## Network Science : Lecture X

# Graph Classification and Clustering 

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# Graph Classification (I) 

## HIV-1 protease inhibitors [Wang et al., 1996] <br> 

Wang S, Milne GW, Yan X, Posey IJ, Nicklaus MC, Graham L, Rice WG. J Med Chem. 1996 May 10;39(10):2047-54.

## Protein Family Classification



## Malware Detection



## Classification in Vector Space

$\square$ Binary Classification Problem
$\square$ Examples: Decision Tree, Naïve Bayes, SVM, ...


Input: $\left\{\left(\mathrm{x}_{1}, \mathrm{y}_{1}\right),\left(\mathrm{x}_{2}, \mathrm{y}_{2}\right), \ldots\right\}$
Output: classification function
e.g., $f(x): w^{t} x+b=0$

$$
\text { or } w_{1} x_{1}+w_{2} x_{2}+b=0
$$

Given a new data point

$$
\begin{aligned}
f(x) & >0 \text { for } y \\
f(x) & =0 \text { for } y
\end{aligned}=-1 .
$$

## Support Vector Machine


which one is better?

## Maximum Margin



If we fix $f(x)=1$ and -1 , then the margin is

## Decision Tree



decision tree

## Decision Tree



## Entropy

$\square$ Let $p_{i}$ be the probability that an arbitrary tuple in D belongs to class $\mathrm{C}_{i}$, estimated by $\mathrm{P}(\mathrm{Y})=\left|\mathrm{C}_{i}\right| /|\mathrm{D}|$
$\square$ Expected information (entropy, $\mathrm{H}(\mathrm{Y})$ ) needed to classify a tuple in D:

$$
H(Y)=-\sum_{i=1}^{m} p_{i} \log _{2}\left(p_{i}\right)
$$



## Information Gain

- Select the attribute with the highest information gain
- Find an attribute that could reduce the entropy -> better predicate the class label



Attribute Selection Measure: Information Gain (ID3/C4.5)


$$
\operatorname{Gain}(A)=H(Y)-H(Y \mid X)
$$

## Graph Classification

## Structure-based Approach

$\square$ Local structures in a graph, e.g., neighbors surrounding a vertex, paths with fixed length
Pattern-based Approach
$\square$ Subgraph patterns from domain knowledge
$\square$ Graph pattern mining
$\square$ Decision Tree (Fan et al. KDD’08)
$\square$ Boosting (Kudo et al. NIPS'04)
$\square$ LAR-LASSO (Tsuda, ICML'07)

## Kernel-based Approach

$\square$ Random walk (Gärtner '02, Kashima et al. '02, ICML'03, Mahé et al. ICML'04)
$\square$ Optimal local assignment (Fröhlich et al. ICML'05)
$\square$ Many others

## Structure/Pattern-based Classification

## Basic Idea

Transform each graph in the dataset into a feature vector,$$
G \rightarrow \mathbf{x}=\left\{x_{1}, x_{2}, \ldots, x_{n}\right\}
$$

where $x_{i}$ is the frequency of the $i$-th structure/pattern in $G$. Each vector is associated with a class label. Classify these vectors in a vector space

## Structure Features

Local structures in a graph, e.g., neighbors surrounding a vertex, paths with fixed lengthEnumerate all of the subgraphs and select the best features?Subgraph patterns from domain knowledge
■ Molecular descriptors
$\square$ Subgraph patterns from data mining

## Decision-Tree

## Basic Idea

$\square$ Partition the data in a top-down manner and construct the tree using the best feature at each step according to some criterionPartition the data set into two subsets, one containing this feature and the other does not


## Kernel

$\square$ Map two objects $x$ and $x^{\prime}$ via mapping $\Phi$ to feature space H .
$\square$ Measure their similarity in H as $\Phi(\mathrm{x}), \Phi\left(\mathrm{x}^{\prime}\right)$.
$\square$ Kernel Trick: Compute inner product in H as kernel in input space

$$
K\left(x, x^{\prime}\right)=<\phi(x), \phi\left(x^{\prime}\right)>
$$

Goal: reuse linear classifier, e.g., support vector machine, by replacing the kernel

