Imperial College London

Lecture 15: Linear Discriminant Analysis

Recommended reading:
Bishop, Chapter 4.1
Hastie et al., Chapter 4.3

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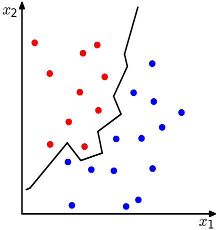
February 22, 2016

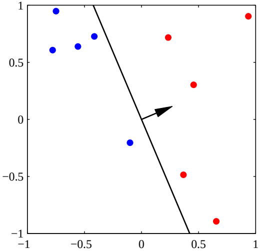
Classification



Adapted from PRML (Bishop, 2006)

- Input vector $\boldsymbol{x} \in \mathbb{R}^D$, assign it to one of K discrete classes $C_k, k = 1, \ldots, K$.
- Assumption: classes are disjoint, i.e., input vectors are assigned to exactly one class
- Idea: Divide input space into decision regions whose boundaries are called decision boundaries/surfaces

Linear Classification

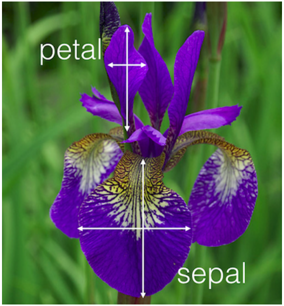


From PRML (Bishop, 2006)

- Focus on linear classification model, i.e., the decision boundary is a linear function of $\boldsymbol{x}$
  - ⏩ Defined by $(D-1)$-dimensional hyperplane
- If the data can be separated exactly by linear decision surfaces, they are called linearly separable
- Implicit assumption: Classes can be modeled well by Gaussians

⏩ Here: Treat classification as a projection problem

Example



- Measurements for 150 Iris flowers from three different species.

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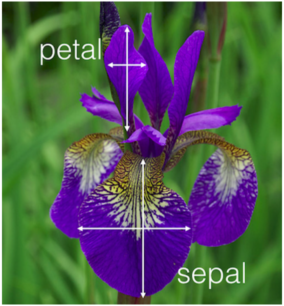

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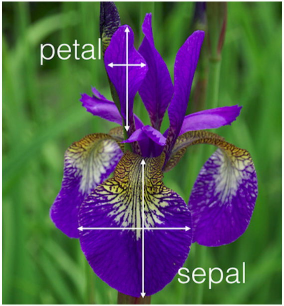

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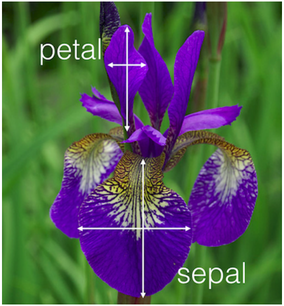

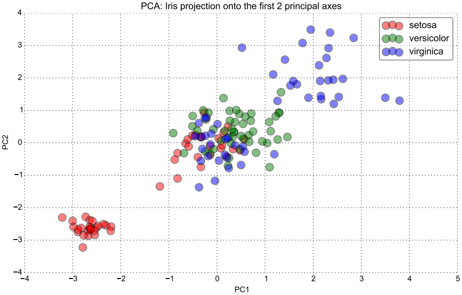

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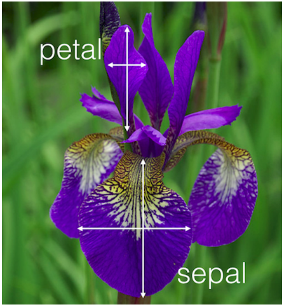

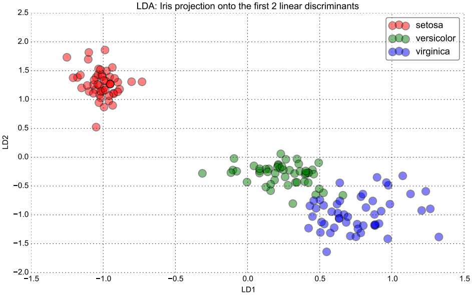

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Orthogonal Projections (Repetition)

- Project input vector $\boldsymbol{x} \in \mathbb{R}^D$ down to a 1-dimensional subspace with basis vector $\boldsymbol{w}$
- With $\|\boldsymbol{w}\| = 1$, we get

