universidade de aveiro

Mining Large Scale Datasets

Mining Network Graphs

(Adapted from CS246@Starford.edu; http://www.mmds.org)

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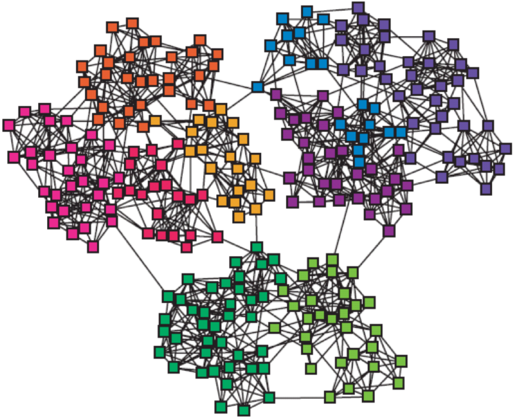
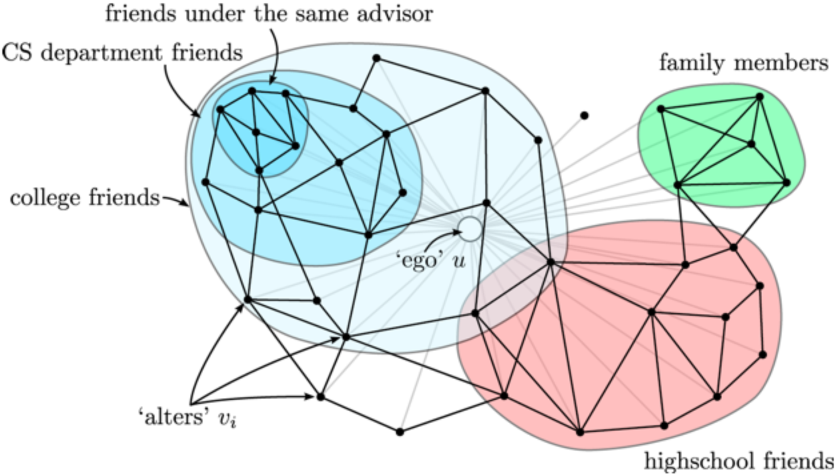
Networks



Analyze networks in terms of modules, cluster, communities

Example: Social circles

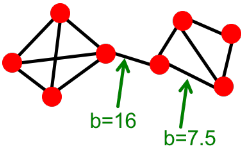


[McAuley, Leskovec: Discovering social circles in ego networks, 2012]

Class roadmap

- Betweenness and Girvan-Newman Algorithm
- Graph cuts
- Spectral graph partitioning

Betweenness

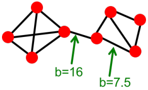


Betweenness of edge (a, b) is the number of pairs of nodes x, y such that the edge (a, b) lies on the shortest path between x and y

Since there can be several shortest paths between x and y, edge (a, b) is credited with the fraction of those shortest paths that include the edge (a, b)

Girvan-Newman Algorithm

Divisive hierarchical clustering based on the notion of edge **betweenness**: Number of shortest paths passing through an edge

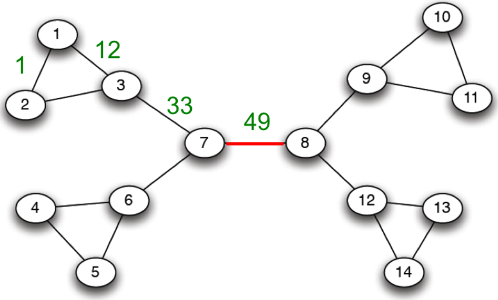


Process: repeat until no edges are left

- Calculate betweenness of edges
- Remove edges with highest betweenness

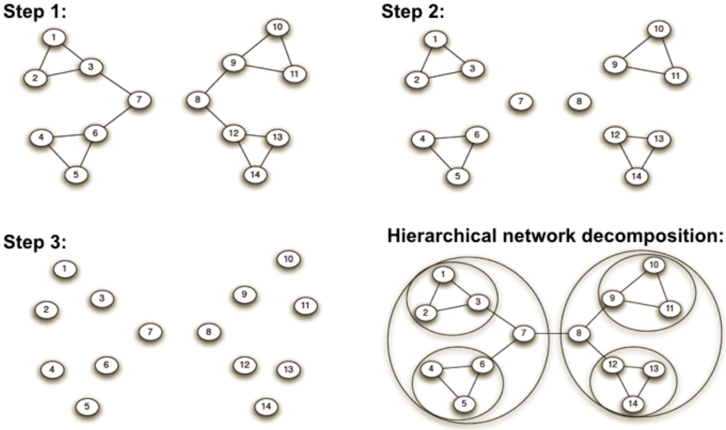
Connected components are communities
Gives a hierarchical decomposition of the network

