Dimension Reduction

CS534

Why dimension reduction?

- High dimensionality – large number of features
  - E.g., documents represented by thousands of words, millions of bigrams
  - E.g., Images represented by thousands of pixels
- Redundant and irrelevant features (e.g., not all words are relevant for classifying/clustering documents)
- Difficult to interpret and visualize
- Curse of dimensionality
  - Distances to nearest and furthest neighbors will become similar as the dimension goes higher

Extract Latent Linear Features

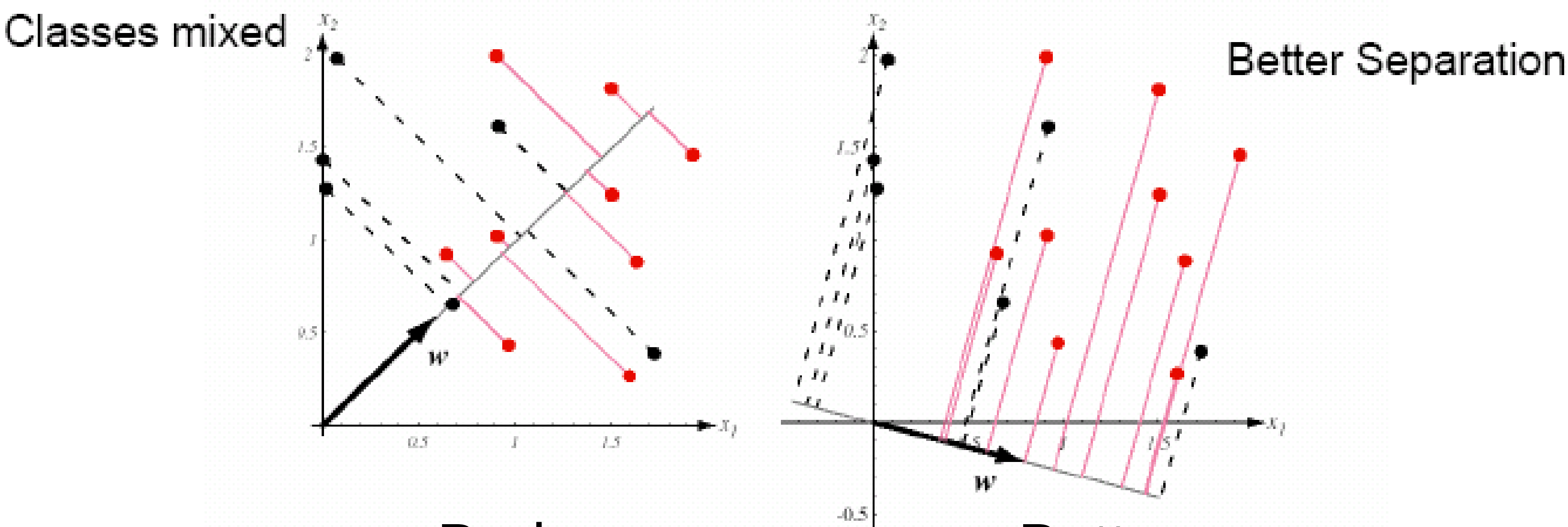
- Linearly project *n*-d data onto a *k*-d space
  - e.g., project space of 10^4 words into 3-dimensions
- There are infinitely many k-d subspaces that we can project the data into, which one should we choose
- This depends on the task at hand
  - If supervised learning: maximize the separation among classes, i.e., Linear discriminant analysis (LDA)
  - If unsupervised, we may wish to retain as much data variance as possible, i.e., principal component analysis (PCA)

LDA: linear discriminant analysis

- Also named Fisher Discriminant Analysis
- It can be viewed as
  - *a dimension reduction* method
  - a generative classifier p(x|y): Gaussian with <u>distinct $\boldsymbol{\mu}$</u> for each class but a <u>shared Σ</u>
- We will look at its **dimension reduction** interpretation and derive it that way

Intuition

- Find a projection direction to maximize the separation between classes



Bad Better

Objectives of LDA

- One way to measure separation is to look at the class means

$$\mathbf{m}_1 = \frac{1}{N_1}\sum_{\mathbf{x}\in c_1}\mathbf{x} \qquad \mathbf{m}_2 = \frac{1}{N_2}\sum_{\mathbf{x}\in c_2}\mathbf{x}$$

Original means

$$m'_1 = \frac{1}{N_1}\sum_{\mathbf{x}\in c_1}\mathbf{w}^T\mathbf{x} \qquad m'_2 = \frac{1}{N_2}\sum_{\mathbf{x}\in c_2}\mathbf{w}^T\mathbf{x}$$

Projected means

A possible goal: find the projection that maximize

$$\left|m'_1 - m'_2\right|^2 = \left|\mathbf{w}^T\mathbf{m}_1 - \mathbf{w}^T\mathbf{m}_2\right|^2$$

subject to $|\mathbf{w}|^2 = 1$?

Objectives of LDA

- Maximizing the mean separation is insufficient
- We also want the data points from the same class to be as close as possible
- This can be measured by the within-class (or interclass) ***scatter*** *(i.e., variance within the class)*

$$s_i^{\,2} = \sum_{x \in c_i} (\mathbf{w}^T \mathbf{x} - m'_i)^2$$

Total within-class scatter for projected class i, where m_i' is the mean of class i after projection

$$s_1^2 + s_2^2$$

Total within-class scatter considering both classes

Combining the two sides

- There are a number of different ways to combine these two sides of the objective
- LDA seeks to optimize the following objective:

$$\underset{\mathrm{w}}{\operatorname{argmax}} \frac{|\mathbf{m}_1' - \mathbf{m}_2'|^2}{S_1^2 + S_2^2}$$

$$|m_1' - m_2'|^2 = |w^T m_1 - w^T m_2|^2$$

$$= w^T (m_1 - m_2)(m_1 - m_2)^T w \quad \boxed{= w^T \Sigma_B w}$$

$$s_1^2 + s_2^2 = w^T (\Sigma_1 + \Sigma_2) w$$

$$\boxed{= w^T \Sigma_w w}$$

$$s_1^2 = \sum_{x \in C_1} (w^T x - w^T m_1)^2 = \sum_x w^T (x - m_1)(x - m_1)^T w$$

$$= w^T \left(\sum_x (x - m_1)(x - m_1)^T \right) w = w^T \Sigma_1 w$$

The LDA Objective

$$J(\boldsymbol{w}) = \frac{\boldsymbol{w}^T \Sigma_B \boldsymbol{w}}{\boldsymbol{w}^T \Sigma_w \boldsymbol{w}}$$

