

CRICOS PROVIDER 00123M

#### ISML\_5: Dimensionality Reduction

Lingqiao Liu

adelaide.edu.au

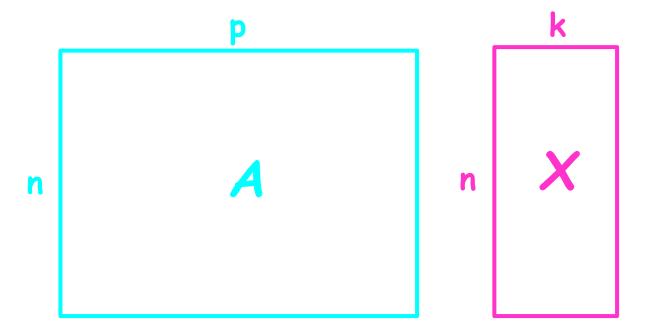
seek LIGHT

#### **Outline**

- Overview of dimensionality reduction
  - The benefits
  - Why we can perform dimensionality reduction
  - Type of dimensionality reduction methods
- Principal component analysis
  - Mathematical basics
  - Decorrelation and dimension selection
  - Eigenface and high-dimensionality issue
- Linear Discriminative Analysis
- Summary

## What is dimensionality reduction

Reduce dimensions of data



#### Extract underlying factors





#### The five factors [edit]

A summary of the factors of the Big Five and their col

- Openness to experience: (inventive/curious vs intellectual curiosity, creativity and a preference for preference for a variety of activities over a strict reexperience.
- Conscientiousness: (efficient/organized vs. eas spontaneous behavior.
- Extraversion: (outgoing/energetic vs. solitary/re talkativeness.
- Agreeableness: (friendly/compassionate vs. an one's trusting and helpful nature, and whether a r
- Neuroticism: (sensitive/nervous vs. secure/conf degree of emotional stability and impulse control;

- Reduce data noise
  - Face recognition
  - Applied to image de-noising



(a) Noisy image



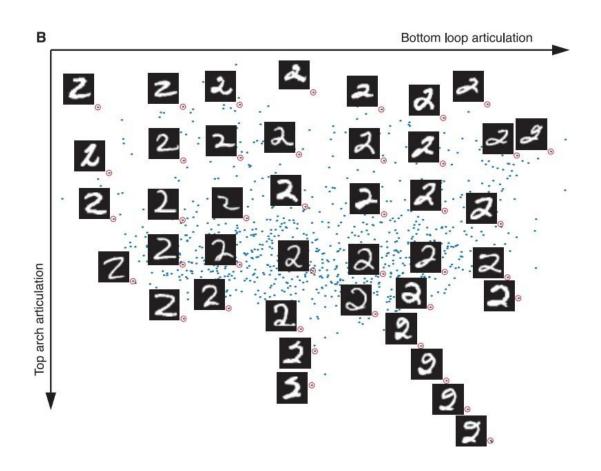
(b) NL means (PSNR=32.90)



(c) Local PCA (PSNR=33.70)

- Reduce the number of model parameters
  - Avoid over-fitting
  - Reduce computational cost

Visualization



## **Dimensionality Reduction**

- General principle:
  - Preserve "useful" information in low dimensional data
- How to define "usefulness"?
  - Many
  - An active research direction in machine learning
- Taxonomy
  - Supervised or Unsupervised
  - Linear or nonlinear
- Commonly used methods:
  - PCA, LDA (linear discriminant analysis), and more.
- Feature Selection vs dimensionality reduction

#### **Outline**

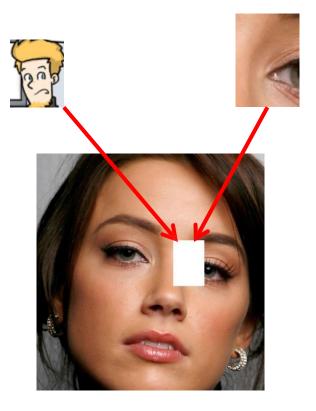
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#### Principal Component Analysis: Motivation

- Principal Component Analysis (PCA) is an unsupervised dimensionality reduction method
  - Transform data to remove redundant information
  - Keep the most informative dimensions after the transformation