Feature Space

$f(x)=w^{t} \phi(x)+b=\sum_{k} \alpha_{k} y_{k} \phi\left(x_{k}\right) \cdot \phi(x)+b=\sum_{k} \alpha_{k} y_{k}\left\langle\phi\left(x_{k}\right), \phi(x)\right\rangle+b$

## The Mercer Condition

$\square$ ls there a mapping $\Phi(x)$ for any symmetric function $K\left(x, x^{\prime}\right)$ ? No
$\square$ The SVM dual formulation requires calculation $K\left(x_{i}, x_{j}\right)$ for each pair of training instances. The array $G_{i j}=K\left(x_{i}, x_{j}\right)$ is called the Gram matrix
$\square$ There is a feature space $\Phi(x)$ when $G$ is always semipositive definite (Mercer condition)
$\square$ A matrix $M$ is semi-positive definite if and only if $x^{t} M x>=0$, for all non-zero vector $x$.

## Graph Kernel

$\square$ Kernels on pairs of graphs
$\square$ A graph kernel makes the whole family of kernel methods applicable to graphs, e.g., support vector machine!
$\square$ More details: Graph Kernel Tutorial: http://www.cs.ucsb.edu/~xyan/tutorial/kdd08_graph.htm, Part II
$\square$ Video lecture is available: http://videolectures.net/kdd08_borgwardt_gmgk/ (Part II)

## Random Walk-based Graph Kernel

$\square$ Random walks are sequences of nodes that allow repetitions of nodes
$\square$ Count the number of matching walks in two graphs
$\square$ Discount contribution of longer walks
$\square$ Two graphs are similar if many walks are matching

## Direct Product Graph

$\square$ Given two graphs, G and H , the vertex set of $\mathrm{G} \times \mathrm{H}$ is the Cartesian product $V(G) \times V(H)$
$\square T w o$ vertices $\left(u, u^{\prime}\right)$ and $\left(v, v^{\prime}\right)$ are adjacent in $G \times H$ if and only if $u$ is adjacent with $v$ and $u^{\prime}$ is adjacent with $v$ '.


## Random Walk-based Graph Kernel

$\square$ Construct direct product graph, $\mathrm{A}_{\mathrm{x}}$ of G and H
$\square$ Count walks in this product graph $A_{x}=\left(\mathrm{V}_{\mathrm{x}}, \mathrm{E}_{\mathrm{x}}\right)$
$\square$ Each walk in the product graph corresponds to one walk in G and H
$\square$ Walks of length $k$ can be computed by looking at the k-th power of the adjacency matrix

$$
K(G, H)=\sum_{i, j=1}^{\left|V_{x}\right|}\left[\sum_{k=1}^{\infty} \lambda^{k} A_{x}^{k}\right]_{i j}
$$

$\square \lambda$ is a decay factor for the sum to converge

## Modular Product of graphs

$\square$ Given two graphs, $G$ and $H$, the vertex set of $G \times H$ is the Cartesian product $V(G) \times V(H)$
$\square$ Two vertices ( $u, u^{\prime}$ ) and $\left(v, v^{\prime}\right)$ are adjacent in $G \times H$ if and only if $u$ is adjacent with $v$ and $u^{\prime}$ is adjacent with $v^{\prime}$, or $u$ is not adjacent with $v$ and $u^{\prime}$ is not adjacent with $v^{\prime}$.
$\square$ Cliques in the modular product graph correspond to isomorphism of induced subgraphs of $G$ and $H$.
$\square$ Specifically, the largest graph that is an induced subgraph of both $G$ and $H$ corresponds to the maximum clique in their modular product.

## Graph Classification (II)

## Task: Classify the Nodes


slides adapted from M. Bilgic

## Content-only Classification



## Relational Classification


$\square \square \square$

## Relational Classification



Use the attributes (content).

## Relational Classification



Use the attributes of the related objects.

## Relational Classification



Use the known labels of the related objects.

## Collective Classification


$\square \square \square$

## Collective Classification



Use the unknown labels of the related objects (during testing).