$\boldsymbol{P} = \boldsymbol{w}\boldsymbol{w}^\top$	Projection matrix, such that $\boldsymbol{P}\boldsymbol{x} = \boldsymbol{p}$
$\boldsymbol{p} = y\boldsymbol{w} \in \mathbb{R}^D$	Projection point ⏩ Discussed in Lecture 14
$y = \boldsymbol{w}^\top \boldsymbol{x} \in \mathbb{R}$	Coordinates with respect to basis $\boldsymbol{w}$ ⏩ Today

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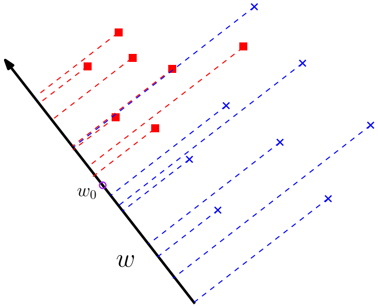
- We will largely focus on the coordinates y in the following
- Projection points equally apply to concepts discussed today
- Coordinates equally apply to PCA (see Lecture 14)

Classification as Projection



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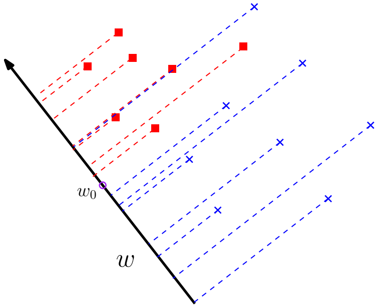

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- Threshold w_0, such that we decide on C_1 if $y \geqslant w_0$ and C_2 otherwise

The Linear Decision Boundary of LDA

- Look at the log-probability ratio

$$\log \frac{p(\mathcal{C}_1|\boldsymbol{x})}{p(\mathcal{C}_2|\boldsymbol{x})} = \log \frac{p(\boldsymbol{x}|\mathcal{C}_1)}{p(\boldsymbol{x}|\mathcal{C}_2)} + \log \frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)}$$

where the decision boundary (for $\mathcal{C}_1$ or $\mathcal{C}_2$) is at 0.

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- Assume Gaussian likelihood $p(\boldsymbol{x}|\mathcal{C}_i) = \mathcal{N}\big(\boldsymbol{x} \mid \boldsymbol{m}_i, \boldsymbol{\Sigma}\big)$ with the same covariance $\boldsymbol{\Sigma}$ in both classes. Decision boundary:

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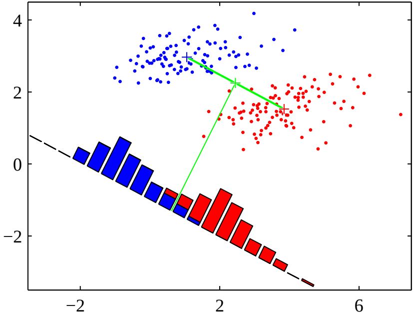
▶▶ Of the form $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ ▶▶ Decision boundary linear in $\boldsymbol{x}$

Potential Issues



From PRML (Bishop, 2006)

- Considerable loss of information when projecting

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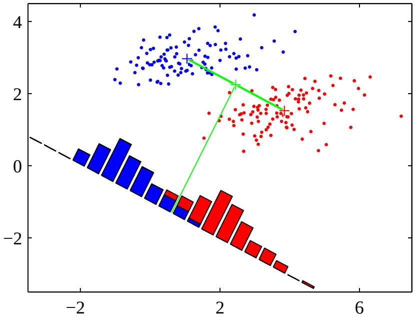

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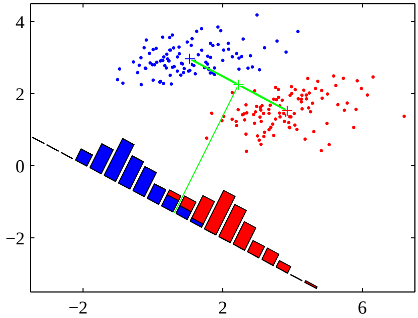

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- Considerable loss of information when projecting
- Even if data was linearly separable in $\mathbb{R}^D$, we may lose this separability (see figure)

⏩ Find good basis vector $\boldsymbol{w}$ that spans the subspace we project onto

Approach: Maximize Class Separation

- Adjust components of basis vector $\boldsymbol{w}$
  - ⏩ Select projection that maximizes the class separation