## Data correlation & information redundancy



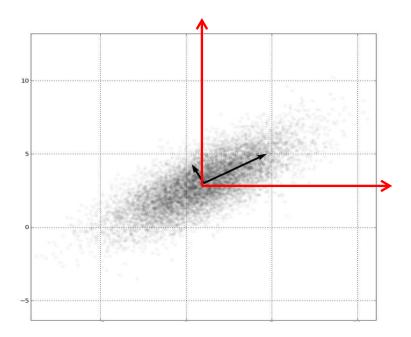


## PCA explained: De-correlating data

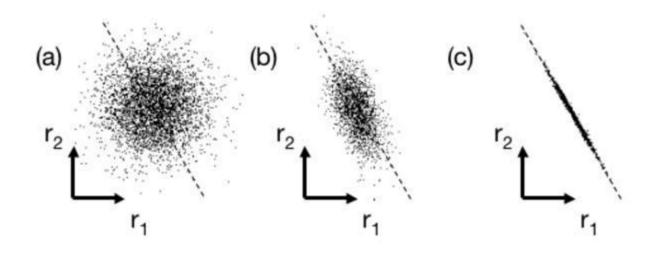
- Dependency vs. Correlation
  - Dependent is a stronger criterion
- Equivalent when data follows Gaussian distribution
- PCA only de-correlates data
  - One limitation of PCA
  - ICA, but it is more complicate

## PCA explained: De-correlating data

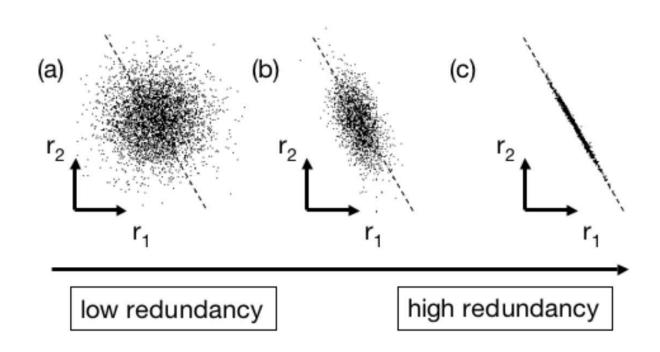
Geometric interpretation of correlation



# Exercise: which figure shows the highest data correlation?

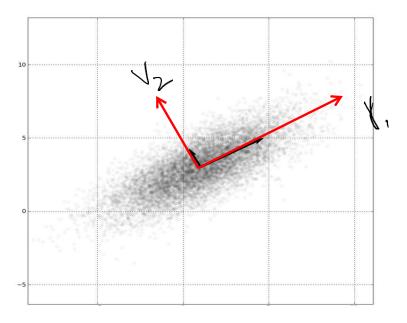


## Exercise: which figure shows the highest data correlation?

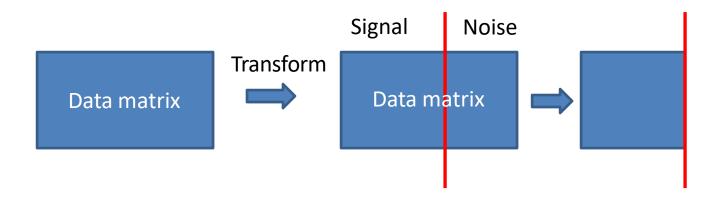


## PCA explained: De-correlating data

 Correlation can be removed by rotating the data point or coordinate



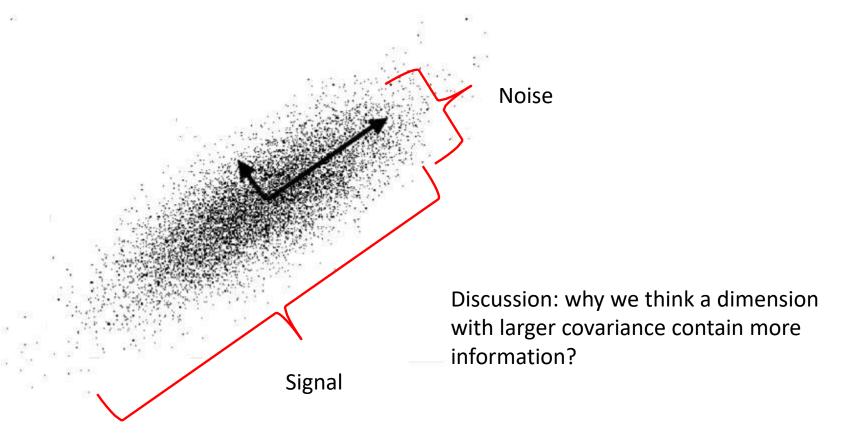
## PCA explained: SNR maximization



Maximize

$$SNR = rac{\sigma_{signal}^2}{\sigma_{noise}^2}.$$

## PCA explained: SNR maximization



## PCA explained

- Target
  - 1: Find a new coordinate system which makes different dimensions zero correlated
  - 2: keep the top-k dimensions with largest variance in the new coordinate system
- Method
  - Rotate the data point or coordinate
- Mathematically speaking...
  - How to rotate?
  - How to express our criterion