## Collective Classification



## Summary - Information Used

$\square$ Content-only classification
■Each object's own attributes only
$\square$ Relational classification
■ Each object's own attributes
■Attributes of the neighbors
■Known labels of the neighbors
$\square$ Collective classification
■Each object's own attributes
■Attributes of the neighbors
■Known labels of the neighbors
■Unknown labels of the neighbors (during testing)

## Content-only Classification

| a 1 | a 2 | a 3 | L |
| :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | R |


| $a 1$ | $a 2$ | $a 3$ | $L$ |
| :--- | :--- | :--- | :--- |
| 1 | 1 | 0 | $G$ |



| a 1 | a 2 | a 3 | L |
| :--- | :--- | :--- | :--- |
| 1 | 0 | 0 | $?$ |



| a1 | a2 | a3 | L |
| :--- | :--- | :--- | :--- |
| 1 | 1 | 1 | B |

## Content-only Classification

| a1 | a2 | a3 | L |
| :---: | :---: | :---: | :---: |
| 1 | 0 | 0 | R |
| 1 | 1 | 0 | R |
| 0 | 1 | 1 | B |
| 0 | 0 | 1 | B |
| 0 | 0 | 1 | G |
| 0 | 0 | 0 | G |
| 0 | 1 | 1 | ? |
| 1 | 0 | 1 | ? |
| 0 | 0 | 0 | ? |
| 0 | 0 | 1 | ? |

Learn a classifier, such as Naïve Bayes, k-NN, Logistic Regression, etc

## Problems



| a 1 | a 2 | a 3 | N 1 | N 2 | N 3 | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | R | R | B | R |

## Problems



| a 1 | a 2 | a 3 | N 1 | N 2 | N 3 | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | R | R | B | R |

How do we order the neighbors?


| a 1 | a 2 | a 3 | N 1 | N 2 | N 3 | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | R | B | R | R |

## Problems



| a 1 | a 2 | a 3 | N 1 | N 2 | N 3 | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | R | R | B | R |



| a 1 | a 2 | a 3 | N 1 | N 2 | N 3 | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | R | B | R | R |

What if different nodes have different number of neighbors?


| a1 | a2 | a3 | N1 | N2 | N3 | N4 | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | $R$ | $R$ | B | R | R |

## Aggregation

$\square$ Main idea:
■Aggregate a set of attributes into a fixed length representation
-Examples
■Count
■Proportion
-Mod
■Exist
■Mean

## Count



| a1 | a2 | a3 | CR | CB | CG | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 2 | 1 | 0 | $R$ |



| a1 | a2 | a3 | CR | CB | CG | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 2 | 1 | 0 | $R$ |



| a1 | a2 | a3 | CR | CB | CG | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 3 | 1 | 0 | $R$ |

## Proportion



| a 1 | a 2 | a 3 | PR | PB | PG | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 0.67 | 0.33 | 0 | R |



| a1 | a2 | a3 | PR | PB | PG | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 0.67 | 0.33 | 0 | $R$ |



| a1 | a2 | a3 | PR | PB | PG | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 0.75 | 0.25 | 0 | $R$ |

## Exist



| a1 | a2 | a3 | ER | EB | EG | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 1 | 1 | 0 | $R$ |



| a1 | a2 | a3 | ER | EB | EG | $L$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 1 | 1 | 0 | $R$ |



| a1 | a2 | a3 | ER | EB | EG | L |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 1 | 0 | 1 | 1 | 0 | $R$ |

## Feature Construction

$\square$ Aggregation is just the tip of the iceberg
$\square$ Which relationships to use?
■In-links
■Out-links
■Both
-Co-citation
$\square$ Which attributes to borrow from the neighbors?
■All
■Specific ones
-Words from only the title

- Age of my friends


## Additional Reading

Lise Getoor's tutorial is available at the lecture repository
http://www.cs.umd.edu/projects/linqs/Tutorials/SDM11/Home .html

## Graph Clustering

## Clustering

Grouping a collection of objects into clusters, such that those within each cluster are more closely related