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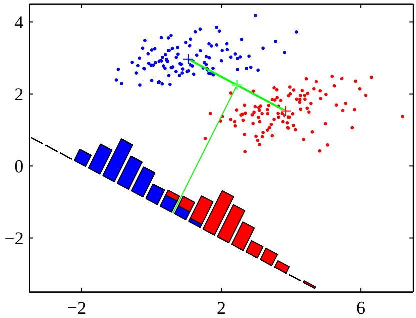
- Measure class separation as the distance of the projected class means:

$$m_2 - m_1 = \boldsymbol{w}^\top \boldsymbol{m}_2 - \boldsymbol{w}^\top \boldsymbol{m}_1 = \boldsymbol{w}^\top (\boldsymbol{m}_2 - \boldsymbol{m}_1)$$

and maximize this w.r.t. $\boldsymbol{w}$ with the constraint $\|\boldsymbol{w}\| = 1$

Maximum Class Separation



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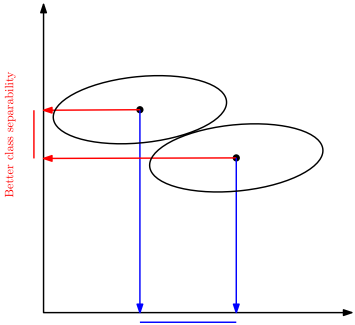

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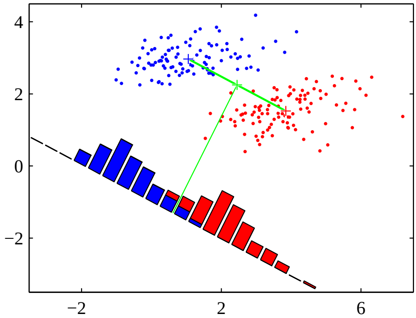

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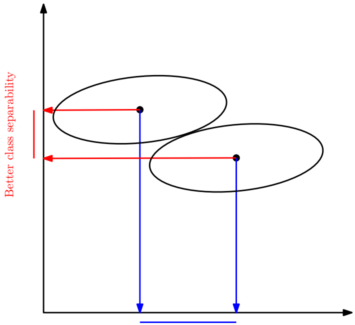

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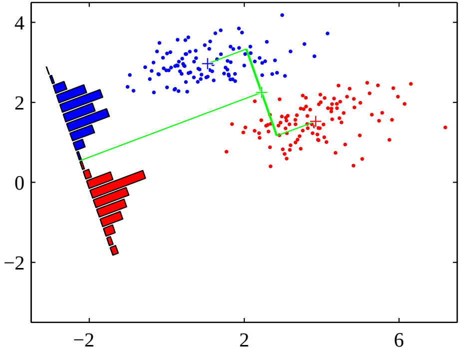
- LDA: Large separation of projected class means **and** small within-class variation (small overlap of classes)

Key Idea of LDA



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- Separate samples of distinct groups by projecting them onto a space that
  - Maximizes their between-class separability while
  - Minimizing their within-class variability

Fisher Criterion

- For each class C_k the within-class scatter (unnormalized variance) is given as

$$s_k^2 = \sum_{n \in C_k} (y_n - m_k)^2 \,, \qquad y_n = \boldsymbol{w}^\top \boldsymbol{x}_n \,, \quad m_k = \boldsymbol{w}^\top \boldsymbol{m}_k$$

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- Maximize the Fisher criterion:

$$J(\boldsymbol{w}) = \frac{\text{Between-class scatter}}{\text{Within-class scatter}} = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2} = \frac{\boldsymbol{w}^\top \boldsymbol{S}_B \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{S}_W \boldsymbol{w}}$$

$$\boldsymbol{S}_W = \sum_k \sum_{n \in C_k} (\boldsymbol{x}_n - \boldsymbol{m}_k)(\boldsymbol{x}_n - \boldsymbol{m}_k)^\top$$

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- $\boldsymbol{S}_W$ is the total within-class scatter and proportional to the sample covariance matrix

