APPLICATIONS OF GRAPH LAPLACEANS: Graph Embeddings, and Dimension Reduction

- **Graph Embeddings, vertex embeddings . The problem**
- **Use of Graph Laplaceans, Laplacean Eigenmaps**
- **Use of similarity graphs: Locally Linear Embeddings**
- **Explicit dimension reduction method: PCA**
- **Explicit graph-based dimension reduction method: LLP, ONPP.**

Graph embeddings

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

➤ Trivial use: visualize a graph $(d = 2)$

➤ Wish: mapping should preserve *similarities* in graph.

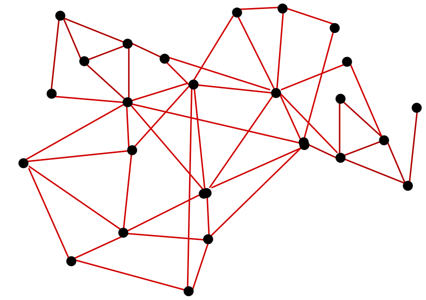
➤ Many applications [clustering, finding missing link, semi-supervised learning, community detection, ...]

➤ We will see two *nonlinear* classical methods: Eigenmaps, LLE ...

➤ ... and two linear (explicit) ones.

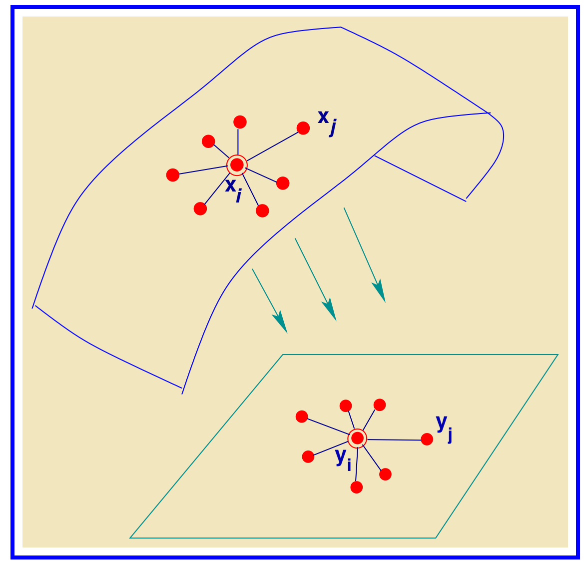
Given: a graph that models some data points $x_1, x_2, \cdots, x_n$ [simplest case: a kNN graph of $x_1, x_2, \cdots, x_n$]

Data: $X = [x_1, x_2, \cdots, x_n] \longrightarrow$ Graph:



➤ 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 to do this. Eigenmaps is one of the best known

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

$$\boxed{L = D - W}$$

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

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

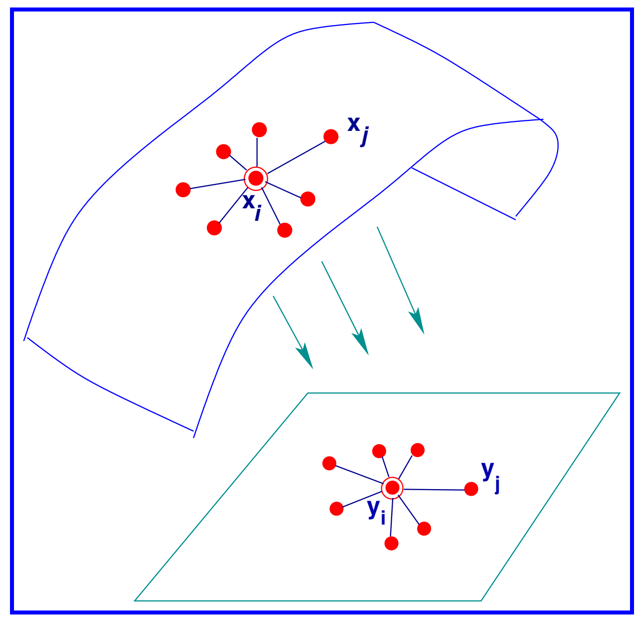
Laplacean Eigenmaps [Belkin-Niyogi '01] *minimizes*

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

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:

$$\min_{\begin{cases} Y \in \mathbb{R}^{d\times n} \\ Y D\, Y^\top = I \end{cases}} \mathrm{Tr}\left[Y(D-W)Y^\top \right] .$$

➤ Solution (sort eigenvalues increasingly):

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

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

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

$$\boxed{(I-W)u_i = \lambda_i u_i \; ; \quad y_i = u_i^\top ; \quad i = 1, \cdots, d}$$