$\Sigma_B = (m_1 - m_2)(m_1 - m_2)^T$
the between-class scatter matrix

$\Sigma_w = \Sigma_1 + \Sigma_2$
the total within-class scatter matrix, where

$$\Sigma_i = \sum_{x \in C_i} (x - m_i)(x - m_i)^T$$

- The above objective is known as generalized Reyleigh quotient, and it's easy to show a w that maximizes $J(w)$ must satisfy $\Sigma_B w = \lambda \Sigma_w w$

- Noticing that $\Sigma_B w = (m_1 - m_2)(m_1 - m_2)^T w$ always take the direction of $m_1 - m_2$

Scalar

- Ignoring the scalars, this leads to:

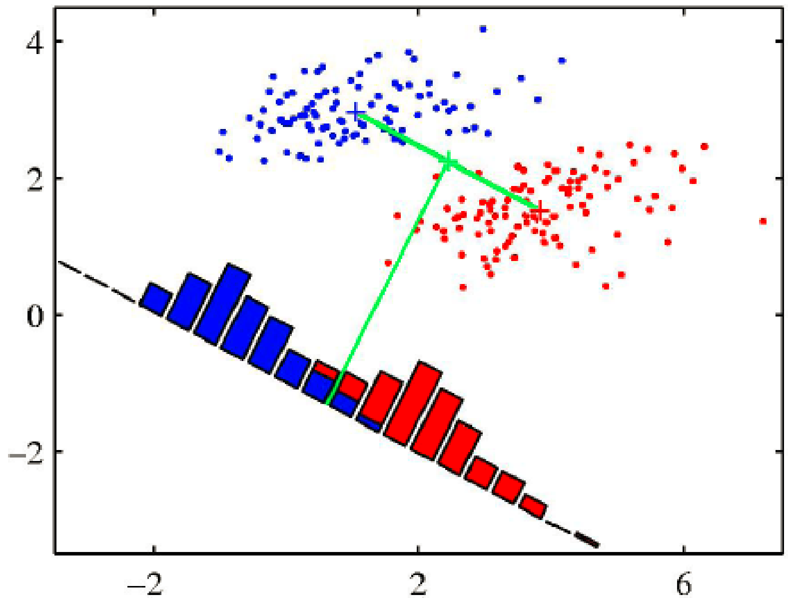
$$(m_1 - m_2) = \Sigma_w w$$

$$w = \Sigma_w^{-1}(m_1 - m_2)$$

LDA for two classes

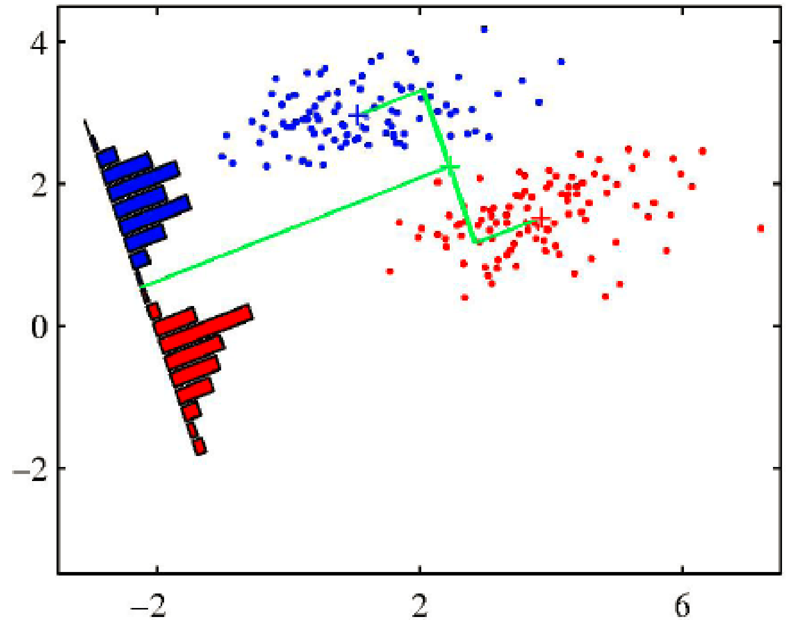
$$w = \Sigma_w^{-1}(m_1 - m_2)$$

Maximize the distance between projected mean



$w = m_1 - m_2$

Maximize $\frac{\text{between scatter}}{\text{within scatter}}$



$w = \Sigma_w^{-1}(m_1 - m_2)$

LDA for Multi-Classes

- Many variants exist. This is one of the commonly used ones:

$$\boxed{J(w) = \frac{w^T \Sigma_B w}{w^T \Sigma_w w}}$$

- Objective remains the same, with slightly different definition for between-class scatter:

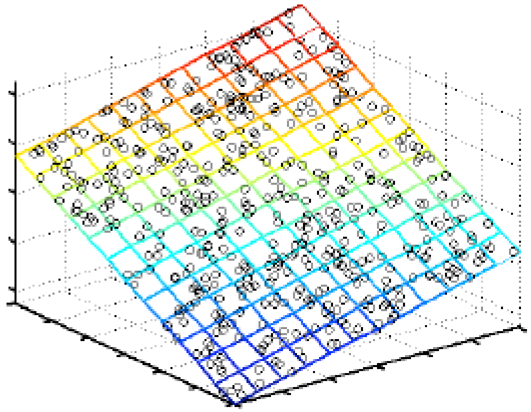
$$\Sigma_B = \frac{1}{k} \sum_{i=1}^{k} (m_i - m)(m_i - m)^T$$

m is the overall mean

- Solution: k-1 eigenvectors of $S_w^{-1} S_B$

Unsupervised Dimension Reduction

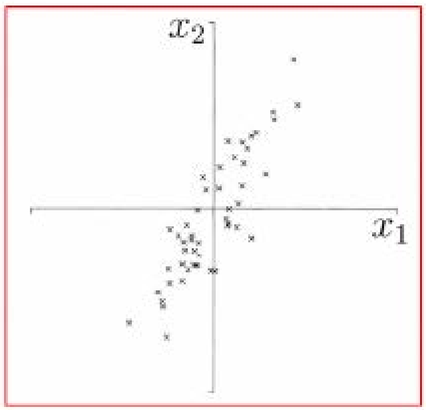
- Consider data without class labels
- Try to find a more compact representation of the data