Girvan-Newman Algorithm: Example

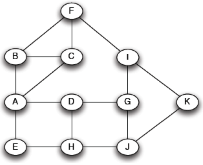


Note: betweenness is recomputed at every step.

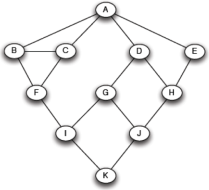
Girvan-Newman Algorithm: Example



Computing betweeness

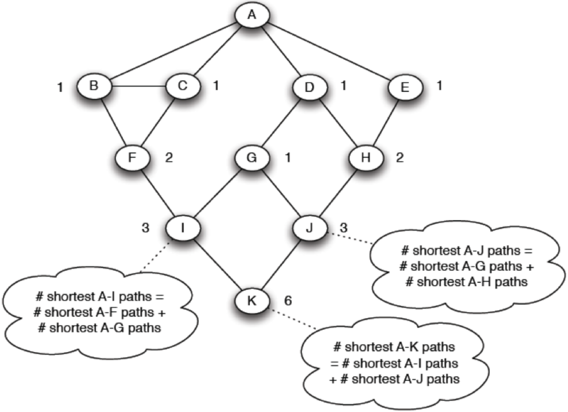


Calculate betweenness of paths starting at node A



Step 1: Breath first search starting from A

Computing betweeness

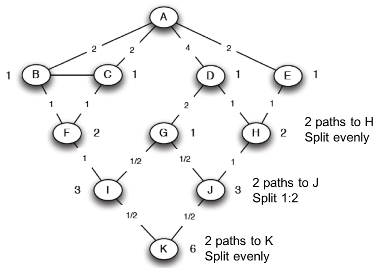


Step 2: Count the number of shortest paths from A to all other nodes of the network

Computing betweeness

Step 3: Compute betweenness by working up the tree

- Each leaf gets a credit of 1
- Non-leaf nodes get credit 1 plus the (weighted) sum of the credits of the edges to the level below
- Weights are defined by the relative number of shortest paths going through the node



Computing betweeness

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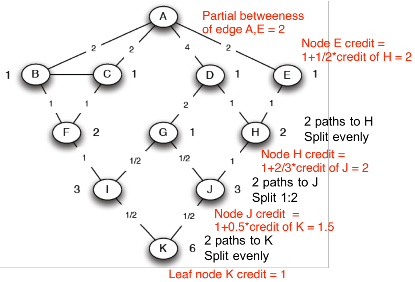
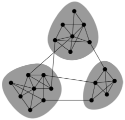


Repeat procedure for each starting node and sum the credits for each edge

Use subset of nodes as starting nodes to speed-up computation

Selecting the number of clusters

Communities:
sets of tightly connected nodes



Modularity Q

A measure of how well a network is partitioned into communities

Given a partitioning of the network into groups

$Q \propto \sum_{s \in S} [(\#\text{ edges in group } s) - (\text{expected }\#\text{ edges in group } s)]$

Modularity

For a partitioning S of graph G with n nodes and m edges

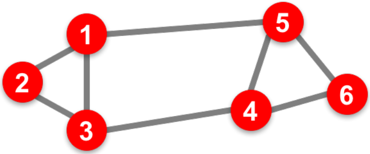
$$Q(G,S) = \frac{1}{2m} \sum_{s \in S} \sum_{i \in s} \sum_{j \in s} \left(A_{ij} - \frac{d_i d_j}{2m} \right)$$

$A_{ij} = 1$ if there is an edge from i to j
d_i degree of node i

Modularity takes values in range [-1,1]

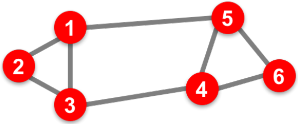
- Positive if the number of edges within groups exceeds the expected number
- $Q > 0.3..0.7$ means significant community structure

Spectral Clustering



Graph partitioning

Undirected graph $G(V, E)$

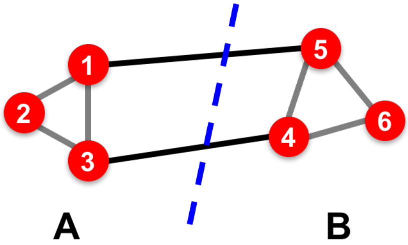


Bi-partitioning task:
Divide vertices into two disjoint groups

- How can we define a “good” partitioning of G?
- How can we efficiently identify such a partition?

