In The Name of Allah

Digital Media Laboratory
Sharif University of Technology

Statistical Pattern Recognition

Feature Extraction

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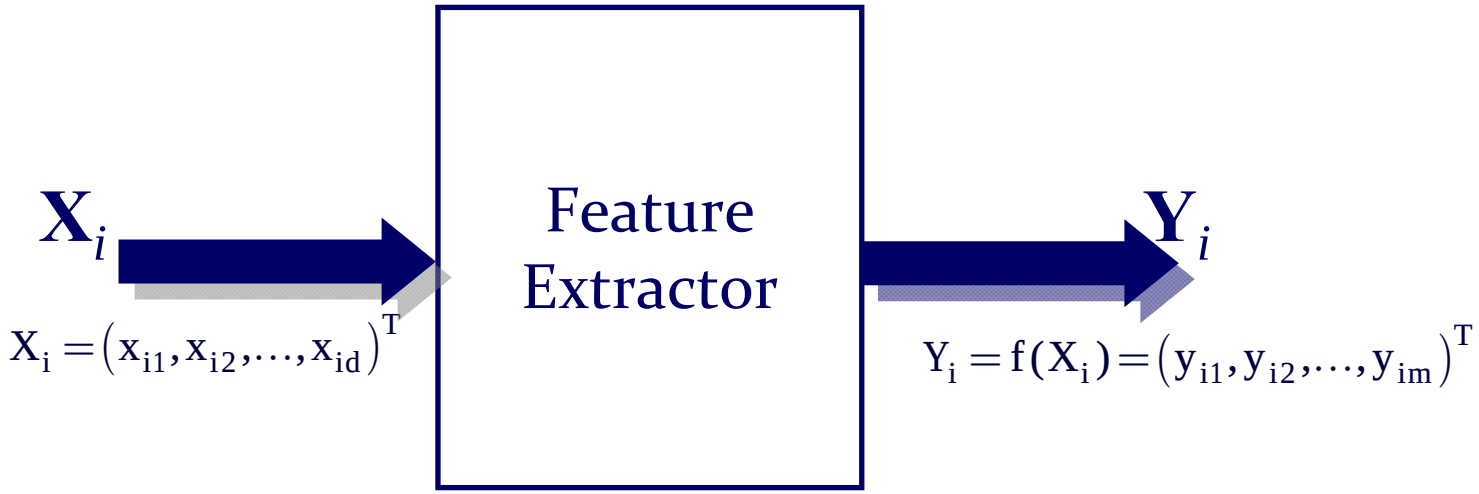
Agenda

- **Dimensionality Reduction**
- **Feature Extraction**
  - **Feature Extraction Approaches**
- **Linear Methods**
  - **Principal Component Analysis (PCA)**
  - **Linear Discriminant Analysis (LDA)**
    - Multiple Discriminant Analysis (MDA)
  - **PCA vs LDA**
  - **Linear Methods Drawbacks**
- **Nonlinear Dimensionality Reduction**
  - **ISOMAP**
  - **Local Linear Embedding (LLE)**
  - **ISOMAP vs. LLE**

Dimensionality Reduction

- **Feature Selection (discussed previous time)**
  - **Select the best subset from a given feature set**
- **Feature Extraction (will be discussed today)**
  - **Create new features based on the original feature set**
  - **Transforms are usually involved**

Feature Extraction



- **For example:**

$$X = [x_1 \quad x_2 \quad x_3 \quad x_4]^T \Rightarrow Y = \begin{bmatrix} x_1 + x_2 \\ x_3 + x_4 \end{bmatrix}$$

Feature Extraction Approaches

- **The best f(x) is most likely a non-linear function, but linear functions are easier to find though**
- **Linear Approaches**
  - **Principal Component Analysis (PCA) → will be discussed**
    - or Karhunen-Loeve Expansion (KLE)
  - **Linear Discriminant Analysis (LDA) → will be discussed**
  - **Multiple Discriminant Analysis (MDA) → will be discussed**
  - **Independent Component Analysis (ICA)**
  - **Project Pursuit**
  - **Factor Analysis**
  - **Multidimensional Scaling (MDS)**

Feature Extraction Approaches

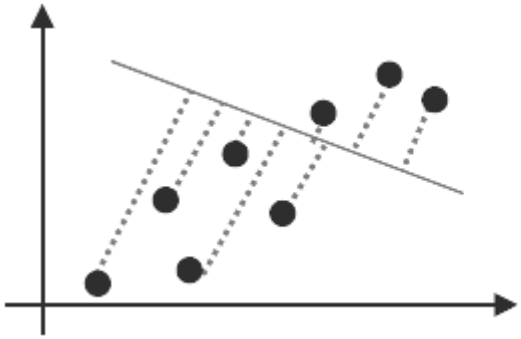
- **Non-linear approach**
  - **Kernel PCA**
  - **ISOMAP**
  - **Locally Linear Embedding (LLE)**
- **Neural Networks**
  - **Feed-Forward Neural Networks**
    - High-dimensional data can be converted to low-dimensional codes by training a multilayer neural network with a small central layer to reconstruct high-dimensional input vectors.
    - Ref: Hinton, G. E. and Salakhutdinov, R. R. (2006) "*Reducing the dimensionality of data with neural networks.*" Science, Vol. 313. no. 5786, pp. 504 - 507, 28 July 2006.
  - **Self-Organizing Map**
    - A Clustering Approach to Dimensionality Reduction
    - Transform data to lower dimensional lattice

