mathrm{C_i}) = assoc(C_i,V) = cut(C_i,V) = \sum_{v_i \in C_i, v_j \in V} w(v_i,v_j) = \sum_{v_i \in C_i} \deg(v_i) =$$



Multi-way Graph Partitioning

- Generalization to $k \geq 2$ clusters
- Partition V into disjoint clusters $C_1, \ldots, C_k$ such that
  - Cut: $\min_{C_1,\ldots,C_k} \sum_{i=1}^{k} cut(C_i, V \backslash C_i)$
  - Ratio Cut: $\min_{C_1,\ldots,C_k} \sum_{i=1}^{k} \frac{cut(C_i, V \backslash C_i)}{|C_i|}$
  - Normalized Cut: $\min_{C_1,\ldots,C_k} \sum_{i=1}^{k} \frac{cut(C_i, V \backslash C_i)}{vol(C_i)}$



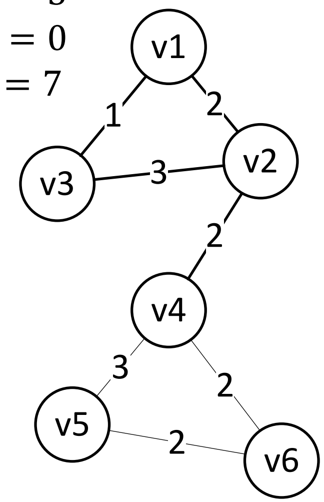
Minimum Cut for $k = 3$

- Finding the optimal solution is NP-hard
- How to compute an approximate solution efficiently?

Graph Laplacian

- Definition: **Laplacian matrix** $\mathrm{L} = D - W$
  - W = (weighted) adjacency matrix, D = degree matrix

$W[2,3] = 3$
$W[2,5] = 0$
$D[2,2] = 7$



- i.e. $L_{uv} = \begin{cases} -W_{uv}, & if\ (u,v) \in E \\ \deg(v), & if\ u = v \\ 0, & otherwise \end{cases}$

- **Observation 1**: For any vector f we have
  $f^T \cdot L \cdot f = \frac{1}{2} \cdot \sum_{(u,v)\in E} W_{uv}(f_u - f_v)^2$

Graph Laplacian

- The Laplacian is a discrete analogue of the Laplacian $\sum_i \frac{\partial^2 f}{\partial x_i^2}$, it measures to what extent a function differs at a point from its values at nearby points
  - Laplace operator often denoted as Δ

- The (discrete) Laplacian is an operator on the n-dimensional vector space of functions $f : V \rightarrow \mathbb{R}$
  - Think about the function f as assigning a "number" to each node

- The Laplacian "transforms" f to another function g, i.e. $\Delta f = g$
  - $g(v) = (\Delta f)(v) = \sum_{(u,v)\in E} W_{uv} \cdot [f(v) - f(u)]$
  - For finite-dimensional graphs, you can simply represent f and g as vectors, e.g. $\boldsymbol{a}$ and $\boldsymbol{b} \Rightarrow \boldsymbol{b} = L \cdot \boldsymbol{a}$

Properties of the Graph Laplacian (I)

- L is symmetric and positive semi-definite
  - Symmetric since D, and W are symmetric (for undirected graphs)
  - From Observation 1 we get PSD: $1x^T Lx \geq 0$, for any x, since it's a quadratic

- The smallest eigenvalue of L is 0, the corresponding eigenvector is the constant one vector $\vec{1}$, (or any $\mathrm{c} \cdot \vec{1}$, for any scalar c)
  - Recall $L\,x = \lambda\,x \quad \Rightarrow \quad x^T Lx = \lambda \quad \Rightarrow \quad \frac{1}{2}\sum_{(u,v)\in E} W_{uv}(x_u - x_v)^2 = \lambda$
  - Trivial solutions set $x = \mathrm{c} \cdot \vec{1}$ and $\lambda = 0$

- L has n non-negative, real-valued eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$
  - In general, any symmetric matrix has real-valued eigenvalues
  - From above $\lambda_1 = 0$ is the smallest eigenvalues ⇒ the rest must be larger
  - To find e.g. the second smallest eigenvalue, one can also use power iteration! (Lanczos algorithm)

Properties of the Graph Laplacian (II)

- Laplacian is additive: $L_{G \cup H} = L_G + L_H$
  - For two graphs G and H on the same vertex set with disjoint edge sets

- Laplacian of an edge, i.e. graph with a single edge (u, v):

$$\mathrm{L}_{(u,v)} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

- Laplacian of a graph is a sum of Laplacians for each edge:
  - $L_G = \sum_{(u,v)\in E} L(u, v)$
  - Allows us to prove properties for a single edge and add them up

Properties of the Graph Laplacian (III)

- **Observation 2**: The number of eigenvectors of L with eigenvalue 0 corresponds to the number of **connected components**.