$3d \Rightarrow 2d$

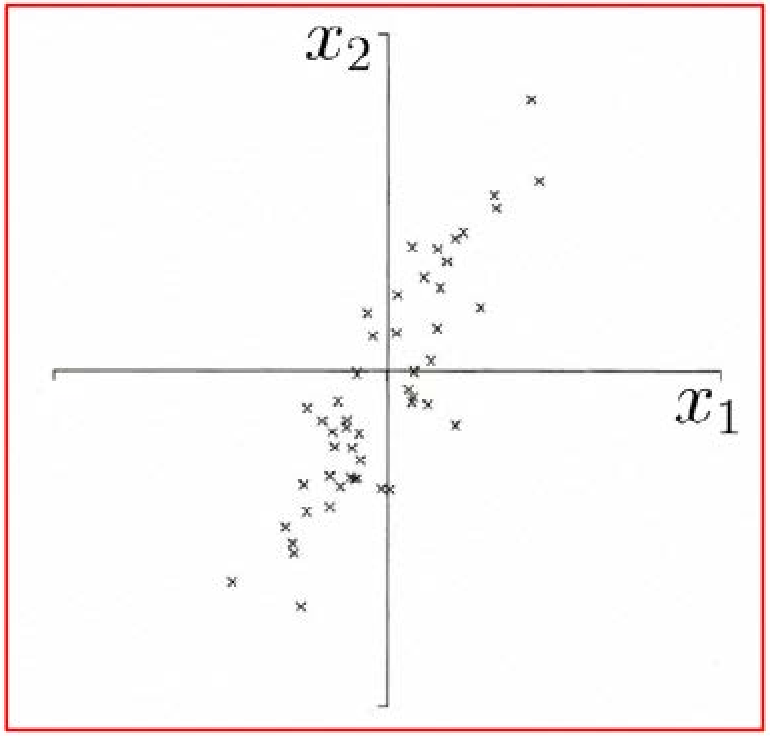
- Assume that the high dimensional data actually resides in a inherent low-dimensional space
- Additional dimensions are just random noise
- Goal is to recover these inherent dimensions and discard noise dimensions

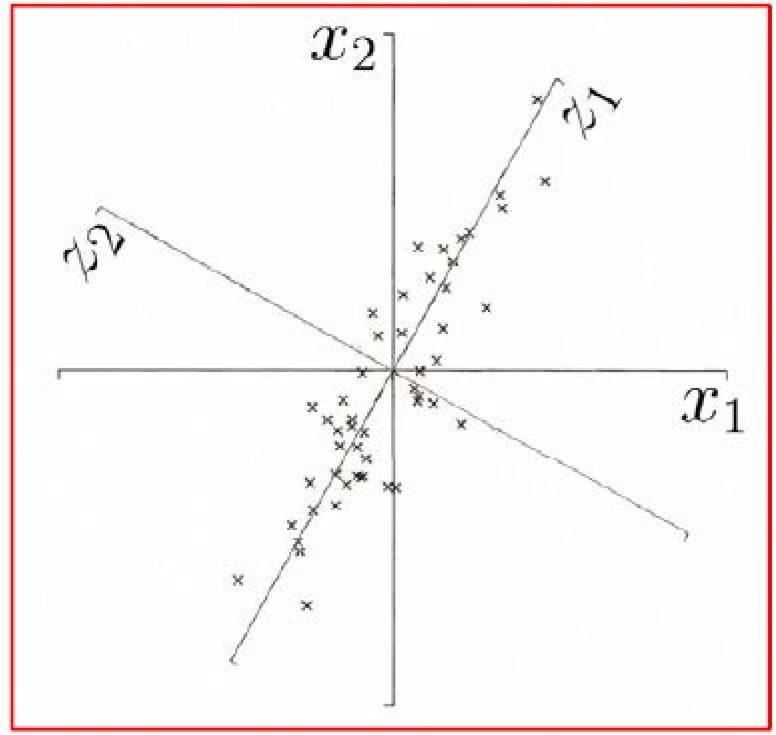
Geometric picture of principal components (PCs)



Goal: to account for the variation in the data in as few dimensions as possible

Geometric picture of principal components (PCs)





- The 1st PC is the projection direction that maximizes the variance of the projected data
- The 2nd PC is the projection direction that is orthogonal to the 1st PC and maximizes the variance …

PCA: variance maximization

- Given n data points: $x_1, \cdots, x_n$
- Consider a linear projection specified by v
- The projection of x onto v is $z = v^T x$
- The variance of the projected data is $var(z) = var(v^T x) = v^T Cov(x) v = v^T \Sigma v$
- The 1st PC maximizes the variance $v^T \Sigma v$ subject to the constraint $v^T v = 1$, where

$$\boxed{\Sigma = Cov(x) = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})^T}$$

Maximizing Variance After Projection

- Goal: $\max v^T \Sigma v$, s.t. $v^T v = 1$
- Lagrange:

$$L = v^T \Sigma v - \lambda(v^T v - 1)$$
$$\frac{\partial L}{\partial v} = 0 \Rightarrow \Sigma v = \lambda v$$