Feature Extraction Approaches

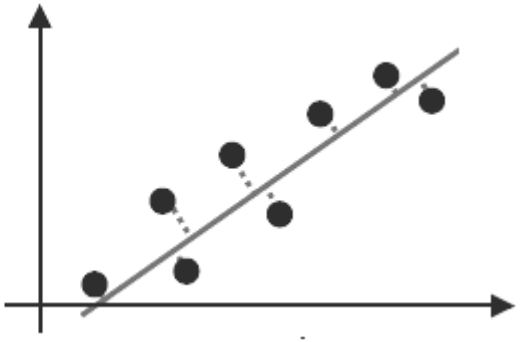
- **Another view**
  - **Unsupervised approaches**
    - PCA
    - LLE
    - Self organized map
  - **Supervised approaches**
    - LDA
    - MDA

Principal Component Analysis (PCA)

- **Main idea:**
  - **seek most accurate data representation in a lower dimensional space**
- **Example in 2-D**
  - **Project data to 1-D subspace (a line) which minimize the projection error**
    - Notice that the good line to use for projection lies is in the direction of largest variance



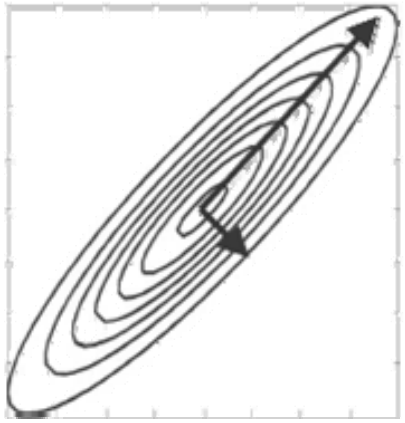
large projection error, bad line to project to



small projection errors, good line to project to

Principal Component Analysis (PCA)

- **Preserves largest variances in the data**
  - **What is the direction of largest variance in data?**
    - Hint: If x has multivariate Gaussian distribution $N(\mu, \Sigma)$, direction of largest variance is given by eigenvector corresponding to the largest eigenvalue of Σ

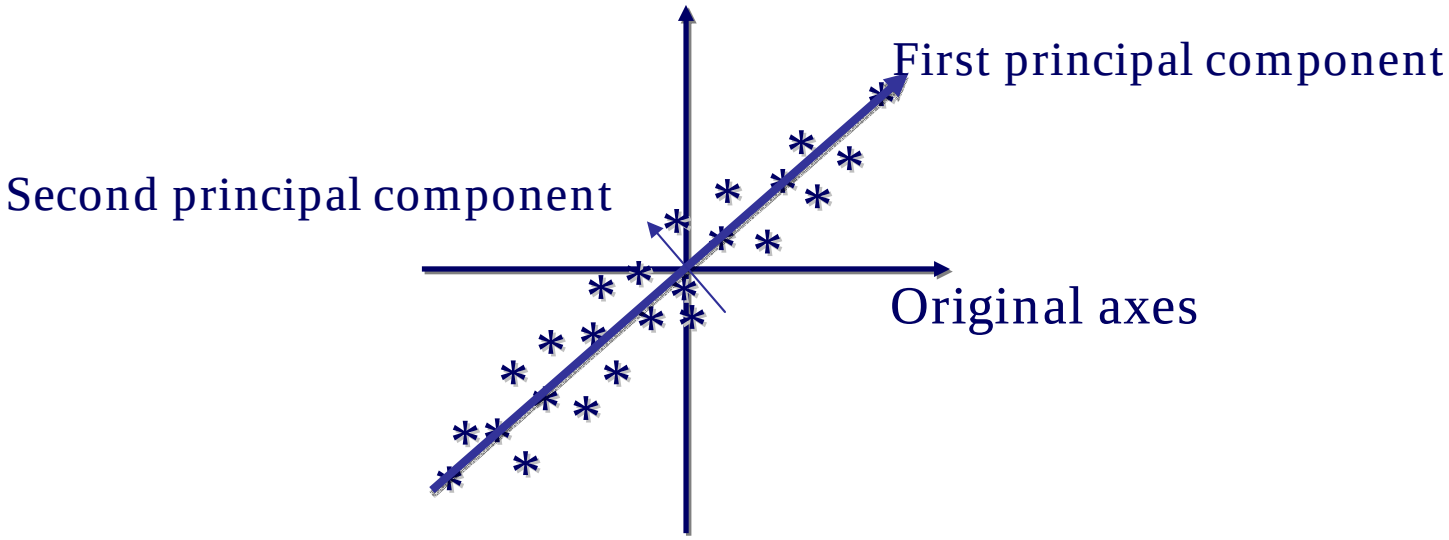


Principal Component Analysis (PCA)

- **We can derive following algorithm (will be discussed in next slides)**
  - **PCA algorithm:**
    - X ← input *nxd* data matrix (each row a d-dimensional sample)
    - X ← subtract mean of X, from each row of X
      - **The new data has zero mean (normalized data)**
    - Σ ← covariance matrix of X
    - Find eigenvectors and eigenvalues of Σ
    - C ← the M eigenvectors with largest eigenvalues, each in a column (a *dxM* matrix) - value of eigenvalues gives importance of each component
    - Y (transformed data) ← transform X using C *(Y = X * C)*
      - **The number of new dimensional is M *(M<<d)***
    - Q: How much is the data energy loss?