0	1	1	0	0	0	0	0	0
1	0	1	0	0	0	0	0	0
1	1	0	0	0	0	0	0	0
0	0	0	0	1	1	0	0	0
0	0	0	1	0	2	0	0	0
0	0	0	1	2	0	0	0	0
0	0	0	0	0	0	0	3	1
0	0	0	0	0	0	3	0	1
0	0	0	0	0	0	1	1	0

Adjacency matrix W

2	0	0	0	0	0	0	0	0
0	2	0	0	0	0	0	0	0
0	0	2	0	0	0	0	0	0
0	0	0	2	0	0	0	0	0
0	0	0	0	3	0	0	0	0
0	0	0	0	0	3	0	0	0
0	0	0	0	0	0	4	0	0
0	0	0	0	0	0	0	4	0
0	0	0	0	0	0	0	0	2

Degree matrix D

2	-1	-1	0	0	0	0	0	0
-1	2	-1	0	0	0	0	0	0
-1	-1	2	0	0	0	0	0	0
0	0	0	2	-1	-1	0	0	0
0	0	0	-1	3	-2	0	0	0
0	0	0	-1	-2	3	0	0	0
0	0	0	0	0	0	4	-3	-1
0	0	0	0	0	0	-3	4	-1
0	0	0	0	0	0	-1	-1	2

Laplacian matrix L

- Let C_k be the set of nodes corresponding to the k-th connected component and Let $f_{C_k}[i] = 1 \; if \; v_i \in C_k, else \; f_{C_k}[i] = 0$
  - e.g. $f_{C_1} = [1,1,1,0,0,0,0,0,0]$, $f_{C_2} = [0,0,0,1,1,1,0,0,0]$ and $f_{C_3} = [0,0,0,0,0,0,1,1,1]$
  - From Observation 1: $f_{C_k}^T L f_{C_k} = 0, \; \forall k \;\; \Rightarrow \;\; f_{C_k}$ are the 'smallest' eigenvectors of L
- Corollary: If the graph is connected $\lambda_2(L) > 0$

Properties of the Graph Laplacian (IV)

- **Algebraic connectivity** of a graph is $\lambda_2(L)$
  - Also known as Fiedler (eigen)value
  - The magnitude reflects how well connected the graph overall is
  - e.g. $\lambda_2(K_n) = n$, where K_n is a complete graph with n nodes

- For every $S \subset V$ we have $\theta(S) = \frac{cut(S,\bar{S})}{|S|} \geq \lambda_2 \left(1 - \frac{|S|}{|V|}\right)$
  - $\theta(S)$ is called the isoperimetric ratio of S
  - $\theta_G \stackrel{\text{def}}{=} \min_{|S| \leq \frac{|V|}{2}} \theta(S) \geq \lambda_2/2$
  - θ_G is called the Cheeger constant of a graph, the conductance of a graph, etc.

- The inequality implies that if λ_2 is big the graph is very well connected
  - the boundary of each *small* set of vertices is at least λ_2 times a value close to 1

Properties of the Graph Laplacian (V)

- Conclusion: The spectrum of L encodes useful information about the graph

- Unfortunately, there exist co-spectral graphs
  - Graphs that are not isomorphic but share the same spectrum
  - Implies that the spectrum doesn't completely characterize the graph

- Co-spectrality can also be useful
  - Find a sparse version of a graph with (approximately) the same spectrum
  - Yields computational benefits for large graphs

The Graph Laplacian and the Minimum Cut

- For $k = 2$ clusters let $f \in \{+1, -1\}^n$ be an indicator vector

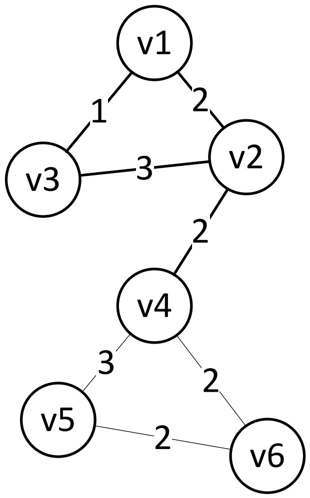
$$f_{C_1}[i] = \begin{cases} +1 & if\ v_i \in C_1 \\ -1 & \text{else}, v_i \in \mathrm{V} \backslash C_1 = C_2 \end{cases}$$