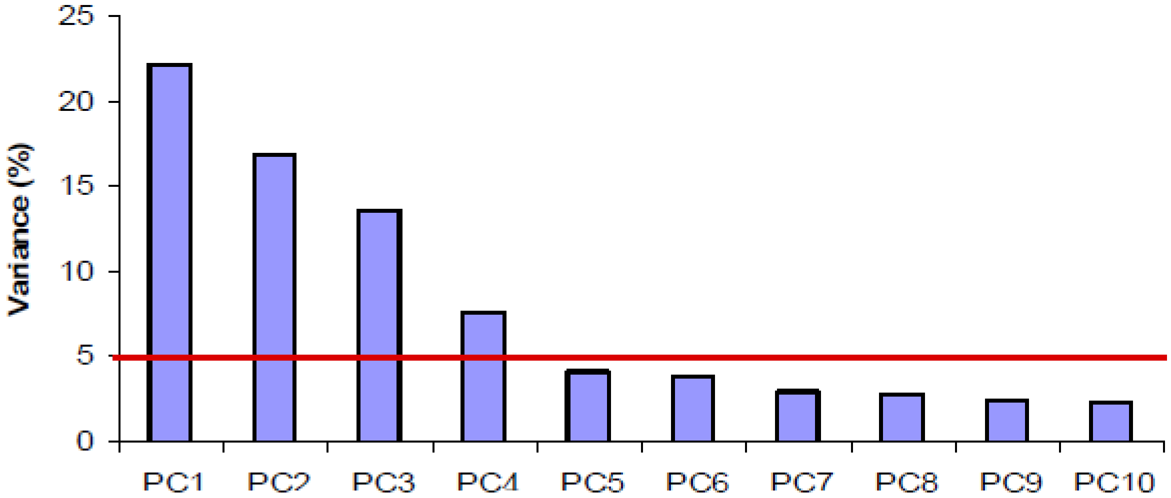
- Thus v is the eigen-vector of Σ with eigen-value λ
- Sample variance of the projected data:

$$v^T \Sigma v = \lambda v^T v = \lambda$$

- The eigen-values λ = the amount of variance captured by each eigen-vector
- Sort all eigen vectors by λ in decreasing order:
  - 1st PC = The first eigen-vector, the projected variance = λ_1
  - 2nd PC = the second eigen-vector, the projected variance = λ_2
  - …

Dimension Reduction Using PCA

- Calculate the covariance matrix of the data Σ
- Calculate the eigen-vectors/eigen-values of Σ
- Rank the eigen-values in decreasing order
- Select a fixed number of eigen-vectors, or just enough to retain a fixed percentage of the variance, (e.g., 75%, the smallest d such that $\frac{\sum_{i=1}^{d} \lambda_i}{\sum_i \lambda_i} \geq 75\%$)



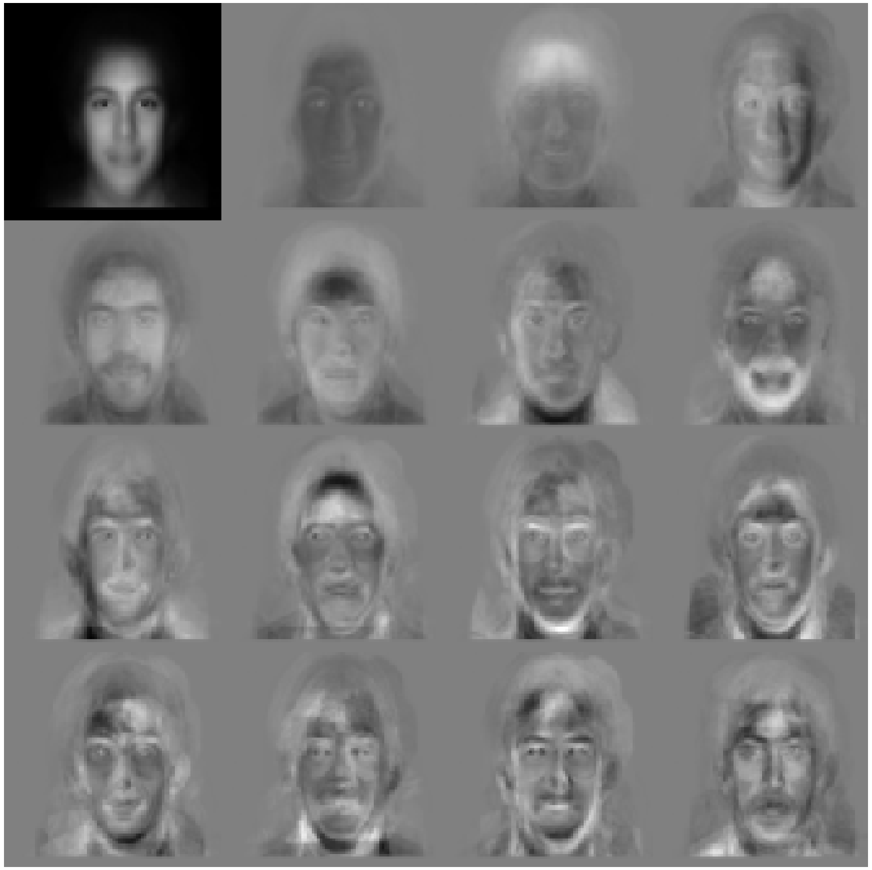
You might loose some info. But if the eigen-values are small, not much is lost.

Example: Face Recognition

- A small image of size 256 x 128 is described by n = 256x128 = 32768 dimensions
- Each face image lies somewhere in this high-dimensional space
- Images of faces are generally similar in overall configuration, thus
  – They cannot be randomly distributed in this space
  – We should be able to describe them in a much low-dimensional space

PCA for Face Images: Eigenfaces

- Database of 128 carefully-aligned faces.
- Here are the mean and the first 15 eigenvectors.
- Each eigenvector can be shown as an image
- These images are face-like, thus called eigenface