## K-Means

$\square$ Squared Euclidean Distance

$$
\mathbf{d}(\mathbf{x}, \mathbf{y})=\|\mathbf{x}-\mathbf{y}\|^{2}
$$

$\square$ Sum of Squared Error Distance

$$
\begin{array}{r}
J=\sum_{k=1}^{K} \sum_{\mathbf{x}_{i} \in C_{k}} \| \mathbf{x}_{i}-\frac{\overline{\mathbf{x}}_{k} \|^{2}}{\nearrow} \\
\overline{\mathbf{x}}_{k}=\frac{1}{n_{i}} \sum_{\mathbf{x}_{i} \in C_{k}} \mathbf{x}_{i}
\end{array}
$$

## K-Means Iterative Optimization

$\square$ Initialize: Randomly partition the data into k initial clusters
$\square$ Step 1: Compute the mean of each cluster
$\square$ Step 2: Assign each point to the closest partition
$\square$ Step 3: If any point changed its cluster membership Then repeat Step 1


## Variants: K-medians and K-medoids

$\square$ Both minimize the sum of the distances from the centroids to the points
$\square K$-medians: Instead of calculating the mean for each cluster to determine its centroid, K-median instead calculates the median.
$\square K$-medoids: It requires that the center of each cluster be a sample point.
$\square$ Both problems can be solved using an iterative method like K-means.

## Graph Clustering: Four Strategies

$\square$ Similar Behavior: $u, v$ are in the same group if and only if $u$ and $v$ have similar connections w.r.t other nodes
$\square$ Graph Cuts
■ Remove some edges => disconnected graph

- The groups are the connected components
$\square$ Embedding: Map nodes to vectors in a Euclidean space, then use standard clustering methods
$\square$ Close Distance: $u, v$ are in the same group if and only if $u$ and $v$ are close to each other


## Greedy Method: $k$-medians clustering



Slides from Delbert Dueck

## Example: Olivetti face images


$\square$ Olivetti face database contains 400 greyscale $64 \times 64$ images from 40 people
■Similarity is based on sum-of-squared distance using a central $50 \times 50$ pixel window
$\square$ Small enough problem to find exact solution

## Olivetti faces: squared error achieved by ONE MILLION runs of $k$-medians clustering

Squared error
k-medians clustering, one million random restarts for each k


# AFFINITY PROPAGATION 

Science, 16 Feb. 2007 joint work with Brendan Frey

## One-sentence summary:

 All data points are simultaneously considered as exemplars, but exchange deterministic messages while a good set of exemplars gradually emerges.
## Affinity Propagation: visualization

All data points are simultaneously considered as exemplars, but exchange deterministic messages while a good set of exemplars gradually emerges.


[^0]
## Affinity Propagation: visualization



## Affinity Propagation

$\square$ TASK:
Identify a subset of data points as exemplars and assign every other data point to one of those exemplars
$\square$ INPUTS:
$\square$ A set of pairwise similarities, $\{s(i, k)\}$, where $s(i, k)$ is a real number indicating how well-suited data point $k$ is as an exemplar for data point $i$

$$
\text { e.g. } s(i, k)=-\left\|x_{i}-x_{k}\right\|^{2}, i \neq k
$$

Need not
be metric!

■For each data point $k$, a real number, $s(k, k)$, indicating the a priori preference that it be chosen as an exemplar

$$
e . g . s(k, k)=p \forall k
$$

## Affinity Propagation: message-passing

$\square$ Affinity propagation can be viewed as data points exchanging messages amongst themselves
■It can be derived as belief propagation (max-product) on a completely-connected factor graph


Sending availabilities, $a$


Responsibilities are how much you think you're in someone else's cluster. Availabilities are how much I think someone is in my cluster.

## Affinity Propagation: update equations



$$
r(i, k) \leftarrow s(i, k)-\max _{k^{\prime} \text { s.t. } k \not k^{\prime} \neq k}\left\{\quad s\left(i, k^{\prime}\right)\right\}
$$

Sending availabilities


$$
a(i, k) \leftarrow \quad \sum_{i^{\prime} \text { s.t. } i^{\notin\{i, k\}}} r\left(i^{\prime}, k\right)
$$

$$
a(k, k) \leftarrow \sum_{i^{\prime} \text { s.t. } i^{\prime} \neq k} \max \left\{0, r\left(i^{\prime}, k\right)\right\}
$$

Making decisions:

$$
\operatorname{argmax}_{k}\{a(i, k)+r(i, k)\}
$$

## Olivetti faces: squared error achieved by Affinity Propadation



## Clustering Objectives

$\square$ Traditional definition of a "good" clustering:

1. Points assigned to the same cluster should be highly similar.
2. Points assigned to different clusters should be highly dissimilar.