- Then you can verify $f_{C_1}^T L f_{C_1} = 4 \cdot cut(C_1, C_2)$
- Thus we can minimize $f_{C_1}^T L f_{C_1}$ to minimize the cut

- However, we established that minimum cut is not ideal
- Can we specify a different indicator that leads to the ratio cut?

Spectral Clustering: 2 Clusters

- Let's focus on minimizing the **ratio cut** for k=2 clusters
  - $\min_{C_1 \subset V} \frac{cut(C_1,C_2)}{|C_1|} + \frac{cut(C_2,C_1)}{|C_2|}$ where $C_2 = V \backslash C_1 =: \overline{C_1}$



- Consider the **indicator vector** f_{C_1} for the cluster C_1, i.e.

$$f_{C_1}[i] = \begin{cases} +\sqrt{\frac{|\overline{C_1}|}{|C_1|}} & if\ v_i \in C_1 \\ -\sqrt{\frac{|C_1|}{|\overline{C_1}|}} & else \end{cases}$$

1. $\sum_i f_{C_1}[i] = 0$ → f_{C_1} is orthogonal to vector $\vec{1}$: $f_{C_1} \perp \vec{1}$
2. $f_{C_1}^T \cdot f_{C_1} = \|f_{C_1}\|_2^2 = |V|$ → length is constant
3. $f_{C_1}^T \cdot L \cdot f_{C_1} = \cdots = |\mathrm{V}| \cdot \left[\frac{cut(C_1,C_2)}{|C_1|} + \frac{cut(C_1,C_2)}{|\overline{C_1}|}\right]$ → |V| ·ratio cut

Spectral Clustering: 2 Clusters

- Minimizing the ratio cut is equivalent to

$\min_{C_1 \subset V} \{ f_{C_1}^T \cdot L \cdot f_{C_1} \}$ subject to $f_{C_1} \perp \vec{1}$ and $\|f_{C_1}\|_2 = \sqrt{|V|}$ and f_{C_1} as defined before

- Discrete optimization problem → still NP-hard in general
- **Idea: Constraint relaxation**
  - drop the discreteness condition (i.e. f_{C_1} can take any values)

- Result: $\min_{f_{C_1} \in R^{|V|}} \{ f_{C_1}^T \cdot L \cdot f_{C_1} \}$ subject to $f_{C_1} \perp \vec{1}$ and $\|f_{C_1}\|_2 = \sqrt{|V|}$

Spectral Clustering: 2 Clusters

- Result: $\min_{f_{C_1} \in R^{|V|}} \{ f_{C_1}^T \cdot L \cdot f_{C_1} \}$ subject to $f_{C_1} \perp \vec{1}$ and $\| f_{C_1} \|_2 = \sqrt{|V|}$
- What is the solution to this problem?

- We have for any symmetric matrix L:
  - $\lambda_1 = \min_{\|x_1\|=1} x_1^T L\, x_1 \quad \lambda_2 = \min_{\|x_2\|=1,\ x_2 \perp x_1} x_2^T L\, x_2 \qquad \lambda_3 = \cdots$

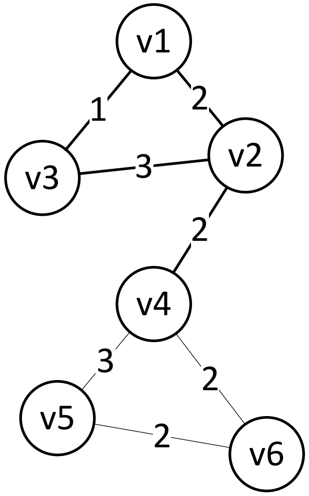
- $\boldsymbol{f_{C_1}}$ **is the second smallest eigenvector of L!**
  - recall: $\vec{1}$ is the smallest eigenvector
  - $L \cdot f_{C_1} = f_{C_1} \cdot \lambda_2 \Leftrightarrow f_{C_1}^T \cdot L \cdot f_{C_1} = |V| \cdot \lambda_2$