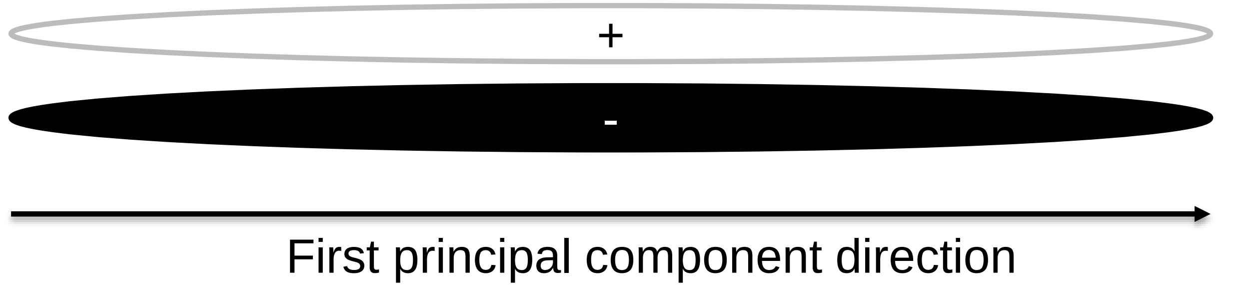


Face Recognition in Eigenface space
(Turk and Pentland 1991)

- Nearest Neighbor classifier in the eigenface space
- Training set always contains 16 face images of 16 people, all taken under the same conditions of lighting, head orientation, and image size
- Accuracy:
  - variation in lighting: 96%
  - variation in orientation: 85%
  - variation in image size: 64%

PCA: A Useful Preprocessing Step

- Helps to reduce the computational complexity
- Helps supervised learning
  - Reduced dimension $\Rightarrow$ simpler hypothesis space
  - Reduced dimension $\Rightarrow$ less over-fitting
- PCA can also be seen as noise reduction
- May loose important information when the small variance directions contain useful information:
  - E.g. for classification

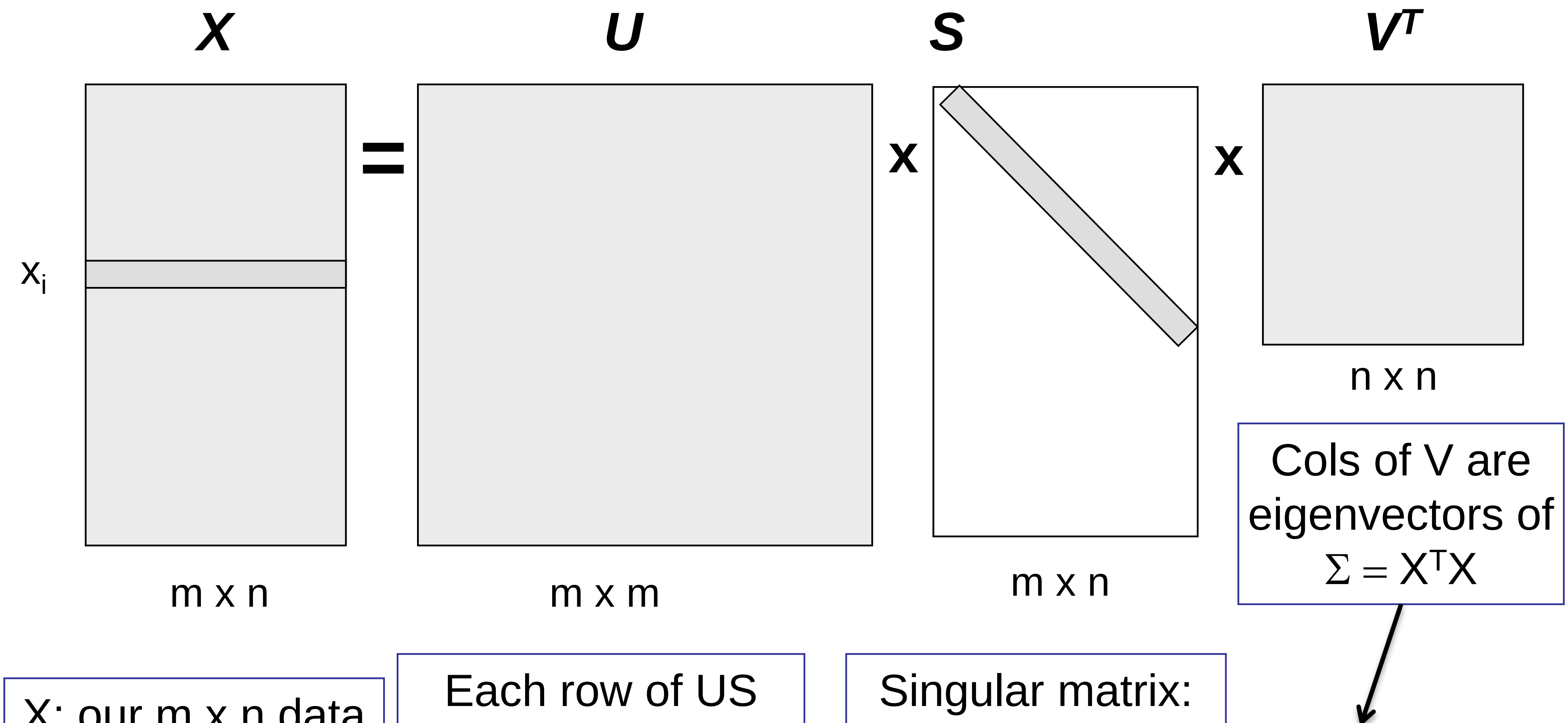


Practical Issue: Scaling Up (Optional)

- Covariance of the image data is BIG!
  - size of $\Sigma = 32768 \times 32768$
  - finding eigenvector of such a matrix is slow.
- SVD comes to rescue!
  - Can be used to compute principal components
  - Efficient implementations available

Singular Value Decomposition: $X=USV^T$

(Optional)