Graph partitioning

What makes a good partition?



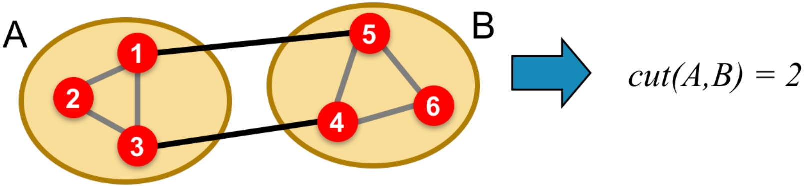
Maximize the number of within-cluster connections
Minimize the number of between-cluster connections

Graph cuts

Express partitioning quality in terms of the “edge cut” of the partition

Cut: Set of edges with only one node in a group

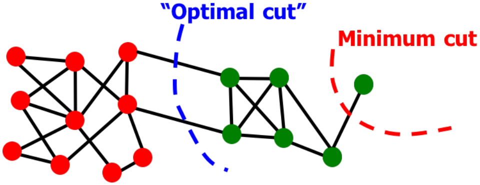
$Cut(A,B) = \sum_{i \in A; j \in B} w_{ij}$ $\qquad$ ($w_{ij} = 1$ for unweighted graphs)



Graph cut criteria: Minimum cut

Minimize weight of connections between groups

$$argmin_{A,B} cut(A, B)$$



Problem:

- Only considers external cluster connections
- Does not consider internal cluster connectivity

Graph cut criteria: Normalized cut

Connectivity between groups relative to the density of each group

$ncut(A, B) = \frac{cut(A,B)}{vol(A)} + \frac{cut(A,B)}{vol(B)}$

$vol(A) = \sum_{i \in A} d_i$ $\qquad$ $(d(i)$ degree of node $i)$

total weight of the edges with at least one endpoint in A

$\hookrightarrow$ Produces more balanced partitions

Graph cut criteria: Conductance

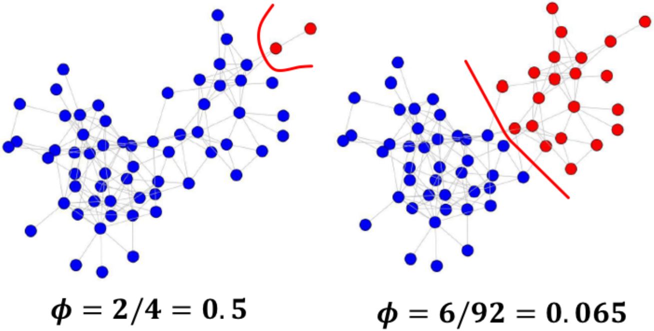
Connectivity of the group to the rest of the network relative to the density of the group

$$\phi(A) = \frac{cut(A)}{min(vol(A), 2m - vol(A))}$$

$vol(A) = \sum_{i \in A} d_i$ $\qquad$ ($d(i)$ degree of node i)

total weight of the edges with at least one endpoint in A

Graph cut criteria: Conductance



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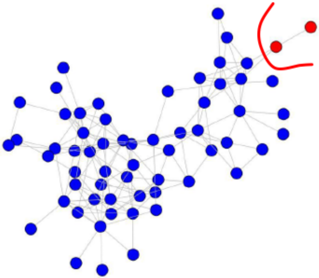
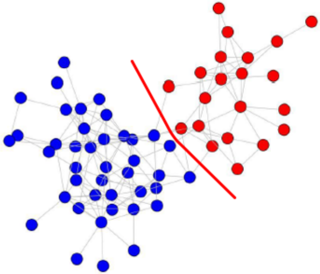
Graph cut criteria: Conductance



$\phi = 2/4 = 0.5$



$\phi = 6/92 = 0.065$

- ↪ Produces more balanced partitions
- ↪ **How do we efficiently find a good partition?**

Spectral Graph Partitioning

Consider

- A: adjacency matrix of undirected G

  $A_{ij} = 1$ if (i, j) if an edge, else 0

- x: vector in $\mathcal{R}^n$ with components $(x_1, ..., x_n)$

  Think of it as a label/value of each node of G

What is the meaning of $A \cdot x$?