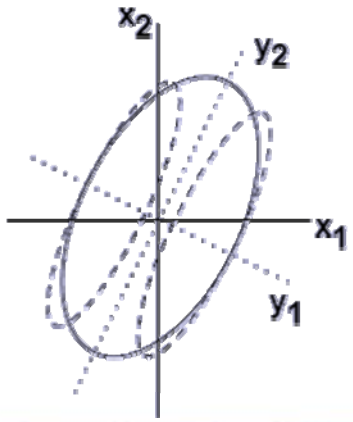
Principal Component Analysis (PCA)

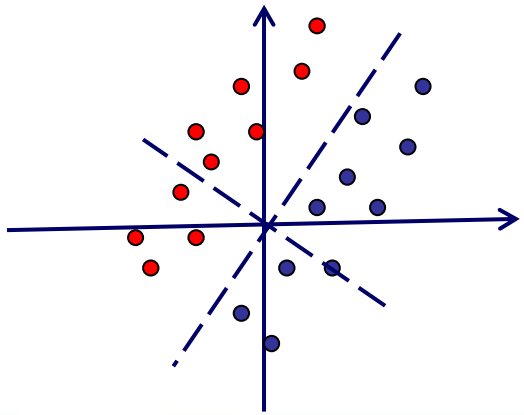
- **Illustration:**



Principal Component Analysis (PCA)

- **Drawbacks**
  - **PCA was designed for accurate data representation, not for data classification**
    - Preserves as much variance in data as possible
    - If directions of maximum variance is important for classification, will work (give an example?)
  - **However the direction of maximum variance may be useless for classification**





PCA Derivation

- **Can be considered in many viewpoints:**
  - **Minimum Error of Projection**
  - **Maximum Information gain**
  - **Or by Neural Nets**
- **The result would be the same!**

PCA Derivation

- We want to find the most accurate representation of d-dimensional data $D=\{x_1,x_2,\ldots,x_n\}$ in some subspace W which has dimension $k < d$
- Let $\{e_1,e_2,\ldots,e_k\}$ be the orthonormal basis for W. Any vector in W can be written as

$$\sum_{i=1}^{k} \alpha_i e_i$$

e_is are d-dimensional vectors in original space.

- Thus x_1 will be represented by some vectors in W: $x_1 \approx \sum_{i=1}^{k} \alpha_{1i} e_i$
- Error of this representation is $error = \left\| x_1 - \sum_{i=1}^{k} \alpha_{1i} e_i \right\|^2$
- Then, the total error is:

$$\begin{aligned} J &= \sum_{j=1}^{n} \left\| x_j - \sum_{i=1}^{k} \alpha_{ji} e_i \right\|^2 \\ &= \sum_{j=1}^{n} \left\| x_j \right\|^2 - 2\sum_{j=1}^{n} x_j^t \left(\sum_{i=1}^{k} \alpha_{ji} e_i \right) + \sum_{j=1}^{n} \sum_{i=1}^{k} \alpha_{ji}^2 \\ &= \sum_{j=1}^{n} \left\| x_j \right\|^2 - 2\sum_{j=1}^{n} \sum_{i=1}^{k} \alpha_{ji} x_j^t e_i + \sum_{j=1}^{n} \sum_{i=1}^{k} \alpha_{ji}^2 \end{aligned}$$

PCA Derivation

- **To minimize J, need to take partial derivatives and also enforce constraint that $\{e_1,e_2,\ldots,e_k\}$ are orthogonal.**

$$J(e_1,\ldots,e_k,\alpha_{11},\ldots,\alpha_{nk}) = \sum_{j=1}^{n}\left\|x_j\right\|^2 - 2\sum_{j=1}^{n}\sum_{i=1}^{k}\alpha_{ji}x_j^t e_i + \sum_{j=1}^{n}\sum_{i=1}^{k}\alpha_{ji}^2$$

- **First take partial derivatives with respect to α_{ml}**

$$\frac{\partial}{\partial\alpha_{ml}}J(e_1,\ldots,e_k,\alpha_{11},\ldots,\alpha_{nk}) = -2x_m^t e_l + 2\alpha_{ml}$$

- **Thus the optimal value for α_{ml} is** $-2x_m^t e_l + 2\alpha_{ml} = 0 \Rightarrow \alpha_{ml} = x_m^t e_l$

- **Plug the optimal value for α_{ml} back into J**

$$\begin{aligned}
J(e_1,\ldots,e_k) &= \sum_{j=1}^{n}\left\|x_j\right\|^2 - 2\sum_{j=1}^{n}\sum_{i=1}^{k}(x_j^t e_i)x_j^t e_i + \sum_{j=1}^{n}\sum_{i=1}^{k}(x_j^t e_i)^2 \\
&= \sum_{j=1}^{n}\left\|x_j\right\|^2 - \sum_{j=1}^{n}\sum_{i=1}^{k}(x_j^t e_i)^2 \\
&= \sum_{j=1}^{n}\left\|x_j\right\|^2 - \sum_{i=1}^{k}e_i^t\left(\sum_{j=1}^{n}(x_j x_j^t)\right)e_i \\
&= \sum_{j=1}^{n}\left\|x_j\right\|^2 - \sum_{i=1}^{k}e_i^t S e_i \;;\quad S = \sum_{j=1}^{n}x_j x_j^t
\end{aligned}$$

PCA Derivation

- **The J is:** $J(e_1,\ldots,e_k) = \sum_{j=1}^{n} \left\| x_j \right\|^2 - \sum_{i=1}^{k} e_i^t S e_i$
- **Minimizing J is equivalent to maximizing** $J' = \sum_{i=1}^{k} e_i^t S e_i$
- **Then, the new problem is maximizing J' with enforce constraints $e_i^t e_i = 1$ for all i**
- **Use the method of Lagrange multipliers, incorporate the constraints with undetermined $\lambda_1, \ldots, \lambda_k$. Need to maximize new function u**

$$u(e_1,\ldots,e_k) = \sum_{i=1}^{k} e_i^t S e_i - \sum_{j=1}^{k} \lambda_j \left(e_j^t e_j - 1 \right)$$

