

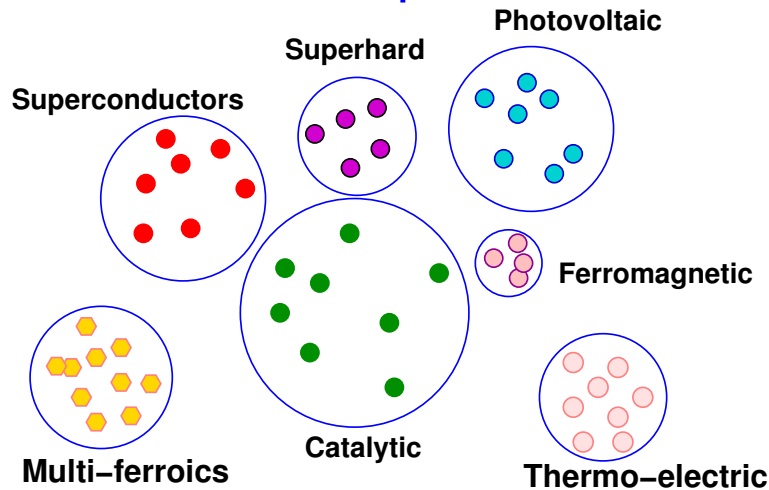
APPLICATIONS OF GRAPH LAPLACEANS: CLUSTERING, EMBEDDING

- *The clustering problem; Basic method: K-means*
- *Similarity graphs; kNN graphs*
- *Measures of separation: edge cuts, normalized cuts, etc*
- *Application: Segmentation*
- *Graph embeddings; Laplacean Eigenmaps*
- *Locally Linear Embeddings (LLE)*
- *Explicit mappings; PCA, LPP, ONPP,..*
- *Building a knn graph*

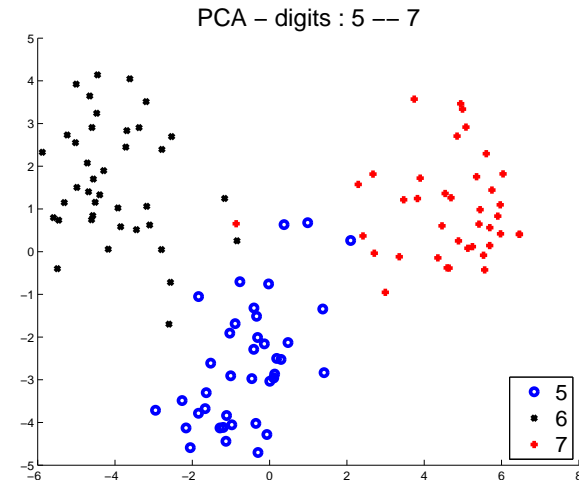
Clustering

➤ Problem: we are given n data items: x_1, x_2, \dots, x_n . Would like to ‘cluster’ them, i.e., group them so that each group or cluster contains items that are similar in some sense.

➤ Example: materials



➤ Example: Digits



➤ Each group is a ‘cluster’ or a ‘class’

➤ ‘Unsupervised learning’

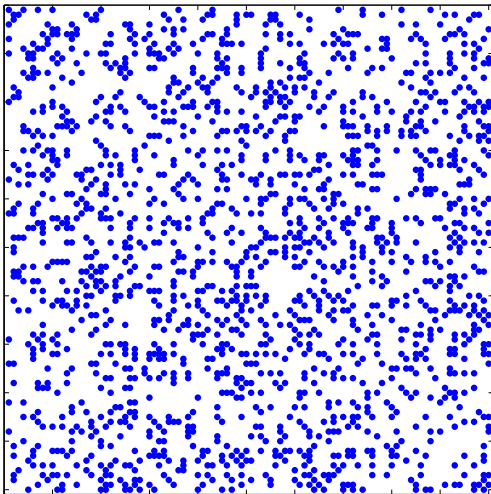
What is 'Unsupervised Learning'?

Ans: Class of methods that do not exploit **labeled data**

- Example of digits: perform a 2-D projection
- Images of same digit tend to cluster (more or less)
- Such 2-D representations are popular for visualization
- Can also try to find natural clusters in data, e.g., in materials
- Basic clustering technique: K-means

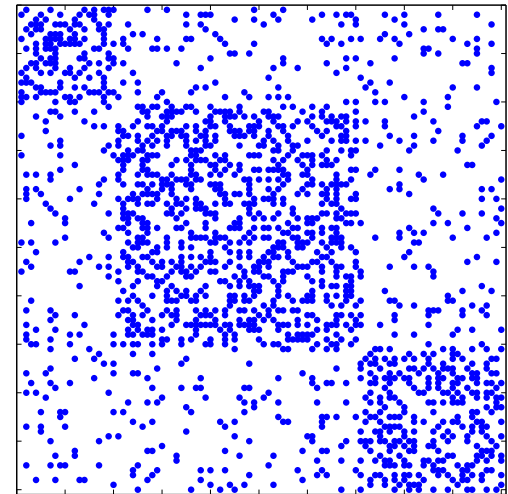
Example: Community Detection

- Communities modeled by an ‘affinity’ graph [e.g., ‘user A sends frequent e-mails to user B ’]. [[data: www-personal.umich.edu/~mejn/netdata/](http://www-personal.umich.edu/~mejn/netdata/)]



← Original Adj. matrix

Goal: Find ordering so blocks are as dense as possible →



- Use ‘blocking’ techniques for sparse matrices
- Advantage of this viewpoint: need not know # of clusters.