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$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & n_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

$$y_i = \sum_{j=1}^{n} A_{ij} x_j = \sum_{(i,j) \in E} x_j$$

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Entry y_i is the sum of labels x_j of the neighbors of x_i

Spectral Graph Partitioning

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & n_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \lambda \cdot \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \qquad A \cdot x = \lambda \cdot x$$

Spectral Graph Theory

- Analyze the spectrum of matrix representing G
- **Spectrum**: Eigenvectors x_i of a graph, ordered by the magnitude (strength) of their corresponding eigenvalues λ_i

  $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$

Spectral Graph Theory

Consider a d-regular graph G

- All nodes have degree d and G is connected

$A \cdot x = \lambda \cdot x$

What are the eigenvectors of G

Spectral Graph Theory

Consider a d-regular graph G

- All nodes have degree d and G is connected

$A \cdot x = \lambda \cdot x$

What are the eigenvectors of G

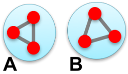
- Consider $x = (1, 1, ...1)$
- $A \cdot x = (d, d, ..., d) = \lambda \cdot x$
- So, $\lambda = d$

- We found the first *eigenpair* of G
  $x = (1, 1, ...1)$, $\lambda = d$

Spectral Graph Theory

What if G is not connected?

- G has 2 components, each d-regular



What are the eigenvectors of G

- x: vector of **1**s on **A** and **0**s on **B** (and vice versa)

  $x' = (1, \dots, 1, 0, \dots, 0)$ then $A \cdot x' = (d, \dots, d, 0, \dots, 0)$

  $x'' = (0, \dots, 0, 1, \dots, 1)$ then $A \cdot x'' = (0, \dots, 0, d, \dots, d)$

- In both cases, $\lambda = d$

Spectral Graph Theory

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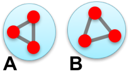

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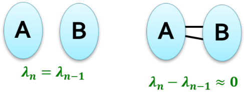
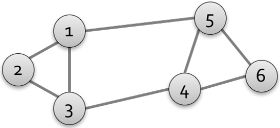
Intuition



second largest eigenvalue λ_2
now has value very close to λ_1

Spectral Graph Theory: Adjacency Matrix

- Adjacency matrix A
  - *nxn* matrix
  - $A = [a_{ij}], a_{ij} = 1$ if edge between nodes i and j

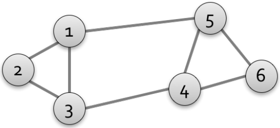


	1	2	3	4	5	6
1	0	1	1	0	1	0
2	1	0	1	0	0	0
3	1	1	0	1	0	0
4	0	0	1	0	1	1
5	1	0	0	1	0	1
6	0	0	0	1	1	0

- Symmetric matrix
- Eigenvectors are real and orthogonal

Spectral Graph Theory: Degree Matrix

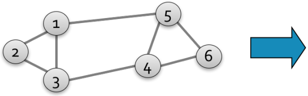
- Degree matrix D
  - nxn diagonal matrix
  - $D = [d_{ii}]$, d_{ii} = degree of node i



	1	2	3	4	5	6
1	3	0	0	0	0	0
2	0	2	0	0	0	0
3	0	0	3	0	0	0
4	0	0	0	3	0	0
5	0	0	0	0	3	0
6	0	0	0	0	0	2

Spectral Graph Theory: Laplacian Matrix

- Laplacian matrix L
  - *nxn* symmetric matrix
  - $L = D - A$



	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
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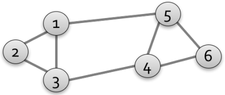

	1	2	3	4	5	6
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- Trivial eigenpair ?