- **Compute the partial derivatives with respect to e_m**

$$\frac{\partial}{\partial e_m} u(e_1,\ldots,e_k) = 2Se_m - 2\lambda_m e_m = 0 \;\Rightarrow\; Se_m = \lambda_m e_m$$

  - **Thus λ_m and e_m are eigenvalues and eigenvectors of scatter matrix S**

PCA Derivation

- **Let's plug e_m back into J and use $Se_m = \lambda_m e_m$**

$$J(e_1,\ldots,e_k) = \sum_{j=1}^{n} \|x_j\|^2 - \sum_{i=1}^{k} e_i^t S e_i$$
$$= \sum_{j=1}^{n} \|x_j\|^2 - \sum_{i=1}^{k} \lambda_i \|e_i\|^2 = \sum_{j=1}^{n} \|x_j\|^2 - \sum_{i=1}^{k} \lambda_i$$

- **The first part of this equation is constant, Thus, to minimize J take for the basis of W the k eigenvectors of S corresponding to the k largest eigenvalues**
  - **The larger the eigenvalue of S, the larger is the variance in the direction of corresponding eigenvector**
  - **This result is exactly what we expected: project x into subspace of dimension k which has the largest variance**
  - **This is very intuitive: restrict attention to directions where the scatter is the greatest**
  - **Thus PCA can be thought of as finding new orthogonal basis by rotating the old axis until the directions of maximum variance are found**

Kernel PCA

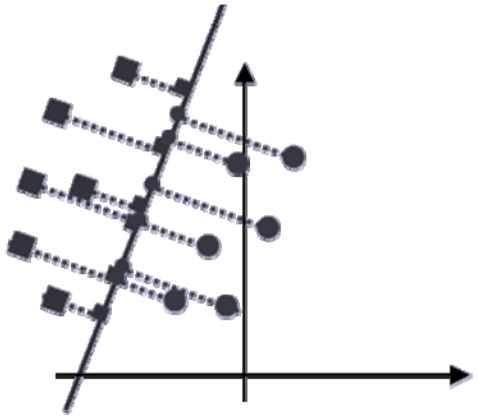
- Assumption behind PCA is that the data points x are multivariate Gaussian
  - Often this assumption does not hold
- However, it may still be possible that a transformation $\phi(x)$ is still Gaussian, then we can perform PCA in the space of $\phi(x)$
- Kernel PCA performs this PCA; however, because of "kernel trick," it never computes the mapping $\phi(x)$ explicitly!
- Kernel methods will be discussed later!

Linear Discriminant Analysis (LDA)

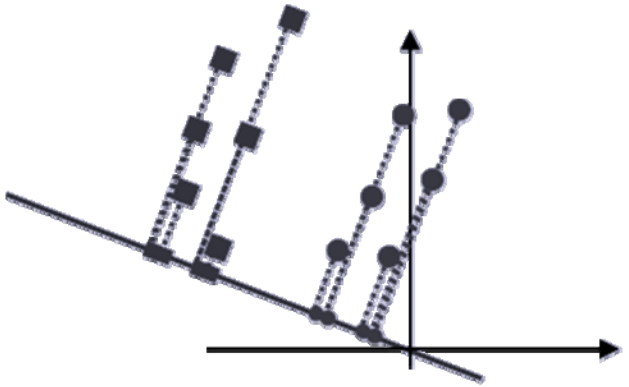
- **LDA, also known as Fisher Discriminant Analysis (FLD)**
- **The objective of LDA is to perform dimensionality reduction while preserving as much of the class discriminatory information as possible**

Linear Discriminant Analysis (LDA)

- **Main idea:**
  - find projection to a line so that samples from different classes are well separated
- **Example in 2-D**
  - Project data to 1-D subspace (a line) which minimize the separation error



bad line to project to,
classes are mixed up



good line to project to,
classes are well separated

Linear Discriminant Analysis (LDA)

- **We can derive following algorithm (will be discussed in next slides)**
  - **LDA algorithm:**
    - X_1, X_2 ← input $n_1$xd and $n_2$xd data matrices belong to class 1 and class 2
    - μ_1, μ_2 ← the means of X_1 and X_2
    - S_1, S_2 ← scatter matrices of X_1 and X_2 (Scatter = n * Σ ; n: size of data)
    - S_w ← within class scatter matrix ($S_w = S_1+S_2$)
    - V ← The direction of V (the new 1-D space) obtains from $V = S_W^{-1}(\mu_1-\mu_2)$
      - **The border would be a point the new space, and a hyperplane in the original space (Why?).**
    - Y (transformed data) ← Project the old data onto new line

LDA Derivation

- Suppose we have 2 classes and d-dimensional samples $x_1, \ldots, x_n$ where
  - n_1 samples come from the first class
  - n_2 samples come from the second class
- The projection of sample x_i onto a line in direction v is given by $v^t x_i$
- How to measure separation between projections of different classes?
- If μ'_1 and μ'_2 be the means of projections of classes 1 and 2, then $|\mu'_1 - \mu'_2|$ seems like a good measure
- the problem with this measure is that it does not consider the variances of the classes
  - we need to normalize that by a factor which is proportional to variance
  - we use the scatter (S) of the data

LDA Derivation

- **The means and scatters of data are (for feature vectors x_is):**

$$\mu_1 = \frac{1}{n_1} \sum_{x_i \in C_1} x_i \qquad \mu_2 = \frac{1}{n_2} \sum_{x_i \in C_2} x_i$$

$$S_1^{\ 2} = \sum_{x_i \in C_1} (x_i - \mu_1)(x_i - \mu_1)^T \qquad S_2^{\ 2} = \sum_{x_i \in C_2} (x_i - \mu_2)(x_i - \mu_2)^T$$