Example of application

Data set from :

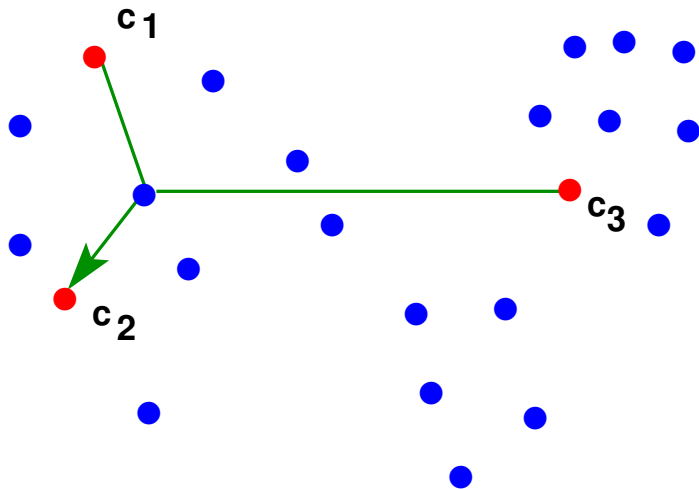
<http://www-personal.umich.edu/~mejn/netdata/>

- Network connecting bloggers of different political orientations [2004 US presidential election]
- ‘Communities’: liberal vs. conservative
- Graph: 1,490 vertices (blogs) : first 758: liberal, rest: conservative.
- Edge: $i \rightarrow j$: a citation between blogs i and j
- Blocking algorithm (Density threshold=0.4): subgraphs [note: density = $|E|/|V|^2$.]
- Smaller subgraph: conservative blogs, larger one: liberals

A basic method: K-means

➤ A basic algorithm that uses Euclidean distance

- 1 Select p initial centers: c_1, c_2, \dots, c_p for classes $1, 2, \dots, p$
- 2 For each x_i do: determine *class* of x_i as $\operatorname{argmin}_k \|x_i - c_k\|$
- 3 Redefine each c_k to be the centroid of class k
- 4 Repeat until convergence



- Simple algorithm
- Works well (gives good results) but can be slow
- Performance depends on initialization

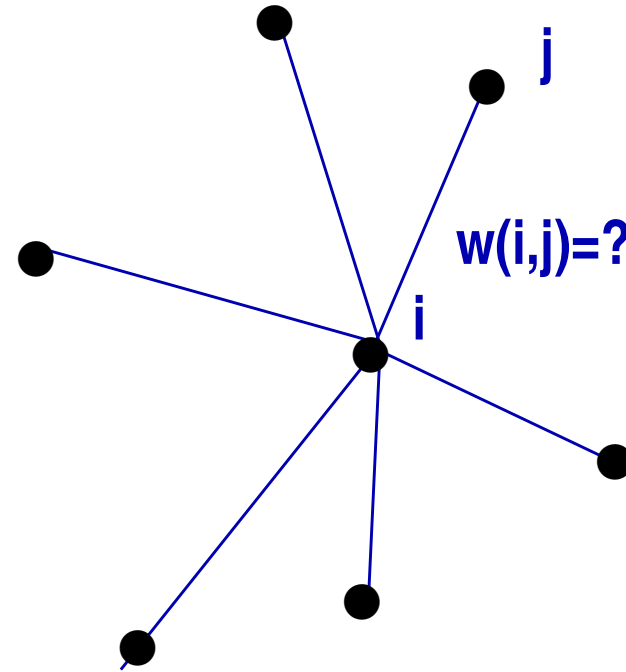
Methods based on similarity graphs

- Class of Methods that perform clustering by exploiting a graph that describes the similarities between any two items in the data.
- Need to:
 1. decide what nodes are in the neighborhood of a given node
 2. quantify their similarities - by assigning a weight to any pair of nodes.

Example: For text data: Can decide that any columns i and j with a cosine greater than 0.95 are 'similar' and assign that cosine value to w_{ij}

First task: build a 'similarity' graph

➤ Goal: to build a **similarity** graph, i.e., a graph that captures similarity between any two items



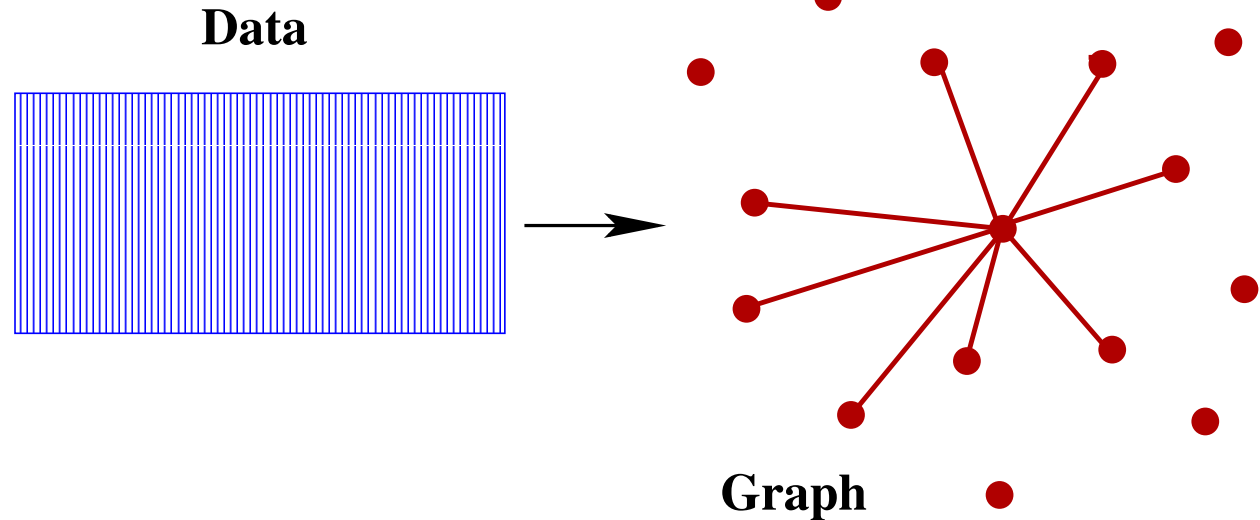
➤ Two methods: K-nearest Neighbor graphs or use Gaussian ('heat') kernel

K-nearest neighbor graphs

- Given: a set of n data points $X = \{x_1, \dots, x_n\} \rightarrow$ vertices
- Given: a **proximity** measure between two data points x_i and x_j – as measured by a quantity $dist(x_i, x_j)$
- Want: For each point x_i a list of the ‘nearest neighbors’ of x_i (edges between x_i and these nodes).
- Note: graph will usually be **directed** \rightarrow need to symmetrize

Nearest neighbor graphs

- For each node, get a few of the nearest neighbors → Graph



- Problem: How to build a nearest-neighbor graph from given data
- We will revisit this later.