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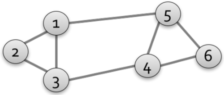

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1	3	-1	-1	0	-1	0
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- Trivial eigenpair
  - $x = (1, ..., 1)$ then $L \cdot x = 0$, so $\lambda = \lambda_1 = 0$

- Important properties
  - Eigenvalues are non-negative real numbers
  - Eigenvectors are real and orthogonal

λ_2 as an optimization problem

Fact: For symmetric matrix M

$$\lambda_2 = \min_x \frac{x^T M x}{x^T x}$$

λ_2 as an optimization problem

Fact: For symmetric matrix M

$$\lambda_2 = \min_x \frac{x^T M x}{x^T x}$$

What is the meaning of $\min_x x^T L x$ for graph G?

$$x^T L x = \sum_{i,j=1}^{n} L_{ij} x_i x_j = \sum_{i,j=1}^{n} \Big(D_{ij} - A_{ij} \Big) x_i x_j$$

$$= \sum_i D_{ii} x_i^2 - \sum_{(i,j) \in E} 2 x_i x_j$$

$$= \sum_{(i,j) \in E} (x_i^2 + x_j^2 - 2 x_i x_j) = \sum_{(i,j) \in E} (x_i - x_j)^2$$

λ_2 as an optimization problem

What we know about x

- x is a unit vector: $\sum_i x_i^2 = 1$
- x is orthogonal to first eigenvector (1, ..., 1):

  $\sum_i x_i \cdot \mathbf{1} = \sum_i x_i = 0$

Note: x is the solution to the λ_2 eigenvector problem

λ_2 as an optimization problem

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$$\lambda_2 = \min_x \frac{x^T L x}{x^T x} = \min_{x_i : \sum x_i = 0} \frac{\sum_{(i,j) \in E} (x_i - x_j)^2}{\sum_i x_i^2}$$

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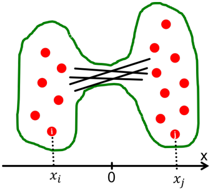
Forces values x_i for nodes i such that few edges cross 0
Forces x_i and x_j to subtract each other



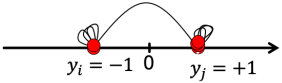
Relation to finding the optimal cut

- Express partition (A,B) as a vector

$$y_i = \begin{cases} +1, & \text{if } i \in A \\ -1, & \text{if } i \in B \end{cases}$$

- Minimize the cut of the partition by finding a vector that minimizes

$$\underset{y \in [-1,+1]^n}{\operatorname{argmin}} f(y) = \sum_{(i,j) \in E} (y_i - y_j)^2$$



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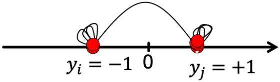
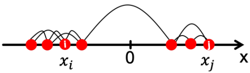


Can be solved if we relax y to allow any real value

Finding the optimal cut: Rayleigh theorem

$$\min_{y \in R^n} f(y) = \sum_{(i,j) \in E} (y_i - y_j)^2 = y^T L y$$



- $\lambda_2 = \min_y f(y)$
  The minimum value of $f(y)$ is given by the 2^{nd} smallest eigenvalue λ_2 of the Laplacian matrix **L**

- $x = \operatorname{argmin}_y f(y)$
  The optimal solution for y is given by the corresponding eigenvector x, referred as the Fiedler vector

Spectral clustering algorithms

Three basic stages

1) Pre-processing

   Construct a matrix representation of the graph

2) Decomposition

   Compute eigenvalues and eigenvectors of the matrix

   Map each point to a lower-dimensional representation based on one or more eigenvectors

3) Grouping

   Assign points to two or more clusters, based on the new representation

Spectral Partitioning Algorithm

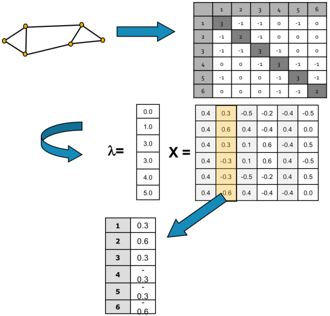
1) Pre-processing

   Build Laplacian matrix L of the graph G

2) Decomposition

   Find eigenvalues λ and eigenvectors x of L

   Map vertices of G to corresponding components of λ_2



Spectral Partitioning Algorithm

1) Pre-processing

   Build Laplacian matrix L of the graph G

	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
4	0	0	-1	3	-1	-1
5	-1	0	0	-1	3	-1
6	0	0	0	-1	-1	2

2) Decomposition

   Find eigenvalues λ and eigenvectors x of L

   Map vertices of G to corresponding components of λ_2

λ=

0.0
1.0
3.0
3.0
4.0
5.0

X =

0.4	0.3	-0.5	-0.2	-0.4	-0.5
0.4	0.6	0.4	-0.4	0.4	0.0
0.4	0.3	0.1	0.6	-0.4	0.5
0.4	-0.3	0.1	0.6	0.4	-0.5
0.4	-0.3	-0.5	-0.2	0.4	0.5
0.4	-0.6	0.4	-0.4	-0.4	0.0

1	0.3
2	0.6
3	0.3
4	-0.3
5	-0.3
6	-0.6

↪ How to find the clusters?