- **The means and scatters of projected data are: (why?)**

$$\mu_1^{'} = v^t \mu_1 \qquad \mu_2^{'} = v^t \mu_1$$

$$S_1^{'2} = \sum_{x_i \in C_1} (v^t x_i - \mu_1^{'})(v^t x_i - \mu_1^{'})^T \qquad S_2^{'2} = \sum_{x_i \in C_2} (v^t x_i - \mu_2^{'})(v^t x_i - \mu_2^{'})^T$$

- **Then we must maximize the following objective function.**

$$J(v) = \frac{\left(\mu_1^{'} - \mu_2^{'}\right)^2}{S_1^{'2} + S_2^{'2}}$$

  - **We can consider another objective functions, too.**

LDA Derivation

- All we need to do now is to express J explicity as a function of v and maximize it
- It is straight forward to see that $S'_1{}^2 = v^t S_1 v$ and $S'_2{}^2 = v^t S_2 v$
- Therefore $S'_1{}^2 + S'_2{}^2 = v^t S_w v$, where $S_w = S_1 + S_2$
- Also it is straight forward to see that $(\mu'_1 - \mu'_2)^2 = v^t S_B v$, where $S_B = (\mu_1 - \mu_2)(\mu_1 - \mu_2)^t$
- then

$$J(v) = \frac{\left(\mu_1^{'} - \mu_2^{'}\right)^2}{S_1^{'2} + S_2^{'2}} = \frac{v^t S_B v}{v^t S_w v}$$

- Maximize J(v) by taking the derivative w.r.t. v and setting it to 0

$$\frac{\partial}{\partial v} J(v) = \frac{\left(\frac{\partial}{\partial v} v^t S_B v\right) v^t S_W v - \left(\frac{\partial}{\partial v} v^t S_W v\right) v^t S_B v}{\left(v^t S_w v\right)^2} = \frac{\left(2 S_B v\right) v^t S_W v - \left(2 S_W v\right) v^t S_B v}{\left(v^t S_w v\right)^2}$$

LDA Derivation

- Need to solve $v^t S_W v(S_B v) - v^t S_B v(S_W v) = 0$, Then

$$\Rightarrow \frac{v^t S_W v(S_B v)}{v^t S_W v} - \frac{v^t S_B v(S_W v)}{v^t S_W v} = 0$$

$$\Rightarrow S_B v - \alpha(S_W v) = 0; \qquad \alpha = J(v) = \frac{v^t S_B v}{v^t S_W v}$$

$$\Rightarrow S_B v = \alpha S_W v$$

- $S_B v$ for any vector v, points in the same direction as $(\mu_1 - \mu_2)$
  - $S_B v = (\mu_1 - \mu_2)(\mu_1 - \mu_2)^t v = (\mu_1 - \mu_2)((\mu_1 - \mu_2)^t v) = \beta(\mu_1 - \mu_2)$
  - Then, $\beta(\mu_1 - \mu_2) = \alpha S_w v$
- If S_W has full rank (the inverse exists), then:

$$v = \gamma\, S_W^{-1}(\mu_1 - \mu_2)$$

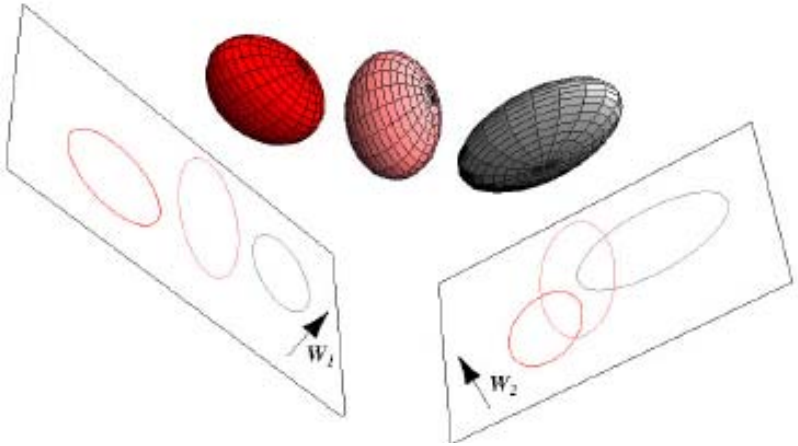
Linear Discriminant Analysis (LDA)

- **LDA Drawbacks**
  - **Reduces dimension only to k = c-1 (unlike PCA) (c is the number of classes - why?)**
    - For complex data, projection to even the best hyperplane may result in inseparable projected samples
  - **Will fail:**
    - If J(v) is always 0: happens if μ1 = μ2 (discriminatory information is not in the mean but rather in the variance of the data)

    - If classes have large overlap when projected to any line

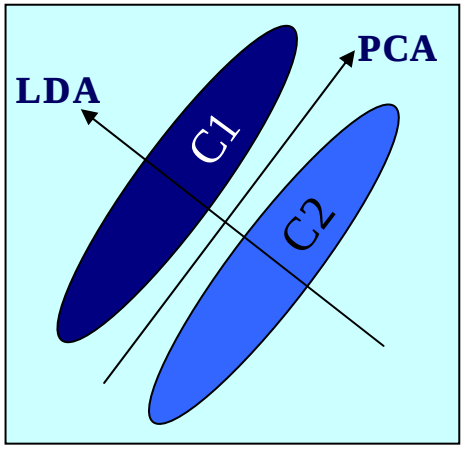
Multiple Discriminant Analysis (MDA)

- Can generalize LDA to multiple classes (how?)
  - Refer to the persian notes on the course page.
- In case of c classes, can reduce dimensionality to 1, 2, 3,…, c-1 dimensions (how and why?).



