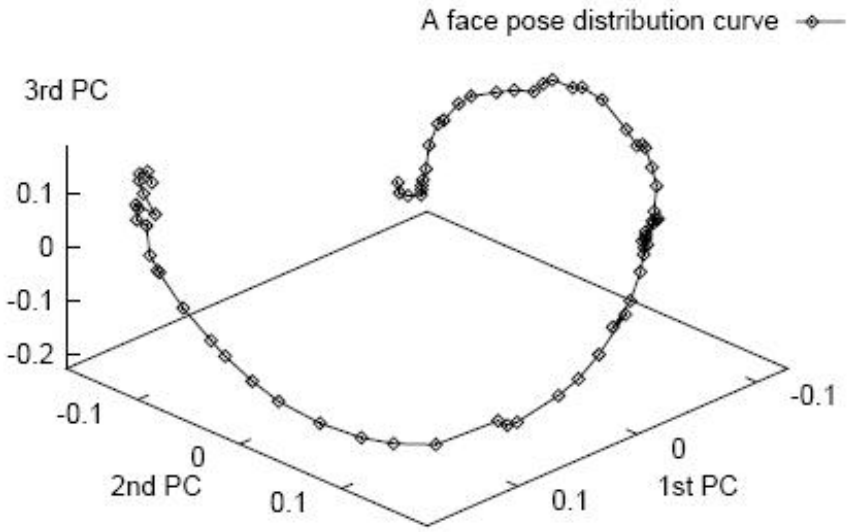
Nonlinear Methods

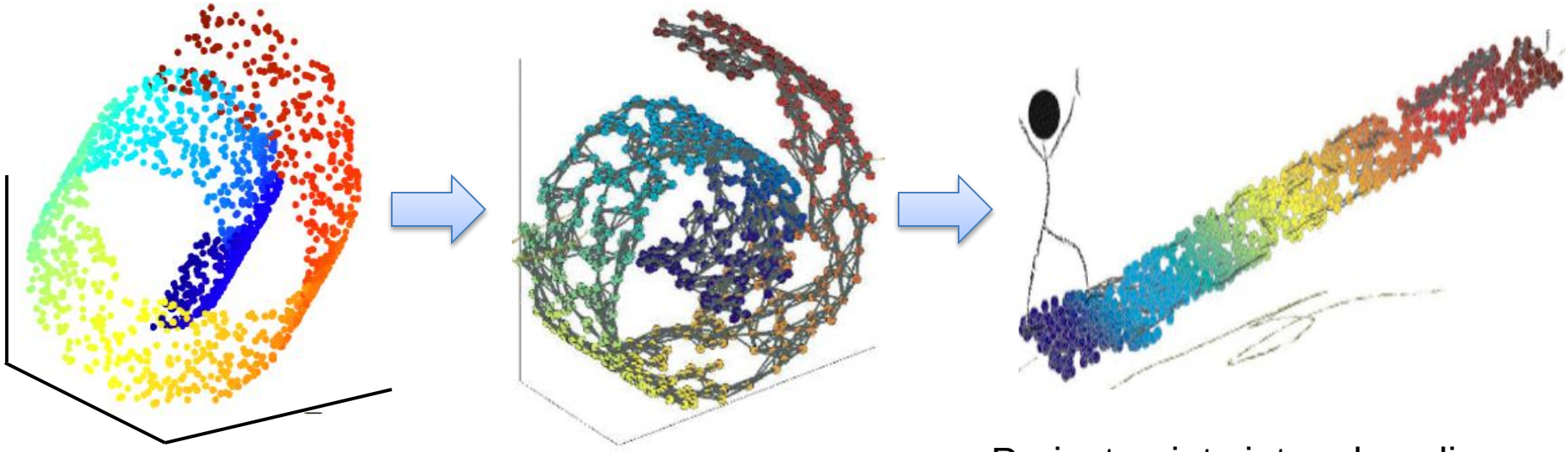
Data often lies on or near a nonlinear low-dimensional curve aka manifold.