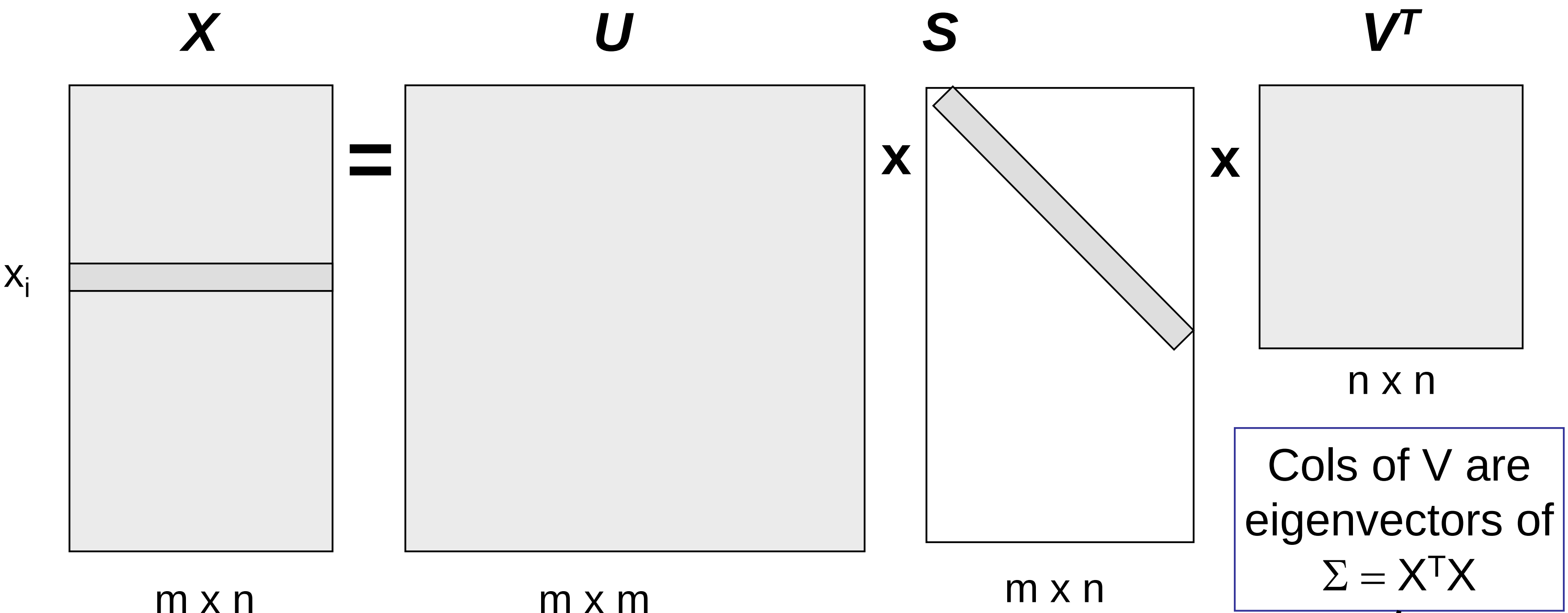
X: our m x n data matrix, one row per data point

Each row of US gives coordinates of a data point in the projected space

Singular matrix: a diagonal matrix, S_i^2 is Σ's i-th eigenvalue

Singular Value Decomposition: $X=USV^T$

(Optional)



X: our m x n data matrix, one row per data point

Each row of US gives coordinates of a data point in the projected space

Singular matrix: a rectangle diagonal matrix, S_i^2 is Σ's i-th eigenvalue

If X is centered, then cols of V are the principal components

SVD for PCA (Optional)

- Create centered data matrix X s.t. $mean(X) = 0_d$

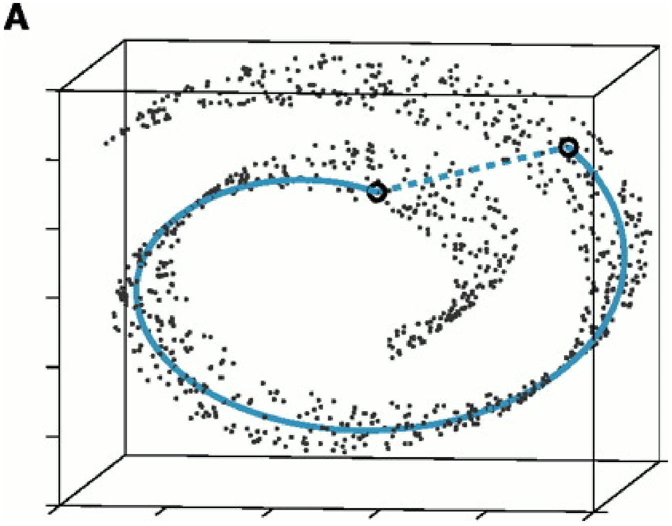
- Solve SVD: $X = USV^T$

- Columns of V are the eigenvectors of Σ sorted from largest to smallest eigenvalues – select the first *k* columns as our principal components

Nonlinear Dimension Reduction

Nonlinear Methods

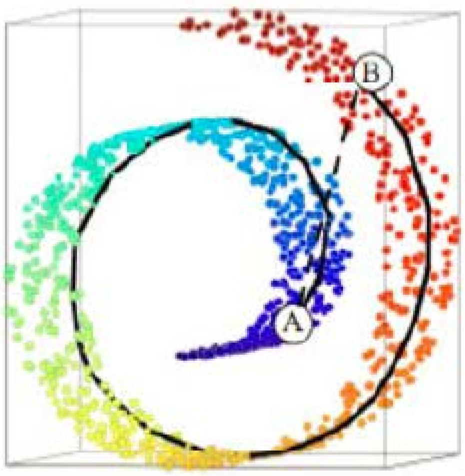
- Data often lies on or near a nonlinear low-dimensional curve
- We call such low dimension structure manifolds



Swiss roll data

ISOMAP: Isometric Feature Mapping
(Tenenbaum et al. 2000)

- A nonlinear method for dimensionality reduction
- Preserves the global, nonlinear geometry of the data by preserving the geodesic distances
- Geodesic: originally geodesic means the shortest route between two points on the surface of the manifold



ISOMAP

- Two steps
  1. Approximate the geodesic distance between every pair of points in the data
     - The manifold is locally linear
     - Euclidean distance works well for points that are close enough
     - For the points that are far apart, their geodesic distance can be approximated by summing up local Euclidean distances

  2. Find a Euclidean mapping of the data that preserves the geodesic distance

Geodesic Distance

- Construct a graph by
  - Connecting i and j if
    - $d(i, j) < \varepsilon$ (ε-isomap) or
    - i is one of j's k nearest neighbors (k-isomap)
  - Set the edge weight equal d(i, j) – Euclidean distance
- Compute the Geodesic distance between any two points as the ***shortest path distance***