PCA vs LDA

- PCA (unsupervised)
  - Uses Total Scatter Matrix
- LDA (supervised)
  - Uses |between-class scatter matrix| / |within-class scatter matrix|

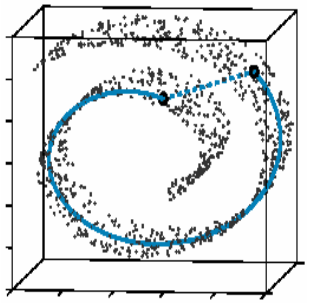


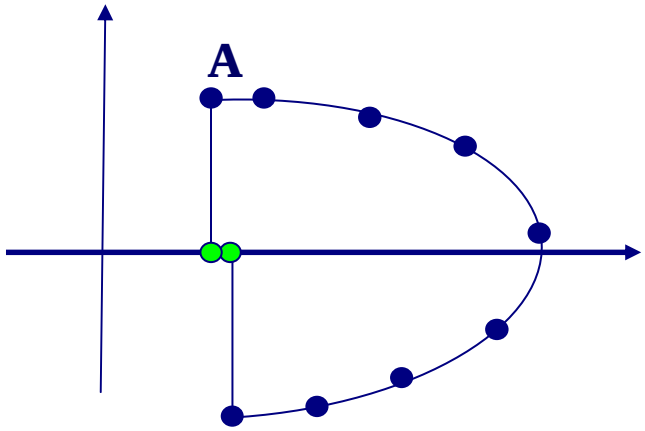
- PCA might outperform LDA when the number of samples per class is small or when the training data non-uniformly sample the underlying distribution
  - With few data, number of samples per class will be too low to have a reasonable estimation for covariance matrix, however the total number of samples may be still sufficient.
- Never knows in advance the underlying distributions for the different classes

Linear Methods Drawbacks

- **Nonlinear Manifolds**
  - **PCA uses the Euclidean distance**
    - Sometimes Euclidean distance is not proper:

manifold **is a topological space which is locally Euclidean**



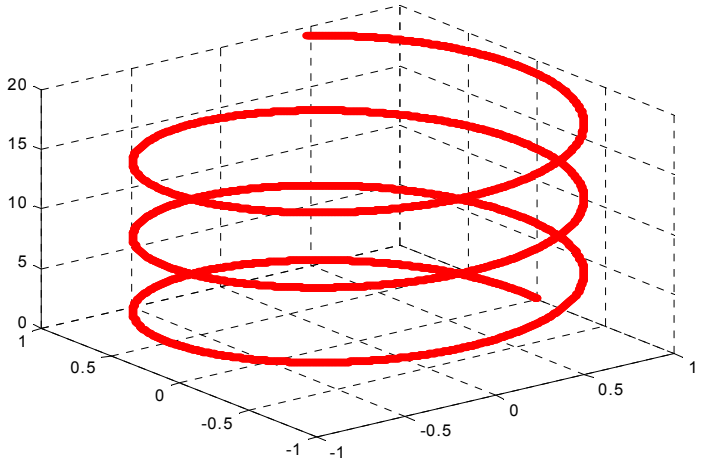


What is important is the geodesic distance

Unroll the manifold

Linear Methods Drawbacks

- **Deficiencies of Linear Methods**
  - **Data may not be best summarized by linear combination of features**
    - Example: PCA cannot discover 1D structure of a helix
    - Question: Does a nonlinear methods can discover a perfect 1D structure for helix? (how?)
      - **Did you realize what the nonlinear dimensionality reduction means ?**

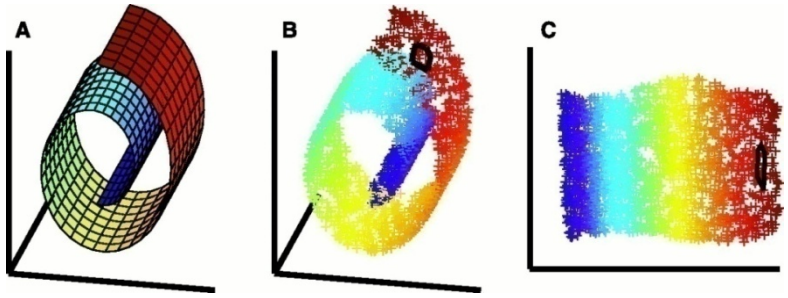


Nonlinear Dimensionality Reduction

- **Many data sets contain essential nonlinear structures that invisible to PCA and LDA.**
- **Resorts to some nonlinear dimensionality reduction approaches.**
  - **Kernel methods (like kernel PCA)**
    - Depend on the kernels
    - Most kernels are not data dependent
  - **Manifold based methods**
    - ISOMAP ← Will be discussed here!
    - Locally Linear Embedding (LLE) ← Will be discussed here!