- Example: $f_{C_1} = [1.1841 \quad 0.6883 \quad 1.0620 \quad -0.6917 \quad -1.0827 \quad -1.1600]^T$

Spectral Clustering: 2 Clusters

- Solution: $\boldsymbol{f_{C_1}}$ **is the second smallest eigenvector of L!**
- Example:
  - $f_{C_1} = [1.1841 \quad 0.6883 \quad 1.0620 \quad -0.6917 \quad -1.0827 \quad -1.1600]^T$

- How to get the actual clustering?
  - simple case: consider the sign of the values in f_{C_1}
  - in general: perform k-means clustering of the values in f_{C_1}



Spectral Clustering: General Case

- General case (k>2): clusters $C_1, \dots, C_k$
- Define indicator vector: $h_C[i] = \begin{cases} \frac{1}{\sqrt{|C|}} & if\ v_i \in C \\ 0 & else \end{cases}$
  - let H=$[h_{C_1}; h_{C_2}; \dots; h_{C_k}]$ // indicator vectors are columns of H

- **Observations:**
  - $H^T H = Id$ // orthonormal matrix
  - $h_{C_i}^T \cdot L \cdot h_{c_i} = \frac{cut(C_i, V \setminus C_i)}{|C_i|}$ and $h_{C_i}^T \cdot L \cdot h_{c_i} = (H^T L H)_{ii}$

➢ $RatioCut(C_1, \dots, C_k) = \sum_{i=1}^{k} \frac{cut(C_i, V \setminus C_i)}{|C_i|} = \sum_{i=1}^{k} (H^T L H)_{ii} = trace(H^T L H)$

Spectral Clustering: General Case

- Minimizing ratio-cut (general case) is equivalent to

  $$\min_{C_1,\ldots,C_k} trace(H^T L H) \text{ subject to } H^T H = Id \text{ and H as defined before}$$

- **Constraint relaxation: allow arbitrary values for H**

➢ Result: $\min_{H \in R^{V \times k}} trace(H^T L H)$ subject to $H^T H = Id$
  - standard trace minimization problem
  - **optimal H = first k smallest eigenvectors of L** // see relation to PCA/SVD

- How to compute the first k smallest eigenvectors?
  - Power iteration yields the largest eigenvalue λ_{max}
  - Shift: Power iteration with $\mathrm{L} - \lambda_{max} I$ yields the smallest eigenvector v_0
  - Deflation: Power iteration with $\mathrm{L} - \lambda_{max} I - \lambda_0 v_0 v_0^T$ yields the second smallest, etc.

Spectral Clustering: Example

0	1	1	0	0	0	0	0	0
1	0	1	0	1	0	0	0	0
1	1	0	0	0	0	0	0	0
0	0	0	0	1	1	0	0	0
0	1	0	1	0	2	0	0	0
0	0	0	1	2	0	0	0	1
0	0	0	0	0	0	0	3	1
0	0	0	0	0	0	3	0	1
0	0	0	0	0	1	1	1	0

Adjacency matrix W

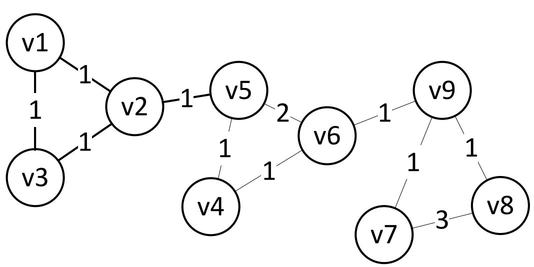
2	0	0	0	0	0	0	0	0
0	3	0	0	0	0	0	0	0
0	0	2	0	0	0	0	0	0
0	0	0	2	0	0	0	0	0
0	0	0	0	4	0	0	0	0
0	0	0	0	0	4	0	0	0
0	0	0	0	0	0	4	0	0
0	0	0	0	0	0	0	4	0
0	0	0	0	0	0	0	0	3

Degree matrix D

2	-1	-1	0	0	0	0	0	0
-1	3	-1	0	0	-1	0	0	0
-1	-1	2	0	0	0	0	0	0
0	0	0	2	-1	-1	0	0	0
0	-1	0	-1	4	-2	0	0	0
0	0	0	-1	-2	4	0	0	-1
0	0	0	0	0	0	4	-3	-1
0	0	0	0	0	0	-3	4	-1
0	0	0	0	0	-1	-1	-1	3