- Mean, Variance, Covariance
- Matrix norm, trace,
- Orthogonal matrix, basis
- Eigen decomposition

• (Sample) Mean

$$\bar{X} = \frac{\sum_{i=1}^{n} X_i}{n}$$

• (Sample) Variance

$$\sigma^2 = \frac{\sum_{i=1}^n (X_i - \bar{X})^2}{n}$$

(Sample) Covariance

$$cov(X,Y) = \frac{\sum_{i=1}^{n} (X_i - \bar{X})(Y_i - \bar{Y})}{n}$$

#### Covariance Matrix

$$C = \begin{pmatrix} cov(x,x) & cov(x,y) & cov(x,z) \\ cov(y,x) & cov(y,y) & cov(y,z) \\ cov(z,x) & cov(z,y) & cov(z,z) \end{pmatrix}$$

$$\mathbf{C} = rac{1}{n} \sum_{i=1}^n (\mathbf{x}_i - \mathbf{ar{x}}) (\mathbf{x}_i - \mathbf{ar{x}})^ op$$
 Or compactly

$$\mathbf{C} = \frac{1}{n} \mathbf{X_c} \mathbf{X_c}^{\top}, \ \mathbf{X_c} \in \mathbf{R}^{d \times n}$$

 $\mathbf{X_c}$  is the centralized data matrix (with mean subtracted)

When C is a diagonal matrix, dimensions of features become zero-correlated

Orthogonal matrix

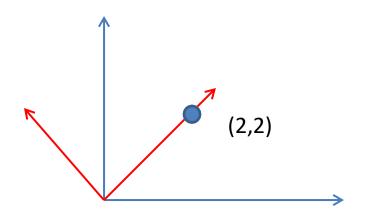
$$Q^{\mathrm{T}}Q = QQ^{\mathrm{T}} = I_{\mathrm{I}}$$

Rotation effect

$$\|\mathbf{Q}\mathbf{x}\|_2 = \|\mathbf{Q}\mathbf{x}\|_F = \sqrt{\operatorname{trace}(\mathbf{x}^T\mathbf{Q}^T\mathbf{Q}\mathbf{x})} = \sqrt{\operatorname{trace}(\mathbf{x}^T\mathbf{x})} = \|\mathbf{x}\|_F$$

$$\mathbf{x} = \mathbf{Q}^T \mathbf{Q} \mathbf{x}$$

- Relationship to coordinate system
  - A point = linear combination of bases
  - Combination weight = coordinate
- Each row (column) of Q = basis
  - Not unique
  - Relation to coordinate rotation
- New coordinate Qx



$$\binom{2}{2} = 2 \binom{1}{0} + 2 \binom{0}{1}$$

$$\binom{2}{2} = 2\sqrt{2} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + 0 \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

New coordinate

#### Eigen-decomposition

• If A is symmetric

$$\mathbf{A} = \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^T \quad Q^{\mathrm{T}} Q = Q Q^{\mathrm{T}} = I_{\mathrm{T}}$$

#### PCA: solution

Target 1: de-correlation

$$\mathbf{C}_X = rac{1}{n} \mathbf{X}_c \mathbf{X}_c^ op$$
 Original covariance matrix of data

$$\mathbf{Y} = \mathbf{P} \mathbf{X_c}$$
 We are looking for transform the centralized data with a matrix P

Require 
$$\mathbf{C}_Y = \frac{1}{n} \mathbf{P} \mathbf{X_c} (\mathbf{P} \mathbf{X_c})^{\top} = \frac{1}{n} \mathbf{P} \mathbf{X_c} \mathbf{X_c}^{\top} \mathbf{P}^{\top}$$
 be a diagonal matrix

#### **PCA**: solution

Target 1: de-correlation

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 be a diagonal matrix

Sounds familiar?