Apply these objectives to our graph representation


1. Maximize weight of within-group connections
2. Minimize weight of between-group connections

Slides Adapted from Royi Itzhak

## Graph Cuts

$\square$ Express partitioning objectives as a function of the "edge cut" of the partition.
$\square C u t$ : Set of edges with only one vertex in a group.

$$
\operatorname{cut}(A, B)=\sum_{i \in A, j \in B} w_{i j}
$$



## Graph Cut Criteria

$\square$ Criterion: Minimum-cut
$\square$ Minimize weight of connections between groups
$\min \operatorname{cut}(A, B)$

- Degenerate case: Optimal cut

- Problem:
- Only considers external cluster connections
- Does not consider internal cluster density


## Graph Cut Criteria (continued)

$\square$ Criterion: Normalized-cut (Shi \& Malik,'97)
■Consider the connectivity between groups relative to the density of each group.

$$
\min \operatorname{Ncut}(A, B)=\frac{\operatorname{cut}(A, B)}{\operatorname{vol}(A)}+\frac{\operatorname{cut}(A, B)}{\operatorname{vol}(B)}
$$

- Normalize the association between groups by volume.
- $\operatorname{Vol}(A)$ : The total weight of the edges originating from group $A$.
- Why use this criterion?
- Produces more balanced partitions.
- Computing an optimal cut is NP-hard


## Spectral Graph Theory

$\square$ Possible approach
-Represent a similarity graph as a matrix
■Apply knowledge from Linear Algebra...

- The eigenvalues and eigenvectors of a matrix provide global information about its structure.

$$
\left[\begin{array}{ccc}
a_{11} & \ldots & a_{1 n} \\
\vdots & & \vdots \\
a_{n 1} & \ldots & a_{n n}
\end{array}\right]\left[\begin{array}{c}
x_{1} \\
\vdots \\
x_{n}
\end{array}\right]=\lambda\left[\begin{array}{c}
x_{1} \\
\vdots \\
x_{n}
\end{array}\right]
$$

- Spectral Graph Theory
- Analyze the "spectrum" of matrix representing a graph.
- Spectrum : The eigenvectors of a graph, ordered by the magnitude of their corresponding eigenvalues.

$$
\Lambda=\left\{\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n}\right\}
$$

## Matrix Representations

$\square$ Adjacency matrix (A)
■ n x $n$ matrix

- $A=\left[w_{i j}\right]$ : edge weight between vertex $x_{i}$ and $x_{j}$

- Symmetric matrix
$\Rightarrow$ Eigenvectors are real and orthogonal


## Matrix Representations (continued)

$\square$ Degree matrix (D)

- $n \times n$ diagonal matrix

■ $D(i, i)=\sum_{j} w_{i j}$ : total weight of edges incident to vertex $x_{i}$


- Important application:
- Normalize adjacency matrix


## Matrix Representations (continued)

$\square$ Laplacian matrix $\quad L=D-A$
■ n x $n$ symmetric matrix


Important properties:

|  | $\mathbf{x}_{\mathbf{1}}$ | $\mathbf{x}_{\mathbf{2}}$ | $\mathbf{x}_{\mathbf{3}}$ | $\mathbf{x}_{\mathbf{4}}$ | $\mathbf{x}_{\mathbf{5}}$ | $\mathbf{x}_{\mathbf{6}}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{x}_{\mathbf{1}}$ | 1.5 | -0.8 | -0.6 | 0 | -0.1 | 0 |
| $\mathbf{x}_{\mathbf{2}}$ | $0-8$ | 1.6 | -0.8 | 0 | 0 | 0 |
| $\mathbf{x}_{\mathbf{3}}$ | 0. | -0.8 | 1.6 | - | 0 | 0 |
| $\mathbf{x}_{\mathbf{4}}$ | 0.8 | 0 | -0.2 | 2.5 | -0.8 | - |
| $\mathbf{x}_{\mathbf{5}}$ | 0.7 |  |  |  |  |  |
| $\mathbf{x}_{\mathbf{6}}$ | 0.1 | 0 | 0 | 0.8 | 1.7 | - |

