Clustering and Classification

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NYU / CUSP - GX 5006

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Learning Strategies

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Situations were data is partially annotated are also common (semi-supervised tasks, more often in classification).

Clustering

Introduction

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- Hierarchical
  - Single Link
  - ⋮
- Partitional
  - K-means
  - Mixture Resolving
  - Spectral Clustering
  - Density-based
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  - Single Link
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- Partitional
  - K-means
  - Mixture Resolving
  - Spectral Clustering (later in this course)
  - Density-based
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Hierarchical Clustering

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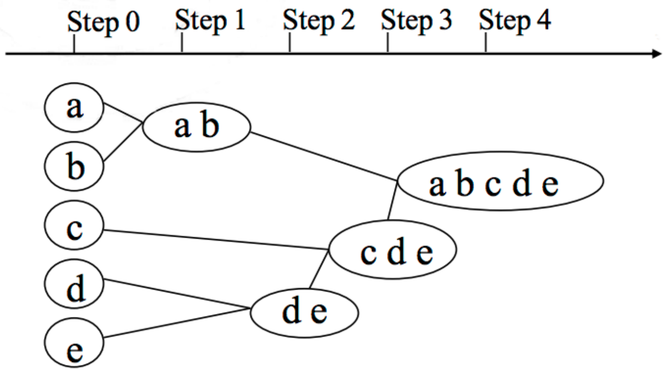

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Step 3 can assume different forms:

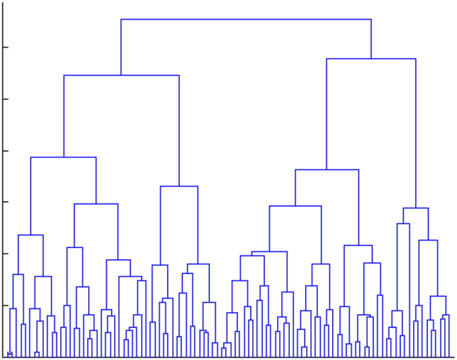
$$d(C_a, C_b) = \min_{i \in C_a, j \in C_b}]\{d(i,j)\} \quad \text{Single Link}$$

$$d(C_a, C_b) = \max_{i \in C_a, j \in C_b} \{d(i,j)\} \quad \text{Complete Link}$$

$$d(C_a, C_b) = \frac{1}{n_a n_b} \sum_{i \in C_a, j \in C_b} \{d(i,j)\} \quad \text{Average Link}$$

Hierarchical Clustering

Dendogram



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$\boldsymbol{\mu}_j$ is simply the average of the $\mathbf{x}_i \in cluster_j$.

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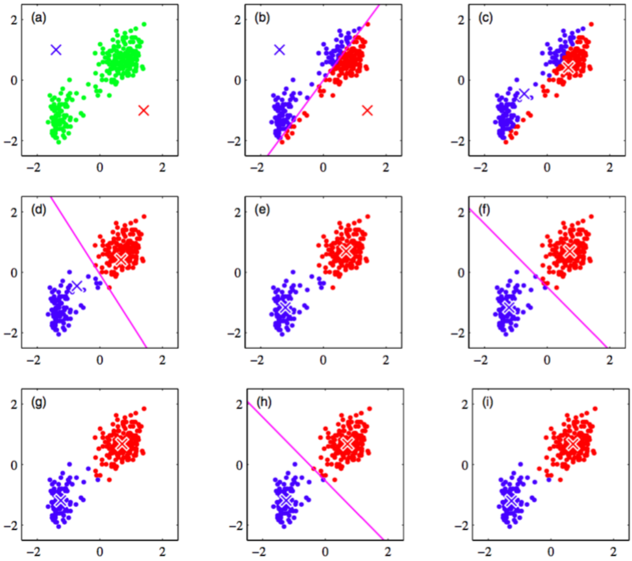

(figure extracted from Bishop's book)

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- There are versions able to handle dynamic data
- The algorithm can be adapted to deal with “distances” (dissimilarities) other than Euclidean distance (see chapter 9 of Bishop’s book).

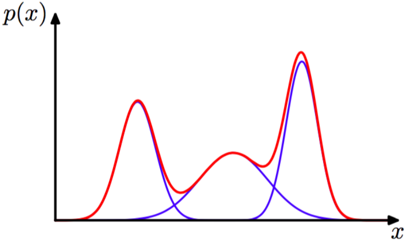
Mixture Resolving

Mixture Resolving

A Gaussian mixture distribution is given by

$$p(\mathbf{x}) = \sum_{i=1}^{k} c_i N(\mathbf{x}|\boldsymbol{\mu}_i, \sigma_i)$$

where $c_i \geq 0$ and $\sum_i c_i = 1$.