#### **PCA**: solution

$$\mathbf{X}_c \in R^{d \times N}$$
$$\mathbf{P} \in R^{d \times d}$$

Target 1: de-correlation

$$\mathbf{C}_X = rac{1}{n} \mathbf{X}_c \mathbf{X}_c^ op$$
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Require 
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 be a diagonal matrix

Sounds familiar? Use eigen decomposition 
$$\mathbf{X_cX_c^\top} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^\top$$
  $Q^TQ = QQ^T = I_1$ 

$$\mathbf{C}_{\mathbf{Y}} = \frac{1}{n} \mathbf{P} \mathbf{X}_{\mathbf{c}} \mathbf{X}_{\mathbf{c}}^{\top} \mathbf{P}^{\top}$$
 set  $\mathbf{P} = \mathbf{Q}^{\top}$   
 $= \frac{1}{n} \mathbf{P} \mathbf{Q} \mathbf{\Lambda} \mathbf{Q}^{\top} \mathbf{P}^{\top}$  so  $\mathbf{C}_{\mathbf{Y}} = \frac{1}{n} \mathbf{\Lambda}$ 

## Recap: Matrix decomposition

- Matrix can be decomposed into the combination (usually product) of special matrices
- Eigen decomposition

$$A = Q\Lambda Q^{-1}$$

where  $\Lambda$  is a diagonal matrix, with its *i*-th diagonal value be the *i*-th eigenvalue of A. Q is a matrix with its *i*th column be the eigenvector corresponding to *i*th eigenvalue.

- When A is symmetric, i.e.  $A = A^{\top}$ 

$$A = Q\Lambda Q^{\top} \qquad Q^{\top}Q = QQ^{\top} = I$$

Related topic: Singular value decomposition

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### A closer look at the covariance matrix of y

- The covariance matrix of the transformed data is a diagonal matrix, what are the diagonal elements?
- From the perspective of covariance matrix

$$\frac{1}{n}[\mathbf{Y}\mathbf{Y}^{\top}]_{\mathbf{i},\mathbf{j}} = \mathbf{E}(\mathbf{y_i}\mathbf{y_j})$$

The i, j th element of the covariance matrix is the covariance between the i-th dimension feature and j-th dimension feature. The i-th diagonal element represents the variance of the feature at the i-th dimension

• From the perspective of Eigen-decomposition, the diagonal matrix corresponding to the eigenvalues of  $\mathbf{X_cX_c^{\top}}$ 

## How to select the most informative dimensions?

• We rank the dimensions by their variance, which is equivalent to rank the dimensions by their corresponding eigen values

$$\mathbf{X_c}\mathbf{X_c^{\top}} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q^{\top}}$$

$$\begin{pmatrix} \mathbf{Q} & \mathbf{A} & \mathbf{Q} \\ \mathbf{Q} \\ \mathbf{Q} & \mathbf{Q} \\ \mathbf{Q} \\ \mathbf{Q} & \mathbf{Q} \\ \mathbf{$$

 Note that the i-th dimension of y is obtained by using the i-th row of P

$$\mathbf{Y} = \mathbf{P}\mathbf{X_c}, \ \mathbf{y}_i = \mathbf{p}_i\mathbf{X_c}$$

 If we only want to have k dimensions, we can simply select the eigen vectors corresponding to the top-k eigenvalues to form the projection matrix P

## PCA: algorithm

- 1. Subtract mean
- 2. Calculate the covariance matrix
- 3. Calculate eigenvectors and eigenvalues of the covariance matrix
- 4. Rank eigenvectors by its corresponding eigenvalues
- 4. Obtain P with its row vectors corresponding to the top k eigenvectors

#### PCA: MATLAB code

```
5
6- Mu = mean(fea);
7- fea = fea - repmat(Mu,[size(fea,1),1]);
8- Cov = fea'*fea;
9- [V,D] = eig(Cov);
10- [value,rank_idx] = sort(diag(D),'descend');
11- P = V(:,rank_idx(1:10));
```

Note fea is with the size of N x d.