Laplacian matrix L

- Smallest eigenvalues of L: 0 ; 0.23 ; 0.7

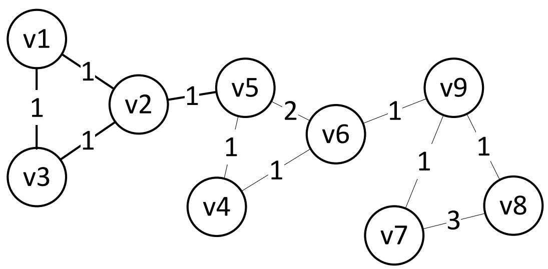


-0.3333	-0.4376	0.2939
-0.3333	-0.3370	0.0890
-0.3333	-0.4376	0.2939
-0.3333	0.0000	-0.5878
-0.3333	-0.0584	-0.3829
-0.3333	0.0584	-0.3829
-0.3333	0.4376	0.2939
-0.3333	0.4376	0.2939
-0.3333	0.3370	0.0890

Eigenvectors of L

Spectral Clustering: Example

- How to find the clusters based on the eigenvectors?
- Represent each vertex by a vector of its corresponding components in the eigenvectors → **spectral embeddings** (see also later in the lecture)
- Clustering (e.g. k-Means) in the **embedding space** yields the final result



k first eigenvectors

-0.3333	-0.4376	0.2939
-0.3333	-0.3370	0.0890
-0.3333	-0.4376	0.2939
-0.3333	0.0000	-0.5878
-0.3333	-0.0584	-0.3829
-0.3333	0.0584	-0.3829
-0.3333	0.4376	0.2939
-0.3333	0.4376	0.2939
-0.3333	0.3370	0.0890

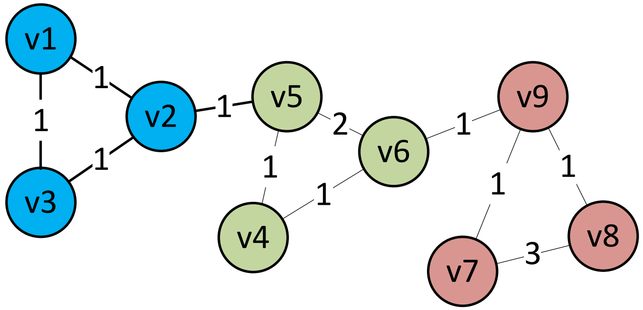
result of k-Means

Representation of vertex v9:
(-0.333,0.337,0.0890)

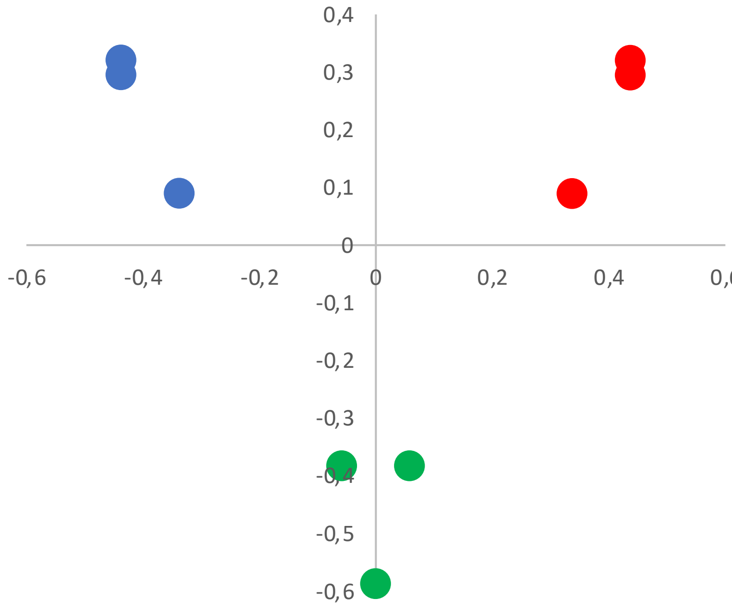
first eigenvector can be ignored since constant anyway

Spectral Clustering: Example of Spectral Embedding

- Also known as **Spectral Layout**



	x axis	y axis
-0.3333	-0.4376	0.2939
-0.3333	-0.3370	0.0890
-0.3333	-0.4376	0.2939
-0.3333	0.0000	-0.5878
-0.3333	-0.0584	-0.3829
-0.3333	0.0584	-0.3829
-0.3333	0.4376	0.2939
-0.3333	0.4376	0.2939
-0.3333	0.3370	0.0890