Laplacian Eigenmaps

Linear methods – Lower-dimensional linear projection that preserves distances between **all** points

Laplacian Eigenmaps (key idea) – preserve **local** information only



Construct graph from data points (capture local information)

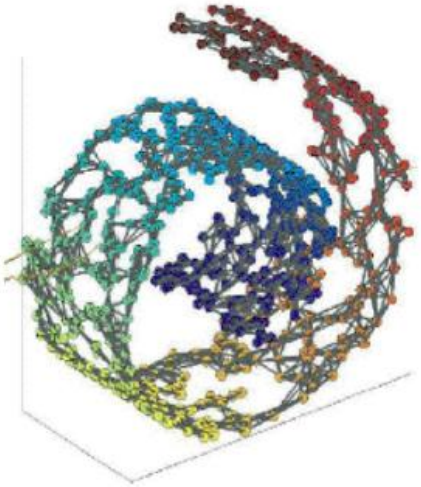
Project points into a low-dim space using “eigenvectors of the graph”

Step 1 - Graph Construction

Similarity Graphs: Model local neighborhood relations between data points

G(V,E) V – Vertices (Data points)

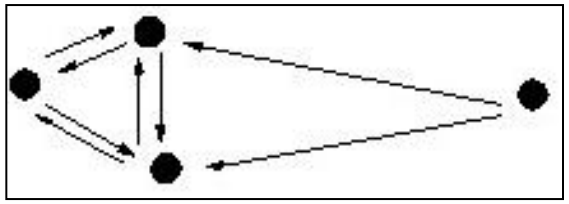
(1) E – Edge if $||x_i - x_j|| \leq \varepsilon$
ε – neighborhood graph



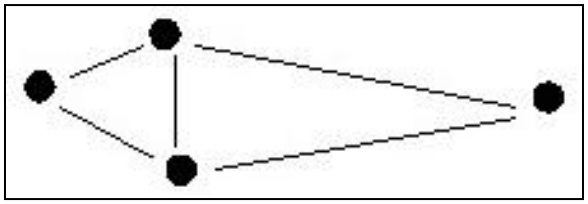
(2) E – Edge if k-NN,

yields directed graph

connect A with B if $A \rightarrow B$ OR $A \leftarrow B$ (symmetric kNN graph)
connect A with B if $A \rightarrow B$ AND $A \leftarrow B$ (mutual kNN graph)



Directed nearest neighbors



(symmetric) kNN graph

mutual kNN graph

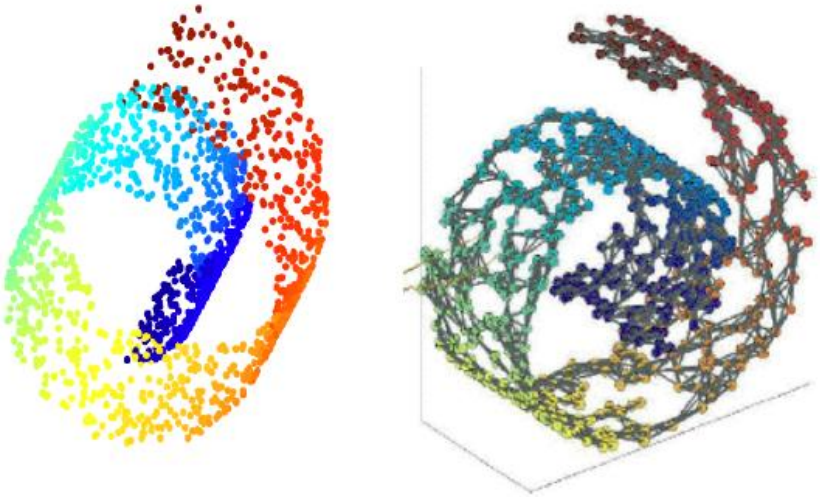
Step 1 - Graph Construction

Similarity Graphs: Model local neighborhood relations between data points

Choice of ε and k :

Chosen so that neighborhood on graphs represent neighborhoods on the manifold (no “shortcuts” connect different arms of the swiss roll)