#### **PCA**: reconstruction

 From a new feature y, we can reconstruct its original feature x

$$\hat{\mathbf{x}} = \mathbf{P}^{\top} \mathbf{y} = \mathbf{P}^{\top} (\mathbf{P} \mathbf{X})$$

Similar to the rotation back operation, e.g.,  $\mathbf{x} = \mathbf{Q}^T \mathbf{Q} \mathbf{x}$ 

 Fun fact, we can also derive PCA algorithm from the following optimization problem

$$\min_{\mathbf{P}} \|\mathbf{X} - \mathbf{P}^T \mathbf{P} \mathbf{X}\|_F^2$$

$$s.t. \ \mathbf{P} \mathbf{P}^T = \mathbf{I}$$

#### PCA: reconstruction

Reighley Quotient

$$\max_{\mathbf{P}} \text{ trace}(\mathbf{P}\mathbf{X}\mathbf{X}^T\mathbf{P}^T)$$

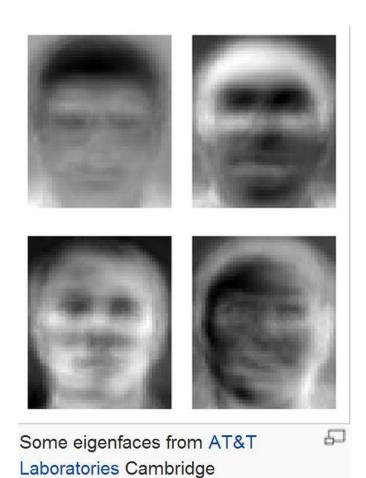
$$s.t. \ \mathbf{P}\mathbf{P}^T = \mathbf{I}$$

• Solution = PCA

## Application: Eigen-face method

- Sirovich and Kirby (1987) showed that PCA could be used on a collection of face images to form a set of basis features.
- Not only limited to face recognition
- Steps
  - Image as high-dimensional feature
  - PCA

## Application: Eigen-face method



## Application: Reconstruction

#### Reconstructed from top-2 eigenvectors









#### **Application: Reconstruction**

#### Reconstructed from top-15 eigenvectors









#### **Application: Reconstruction**

#### Reconstructed from top-40 eigenvectors









## Application: Eigen-face method

From large to small eigenvalues



## high dimensionality issue

- For high-dimensional data large
- The number of samples is relatively small,  $\mathbf{X_c}\mathbf{X_c^{\top}} \in \mathbf{R^{d \times d}}$  can be too large
- Solution: a useful relation

Suppose  $d\gg N$  , we first consider the eigen value and vectors of the matrix  $\mathbf{X}^T\mathbf{X}$ 

$$\mathbf{X}^T \mathbf{X} \mathbf{v} = \lambda \mathbf{v}$$

Multiply X on both side of equation

$$\mathbf{X}\mathbf{X}^{T}(\mathbf{X}\mathbf{v}) = \lambda(\mathbf{X}\mathbf{v})$$

If we define  $\mathbf{11} = \mathbf{X}\mathbf{v}$ 

Then we know 
$$\mathbf{X}\mathbf{X}^T\mathbf{u} = \lambda\mathbf{u}$$

## high dimensionality issue

- For high-dimensional data large
- The number of samples is relatively small,  $X_cX_c^{\top} \in \mathbb{R}^{d \times d}$ can be too large
- Solution: a useful relation

Suppose  $d\gg N$  , we first consider the eigen value and vectors of the matrix  ${f X}^T{f X}$ 

$$\mathbf{X}^T \mathbf{X} \mathbf{v} = \lambda \mathbf{v}$$

Kernel matrix

Multiply X on both side of equation

$$\mathbf{X}\mathbf{X}^{T}(\mathbf{X}\mathbf{v}) = \lambda(\mathbf{X}\mathbf{v})$$

 $\mathbf{u} = \mathbf{X}\mathbf{v}$ If we define

Then we know

$$\mathbf{X}\mathbf{X}^T\mathbf{u} = \lambda\mathbf{u}$$

The definition of the eigen system of covariance matrix

## High dimensionality issue

- 1. Centralize data
- 2. Calculate the kernel matrix
- 3. Perform Eigen-decomposition on the kernel matrix and obtain its eigenvector  ${f v}$
- 4. Obtain the Eigenvector of the covariance matrix by  $\mathbf{u} = \mathbf{X}\mathbf{v}$
- Question? How many eigenvectors you can obtain in this way?