Two types of nearest neighbor graph often used:

ϵ -graph:

Edges consist of pairs (x_i, x_j) such that $\rho(x_i, x_j) \leq \epsilon$

k NN graph:

Nodes adjacent to x_i are those nodes x_ℓ with the k with smallest distances $\rho(x_i, x_\ell)$.

- ϵ -graph is undirected and is geometrically motivated. Issues: 1) may result in disconnected components 2) what ϵ ?
- k NN graphs are directed in general (can be trivially fixed).
- k NN graphs especially useful in practice.

Similarity graphs: Using 'heat-kernels'

Define weight between i and j as:

$$w_{ij} = f_{ij} \times \begin{cases} e^{-\frac{\|x_i - x_j\|^2}{\sigma_X^2}} & \text{if } \|x_i - x_j\| < r \\ 0 & \text{if not} \end{cases}$$

- Note $\|x_i - x_j\|$ could be any measure of distance...
- f_{ij} = optional = some measure of similarity - other than distance
- Only nearby points kept.
- Sparsity depends on parameters

Edge cuts, ratio cuts, normalized cuts, ...

- Assume now that we have built a ‘similarity graph’
- Setting is identical with that of graph partitioning.
- Need a Graph Laplacean: $L = D - W$ with $w_{ii} = 0, w_{ij} \geq 0$ and $D = \text{diag}(W * \text{ones}(n, 1))$ [in matlab notation]

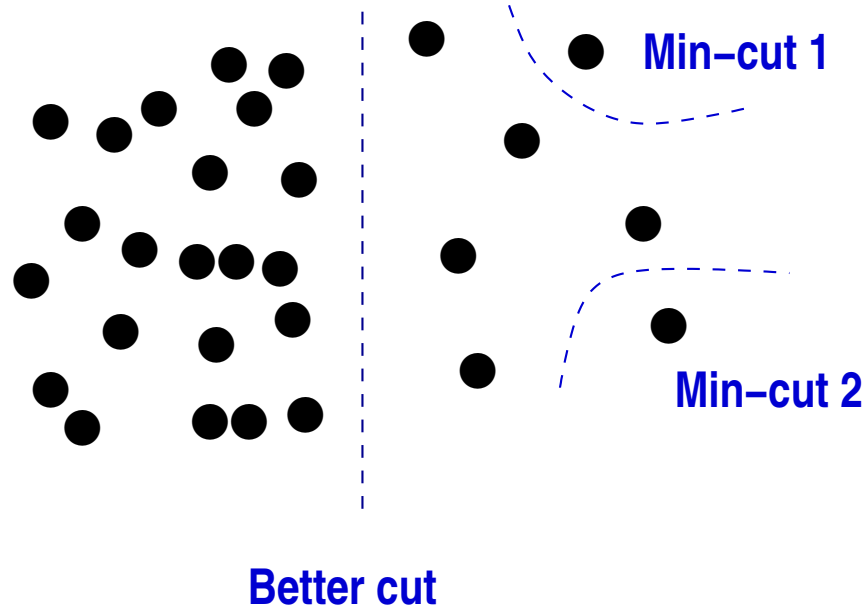
- Partition vertex set V in two sets A and B with

$$A \cup B = V, \quad A \cap B = \emptyset$$

- Define

$$\text{cut}(A, B) = \sum_{u \in A, v \in B} w(u, v)$$

- First (naive) approach: use this measure to partition graph, i.e.,
... Find A and B that minimize $cut(A, B)$.
- Issue: Small sets, isolated nodes, big imbalances,



- Standard Graph Partitioning approach: Find A, B by solving

$$\text{Minimize } \textit{cut}(A, B), \text{ subject to } |A| = |B|$$

- Condition $|A| = |B|$ not too meaningful in some applications - too restrictive in others.
- Minimum Ratio Cut approach. Find A, B by solving:

$$\text{Minimize } \frac{\textit{cut}(A, B)}{|A| \cdot |B|}$$

- Difficult to find solution (original paper [Wei-Cheng '91] proposes several heuristics)
- Approximate solution : spectral .

Theorem [Hagen-Kahng, 91] If λ_2 is the 2nd smallest eigenvalue of L , then a lower bound for the cost c of the optimal ratio cut partition, is:

$$c \geq \frac{\lambda_2}{n}.$$

Proof: Consider an optimal partition A, B and let $p = |A|/n, q = |B|/n$. Note that $p + q = 1$. Let x be the vector with coordinates

$$x_i = \begin{cases} q & \text{if } i \in A \\ -p & \text{if } i \in B \end{cases}$$

Note that $x \perp \mathbf{1}$. Also if $(i, j) ==$ an edge-cut then $|x_i - x_j| = |q - (-p)| = |q + p| = 1$, otherwise $x_i - x_j = 0$. Therefore:

$$x^T L x = \sum_{(i,j) \in E} w_{ij} (x_i - x_j)^2 = w(A, B).$$

In addition: $\|x\|^2 = pq^2n + qp^2n = pq(p + q)n = pqn = \frac{|A| \cdot |B|}{n}$.