Mostly ad-hoc



Step 1 - Graph Construction

Similarity Graphs: Model local neighborhood relations between data points

G(V,E,W) V – Vertices (Data points) E – Edges (nearest neighbors)

W - Edge weights

E.g. 1 if connected, 0 otherwise (Adjacency graph)

Gaussian kernel similarity function (aka Heat kernel)

$$W_{ij} = e^{-\frac{\|x_i - x_j\|^2}{2\sigma^2}}$$

$\sigma^2 \to \infty$ results in adjacency graph

Step 2 – Embed using Graph Laplacian

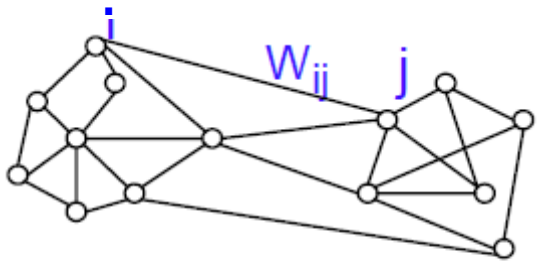
- Graph Laplacian (unnormalized version)

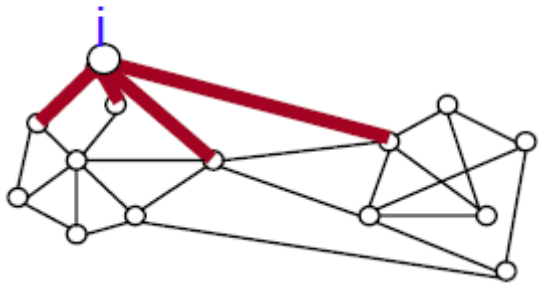
$$L = D - W$$

W – Weight matrix

D – Degree matrix = $diag(d_1, \ldots, d_n)$

$d_i = \sum_j w_{ij}$ degree of a vertex





Note: If graph is connected,

1 is an eigenvector

$$\mathbf{L1} = \begin{bmatrix} d_1 - \sum_j w_{1j} \\ d_2 - \sum_j w_{2j} \\ \ldots \\ d_n - \sum_j w_{nj} \end{bmatrix} = 0$$

Step 2 – Embed using Graph Laplacian

- Graph Laplacian (unnormalized version)

$$L = D - W$$

Solve generalized eigenvalue problem $\mathbf{Lf} = \lambda \mathbf{Df}$

Order eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_n$

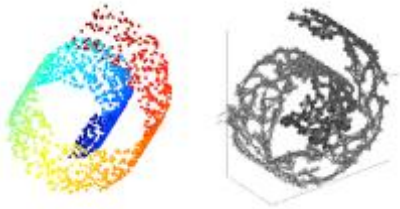
To embed data points in d-dim space, project data points onto eigenvectors associated with $\lambda_2, \lambda_3, \ldots, \lambda_{d+1}$