Locally Linear Embedding (Roweis-Saul-00)

➤ LLE is very similar to Eigenmaps. Main differences:

1) Graph Laplacean matrix is replaced by an 'affinity' graph

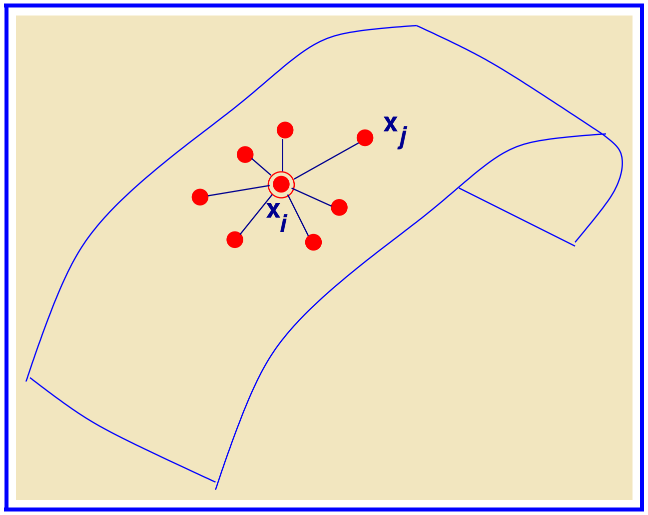
2) Objective function is changed: want to preserve graph

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

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

➤ Optimal weights computed ('local calculation') by minimizing

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



2. Mapping:

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

Minimize:

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

Solution:

$$\boxed{(I - W^\top)(I - W)u_i = \lambda_i u_i; \qquad y_i = u_i^\top.}$$

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

Implicit vs explicit mappings

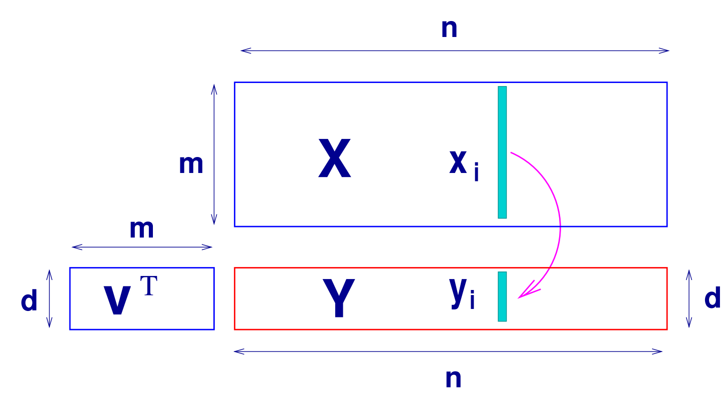
➤ Background: Principal Component Analysis (PCA)

Dimension reduction via PCA: We are given a data set $\boldsymbol{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n]$, and want a linear mapping from $\boldsymbol{X}$ to $\boldsymbol{Y}$, expressed as:

$$\boxed{\boldsymbol{Y} = \boldsymbol{V}^\top \boldsymbol{X}}$$

$$\boldsymbol{X} \in \mathbb{R}^{m \times n}; \quad \boldsymbol{V} \in \mathbb{R}^{m \times d} \quad \to \quad \boldsymbol{Y} \in \mathbb{R}^{d \times n}$$

➤ $\boldsymbol{m}$-dimens. objects ($\boldsymbol{x}_i$) 'flattened' to $\boldsymbol{d}$-dimens. space ($\boldsymbol{y}_i$)



➤ In PCA $\boldsymbol{V}$ is orthogonal ($\boldsymbol{V}^T \boldsymbol{V} = \boldsymbol{I}$)

➤ In *Principal Component Analysis* $\boldsymbol{V} \in \mathbb{R}^{m \times d}$ is computed to maximize variance of projected data:

$$\max_{\boldsymbol{V}\ ;\ \boldsymbol{V}^\top \boldsymbol{V} = \boldsymbol{I}} \quad \sum_{i=1}^{d} \left\| \boldsymbol{y}_i - \frac{1}{n} \sum_{j=1}^{n} \boldsymbol{y}_j \right\|_2^2, \quad \boldsymbol{y}_i = \boldsymbol{V}^\top \boldsymbol{x}_i.$$

➤ Leads to maximizing

$$\text{Tr}\left[\boldsymbol{V}^\top (\boldsymbol{X} - \boldsymbol{\mu} \boldsymbol{e}^\top)(\boldsymbol{X} - \boldsymbol{\mu} \boldsymbol{e}^\top)^\top \boldsymbol{V}\right], \quad \boldsymbol{\mu} = \tfrac{1}{n} \Sigma_{i=1}^{n} \boldsymbol{x}_i$$