Therefore, by the Courant-Fischer theorem:

$$\lambda_2 \leq \frac{(Lx, x)}{(x, x)} = n \times \frac{w(A, B)}{|A| \cdot |B|} = n \times c.$$

Hence result. ■

➤ Idea is to use eigenvector associated with λ_2 to determine partition, e.g., based on sign of entries. Use the ratio-cut measure to actually determine where to split.

Normalized cuts [Shi-Malik,2000]

- Recall notation $w(X, Y) = \sum_{x \in X, y \in Y} w(x, y)$ - then define:

$$\text{ncut}(A, B) = \frac{\text{cut}(A, B)}{w(A, V)} + \frac{\text{cut}(A, B)}{w(B, V)}$$

- Goal is to avoid small sets A, B

 What is $w(A, V)$ in the case when $w_{ij} == 1$?

- Let x be an indicator vector:

$$x_i = \begin{cases} 1 & \text{if } i \in A \\ 0 & \text{if } i \in B \end{cases}$$

- Recall that: $x^T L x = \sum_{(i,j) \in E} w_{ij} |x_i - x_j|^2$ (note: each edge counted once)

➤ Therefore:

$$\text{cut}(A, B) = \sum_{x_i=1, x_j=0} w_{ij} = x^T L x$$

$$w(A, V) = \sum_{x_i=1} d_i = x^T W \mathbf{1} = x^T D \mathbf{1}$$

$$w(B, V) = \sum_{x_j=0} d_j = (\mathbf{1} - x)^T W \mathbf{1} = (\mathbf{1} - x)^T D \mathbf{1}$$

➤ Goal now: to minimize ncut

$$\min_{A, B} \text{ncut}(A, B) = \min_{x_i \in \{0,1\}} \frac{x^T L x}{x^T D x} + \frac{x^T L x}{(\mathbf{1} - x)^T D x}$$

➤ Let

$$k = \frac{\sum_{x_i > 0} d_i}{\sum_i d_i}; \quad b = \frac{k}{1 - k}; \quad \text{and:} \quad \mathbf{y} = (\mathbf{1} + \mathbf{x}) - b(\mathbf{1} - \mathbf{x})$$

➤ Then it can be shown that we need to solve:

$$\begin{aligned} & \min_{y_i \in \{1, -b\}} \frac{\mathbf{y}^T \mathbf{L} \mathbf{y}}{\mathbf{y}^T \mathbf{D} \mathbf{y}} \\ & \text{Subject to} \quad \mathbf{y}^T \mathbf{D} \mathbf{1} = 0 \end{aligned}$$

➤ + Relax \rightarrow need to solve Generalized eigenvalue problem

$$\mathbf{L} \mathbf{y} = \lambda \mathbf{D} \mathbf{y}$$

➤ $\mathbf{y}_1 = \mathbf{1}$ is eigenvector associated with eigenvalue $\lambda_1 = 0$


➤ \mathbf{y}_2 associated with second eigenvalue solves problem.

A few properties

2 Show that

$$ncut(A, B) = \sigma \times \frac{cut(A, B)}{w(A, V) \times w(B, V)}$$

where σ is a constant

3 How do ratio-cuts and normalized cuts compare when the graph is d -regular (same degree for each node).

Extension to more than 2 clusters

➤ Just like graph partitioning we can:

1. Apply the method recursively [Repeat clustering on the resulted parts]
2. or compute a few eigenvectors and run K-means clustering on these eigenvectors to get the clustering.

Application: Image segmentation

- First task: obtain a graph from pixels.
- Common idea: use “Heat kernels”
- Let F_j = feature value (e.g., brightness), and Let X_j = spatial position.

Then define

$$w_{ij} = e^{-\frac{\|F_i - F_j\|^2}{\sigma_I^2}} \times \begin{cases} e^{-\frac{\|X_i - X_j\|^2}{\sigma_X^2}} & \text{if } \|X_i - X_j\| < r \\ 0 & \text{else} \end{cases}$$

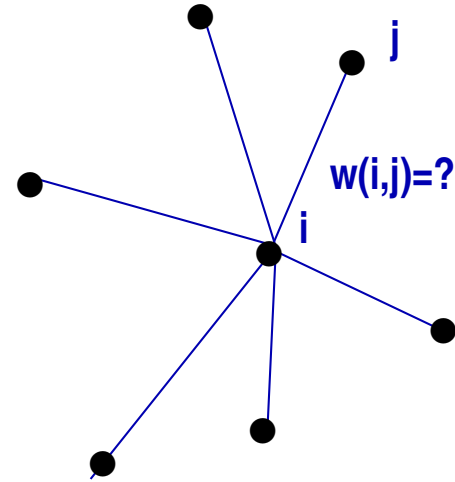
- Sparsity depends on parameters

 Run *test_mir* and *test_jump*

Spectral clustering: General approach

1 Given: Collection of data samples $\{x_1, x_2, \dots, x_n\}$

2 Build a **similarity** graph between items

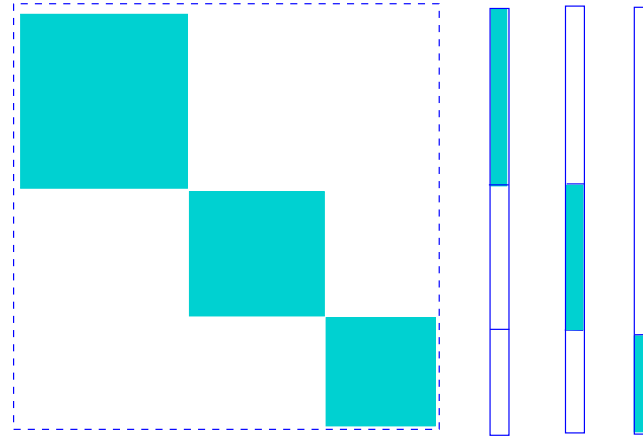
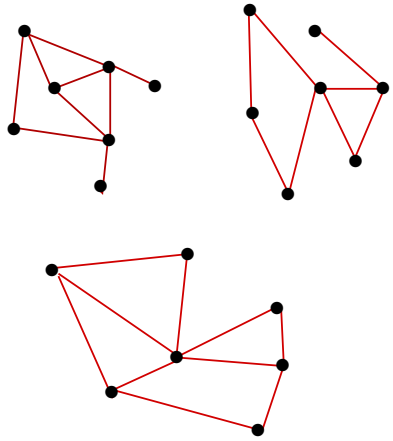


3 Compute (smallest) eigenvector (s) of resulting graph Laplacean

4 Use k-means on eigenvector (s) of Laplacean

➤ For Normalized cuts solve generalized eigen problem.