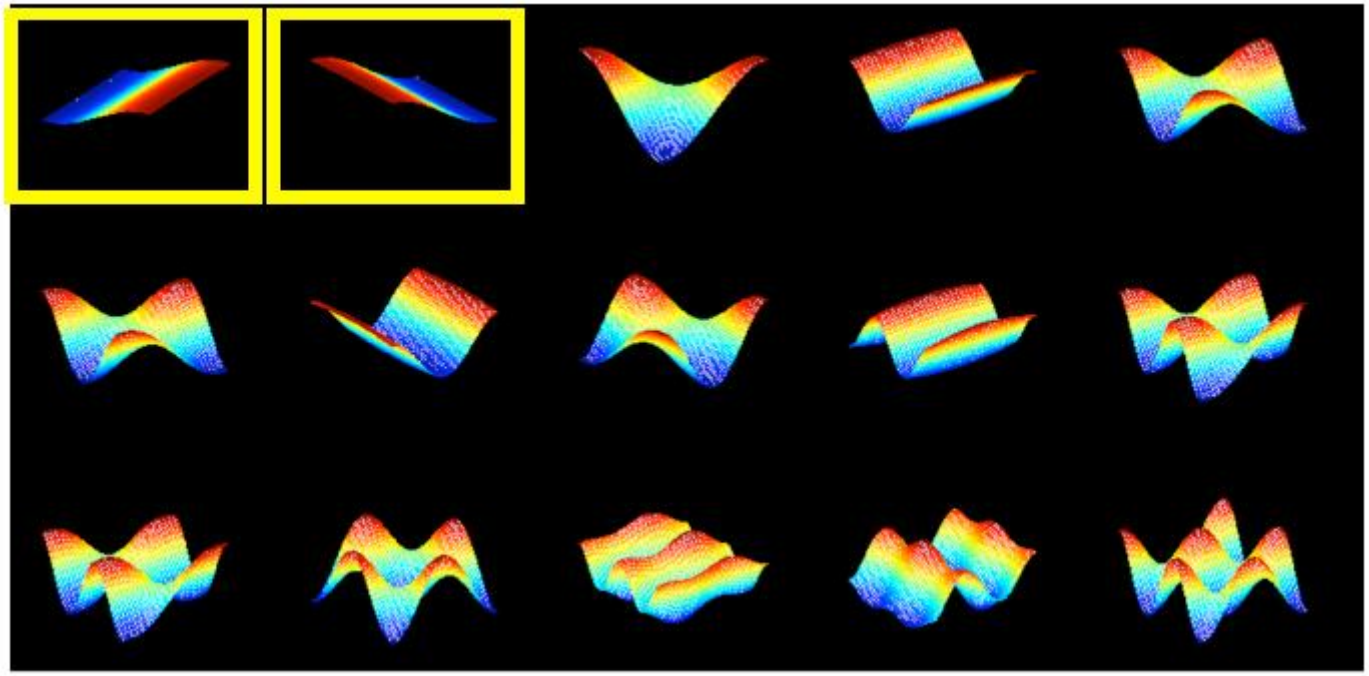
ignore 1st eigenvector – same embedding for all points

Original Representation		Transformed representation
data point		projections
x_i	→	$(f_2(i), \ldots, f_{d+1}(i))$
(D-dimensional vector)		(d-dimensional vector)

Understanding Laplacian Eigenmaps

- Best projection onto a 1-dim space
  - Put all points in one place (1st eigenvector – all 1s)
  - If two points are close on graph, their embedding is close (eigenvector values are similar – captured by smoothness of eigenvectors)





Laplacian eigenvectors of swiss roll example (for large # data points)

Step 2 – Embed using Graph Laplacian

- Justification – points connected on the graph stay as close as possible after embedding

$$\min_{\mathbf{f}} \sum_{ij} w_{ij}(\mathbf{f}_i - \mathbf{f}_j)^2 \equiv \min_{\mathbf{f}} \mathbf{f}^T \mathbf{L} \mathbf{f}$$

RHS = $\mathbf{f}^T(D-W)\,\mathbf{f} = \mathbf{f}^T D\,\mathbf{f} - \mathbf{f}^T W\,\mathbf{f} = \sum_i d_i f_i^2 - \sum_{i,j} f_i f_j w_{ij}$

$$= \frac{1}{2}\left(\sum_i (\sum_j w_{ij}) f_i^2 - 2\sum_{ij} f_i f_j w_{ij} + \sum_j (\sum_i w_{ij}) f_j^2\right)$$

$$= \frac{1}{2}\sum_{ij} w_{ij}(f_i - f_j)^2$$ **= LHS**

Step 2 – Embed using Graph Laplacian

- Justification – points connected on the graph stay as close as possible after embedding

$$\min_{\mathbf{f}} \sum_{ij} w_{ij}(\mathbf{f}_i - \mathbf{f}_j)^2 \equiv \min_{\mathbf{f}} \mathbf{f}^T \mathbf{L} \mathbf{f} \qquad s.t.\ \mathbf{f}^T \mathbf{D} \mathbf{f} = 1$$