Spectral Partitioning Algorithm

3) Grouping

   Sort components of reduced 1-dimensional vector

   Identify clusters by splitting the sorted vector in two

Select the splitting point

- Split at **0** or median value
- More expensive approach
  - Sweep over ordering of nodes induced by the eigenvector and attempt to minimize the normalized cut in 1 dimension

1	0.3
2	0.6
3	0.3
4	-0.3
5	-0.3
6	-0.6

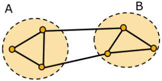
Split at 0:

Cluster A: Positive points

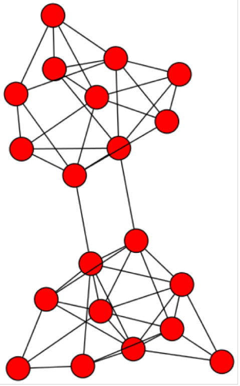
Cluster B: Negative points

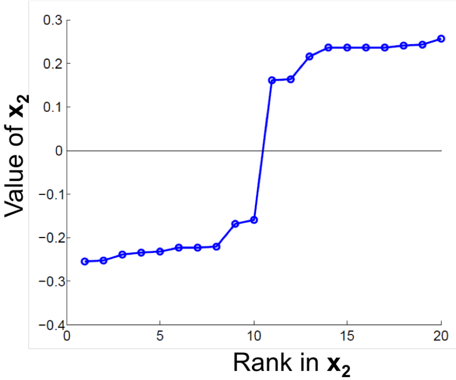
1	0.3
2	0.6
3	0.3

4	-0.3
5	-0.3
6	-0.6

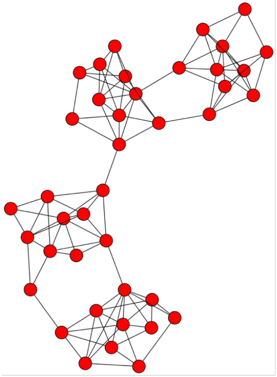


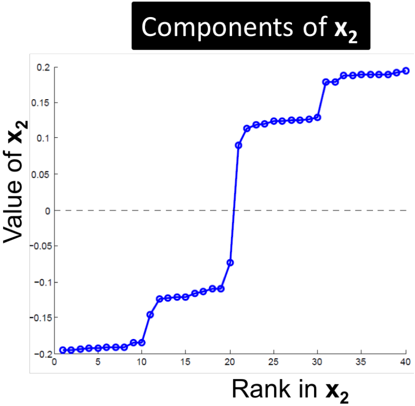
Spectral partitioning: example



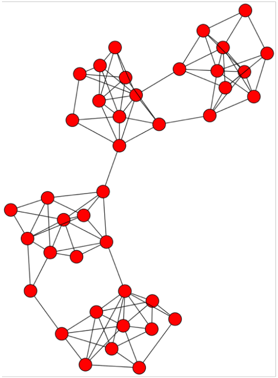


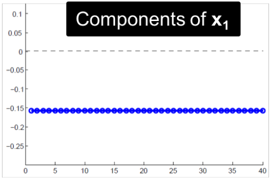
Spectral partitioning: example

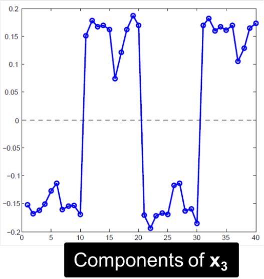




Spectral partitioning: example







k-way spectral partitioning

- How do we partition a graph into k clusters?
- Two basic approaches:
  - Recursive bi-partitioning [Hagen et al., '92]
    Recursively apply bi-partitioning algorithm in a hierarchical divisive manner
    Disadvantages: Inefficient, unstable
  - Cluster using multiple eigenvectors [Shi-Malik, '00]
    Build a reduced space from multiple eigenvectors
    Commonly used in recent papers; better results