Generalization to k Classes

For k classes, we define the between-class scatter matrix as

$$\boldsymbol{S}_B = \sum\nolimits_k N_k(\boldsymbol{m}_k - \boldsymbol{\mu})(\boldsymbol{m}_k - \boldsymbol{\mu})^\top, \qquad \boldsymbol{\mu} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x}_i$$

where $\boldsymbol{\mu}$ is the global mean of the data set

Finding the Projection

Objective

Find $\boldsymbol{w}^*$ that maximizes

$$J(\boldsymbol{w}) = \frac{\boldsymbol{w}^\top \boldsymbol{S}_B \boldsymbol{w}}{\boldsymbol{w}^\top \boldsymbol{S}_W \boldsymbol{w}}$$

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- The projection vector $\boldsymbol{w}$ is the eigenvector of $\boldsymbol{S}_W^{-1} \boldsymbol{S}_B$.
- Choose the eigenvector that corresponds to the maximum eigenvalue (similar to PCA) to maximize class separability

Algorithm

1. Mean normalization

- $\boldsymbol{X} \in \mathbb{R}^{n \times D}$: ith row represents the ith sample

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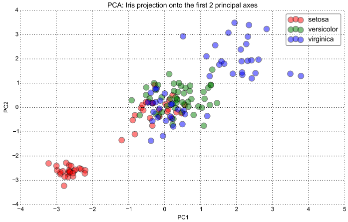
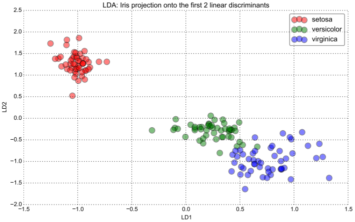
6. Project samples onto the new subspace using $\boldsymbol{W}$ and compute the new coordinates as $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{W}$

- $\boldsymbol{X} \in \mathbb{R}^{n \times D}$: ith row represents the ith sample
- $\boldsymbol{Y} \in \mathbb{R}^{n \times k}$: Coordinate matrix of the n data points w.r.t. eigenbasis $\boldsymbol{W}$ spanning the k-dimensional subspace

PCA vs LDA





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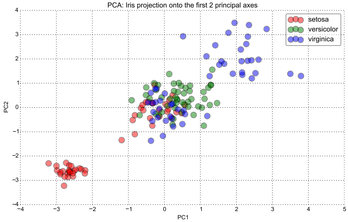

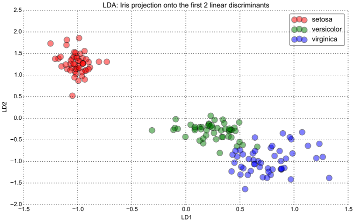

- Similar to PCA, we can use LDA for dimensionality reduction by looking at an eigenvalue problem
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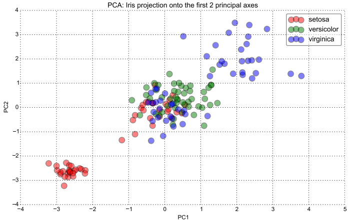
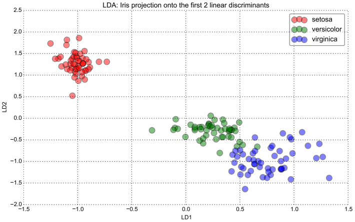
PCA vs LDA





- Similar to PCA, we can use LDA for dimensionality reduction by looking at an eigenvalue problem
- LDA: Magnitude of the eigenvalues in LDA describe importance of the corresponding eigenspace with respect to classification performance
- PCA: Magnitude of the eigenvalues in LDA describe importance of the corresponding eigenspace with respect to minimizing reconstruction error

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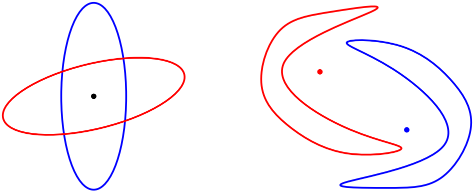
  ⏩ Shrinkage (Copas, 1983)
- LDA explicitly attempts to model the difference between the classes of data. PCA on the other hand does not take into account any difference in class

Limitations of LDA



- LDA's most disriminant features are the means of the data distributions
- LDA will fail when the discriminatory information is not the mean but the variance of the data.
- If the data distributions are very non-Gaussian, the LDA projections will not preserve the complex structure of the data that may be required for classification

▶▶ Nonlinear LDA (e.g., Mika et al., 1999; Baudat & Anouar, 2000)

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