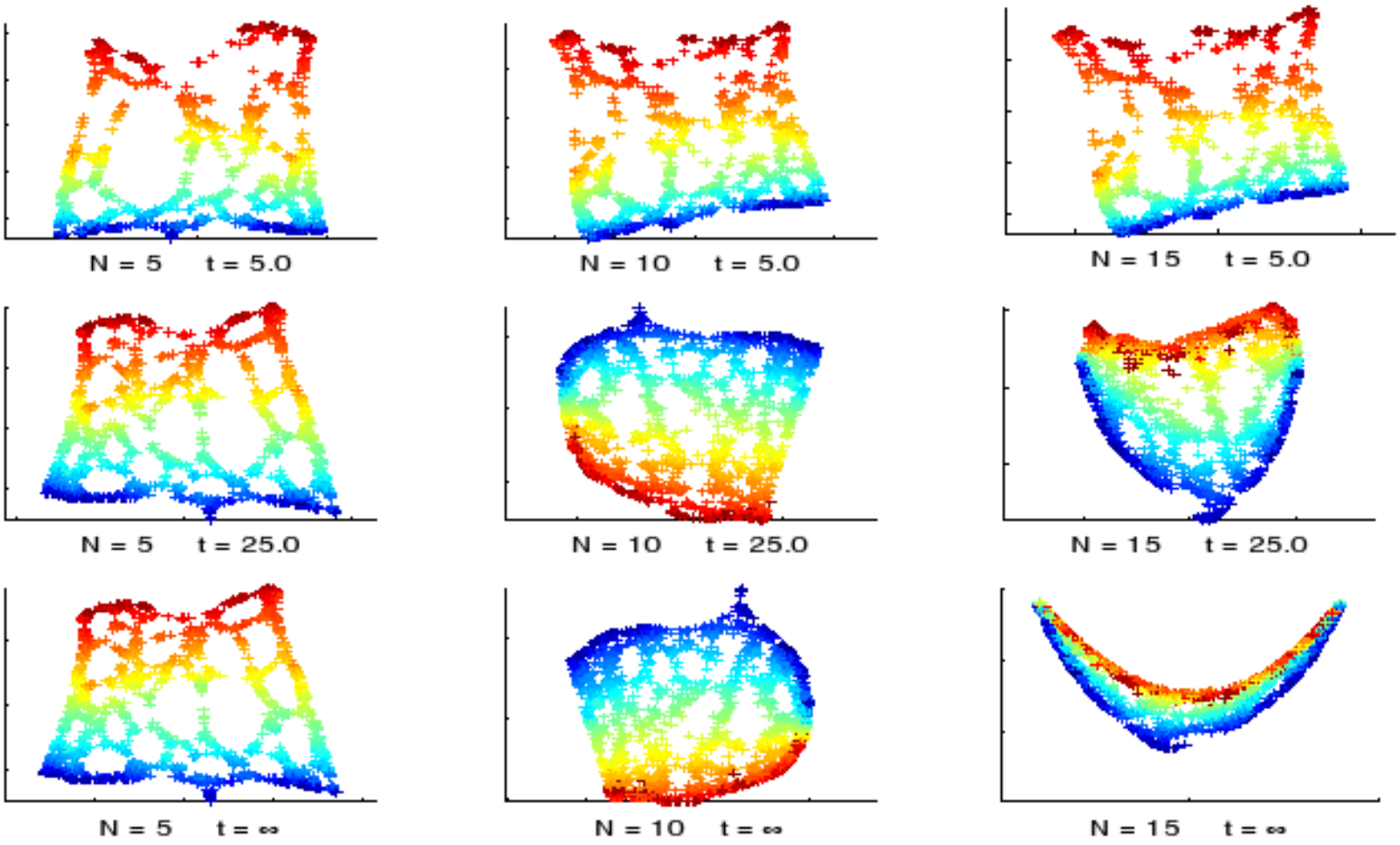
constraint removes arbitrary scaling factor in embedding

Lagrangian: $\min_{\mathbf{f}} \mathbf{f}^{\mathbf{T}} \mathbf{L} \mathbf{f} - \lambda \mathbf{f}^{\mathbf{T}} \mathbf{D} \mathbf{f}$