#### **Mathematic Basics**

- Rank of a matrix
  - In linear algebra, the rank of a matrix A is the dimension of the vector space generated (or spanned) by its columns
  - It is identical to the dimension of the vector space spanned by its rows  $\max_{n \in \mathbb{N}} h(\mathbf{A}) < \min_{n \in \mathbb{N}} \{m, n\} \quad \mathbf{A} \in \mathbb{R}^{m \times n}$

 $rank(\mathbf{A}) < min\{m, n\}, \quad \mathbf{A} \in \mathbb{R}^{m \times n}$ 

Important relationship

if 
$$\mathbf{A} = \mathbf{BC}$$
  
 $\operatorname{rank}(\mathbf{A}) \leq \min \{ \operatorname{rank}(\mathbf{B}), \operatorname{rank}(\mathbf{C}) \}$ 

Relationship to the eigenvalues
 the rank of a matrix equals to the number of non-zero
 eigenvalues of the matrix.

## Back to the previous question

So the rank of

$$rank(\mathbf{X}\mathbf{X}^{\top}) \le rank(\mathbf{X}) \le \min\{d, N\}$$
  
 $rank(\mathbf{X}^{\top}\mathbf{X}) \le rank(\mathbf{X}) \le \min\{d, N\}$ 

• So at most  $min\{d, N\}$  meaningful projections from PCA

The eigen vector corresponding to 0 eigenvalue is meaningless in PCA

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## Discriminative dimensionality reduction

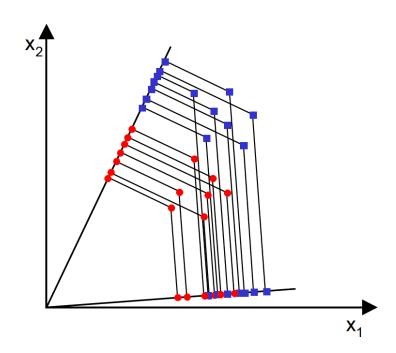
- General principle:
  - Preserve "useful" information in low dimensional data
  - PCA: measure ``usefulness'' through reconstruction error or covariance structure.
  - Useful for reconstruction ≠ useful for classification
- General principle for discriminative dimensionality reduction
  - Preserve "discriminative" information in low dimensional data

# Linear Discriminant Analysis: Basic idea

- Linear Discriminant Analysis (LDA)
  - Discriminative dimensionality reduction
  - Linear dimensionality reduction  $\mathbf{P}\mathbf{X}$
- Supervised information
  - Class label
  - Data from the same class => Become close
  - Data from different classes => far from each other

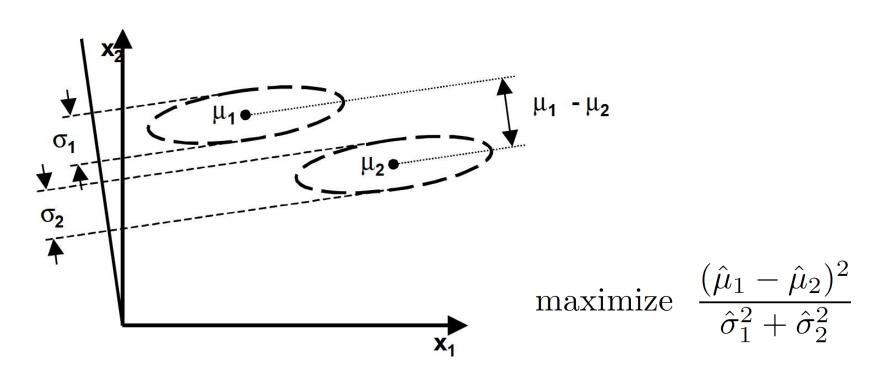
## Linear Discriminant Analysis (LDA): Objective

• Two classes:



## Linear Discriminant Analysis: Objective

• Two classes:



### Linear Discriminant Analysis (LDA): Objective

Mean after projection:

$$\hat{\mu} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{p}^{T} \mathbf{x}_{i} = \mathbf{p}^{T} \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_{i} = \mathbf{p}^{T} \mu$$

Variance after projection:

$$\hat{\sigma}^2 = \frac{1}{N} \sum_{i=1}^N (\mathbf{p}^T \mathbf{x}_i - \mathbf{p}^T \mu)^2$$

$$= \frac{1}{N} \sum_{i=1}^N \mathbf{p}^T (\mathbf{x}_i - \mu) (\mathbf{x}_i - \mu)^T \mathbf{p}$$

$$= \mathbf{p}^T \left( \frac{1}{N} \sum_{i=1}^N (\mathbf{x}_i - \mu) (\mathbf{x}_i - \mu)^T \right) \mathbf{p}$$

## Linear Discriminant Analysis (LDA), Objective

Mean distance

$$(\mathbf{p}^T \mu_1 - \mathbf{p}^T \mu_2)^2 = \mathbf{p}^T (\mu_1 - \mu_2) (\mu_1 - \mu_2)^T \mathbf{p}$$

