Classification: LDA, QDA, knn, cross-validation

TMA4300: Computer Intensive Statistical Methods
(Spring 2016)

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*Slides are based on lecture notes kindly provided by Håkon Tjelmeland.

Last part of this course

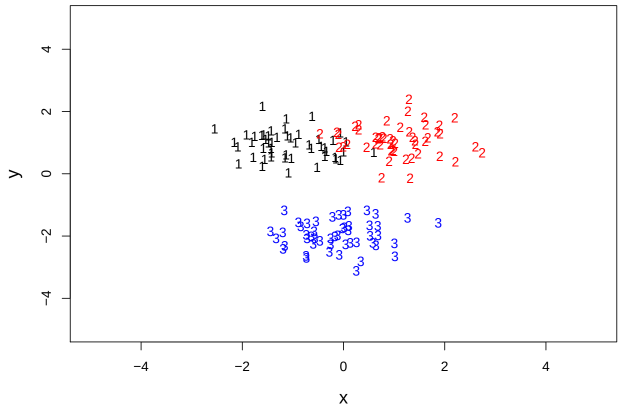
⇒ Not closely related to the two first parts

⇒ Three topics (not closely related to each other):

- Classification problem
- Bootstrapping
- Expectation-Maximization algorithm

Classification

Situation: Have observations $x_1, \ldots, x_n$ and corresponding class labels $y_1, \ldots, y_n$, where $y_i \in \{0, 1, \ldots, J-1\}$ (Training data)



New observation: x_0

Classification of the new observation

- Goal: Classify the new observation x_0 to one of the J possible classes.
- Alternatively, want to assign probabilities

$$\pi_j(x_0) = \mathrm{P}(y_0 = j | X = x_0)$$

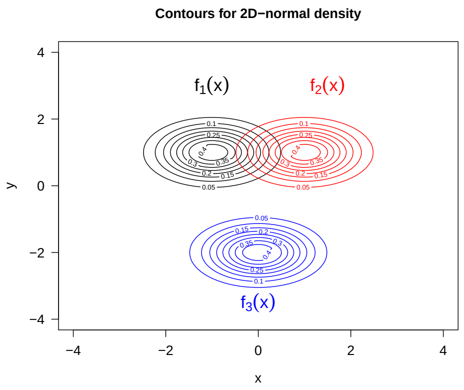
for $j = 0, \ldots, J-1$.

Example: x denotes the results of a medical test with $y \in \{0, 1, 2\}$ where ($y = 0$: healthy, $y = 1$: disease 1, $y = 2$: disease 2).

Model

- We assume a distribution for x that depends on the class y:

$$f(x|y=j) = f_j(x)$$



- and prior probabilities for class j: $p_j = P(y=j)$.

Model (II)

Thus, we assume a joint distribution for x and y:

$$f(x, y=j) = p_j f_j(x)$$

Comment: Must estimate $f_j(x)$ from training data

$$(x_1, y_1), \ldots, (x_n, y_n),$$

perhaps also estimate $p_0, \ldots, p_{J-1}$. For now, assume $p_0, \ldots, p_{J-1}, f_0(x), \ldots, f_{J-1}(x)$ known.

What is then $\pi_j(x_0)$ and $\hat{y}_0$?

Use Bayes rule

$$\begin{aligned}
\pi_j(x_0) &= \mathrm{P}(y_0 = j | X = x_0) \\
&= \frac{\mathrm{P}(y_0 = j, x_0)}{f(x_0)} \\
&= \frac{\mathrm{P}(y_0 = j, x_0)}{\sum_{i=0}^{J-1} \mathrm{P}(y_0 = i, x_0)} \\
&= \frac{p_j f_j(x_0)}{\sum_{i=0}^{J-1} p_i f_i(x_0)}.
\end{aligned}$$

For classification, need to consider the *cost* of misclassification. Some misclassification may be more *costly* than others.

Example: More *costly* to classify a person as healthy when he/she really has disease, than vice versa.

Cost function

Assume a cost function:

- $c(i|j)$: cost of classifying a subject to class i when the true class is j.
- In particular, $c(i|i) = 0$, for $i = 0, \ldots, J-1$.

Then, it is natural to make the classification by minimising the expected cost.