➤ Recall observation made earlier:

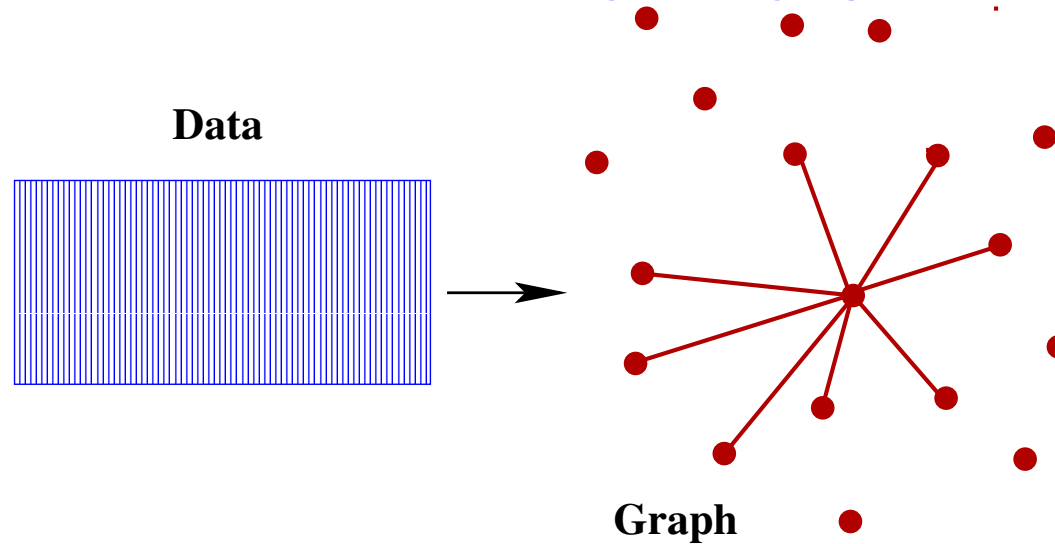


➤ Alg. Multiplicity of eigenvalue zero = # connected components.

KNN GRAPHS

Building a nearest neighbor graph

- Question: How to build a nearest-neighbor graph from given data?



- Will demonstrate the power of a divide a conquer approach combined with the Lanczos algorithm.

Recall: Two common types of nearest neighbor graphs

ϵ -graph:

Edges consist of pairs (x_i, x_j) such that $\rho(x_i, x_j) \leq \epsilon$

k NN graph:

Nodes adjacent to x_i are those nodes x_ℓ with the k with smallest distances $\rho(x_i, x_\ell)$.

- ϵ -graph is undirected and is geometrically motivated. Issues: 1) may result in disconnected components 2) what ϵ ?
- k NN graphs are directed in general (can be trivially fixed).
- k NN graphs especially useful in practice.

Divide and conquer KNN: key ingredient

- Key ingredient is *Spectral bisection*
- Let the data matrix $X = [x_1, \dots, x_n] \in \mathbb{R}^{d \times n}$
- Each column == a data point.
- Center the data: $\hat{X} = [\hat{x}_1, \dots, \hat{x}_n] = X - ce^T$
where c == centroid; $e = \text{ones}(d, 1)$ (matlab)

Goal: Split \hat{X} into halves using a hyperplane.

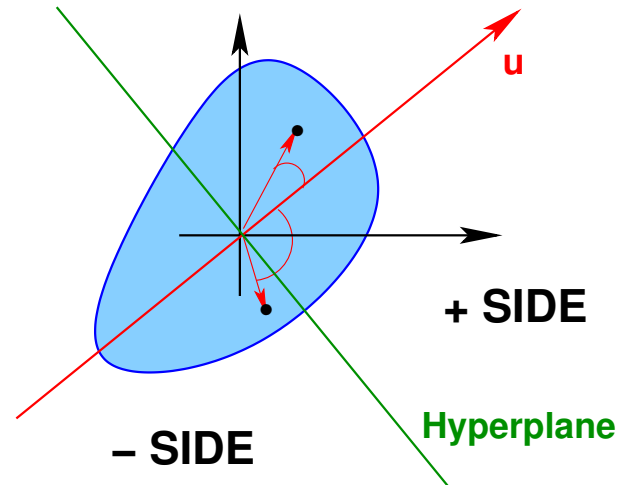
Method: Principal Direction Divisive Partitioning D. Boley, '98.

Idea: Use the (σ, u, v) = largest singular triplet of \hat{X} with:

$$u^T \hat{X} = \sigma v^T.$$

- Hyperplane is defined as $\langle u, x \rangle = 0$, i.e., it splits the set of data points into two subsets:

$$X_+ = \{x_i \mid u^T \hat{x}_i \geq 0\} \quad \text{and} \quad X_- = \{x_i \mid u^T \hat{x}_i < 0\}.$$



- Note that $u^T \hat{x}_i = u^T \hat{X} e_i = \sigma v^T e_i \rightarrow$

$$\mathbf{X}_+ = \{x_i \mid v_i \geq 0\} \quad \text{and} \quad \mathbf{X}_- = \{x_i \mid v_i < 0\},$$

where v_i is the i -th entry of v .