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Given a data set $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, a mixture solving algorithm aims to find parameters c_i, $\boldsymbol{\mu}_i$, Σ_i and a "responsibility" (membership) function γ_{ij} so as to maximize the likelihood

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Such optimization can be accomplish via an Expectation Maximization strategy (chapter 9 of Bishop's book).

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Steps E and M are repeated until convergence.

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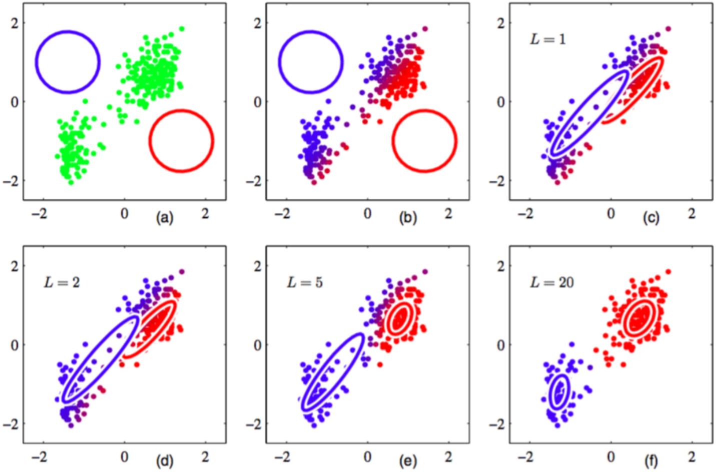

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The convergence of Mixture Resolving is slower.
K-means is typically used to set initial conditions !!

Classification

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- Logistic Regression
- Bayesian Classifier
- SVM
- Neural Networks
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- SVM (next class)
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- ⋮

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$\mathbf{x}$ should be assigned to the class y that satisfies

$$\arg\max_y \log(p(y|\mathbf{x}))$$

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Thus, assuming a single covariance matrix for all Gaussians, the decision boundary is linear

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The *Linear Discriminant Analysis* (LDA) algorithm simply estimates the parameters from the training data as (approximates the MLE solution):

$$\hat{p}(y) = \frac{n_y}{n}$$

$$\hat{\boldsymbol{\mu}}_y = \frac{1}{n_y} \sum_{\mathbf{x}_i \in y} \mathbf{x}_i$$

$$\hat{\Sigma} = \frac{1}{n-k} \sum_{y} \sum_{\mathbf{x}_i \in y} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_y)(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_y)^\top$$

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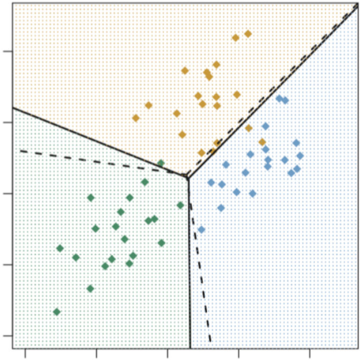
Since the covariance is constant for all classes, LDA has a linear decision boundary



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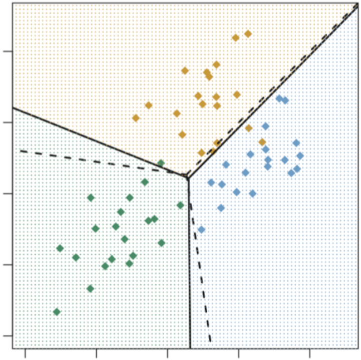
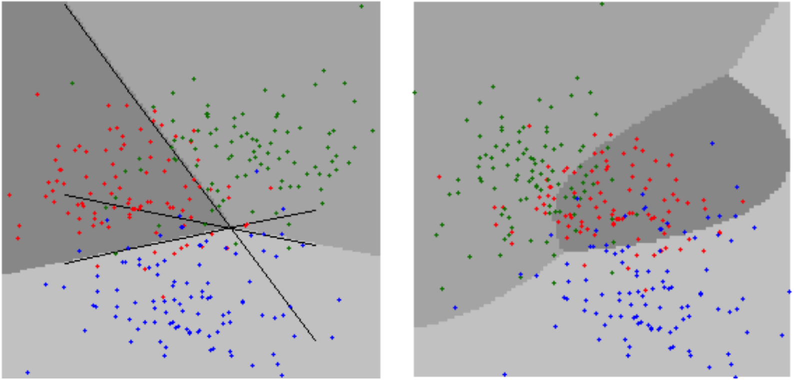


This is one of the main limitations when using a single covariance matrix. Non-linear boundaries can be obtained solving the MLE problem with distinct covariance matrices for each class.