See blackboard

Bayes classifier:

$$\hat{y}_0 = \mathrm{argmax}_i \{p_i f_i(x_0)\}$$

Practical challenge

$p_0, \dots, p_{J-1}, f_0(x), \dots, f_{J-1}(x)$ are unknown. Different possibilities exist:

i) estimate the unknown properties from the training data:

$$\hat{p}_j = \frac{\#\{y_i = j\}}{n}$$

a) Estimate each $f_j(x)$ by density estimation, or

b) assume parametric form for $f_j(x)$ and estimate its parameters.

ii) Bayesian modelling: Put prior distributions on the unknown quantities. For example

$$(p_0, \dots, p_{J-1}) \sim \text{Dirichlet}$$

$$x|y = j \sim \mathcal{N}(\mu_j, \mathbf{\Sigma}_j)$$

$$\text{hyper-priors on } \mu_j, \mathbf{\Sigma}_j$$

Discriminant analysis

We will now only consider alternative i) b).

Assume

$$x|y = j \sim \mathcal{N}(\mu_j, \mathbf{\Sigma}_j)$$

Two (extreme) alternatives:

- assume $\mathbf{\Sigma}_0 = \mathbf{\Sigma}_1 = \dots = \mathbf{\Sigma}_{J-1} = \mathbf{\Sigma}$
- different covariance matrices (more parameters to estimate)

Linear discriminant analysis (LDA)

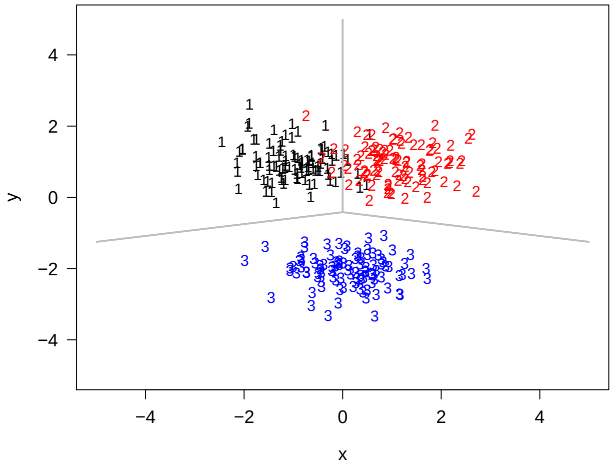
Consider first $\mathbf{\Sigma}_0 = \mathbf{\Sigma}_1 = \dots = \mathbf{\Sigma}_{J-1} = \mathbf{\Sigma}$. Then for given parameters, the Bayes decision rule becomes (i.e. using "0/1-loss"):

$$\begin{aligned}
\hat{y}_0 &= \text{argmax}_i \left\{ p_i \cdot \frac{1}{(2\pi)^{1/2}} \frac{1}{\sqrt{|\mathbf{\Sigma}|}} \exp\left(-\frac{1}{2}(x_0 - \mu_i)^\top \mathbf{\Sigma}^{-1}(x_0 - \mu_i) \right) \right\} \\
&= \text{argmax}_i \left\{ -\frac{1}{2}(x_0 - \mu_i)^\top \mathbf{\Sigma}^{-1}(x_0 - \mu_i) + \log(p_i) \right\} \\
&= \text{argmax}_i \left\{ x_0^\top \mathbf{\Sigma}^{-1}\mu_i - \frac{1}{2}\mu_i^\top \mathbf{\Sigma}^{-1}\mu_i + \log(p_i) \right\} \\
&= \text{argmax}_i \left\{ \hat{\delta}_i(x_0) \right\}
\end{aligned}$$

with $\hat{\delta}_i(x_0) = x_0^\top \mathbf{\Sigma}^{-1}\mu_i - \frac{1}{2}\mu_i^\top \mathbf{\Sigma}^{-1}\mu_i + \log(p_i)$.

LDA (cont.)

Note: $\hat{\delta}_i(x_0)$ is linear in x_0. Thus the Bayes decision borders between the classification regions become lines/hyper-planes.



LDA: Example

Note: $\hat{\delta}_i(x_0)$ is linear in x_0. Thus the borders between the classification regions become lines/hyper-planes.

Example

- The center of mass of the individual classes are at:

$$\boldsymbol{\mu}_1 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \boldsymbol{\mu}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \boldsymbol{\mu}_3 = \begin{pmatrix} 0 \\ -2 \end{pmatrix} .$$

- The joint covariance matrix has the form $\boldsymbol{\Sigma} = \begin{pmatrix} 0.5 & 0 \\ 0 & 0.25 \end{pmatrix}$.
- The a-priori probabilities are equal: $p_1 = p_2 = p_3 = \frac{1}{3}$.