➤ In practice: replace above criterion by

$$\mathbf{X}_+ = \{x_i \mid v_i \geq \text{med}(v)\} \ \& \ \mathbf{X}_- = \{x_i \mid v_i < \text{med}(v)\}$$

where $\text{med}(v) == \text{median of the entries of } v$.

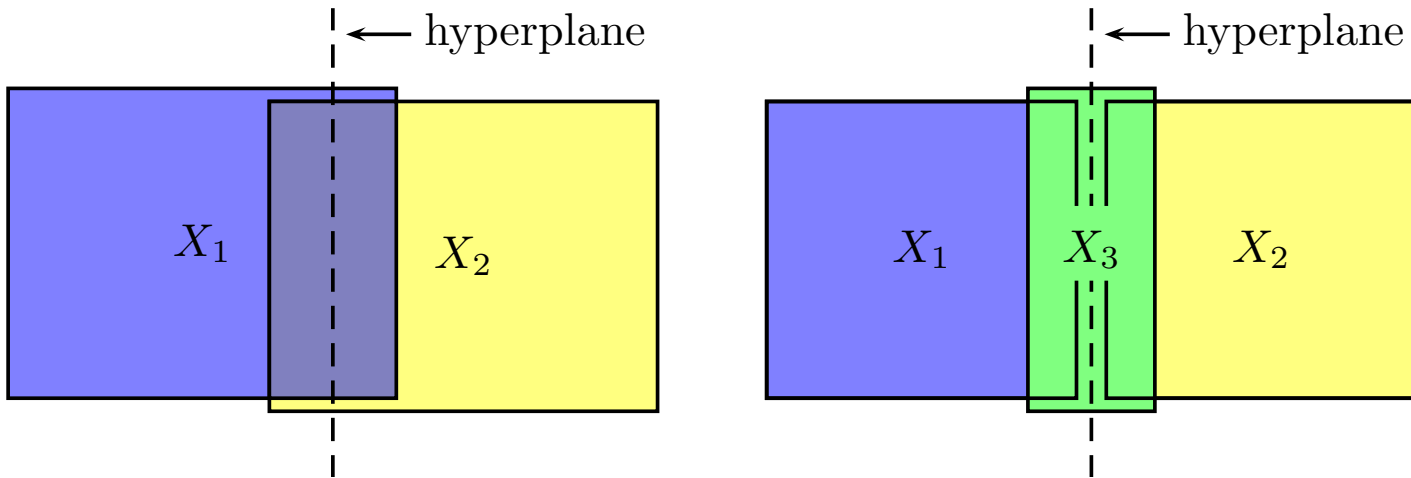
➤ For largest singular triplet (σ, u, v) of \hat{X} : use Golub-Kahan-Lanczos algorithm or Lanczos applied to $\hat{X}\hat{X}^T$ or $\hat{X}^T\hat{X}$

➤ Cost (assuming s Lanczos steps) : $O(n \times d \times s)$; Usually: d very small

Two divide and conquer algorithms

Overlap method: divide current set into two overlapping subsets X_1, X_2

Glue method: divide current set into two disjoint subsets X_1, X_2 plus a third set X_3 called gluing set.



➤ Exploit recursivity

The Overlap Method

➤ Divide current set X into two overlapping subsets:

$$X_1 = \{x_i \mid v_i \geq -h_\alpha(S_v)\} \quad \text{and} \quad X_2 = \{x_i \mid v_i < h_\alpha(S_v)\},$$

- where $S_v = \{|v_i| \mid i = 1, 2, \dots, n\}$.
 - and $h_\alpha(\cdot)$ is a function that returns an element larger than $(100\alpha)\%$ of those in S_v .
- Rationale: to ensure that the two subsets overlap $(100\alpha)\%$ of the data, i.e.,

$$|X_1 \cap X_2| = \lceil \alpha |X| \rceil .$$

The Glue Method

Divide the set X into two disjoint subsets X_1 and X_2 with a gluing subset X_3 :

$$X_1 \cup X_2 = X, \quad X_1 \cap X_2 = \emptyset, \quad X_1 \cap X_3 \neq \emptyset, \quad X_2 \cap X_3 \neq \emptyset.$$

Criterion used for splitting:

$$X_1 = \{x_i \mid v_i \geq 0\}, \quad X_2 = \{x_i \mid v_i < 0\}, \\ X_3 = \{x_i \mid -h_\alpha(S_v) \leq v_i < h_\alpha(S_v)\}.$$

Note: gluing subset X_3 here is just the intersection of the sets X_1, X_2 of the overlap method.

Theorem The time complexity for the overlap method is

$$T_o(n) = \Theta(dn^{t_o}), \quad \text{where:} \quad t_o = \log_{2/(1+\alpha)} 2 = \frac{1}{1 - \log_2(1 + \alpha)}.$$

Theorem The time complexity for the glue method is

$$T_g(n) = \Theta(dn^{t_g}/\alpha), \quad \text{where} \quad t_g \equiv \text{sol. to the equ.:} \quad \frac{2}{2^t} + \alpha^t = 1.$$

Example: When $\alpha = 0.1$, then $t_o = 1.16$ while $t_g = 1.12$.

Reference:

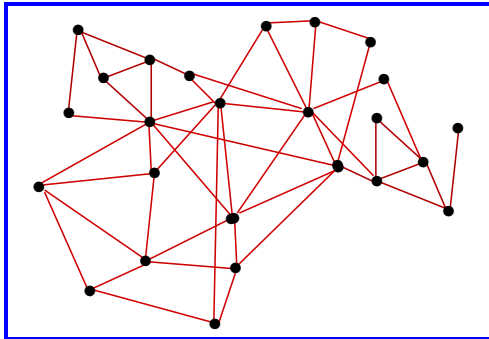
Jie Chen, Haw-Ren Fang and YS, "Fast Approximate k NN Graph Construction for High Dimensional Data via Recursive Lanczos Bisection" JMLR, vol. 10, pp. 1989-2012 (2009).