➤ Solution $\boldsymbol{V} = \{$ dominant eigenvectors $\}$ of the covariance matrix

Explicit (linear) vs. Implicit (nonlinear) mappings:

➤ In PCA the mapping $\boldsymbol{\Phi}$ from high-dimensional space ($\mathbb{R}^m$) to low-dimensional space ($\mathbb{R}^d$) is explicitly known:

$$\boldsymbol{y = \Phi(x) \equiv V^T x}$$

➤ In Eigenmaps and LLE we only know

$$\boldsymbol{y_i = \phi(x_i), i = 1, \cdots, n}$$

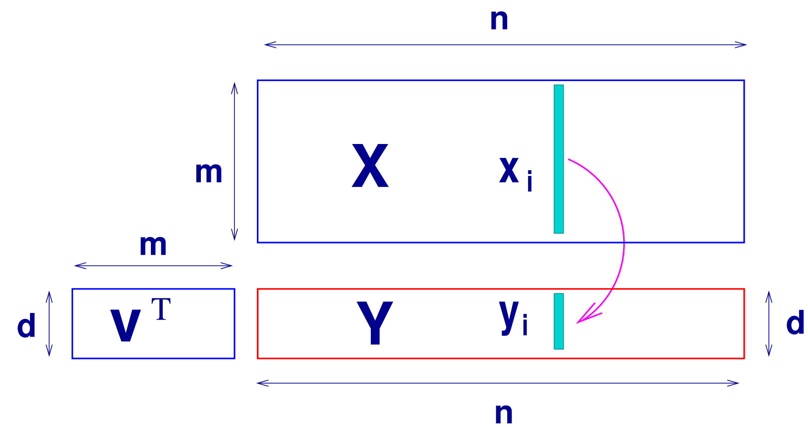
➤ Mapping $\boldsymbol{\phi}$ is now implicit: Very difficult to compute $\boldsymbol{\phi(x)}$ for an $\boldsymbol{x}$ that is not in the sample (i.e., not one of the $\boldsymbol{x_i}$'s)

➤ Inconvenient for classification. Thus is known as the "The out-of-sample extension" problem

Locally Preserving Projections (He-Niyogi-03)

➤ LPP is a linear dimensionality reduction technique

➤ Recall the setting:
Want $V \in \mathbb{R}^{m \times d}$; $Y = V^\top X$



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

➤ Optimization problem is to solve

$$\min_{\boldsymbol{Y} \in \mathbb{R}^{d\times n},\ \boldsymbol{Y}\boldsymbol{D}\boldsymbol{Y}^\top = \boldsymbol{I}} \quad \Sigma_{i,j} w_{ij} \left\| \boldsymbol{y}_i - \boldsymbol{y}_j \right\|^2, \quad \boldsymbol{Y} = \boldsymbol{V}^\top \boldsymbol{X}.$$

➤ Difference with eigenmaps: $\boldsymbol{Y}$ is an explicit projection of $\boldsymbol{X}$

➤ Solution (sort eigenvalues increasingly)

$$\boldsymbol{X}\boldsymbol{L}\boldsymbol{X}^\top \boldsymbol{v}_i = \lambda_i \boldsymbol{X}\boldsymbol{D}\boldsymbol{X}^\top \boldsymbol{v}_i \quad \boldsymbol{y}_{i,:} = \boldsymbol{v}_i^\top \boldsymbol{X}$$

➤ 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 (orthogonoal) version of LLE obtained by writing $\boldsymbol{Y}$ in the form $\boldsymbol{Y} = \boldsymbol{V}^\top \boldsymbol{X}$

➤ Same graph as LLE. Objective: preserve the affinity graph (as in LLE) *but* with the constraint $\boldsymbol{Y} = \boldsymbol{V}^\top \boldsymbol{X}$

➤ Problem solved to obtain mapping:

$$\min_{\boldsymbol{V}} \mathrm{Tr}\left[\boldsymbol{V}^\top \boldsymbol{X}(\boldsymbol{I} - \boldsymbol{W}^\top)(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{X}^\top \boldsymbol{V}\right]$$

s.t. $\boldsymbol{V}^T \boldsymbol{V} = \boldsymbol{I}$

➤ In LLE replace $\boldsymbol{V}^\top \boldsymbol{X}$ by $\boldsymbol{Y}$

More recent methods

➤ Quite a bit of recent work - e.g., methods: node2vec, DeepWalk, GraRep, ...

See the following papers:

[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 Qiongkai 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 1317, 2013, Rio de Janeiro, Brazil]

... among many others