Bayes Classifier



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Therefore,

$$p(y|\mathbf{x}) \propto p(\mathbf{x}|y)\, p(y) = p(y) \prod_{j=1}^{d} p(x_j|y)$$

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Naive Bayes assume a joint density distribution for

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Recalling that $\mathbf{x} \in \mathbb{R}^d$, the Naive Bayes classifier assumes that

$$p(\mathbf{x}|y) \sim \prod_{j=1}^{d} p(x_j|y)$$

the attributes of each data instances are independent (notice x_j is not bold, it is a scalar representing the j-th attribute of $\mathbf{x}$).

Therefore,

$$p(y|\mathbf{x}) \propto p(\mathbf{x}|y)\, p(y) = p(y) \prod_{j=1}^{d} p(x_j|y)$$

The class y to be assigned to $\mathbf{x}$ is the one satisfying

$$\arg\min_{y} p(y) \prod_{j=1}^{d} p(x_j|y)$$

Naive Bayes Classifier: Discrete Case

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x_i	age	income	job status	gender	class
1	20-30	medium	manager	male	ok
2	40-50	high	engineer	female	rich
3	20-30	medium	student	male	ok
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
n	60-70	medium	retired	male	poor

Naive Bayes Classifier: Discrete Case

$p(poor) = \frac{\#poor}{n}$, $p(ok) = \frac{\#ok}{n}$, $p(rich) = \frac{\#rich}{n}$
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$$\arg\min_y p(y) \prod_{j=1}^{d} p(x_j|y)$$

Laplace correction (add 1 in each count) makes possible to deal with zero conditionals.

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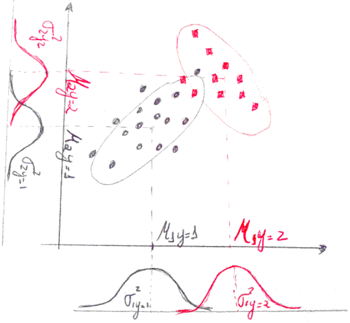

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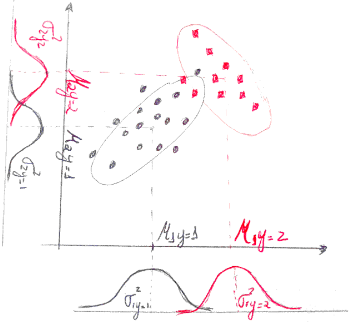

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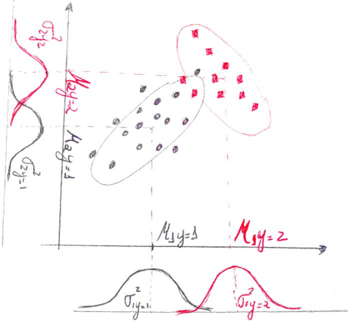

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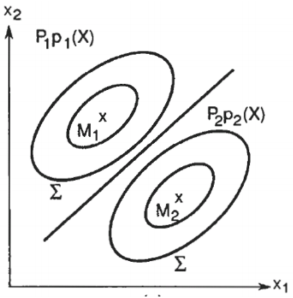
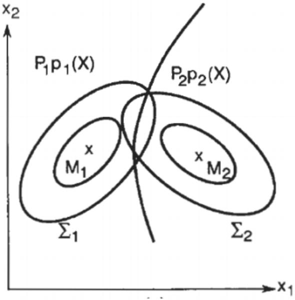
which results in:

$$\hat{\mu}_{jy} = \frac{1}{n_y} \sum_{\mathbf{x} \in y} x_j \quad \hat{\sigma}^2_{iy} = \frac{1}{n_y} \sum_{\mathbf{x} \in y} (x_j - \hat{\mu}_{jy})^2$$

Naive Bayes Classifier: Gaussian

Decision Boundary





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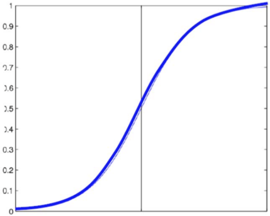
Considering two classes $y \in \{0, 1\}$, the logistic regression assumption is:

$$p(y|\mathbf{x}) = \frac{1}{1 + \exp(-(\beta_0 + \mathbf{x}^\top \boldsymbol{\beta_1}))}$$



$\beta_0 + \mathbf{x}^\top \boldsymbol{\beta_1} \geq 0$ means $\mathbf{x}$ to class 1 and to class 0 otherwise (linear decision boundary).

Logistic Regression

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Parameters β_0 and $\boldsymbol{\beta}_1$ can be obtained by MLE.

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The maximization has no analytical formula and a gradient descent is typically applied to numerical approximation of the parameters.

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