GRAPH EMBEDDINGS

Graph embeddings

- We have seen how to build a graph to represent data
- *Graph embedding* does the opposite: maps a graph to data

Given: a graph that models some data (e.g., a kNN graph)



→ Data: $Y = [y_1, y_2, \dots, y_n]$ in \mathbb{R}^d

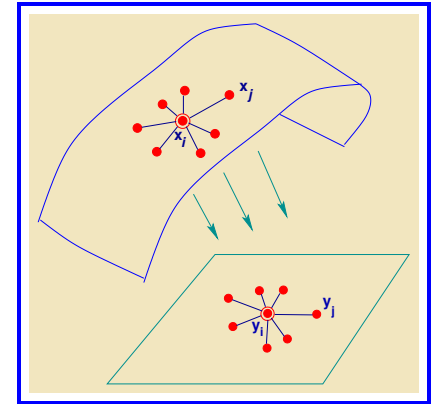
- Trivial use: visualize a graph ($d = 2$)
- Wish: mapping should preserve *similarities* in graph.

Vertex embedding: map every vertex x_i to a vector $y_i \in \mathbb{R}^d$

➤ Many applications [clustering, finding missing link, semi-supervised learning, community detection, ...]

➤ Graph captures similarities, closeness, ..., in data

Objective: Build a mapping of each vertex i to a data point $y_i \in \mathbb{R}^d$



➤ Many methods do this

➤ **Eigenmaps** and **LLE** are two of the best known

- Eigenmaps uses the *graph Laplacean*
- Recall: Graph Laplacean is a matrix defined by :

$$L = D - W$$

$$\begin{cases} w_{ij} \geq 0 & \text{if } j \in Adj(i) \\ w_{ij} = 0 & \text{else} \end{cases} \quad D = \text{diag} \left[d_{ii} = \sum_{j \neq i} w_{ij} \right]$$

with $Adj(i)$ = neighborhood of i (excludes i)

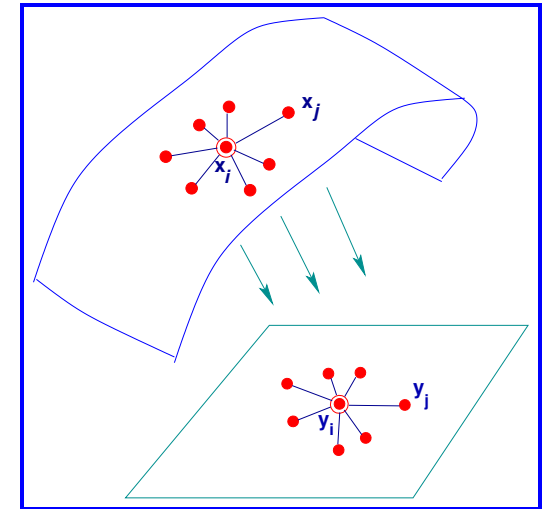
- Remember that vertex i represents data item x_i . We will use i or x_i to refer to the vertex.
- We will find the y_i 's by solving an optimization problem.

The Laplacean eigenmaps approach

Laplacean Eigenmaps [Belkin-Niyogi '01] *minimizes*

$$\mathcal{F}(Y) = \sum_{i,j=1}^n w_{ij} \|y_i - y_j\|^2 \quad \text{subject to} \quad YDY^T = I$$

- Motivation:** if $\|x_i - x_j\|$ is small (orig. data), we want $\|y_i - y_j\|$ to be also small (low-Dim. data)
- Original data used indirectly through its graph
 - Objective function can be translated to a trace (see Property 3 in Lecture notes 9) and will yield a sparse eigenvalue problem



➤ Problem translates to:

$$\begin{cases} \min & \text{Tr} [Y(D - W)Y^\top] \\ Y \in \mathbb{R}^{d \times n} \\ YDY^\top = I \end{cases} .$$

➤ Solution (sort eigenvalues increasingly):

$$(D - W)u_i = \lambda_i D u_i ; \quad y_i = u_i^\top ; \quad i = 1, \dots, d$$

➤ An $n \times n$ sparse eigenvalue problem [In 'sample' space]

➤ Note: can assume $D = I$. Amounts to rescaling data. Problem becomes

$$(I - W)u_i = \lambda_i u_i ; \quad y_i = u_i^\top ; \quad i = 1, \dots, d$$

Locally Linear Embedding (Roweis-Saul-00)

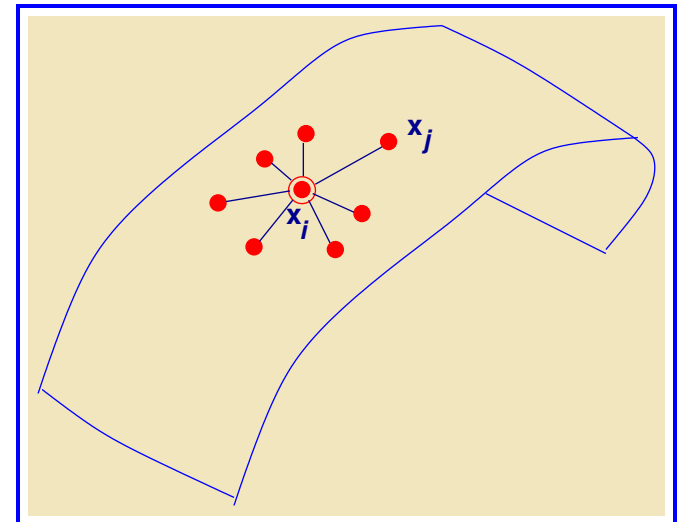
- LLE is very similar to Eigenmaps. Main differences:
 - 1) Graph Laplacean matrix is replaced by an ‘affinity’ graph
 - 2) Objective function is changed: want to preserve graph