Wrap constraint into the objective function

$\partial / \partial \mathbf{f} = 0 \qquad (\mathbf{L} - \lambda \mathbf{D})\mathbf{f} = 0 \qquad \boxed{\mathbf{L}\mathbf{f} = \lambda \mathbf{D}\mathbf{f}}$

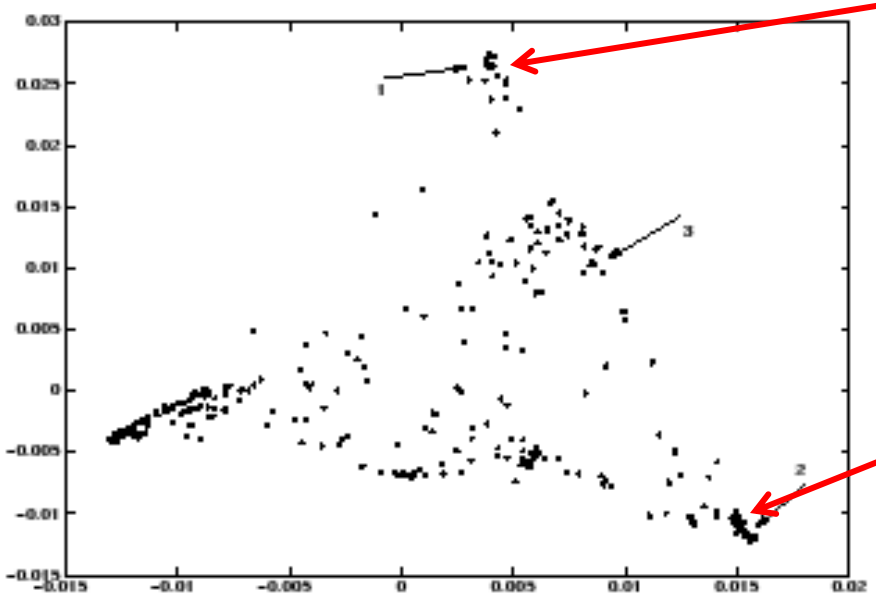
Example – Unrolling the swiss roll



N=number of nearest neighbors, t = the heat kernel parameter (Belkin & Niyogi'03)

Example – Understanding syntactic structure of words

- 300 most frequent words of Brown corpus
- Information about the frequency of its left and right neighbors (600 Dimensional space.)
- The algorithm run with N = 14, t = 1



verbs

be
find
make
say
look
get
take
give
see
do
help
become
go
know

prepositions

in
on
upon
under
along
during
at
from
than
of
against
between
toward
among

PCA vs. Laplacian Eigenmaps

PCA	Laplacian Eigenmaps
Linear embedding	Nonlinear embedding
based on largest eigenvectors of D x D correlation matrix $\Sigma = XX^T$ between features	based on smallest eigenvectors of n x n Laplacian matrix $L = D - W$ between data points
eigenvectors give latent features - to get embedding of points, project them onto the latent features	eigenvectors directly give embedding of data points
$x_i \rightarrow [v_1^T x_i, v_2^T x_i, \ldots v_d^T x_i]^T$	$x_i \rightarrow [f_2(i), \ldots, f_{d+1}(i)]^T$
D x1 d x1	D x1 d x1

Dimensionality Reduction Methods

- Feature Selection - Only a few features are relevant to the learning task

  Score features (mutual information, prediction accuracy, domain knowledge)
  Regularization

- Latent features – Some linear/nonlinear combination of features provides a more efficient representation than observed feature

  Linear: Low-dimensional linear subspace projection

  PCA (Principal Component Analysis),
  MDS (Multi Dimensional Scaling),

  Factor Analysis, ICA (Independent Component Analysis)

  Nonlinear: Low-dimensional nonlinear projection that preserves local information along the manifold

  Laplacian Eigenmaps

  ISOMAP, Kernel PCA, LLE (Local Linear Embedding),

  Many, many more …