Spectral Clustering: Remarks

- Spectral clustering using **unnormalized Laplacian** $L = D - W$
  - approximation of ratio cut
- Spectral clustering using **normalized Laplacian** $L_{sym} = D^{-1/2}\, L\, D^{-1/2}$
  - approximation of normalized cut

- Drawback: No guarantee to achieve a result close to optimal cut!
  - but often performs very well in practice

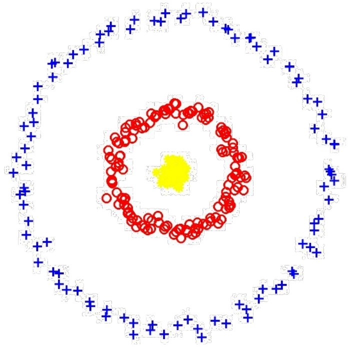
Spectral Clustering for Numerical Data

- Spectral clustering is also used for other data types, e.g. numerical data

- **Step 1: Construct similarity graph**
  - requires similarity function between data instances
    - frequently used: Gaussian radial basis function kernel $sim(x, x') = e^{-\gamma \cdot \|x-x'\|^2}$
  - different variants of similarity graphs possible:
    - k-NN graph: connect two points if at least one of them is k-NN of the other
      i.e. $(u, v) \in E \Leftrightarrow u \in NN_v(k) \vee v \in NN_u(k)$
    - neighborhood graph: connects all points whose distance is in specific range
      i.e. $(u, v) \in E \Leftrightarrow sim(u, v) \geq \delta$

- **Step 2: Apply spectral clustering on similarity graph**

- Strong advantage of spectral clustering:
  able to detect clusters of complex shapes



Roadmap

- **Chapter: Graphs**
  1. Graphs & Networks
  2. Generative Models
  3. Ranking
  4. **Clustering**
     - Introduction
     - Cuts & Spectral Clustering
     - **Probabilistic Approaches**
  5. Classification (Semi-Supervised Learning)
  6. Node/Graph Embeddings
  7. Graph Neural Networks (GNNs)

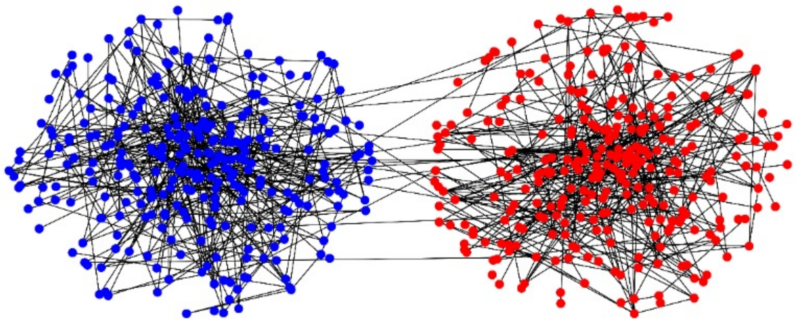
Probabilistic Community Detection

- Optimization view on graph clustering
  - find a community assignment that **optimizes** some criterion (e.g. minimum cut, maximum modularity)
- Alternatively: Probabilistic view
  - consider the graph as a realization (**sample**) drawn from a generative model
  - the generative process is controlled by a set of **parameters**
  - **communities** are explicitly modeled within the generative process
    - seen before: PPM, SBM
  - finding a “good” community assignment ⇔ performing **inference** in the model
- Advantages of the probabilistic view
  - capture uncertainty
  - handle missing / noisy data
  - generate new data (e.g. link prediction)

Recap: Planted Partition Model (PPM)

- We start with a set of nodes V, partitioned into 2 communities C_1, C_2
  - denote community assignment of node i as $z_i \in \{-1, 1\}$ – latent variables
- We generate an edge between every pair of nodes with probability

$$Pr\left(A_{ij} = 1 \middle| z_i, z_j\right) = \begin{cases} p & \text{if } z_i = z_j \\ q & \text{if } z_i \neq z_j \end{cases}$$



Graph generated by a PPM with
$N = 600, p = 6/600, q = 0.1/600$
$z_i = -1$ for blue nodes, $z_i = 1$ for red nodes

Inference in PPM

- The likelihood of a community assignment $\boldsymbol{z} \in \{-1,1\}^N$ for an observed symmetric adjacency matrix $\boldsymbol{A} \in \{0,1\}^{N\times N}$ is

$$\Pr(\boldsymbol{A}|\boldsymbol{z}) = \prod_{i<j} \left[p^{A_{ij}}(1-p)^{1-A_{ij}}\right]^{\mathbb{I}(z_i=z_j)} \left[q^{A_{ij}}(1-q)^{1-A_{ij}}\right]^{\mathbb{I}(z_i\neq z_j)}$$

- Assume that p and q are known.