1. Graph: Each x_i is written as a convex combination of its k nearest neighbors:

$$x_i \approx \sum w_{ij} x_j, \quad \sum_{j \in N_i} w_{ij} = 1$$

➤ Optimal weights computed (‘local calculation’) by minimizing

$$\|x_i - \sum w_{ij} x_j\| \quad \text{for } i = 1, \dots, n$$



2. Mapping:

The y_i 's should obey the same 'affinity' as x_i 's \rightsquigarrow

Minimize:

$$\sum_i \left\| y_i - \sum_j w_{ij} y_j \right\|^2 \quad \text{subject to: } Y \mathbf{1} = 0, \quad Y Y^\top = I$$

Solution:

$$(I - W^\top)(I - W)u_i = \lambda_i u_i; \quad y_i = u_i^\top.$$

➤ $(I - W^\top)(I - W)$ replaces the graph Laplacean of eigenmaps

Implicit vs explicit mappings

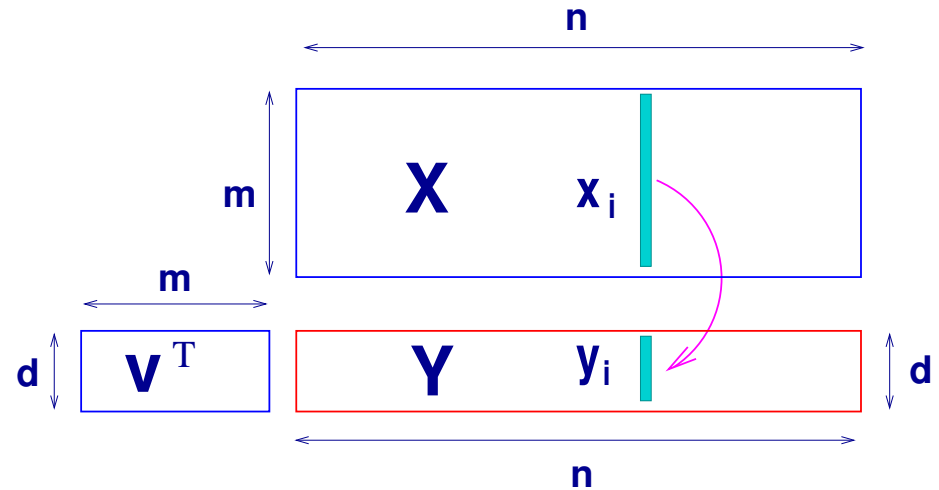
- In Eigenmaps and LLE we only determine a set of y'_i 's in \mathbb{R}^d from the data points $\{x_i\}$.
- The mapping $y_i = \phi(x_i), i = 1, \dots, n$ is implicit
- Difficult to compute a y for an x that is not one of the x_i 's
- Inconvenient for classification. Thus is known as the “The out-of-sample extension” problem
- In **Explicit** (also known as **linear**) methods: mapping ϕ is known explicitly (and it is linear.)

Locally Preserving Projections (He-Niyogi-03)

➤ LPP is a **linear** dimensionality reduction technique

➤ Recall the setting:

Want $V \in \mathbb{R}^{m \times d}$; $Y = V^T X$



➤ Starts with the same neighborhood graph as Eigenmaps: $L \equiv D - W =$ graph 'Laplacian'; with $D \equiv \text{diag}(\{\sum_i w_{ij}\})$.

- Optimization problem is to solve

$$\min_{Y \in \mathbb{R}^{d \times n}, YDY^\top = I} \sum_{i,j} w_{ij} \|y_i - y_j\|^2, \quad Y = V^\top X.$$

- Difference with eigenmaps: Y is an explicit projection of X
- Solution (sort eigenvalues increasingly)

$$XLX^\top v_i = \lambda_i XDX^\top v_i \quad y_{i,:} = v_i^\top X$$

- Note: essentially same method in [Koren-Carmel'04] called 'weighted PCA' [viewed from the angle of improving PCA]

ONPP (Kokiopoulou and YS '05)

- Orthogonal Neighborhood Preserving Projections
- A linear (orthogonal) version of LLE obtained by writing Y in the form $Y = V^T X$
- Same graph as LLE. Objective: preserve the affinity graph (as in LLE) *but* with the constraint $Y = V^T X$
- Problem solved to obtain mapping:

$$\begin{aligned} \min_V \text{Tr} [V^T X (I - W^T) (I - W) X^T V] \\ \text{s.t. } V^T V = I \end{aligned}$$

- In LLE replace $V^T X$ by Y

More recent methods

➤ Quite a bit of recent work - e.g., methods: node2vec, DeepWalk, GraRep, ... See the following papers ... among many others :

[1] *William L. Hamilton, Rex Ying, and Jure Leskovec Representation Learning on Graphs: Methods and Applications arXiv:1709.05584v3*

[2] *Shaosheng Cao, Wei Lu, and Qionghai Xu GraRep: Learning Graph Representations with Global Structural Information, CIKM, ACM Conference on Information and Knowledge Management, 24*

[3] *Amr Ahmed, Nino Shervashidze, and Shravan Narayanamurthy, Distributed Large-scale Natural Graph Factorization [Proc. WWW 2013, May 13–17, 2013, Rio de Janeiro, Brazil]*

Example: Graph factorization

- Line of work in Papers [1] and [3] above + others
- Instead of minimizing $\sum w_{ij} \|y_i - y_j\|_2^2$ as before

... try to minimize

$$\sum_{ij} |w_{ij} - y_i^T y_j|^2$$

- In other words solve: $\min_Y \|W - Y^T Y\|_F^2$
- Referred to as *Graph factorization*
- Common in knowledge graphs