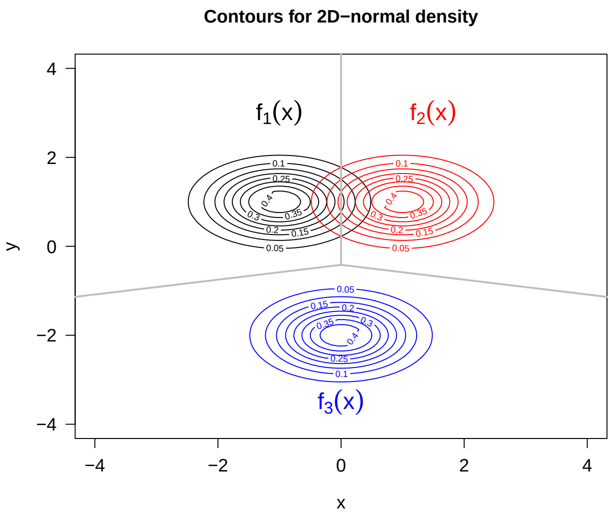
LDA: Example (II)

For the *line of separation due to Bayes' rule* we get:

$$x^\top \boldsymbol{\Sigma}^{-1} \mu_i - \frac{1}{2}\mu_i^\top \boldsymbol{\Sigma}^{-1} \mu_i + \log(p_i) = x^\top \boldsymbol{\Sigma}^{-1} \mu_j - \frac{1}{2}\mu_j^\top \boldsymbol{\Sigma}^{-1} \mu_j + \log(p_j) .$$

- $-2x_1 + 4x_2 - 3 = 2x_1 + 4x_2 - 3$,
  i.e. $x_1 = 0$ is line of separation between classes 1 and 2.
- $-2x_1 + 4x_2 - 3 = -8x_2 - 8$,
  i.e. $x_2 = \frac{1}{6}x_1 - \frac{5}{12}$ is line of separation between classes 1 and 3.
- $2x_1 + 4x_2 - 3 = -8x_2 - 8$,
  i.e. $x_2 = \frac{-1}{6}x_1 - \frac{5}{12}$ is line of separation between classes 2 and 3.
- All lines meet at point $\left(0, \quad -\frac{5}{12}\right)$.

LDA: Example (III)



Practical comments

In practice we estimate $p_0, \ldots, p_{J-1}, \mu_0, \ldots, \mu_{J-1}, \boldsymbol{\Sigma}$ by

$$\hat{p}_j = \frac{\sum_{i=1}^n 1(y_i = j)}{n}$$

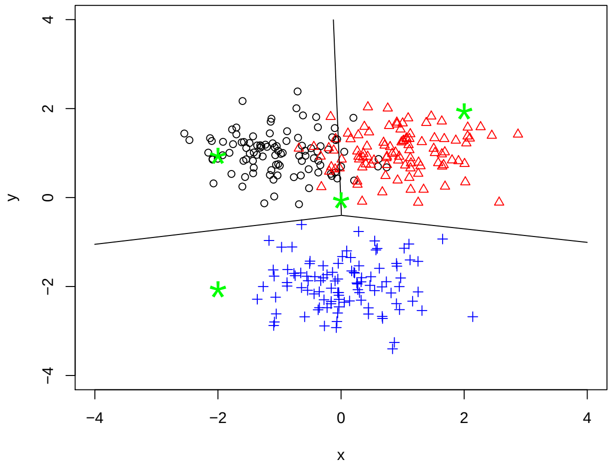
$$\hat{\mu}_j = \frac{\sum_{i=1}^n 1(y_i = j) x_i}{\sum_{i=1}^n 1(y_i = j)}$$

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n-J} \sum_{i=1}^n (x_i - \hat{\mu}_{y_i})(x_i - \hat{\mu}_{y_i})^\top$$

where $1(\cdot)$ is the indicator function. Then we use

$$\hat{\delta}_i(x_0) = x_0^\top \hat{\boldsymbol{\Sigma}}^{-1} \hat{\mu}_i - \frac{1}{2}\hat{\mu}_i^\top \hat{\boldsymbol{\Sigma}}^{-1} \hat{\mu}_i + \log(p_i)$$

Result of lda-function in R



Projections are done using the `predict()` function (see R-code).