- Given an observed $\boldsymbol{A}$, what is the most likely community assignment $\boldsymbol{z}^*$ that produced it?
  - Community detection problem ⇔ probabilistic inference problem!
  - Simplest solution – maximum-a-posteriori estimation

$$\boldsymbol{z}^* = \underset{\boldsymbol{z}\in\{-1,1\}^N}{\arg\max} \Pr(\boldsymbol{z}|\boldsymbol{A})$$

PPM and Spectral Clustering (I)

- How do we find the ML estimate of $\boldsymbol{z}$ for the planted partition model?
  - no closed-form solution
  - $\boldsymbol{z}$ is discrete $\Rightarrow$ gradient descent doesn't work
- Let's assume that we have a uniform prior over the communities and that they are balanced: $|C_1| = |C_2| = \frac{N}{2}$
  - equivalent to the constraint $\sum_i z_i = 0$
- Let's denote the number of edges whose endpoints are in different communities as

$$E_{cut}(\boldsymbol{z}) = |\{(i,j) \in E \ \text{ s.t. } \ z_i \neq z_j\}| = \sum_{(i,j)\in E} \mathbb{I}(z_i \neq z_j)$$

- We can show that the likelihood of the PPM is proportional to

$$\Pr(\boldsymbol{z}|\boldsymbol{A}) \propto \Pr(\boldsymbol{A}|\boldsymbol{z}) \propto \left(\frac{(1-p)q}{(1-q)p}\right)^{E_{cut}(\boldsymbol{z})}$$

PPM and Spectral Clustering (II)

- We can show that the likelihood of the PPM is proportional to

$$\Pr(\boldsymbol{A}|\boldsymbol{z}) \propto \left(\frac{(1-p)q}{(1-q)p}\right)^{E_{cut}(\boldsymbol{z})}$$

- Since $p > q$, maximizing the likelihood is equivalent to finding a minimum balanced cut!
- How can we solve that? ⇒ Spectral clustering!

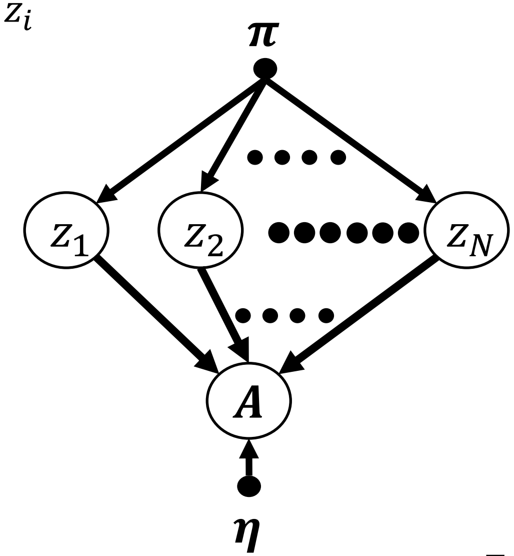
➢ MLE in PPM (under some assumptions) ⇔ minimum cut ⇔ spectral clustering

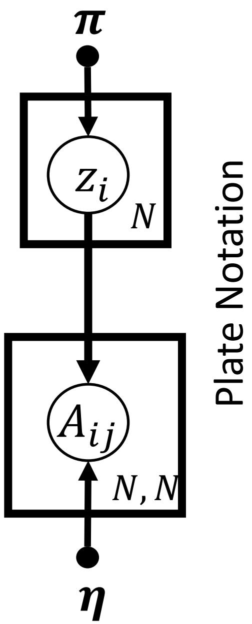
Recap: Stochastic Block Model (SBM)

- **Stochastic block model** generalizes the PPM to graphs with arbitrary numbers and sizes of communities, and varying edge densities.