- Eigenvalues are non-negative real numbers
- Eigenvectors are real and orthogonal
- Eigenvalues and eigenvectors provide an insight into the connectivity of the graph...


## Find An Optimal Min-Cut (Hall'70, Fiedler'73)

$\square$ Express a bi-partition $(A, B)$ as a vector $\quad p_{i}=\left\{\begin{array}{l}+1 \text { if } x_{i} \in \mathrm{~A} \\ -1 \text { if } x_{i} \in \mathrm{~B}\end{array}\right.$

- We can minimize the cut of the partition by finding a non-trivial vector $p$ that minimizes the function

$$
f(p)=\sum_{i, j \in V} w_{i j}\left(p_{i}-p_{j}\right)^{2}=p^{T} L_{\mathbb{R}} p
$$

- The Rayleigh Theorem shows:
- The minimum value for $f(p)$ is given by the $\underline{2}^{\text {nd }}$ smallest eigenvalue of the Laplacian $L$.
- The optimal solution for $p$ is given by the corresponding eigenvector $\mathrm{x}_{2}$, referred as the Fiedler Vector.


## So far...

$\square$ How can we define a "good" partition of a graph?

- Minimize a given graph cut criterion.

How can we efficiently identify such a partition? - Approximate using information provided by the eigenvalues and eigenvectors of a graph.
$\Rightarrow$ Spectral Clustering (Simon et. al,'90)

## Spectral Clustering Algorithms

$\square$ Three basic stages:

1. Pre-processing

- Construct a matrix representation of the dataset.

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 Bi-partitioning Algorithm (Simon,'90)

1. Pre-processing

Build Laplacian matrix $L$ of the graph


| $\mathbf{x}_{\mathbf{1}}$ | 1.5 | -0.8 | -0.6 | 0 | -0.1 | 0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{x}_{\mathbf{2}}$ | -0.8 | 1.6 | -0.8 | 0 | 0 | 0 |
| $\mathbf{x}_{\mathbf{3}}$ | -0.6 | -0.8 | 1.6 | -0.2 | 0 | 0 |
| $\mathbf{x}_{\mathbf{4}}$ | -0.8 | 0 | -0.2 | 2.5 | -0.8 | -0.7 |
| $\mathbf{x}_{\mathbf{5}}$ | -0.1 | 0 | 0 | 0.8 | 1.7 | -0.8 |
| $\mathbf{x}_{\mathbf{6}}$ | 0 | 0 | 0 | -0.7 | -0.8 | 1.5 |

2. Decomposition

Find eigenvalues $\Lambda$ and eigenvectors $X$ of the matrix $L$



How do we find the clusters?

## Spectral Bi-partitioning (continued)

$\square \quad$ Grouping

- Sort components of reduced 1-dimensional vector.
- Identify clusters by splitting the sorted vector in two.
$\square \quad$ How to choose a splitting point?
- Naïve approaches:
- Split at 0, mean or median value
- More expensive approaches
- Attempt to minimize normalised cut criterion in 1-dimension

| $x_{1}$ | 0.2 |
| :--- | :---: |
| $x_{2}$ | 0.2 |
| $x_{3}$ | 0.2 |
| $x_{4}$ | -0.4 |
| $x_{5}$ | -0.7 |
| $x_{6}$ | -0.7 |

## Split at 0

Cluster A: Positive points
Cluster B: Negative points

| $x_{1}$ | 0.2 |
| :--- | :--- |
| $x_{2}$ | 0.2 |
| $x_{3}$ | 0.2 |


| $x_{4}$ | -0.4 |
| :---: | :---: |
| $x_{5}$ | -0.7 |
| $x_{6}$ | -0.7 |

## K-Eigenvector Clustering

$\square$ K-eigenvector Algorithm (Ng et al.,'01)

1. Pre-processing

- Construct the scaled adjacency matrix

$$
A^{\prime}=D^{-1 / 2} A D^{-1 / 2}
$$

2. Decomposition

- Find the eigenvalues and eigenvectors of $A^{\prime}$.
- Build embedded space from the eigenvectors corresponding to the $k$ largest eigenvalues.