Between class Scatterness, within class Scatterness

$$\mathbf{S}_{b} = (\mu_{1} - \mu_{2}) (\mu_{1} - \mu_{2})^{T}$$

$$\mathbf{S}_{w} = \sum_{i=1,2} \frac{1}{N_{j}} \sum_{i=1}^{N_{j}} (\mathbf{x}_{i} - \mu) (\mathbf{x}_{i} - \mu)^{T}$$

# Linear Discriminant Analysis (LDA): Solution

Objective

maximize 
$$\frac{\mathbf{p}^T \mathbf{S}_b \mathbf{p}}{\mathbf{p}^T \mathbf{S}_w \mathbf{p}}$$

Solution

maximize 
$$\frac{\mathbf{p}^{T}\mathbf{S}_{b}\mathbf{p}}{\mathbf{p}^{T}\mathbf{S}_{w}\mathbf{p}}$$
 maximize  $\mathbf{p}^{T}\mathbf{S}_{b}\mathbf{p}$ 

$$s.t. \ \mathbf{p}^{T}\mathbf{S}_{w}\mathbf{p} = 1$$

$$L = \mathbf{p}^{T}\mathbf{S}_{b}\mathbf{p} - \lambda(\mathbf{p}^{T}\mathbf{S}_{w}\mathbf{p} - 1)$$

$$\frac{\partial L}{\partial \mathbf{p}} = 0 \quad \Rightarrow \quad \mathbf{S}_{w}^{-1}\mathbf{S}_{b}\mathbf{p} = \lambda\mathbf{p}$$

## Linear Discriminant Analysis (LDA), Solution

- Eigenvectors corresponding to the largest eigenvalues of  $\mathbf{S}_w^{-1}\mathbf{S}_b$ 
  - Why?  $\text{maximize } \mathbf{p}^T \mathbf{S}_b \mathbf{p} \\
     s.t. \ \mathbf{p}^T \mathbf{S}_w \mathbf{p} = 1$   $\frac{\partial L}{\partial \mathbf{p}} = 0 \Rightarrow \mathbf{S}_w^{-1} \mathbf{S}_b \mathbf{p} = \lambda \mathbf{p}$

At optimum, we have  $\mathbf{p}^{*\top}\mathbf{S}_b\mathbf{p}^*=\lambda$ 

- Implementation details
  - What if  $S_{yy}$  is not invertible?

Use  $(\mathbf{S}_w + \lambda \mathbf{I})^{-1}$  instead

## Linear Discriminant Analysis, Multiclass

Generalized to multiple classes

$$\mathbf{S}_{b} = \sum_{i=1,j=1}^{C} (\mu_{i} - \mu_{j}) (\mu_{i} - \mu_{j})^{T} = \sum_{i} (\mu_{i} - \mu) (\mu_{i} - \mu)^{T}$$

$$\mathbf{S}_{w} = \sum_{j=1}^{C} \sum_{i \in \mathcal{C}_{j}} (\mathbf{x}_{i} - \mu) (\mathbf{x}_{i} - \mu)^{T}$$

$$\max imize \quad \frac{\operatorname{trace} (\mathbf{P}^{T} \mathbf{S}_{b} \mathbf{P})}{\operatorname{trace} (\mathbf{P}^{T} \mathbf{S}_{w} \mathbf{P})}$$

- Solution:
  - Top c eigenvectors of  $\mathbf{S}_w^{-1}\mathbf{S}_b$
  - Discussion: how many projections you can have?

## Linear Discriminant Analysis, Multiclass

Generalized to multiple classes

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- Solution:
  - Top c eigenvectors of  $\mathbf{S}_w^{-1}\mathbf{S}_b$
  - Discussion: how many projections you can have?

Check the rank of 
$$\mathbf{S}_w^{-1}\mathbf{S}_b$$

$$rank(\mathbf{S}_w^{-1}\mathbf{S}_b) \le rank(\mathbf{S}_b) \le C$$

### Summary

- The benefit of dimensionality reduction
- Principal component analysis
  - Two basic steps: decorrelation and select the dimensions with top variances
  - How to perform data transformation?
  - Its application, eigen face. The meaning behind eigen vectors
  - High dimensionality issue
- Linear discriminative component analysis
  - Basic objective
  - Two-class case
  - Multi-class case