$\boldsymbol{\pi} = [\pi_1, \pi_2, \dots, \pi_k]$

- Random variables:
  - $z_i \in \{1, \dots, K\}$: node i belongs to block/community z_i
  - $\boldsymbol{A} \in \{0,1\}^{N \times N}$: adjacency matrix





- Model parameters:
  - $\boldsymbol{\pi} = [\pi_1, \dots, \pi_K]$: community proportions
  - η_{uv}: edge probability between two nodes that are in communities u and v.

- Conditional distributions:
  - $\Pr(z_i = k) = \pi_k$
  - $\Pr(A_{ij} | z_i, z_j) = \text{Bernoulli}(\eta_{z_i z_j})$

$$\boldsymbol{\eta} = \begin{bmatrix} \eta_{11} & \cdots & \eta_{1K} \\ \vdots & \ddots & \vdots \\ \eta_{K1} & \cdots & \eta_{KK} \end{bmatrix}$$

Inference in SBM

- Assume that $\boldsymbol{\eta}$ and $\boldsymbol{\pi}$ are known. What is the distribution of $\boldsymbol{z}$ given $\boldsymbol{A}$?
$$\Pr(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{\eta},\boldsymbol{\pi}) = \frac{\Pr(\boldsymbol{A}|\boldsymbol{z},\boldsymbol{\eta},\boldsymbol{\pi})\Pr(\boldsymbol{z}|\boldsymbol{\pi})}{\Pr(\boldsymbol{A}|\boldsymbol{\eta},\boldsymbol{\pi})}$$
- The normalizing constant $\Pr(\boldsymbol{A}|\boldsymbol{\eta},\boldsymbol{\pi})$ is intractable and requires $O(K^N)$ operations to compute.
- We can use, e.g., variational inference to find an approximate solution
  - find a distribution $q(\boldsymbol{z})$ that is similar to the true posterior $\Pr(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{\eta},\boldsymbol{\pi})$ (e.g. with a mean-field assumption)
$$\Pr(\boldsymbol{z}|\boldsymbol{A},\boldsymbol{\eta},\boldsymbol{\pi}) \approx q(\boldsymbol{z}|\boldsymbol{\Psi}) = \prod_{i=1}^{N} q(\boldsymbol{z}_i|\boldsymbol{\psi}_i)$$

Learning in SBM

- If both $\boldsymbol{z}$ and $\boldsymbol{A}$ are observed, the MLE for $\boldsymbol{\eta}$ and $\boldsymbol{\pi}$ is simple counting

$$\pi_k^{MLE} = \frac{\#\text{ nodes in cluster } k}{N} =: \frac{N_k}{N}$$

$$\eta_{uv}^{MLE} = \frac{\text{observed \# edges between } u \text{ and } v}{\text{possible \#edges between } u \text{ and } v} = \frac{\sum_{(i,j)\in E} \mathbb{I}(z_i = u)\mathbb{I}(z_j = v)}{P_{uv}}$$

where $P_{uv} = \begin{cases} \binom{N_u}{2} & \text{if } u = v \\ N_u \cdot N_v & \text{if } u \neq v \end{cases}$ is the number of possible edges between clusters u and v

- If only $\boldsymbol{A}$ is observed, we can use again variational inference
  - i.e. optimize the ELBO w.r.t. $q(\boldsymbol{z})$ as well as $\boldsymbol{\eta}$ and $\boldsymbol{\pi}$

Summary

- Graph Laplacian and its spectrum captures the connectivity structure of the graph
- Spectral clustering finds a partition of the graph that minimizes the number of edges between different parts, a minimum cut.
  - relax an NP-hard problem to a continuous trace minimization problem
  - optimal solution is given by the eigenvectors of the graph Laplacian
- Clustering can be framed as inference in a generative model such as the Stochastic Block Model or its special case PPM.
  - advantages: handles uncertainty, more robust against noise, finds a generative model
  - disadvantages: inference is intractable, doesn't model all known patterns

Questions

- How can you find the connected components of a graph from its Laplacian?

- Consider a graph with n arbitrarily connected nodes and k disconnected nodes. What are the first $k + 1$ clusters that spectral clustering finds? Why?

Reading Material

- Aggarwal,C., Wang, H.: Managing and Mining Graph Data, Chapter 9 and 10
- Fortunato, S.: Community detection in graphs, in Physics Reports, 2010
- Tutorial and overview about different spectral clustering approaches: "Von Luxburg, U.: A tutorial on spectral clustering"