Compute the Low-Dimensional Mapping

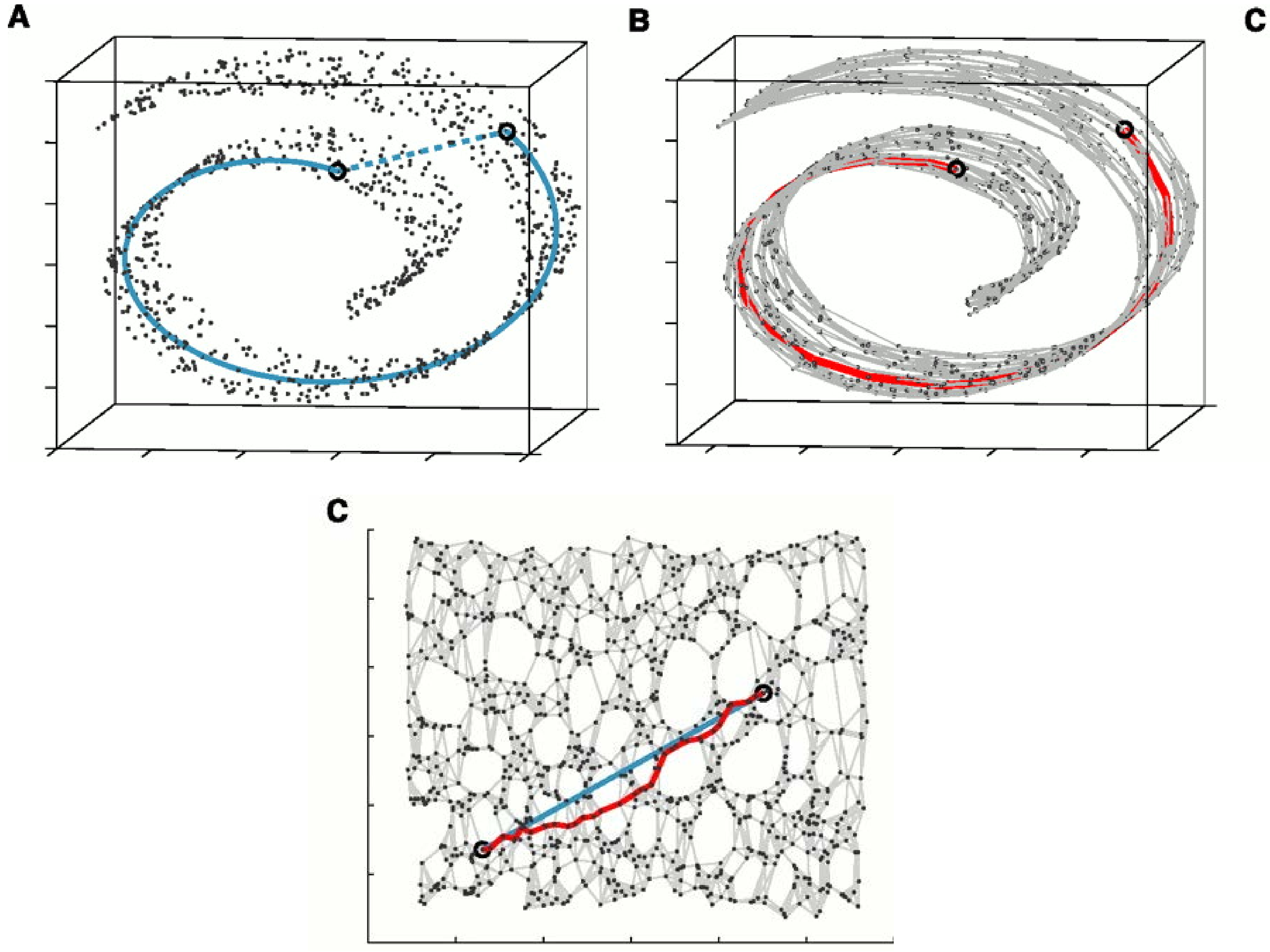
- We can use **Multi-Dimensional scaling** (MDS), a class of statistical techniques that

Given:

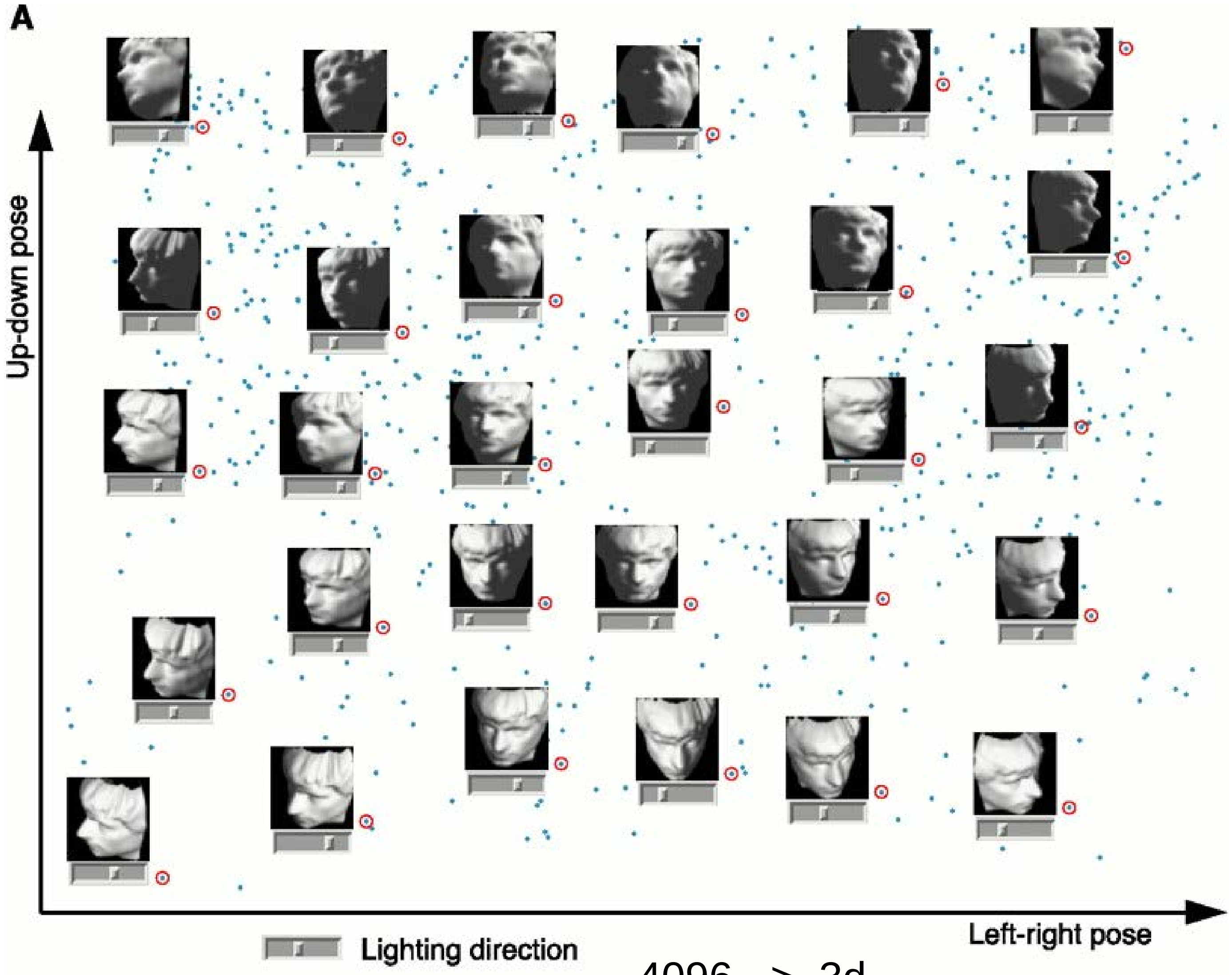
n x *n* matrix of dissimilarities between *n* objects