Quadratic discriminant analysis (QDA)

Consider next the case where the covariance matrices are different (still assuming 0/1-loss). Thus,

$$x|y = j \sim \mathcal{N}(\mu_j, \mathbf{\Sigma}_j)$$

Then

$$\hat{y}_0 = \text{argmax}_i \left\{ p_i \cdot \frac{1}{(2\pi)^{1/2}} \frac{1}{\sqrt{|\mathbf{\Sigma}_i|}} \exp\left(-\frac{1}{2}(x_0 - \mu_i)^\top \mathbf{\Sigma}_i^{-1} (x_0 - \mu_i) \right) \right\}$$

$$= \text{argmax}_i \left\{ \underbrace{-\frac{1}{2}(x_0 - \mu_i)^\top \mathbf{\Sigma}_i^{-1}(x_0 - \mu_i) + \log(p_i) - \frac{1}{2}\log|\mathbf{\Sigma}_i|}_{=\hat{\delta}_i(x_0)} \right\}$$

Thus, $\hat{\delta}_i(x_0)$ is quadratic in x_0 and the Bayes decision borders between the classification regions become quadratic.

k-nearest neighbour (KNN) classification

Assume we do not want to do any assumptions about $f_i(x_0)$ except that it is *smooth*. Reasonable to estimate $p_i f_i(x_0)$ by $\widehat{p_i f_i(x_0)} \approx$ number of data points (in the training set) "close to" x_0 that have $y_j = i$.

How to define "close to"?

Not a good idea: "close to" means $||x_i - x_0|| \leq R$, because the set may be empty for some x_0, and very large for others.

KNN classification

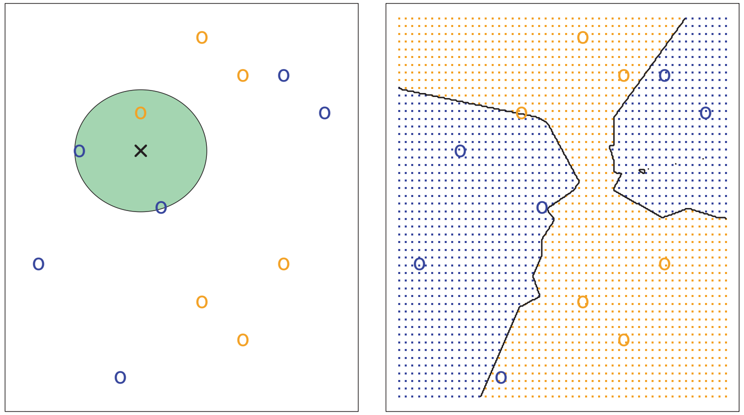
Let R depend on x_0 (and the training set), so that the number of training values with $||x_i - x_0|| \leq R$ is equal to k for all x_0. Then we get the k-nearest-neighbour classifier.

Algorithm:

1. find the k x_i's closest to x_0 (in some norm)
2. choose $\hat{y}_0$ by majority vote among these k neighbours.

Here, k is a tuning parameter.

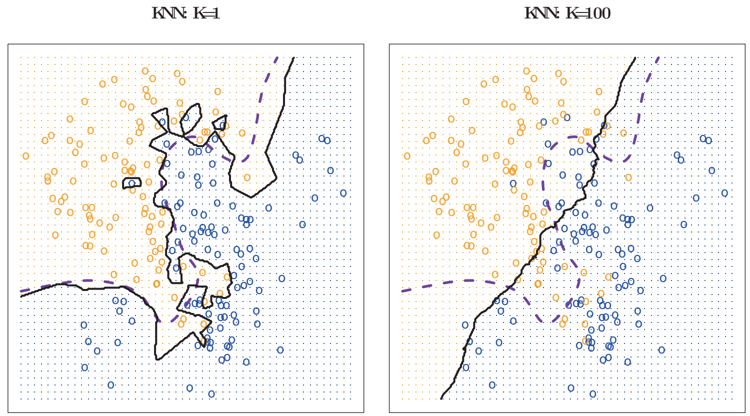
KNN classification - Example K=3



(James, Witten, Tibshirani, Hastie (2014), An Introduction to Statistical Learning, Springer, p.40)

Show animation in R: `knn.ani` in animation package.

k-nearest-neighbour classifiers



(James, Witten, Tibshirani, Hastie (2014), An Introduction to Statistical Learning, Springer, p.41)

Cross-validation

Consider a classification problem:

Have observed $(x_1, y_1), \ldots, (x_n, y_n) \leftarrow$ training data. Have one (or more) classification rule(s):

$$\hat{y}(x_0; (x_1, y_1), \ldots, (x_n, y_n))$$

How can we evaluate how good the rule is? Alternatively, how can we decide which rule is the best?