3. Grouping

- Apply k-means to reduced $n x k$ space to produce $k$ clusters.


## Aside: How to select $k$ ?

$\square$ Eigengap: the difference between two consecutive eigenvalues.
$\square$ Most stable clustering is generally given by the value $k$ that maximizes the expression

$$
\Delta_{k}=\left|\lambda_{k}-\lambda_{k-1}\right|
$$

## Largest eigenvalues of Cisi/Medline data

$\max \Delta_{k}=\left|\lambda_{2}-\lambda_{1}\right|$
$\Rightarrow$ Choose $k=2$


## Random Walk with Restart



## Random Walk with Restart



Nearby nodes, higher scores
More red, more relevant

|  | Node 4 |
| :--- | :--- |
| Node 1 | 0.13 |
| Node 2 | 0.10 |
| Node 3 | 0.13 |
| Node 4 | 0.22 |
| Node 5 | 0.13 |
| Node 6 | 0.05 |
| Node 7 | 0.05 |
| Node 8 | 0.08 |
| Node 9 | 0.04 |
| Node 10 | 0.03 |
| Node 11 | 0.04 |
| Node 12 | 0.02 |

ranking vector

## Random Walk with Restart

$\square$ The walk distribution satisfies a simple equation:

$$
\boldsymbol{\pi}=(1-c) \mathbf{P} \boldsymbol{\pi}+c \mathbf{e}
$$

$\square \mathbf{P}$ : Transition matrix
$\square C$ : Restart probability
$\square e: S t a r t$ node
$\square \boldsymbol{\pi}$ : Ranking vector
$\square$ Solution: $\quad \boldsymbol{\pi}=c(I-(1-c) \mathbf{P})^{-1} \mathbf{e}$

## Example of RWR

## Iterative update until convergence

$$
\boldsymbol{\pi}^{t}=(1-c) \mathbf{P} \boldsymbol{\pi}^{t-1}+c \mathbf{e}
$$

$\left(\begin{array}{l}0.13 \\ 0.10 \\ 0.13 \\ 0.22 \\ 0.13 \\ 0.05 \\ 0.05 \\ 0.08 \\ 0.04 \\ 0.03 \\ 0.04 \\ 0.02\end{array}\right)=0.9 \times\left(\begin{array}{cccccccccccc}0 & 1 / 3 & 1 / 3 & 1 / 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 / 3 & 0 & 1 / 3 & 0 & 0 & 0 & 0 & 1 / 4 & 0 & 0 & 0 & 0 \\ 1 / 3 & 1 / 3 & 0 & 1 / 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 / 3 & 0 & 1 / 3 & 0 & 1 / 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 / 3 & 0 & 1 / 2 & 1 / 2 & 1 / 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 / 4 & 0 & 1 / 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 / 4 & 1 / 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 / 3 & 0 & 0 & 1 / 4 & 0 & 0 & 0 & 1 / 2 & 0 & 1 / 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 / 4 & 0 & 1 / 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 / 2 & 0 & 1 / 3 & 1 / 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 / 4 & 0 & 1 / 3 & 0 & 1 / 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 / 3 & 1 / 3 & 0\end{array}\right)\left(\begin{array}{l}0.13 \\ 0.10 \\ 0.13 \\ 0.22 \\ 0.13 \\ 0.05 \\ 0.05 \\ 0.08 \\ 0.04 \\ 0.03 \\ 0.04 \\ 0.02\end{array}\right)+0.1 \times\left(\begin{array}{l}0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0\end{array}\right)$

$\mathrm{n} \times 1$
$\mathrm{n} \times \mathrm{n}$
$\mathrm{n} \times 1$

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