Outputs: a coordinate configuration of the data in a low-dimensional space R^d whose Euclidean distances closely match given dissimilarities.

ISOMAP on Swiss Roll Data

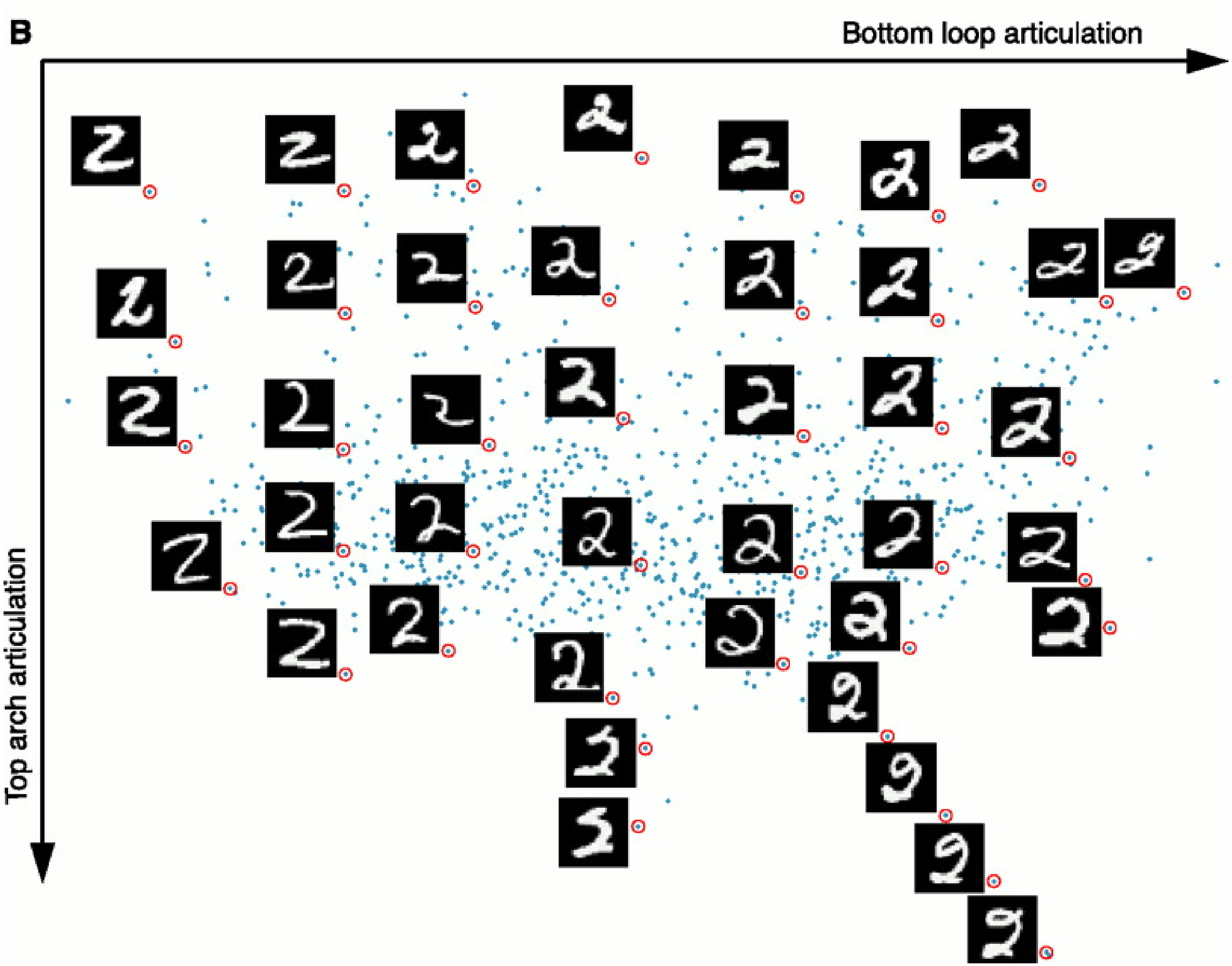


ISOMAP Examples



4096 -> 3d

ISOMAP Examples



Summary of ISOMAP

- Preserve global nonlinear structure by approximating geodesic distance
- Sensitive to the parameters used in the graph construction
  - K: for k-isomap
  - ϵ: for ϵ-isomap
- If data is overly sparse, the shortest path approximation to the geodesic distances can be poor