ISOMAP

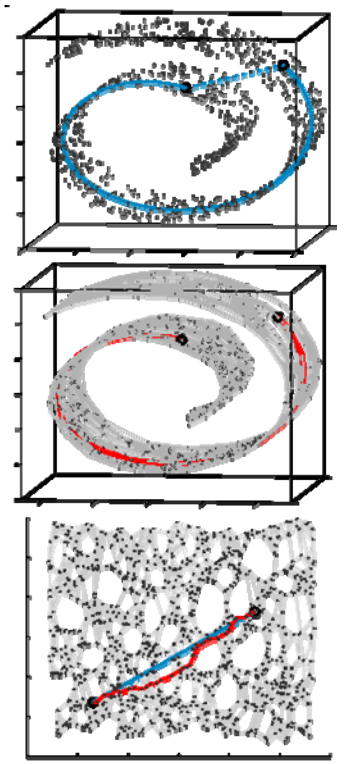
- **A non-linear approach for manifold learning (dimensionality reduction)**
  - **Estimate the geodesic distance between points, by finding shortest paths in a graph with edges connecting neighboring data points**



  - **Looking for new data points in a low dimensional space (d-dimensional) that preserve the geodesic distances.**

ISOMAP

- **Construct neighborhood graph G**
  - **In neighborhood graph, each sample is connected to *K* nearest neighbors.**
  - **Steps to form neighborhood graph matrix (D_G)**
    - Create binary *NxN* adjacency matrix so that each sample be connected to *K* nearest neighbors
    - Compute all-pairs shortest path in D_G
      - **Now D_G is *NxN* geodesic distance matrix of two arbitrary points along the manifold**
- **Use D_G as distance matrix in MDS.**



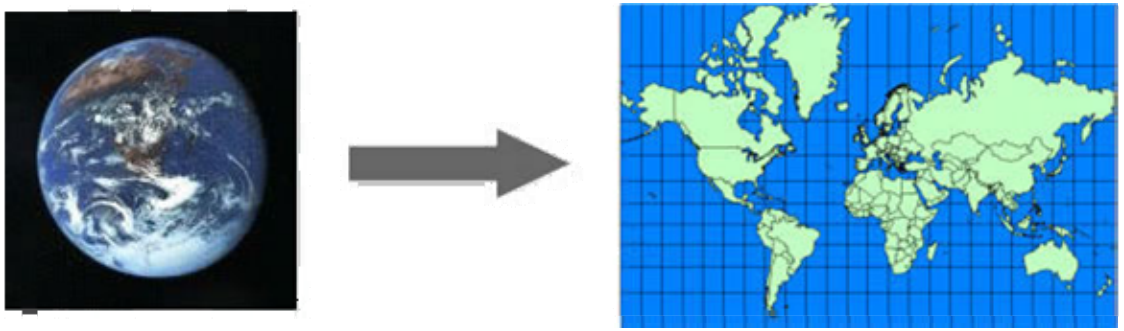
ISOMAP

- **Multi Dimensional Scaling (MDS)**
  - **MDS attempts to find an embedding from the K objects in $\mathbb{R}^N$, such that distances are preserved.**

$$\min_{x_1,\ldots,x_K} \sum_{i<j} (\|x_i - x_j\| - D_{ij})^2$$

  - **Use D as distance matrix in MDS**
    - The result of MDS is a N-dimensional Euclidean space X that minimizes the cost function

An example of multi dimensional scaling



ISOMAP

- **Multi Dimensional Scaling (MDS)**
  - **The top d eigenvectors of the dissimilarity matrix, represent the coordinates in the new d-dimensional Euclidean space.**

- **For more information visit the ISOMAP home page: http://isomap.stanford.edu/**

ISOMAP

- **Advantages**
  - **Nonlinear**
  - **Globally optimal**
  - **Still produces globally optimal low-dimensional Euclidean representation even though input space is highly folded, twisted, or curved.**
  - **Guarantee asymptotically to recover the true dimensionality.**
- **Disadvantages**
  - **May not be stable, dependent on topology of data**
    - Sensitive to noise (short circuits)
  - **Guaranteed asymptotically to recover geometric structure of nonlinear manifolds**
    - As *N* increases, pair wise distances provide better approximations to geodesics, but cost more computation
    - If *N* is small, geodesic distances will be very inaccurate.

Local Linear Embedding (LLE)

- **ISOMAP is a global approach**
  - **It uses geodesic distances and needs a graph traversal to compute them**
  - **Can we have the same functionality with a local approach?**

- **Local Linear Embedding (LLE)**
  - **A local approach to dimensionality reduction**
  - **LLE doesn't use geodesic distances.**

Local Linear Embedding (LLE)

- **Main idea:**
  - Finding a nonlinear manifold by stitching together small linear neighborhoods.
  - Assumption: manifold is approximately “linear” when viewed locally, that is, in a small neighborhood
- **ISOMAP does this by doing a graph traversal.**

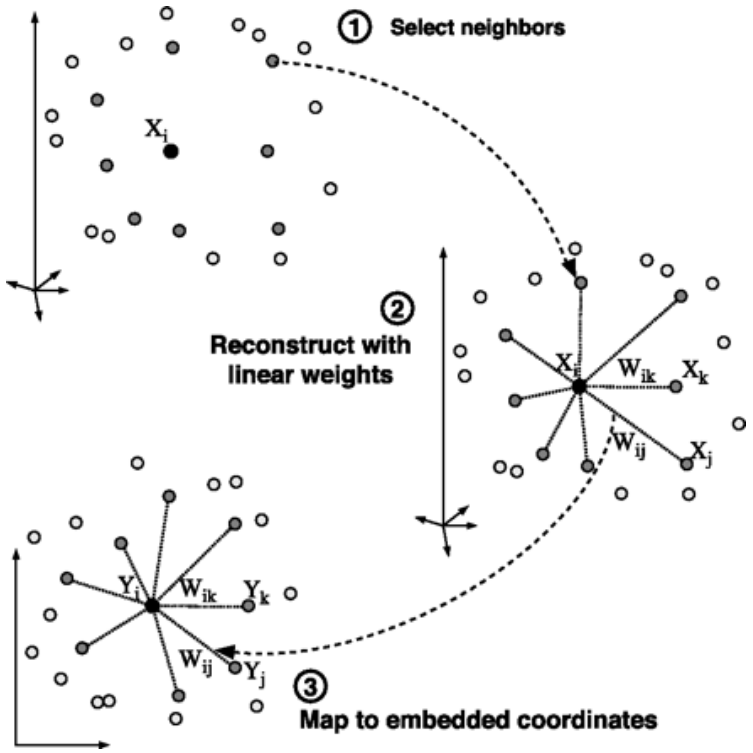
Local Linear Embedding (LLE)