Misclassification rate

It is reasonable to focus on

- the misclassification rate

$$P(y_0 \neq \hat{y}(x_0; (x_1, y_1), \ldots, (x_n, y_n)))$$

, or

- expected cost (from misclassification)

$$E[c(\hat{y}(x; (x_1, y_1), \ldots, (x_n, y_n))|y)]$$

Apparent error rate

The apparent misclassification rate classifies each member of the training sample and becomes

$$\frac{1}{n}\sum_{i=1}^{n} 1(y_i \neq \hat{y}(x_i; (x_1, y_1), \ldots, (x_n, y_n))$$

This estimate becomes clearly too optimistic because we use the same data to "train" the classifier and to estimate the misclassification rate.

We have to take into account:

- the assumed (parametric) model may be wrong.
- uncertainty in the parameter estimates
- inherent randomness

If we have a lot of training data ...

...the effect of parameter uncertainty is negligible and we can do the following:

1. divide the (training) data in two parts: training and test set
2. establish classifier from training set data
3. do classification for data in test data set, and estimate misclassification rate by the fraction of misclassification in test set.

Note: If we do not have so many training data this procedure will overestimate the misclassification rate, i.e. too pessimistic.

Idea k-fold cross validation

- Cross-validation can be use to estimate the misclassification rate of a statistical classification method.
- k-fold cross-validation involves randomly dividing the set of observations into k groups, or folds, $A_1, \ldots, A_k$ of approximately equal size.
- For the j-th fold (test set), we fit the model to the other $k-1$ folds (training set) of the data, and count the number of misclassifications of the fitted model when predicting the j-th part of the data.
- We do this for $j = 1, 2, \ldots, k$ and combine the k estimates
- Leave-one-out cross validation is a special case.

Leave-one-out cross validation (CV)

Let $\hat{y}(x) = \hat{y}(x; (x_1, y_1), \ldots, (x_n, y_n))$ denote our classifier based on all training data. Let

$$\hat{y}_{-i}(x) = \hat{y}(x; (x_1, y_1), \ldots, (x_{i-1}, y_{i-1}), (x_{i+1}, y_{i+1}), \ldots, (x_n, y_n))$$

be our classifier based on all training data except (x_i, y_i).

Estimate the misclassification rate by:

$$\frac{1}{n}\sum_{i=1}^{n} 1(y_i \neq \hat{y}_{-i}(x_i))$$

Leave-one-out CV is computationally expensive. A cheaper variant is K-fold CV

K-fold CV

Divide at random training data into K sets $A_1, \dots, A_K$ of equal size (or as close as possible). Let

$$\hat{y}_{-A_k}(x) = \hat{y}(x; (x_i, y_i), i \in \bigcup_{j \neq k} A_j)$$

and estimate the misclassification rate by

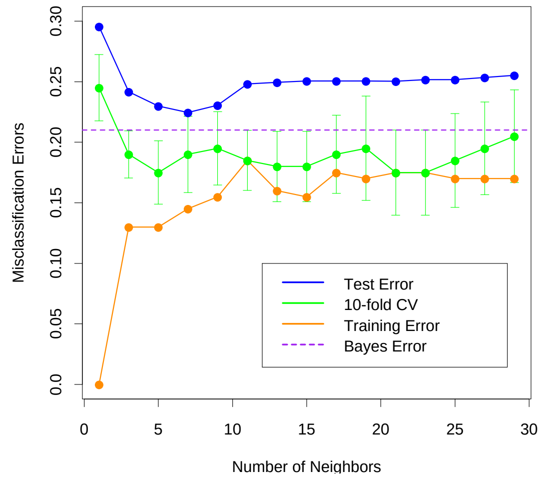
$$\frac{1}{n} \sum_{k=1}^{K} \left[\sum_{i \in A_k} 1(y_i \neq \hat{y}_{-A_k}(x_i)) \right].$$

Often, $K = 5$ or $K = 10$ is used.

Note: The tuning parameter k in the knn-classifier can be chosen using CV.

Show animation in R: `cv.ani` in animation package.

Misclassification as function of k



Hastie, Tibshirani, Friedman, "The elements of statistical learning", 2nd ed., p. 467