✧ LLE procedure

1) Compute the k nearest neighbors for each sample

2) Reconstruct each point using a linear combination of its neighbors

3) Find a low dimensional embedding which minimizes reconstruction loss



Local Linear Embedding (LLE)

- **Each data point is constructed by its K neighbors (Step 2):**

$$\hat{\vec{X}}_i = \sum_{j=1}^{K} W_{ij} \vec{X}_j \; ; \qquad \sum_{j=1}^{K} W_{ij} = 1$$

  - **W_{ij} summarizes the contribution of j-th data point to the i-th data reconstruction**
  - **To obtain the weights we must solve the following optimization problem:**

$$\varepsilon(W) = \min_W || X_i - \sum_{j=1}^{K} W_{ij} X_j ||^2; \qquad \sum_{j=1}^{K} W_{ij} = 1$$

- **Find a low dimensional embedding which minimizes reconstruction loss (Step 3):**

$$\varphi(Y) = \min_Y || Y_i - \sum_{j=1}^{K} W_{ij} Y_j ||^2$$

Local Linear Embedding (LLE)

- **The weights that minimize the reconstruction errors are invariant to rotation, rescaling and translation of the data points.**
  - **Invariance to translation is enforced by adding the constraint that the weights sum to one (Why?).**
  - **The weights characterize the intrinsic geometric properties of each neighborhood.**
- **The same weights that reconstruct the data points in D dimensions should reconstruct it in the manifold in d dimensions (d<D).**
  - **Local geometry is preserved**

Local Linear Embedding (LLE)

- **Meaning of W: a linear representation of every data point by its neighbors**
  - **This is an intrinsic geometrical property of the manifold**
  - **A good projection should preserve this geometric property as much as possible**
- **In LLE, we must solve two optimization problems:**
  - **First optimization problem: finding W**
    - It is a “Constrained Least Square” problem
    - It is also a convex optimization problem
  - **Second optimization problem: finding vectors Y**
    - It is a “Least Square” problem
    - It is also a convex optimization problem, too.

Local Linear Embedding (LLE)

- **Optimization problem 1: Obtaining W**
  - **Compute the optimal weight for each point individually:**

$$\varepsilon = | x_i - \sum_{x_j \in Neighbors\ of\ x_i} w_{ij} x_j |^2 = | \sum_j w_{ij} (x_i - x_j) |^2 = \sum_j \sum_j w_{ij} w_{ik} C_{jk}$$

$$C_{jk} = (x_j - x_k)^T (x_j - x_k)$$

  - **This error can be minimized in closed form, using Lagrange multipliers to enforce the constraint that $\sum_j w_{ij} = 1$ in terms of the C, the optimal weights are given by:**
    - W_{ij} is Zero for all non-neighbors of x

$$w_{ij} = \frac{\sum_k C_{jk}^{-1}}{\sum_p \sum_q C_{pq}^{-1}}$$

Local Linear Embedding (LLE)

- **Optimization problem 2: Obtaining Y**
  - **The following is a more direct and simpler derivation for Y:**

$$\Phi(Y)=\sum_i\left\|Y_i-\sum_j W_{ij}Y_j\right\|^2=\sum_i\left\|Y_i-[Y_1;Y_2;\cdots;Y_n]W_i^T\right\|^2$$

$$=\left\|[Y_1;Y_2;\cdots;Y_n]-[Y_1;Y_2;\cdots;Y_n][W_1^T;W_2^T;\cdots;W_n^T]\right\|^2$$

$$=\left\|Y-YW^T\right\|_F^2=\left\|Y(I-W^T)\right\|_F^2=\text{trace}(Y(I-W)^T(I-W)Y^T)$$

$$=\text{trace}(YMY^T),\quad \text{where } Y=[Y_1;Y_2;\cdots;Y_n],\quad M=(I-W)^T(I-W)$$

Which $\|.\|_F$ indicates the Frobenius norm, i.e. $\|A\|_F=\sqrt{\sum_{i=1}^m\sum_{j=1}^n|a_{ij}|^2}=\sqrt{trace(AA^T)}$

- **Y is given by the eigenvectors of the lowest *d* non-zero eigenvalues of the matrix**

$$M=(I-W)^T(I-W)$$

- **For more information visit the LLE home page: http://cs.nyu.edu/~roweis/lle/**

Local Linear Embedding (LLE)

- **Some Limitations of LLE**
  - **require dense data points on the manifold for good estimation**
  - **A good neighborhood seems essential to their success**
    - How to choose k?
      - **Too few neighbors: Result in rank deficient tangent space and lead to over-fitting**
      - **Too many neighbors: Tangent space will not match local geometry well**

ISOMAP vs. LLE

- **ISOMAP preserves the neighborhoods and their geometric relation better than LLE.**
- **LLE requires massive input data sets and it must have same weight dimension.**
- **Merit of ISOMAP is fast processing time with Dijkstra's algorithm.**
- **ISOMAP is more practical than LLE.**

Any Question?

End of Lecture 4

Thank you!

Spring 2012

http://ce.sharif.edu/courses/90-91/2/ce725-1/