ML01 – Introduction to Machine Learning

Linear and Quadratic Classification

Thierry Denœux

tdenoeux@utc.fr
https://www.hds.utc.fr/~tdenoeux

Université de technologie de Compiègne

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Overview

1 Introduction to classification
- Basic notions
- Bayes classifier
- Voting K-NN rule

2 Linear and quadratic discriminant analysis
- Model
- Case of binary classification
- Related models

3 Logistic regression and related models
- Binary logistic and probit regression
- Multinomial logistic regression
- Ordered probit and logit regression

4 Appendix

Classification

- In classification problems, the response variable Y is nominal, i.e., it takes valued in a finite and unordered set $\mathcal{C}$, e.g.
  - Email is one of $\mathcal{C} = \{\text{spam}, \text{email}\}$
  - Facial expression is one of $\mathcal{C} = \{\text{sadness}, \text{joy}, \text{disgust}, \ldots\}$
  - Object is one of $\mathcal{C} = \{\text{pedestrian}, \text{car}, \text{bike}, \ldots\}$, etc.
- The elements in $\mathcal{C}$ are called classes. They are arbitrarily numbered $1, 2, \ldots, c$.
- Our goals are to:
  - Build a classifier $C : \mathbb{R}^p \to \mathcal{C}$ that predicts the class a future predictor vector X.
  - Assess the uncertainty in each classification
  - Understand the roles of the different predictors
- In this chapter, we will also see how to handle the case where Y is an ordinal variable, i.e., the elements of $\mathcal{C}$ are ordered. This learning task is called ordinal regression/classification.

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1. Introduction to classification
   - Basic notions
   - Bayes classifier
   - Voting K-NN rule
2. Linear and quadratic discriminant analysis
   - Model
   - Case of binary classification
   - Related models
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   - Binary logistic and probit regression
   - Multinomial logistic regression
   - Ordered probit and logit regression
4. Appendix

Formalization

- We have a feature (predictor) vector X, and a discrete response variable Y, both random.
- To represent the joint distribution of (X, Y), we can give:
  1. The marginal distribution of Y. We use the notation
  $$\pi_k = \mathbb{P}(Y = k),$$
  and we call π_k the prior probability of class k. We have
  $$\sum_{k=1}^{c} \pi_k = 1$$
  2. The conditional probability density functions (pdf's) of X given $Y = k$, for $k = 1, \ldots, c$. We use the notation
  $$p_k(x) = p(x \mid Y = k)$$

Formalization (continued)

We can then compute

- The marginal (mixture) pdf of X as

$$p(x) = \sum_{k=1}^{c} p_k(x)\pi_k$$

- The conditional distribution of Y given $X = x$ using Bayes' theorem. Let

$$P_k(x) = \mathbb{P}(Y = k \mid X = x)$$

  denote the posterior (conditional) class probabilities. We have

$$\boxed{P_k(x) = \frac{p_k(x)\pi_k}{p(x)}, \quad k = 1, \ldots, c}$$

Example

- Consider a classification problem with $c = 3$ classes and $p = 1$ feature.
- Assume that

$$\pi_1 = 0.3, \quad \pi_2 = 0.5, \quad \pi_3 = 0.2$$

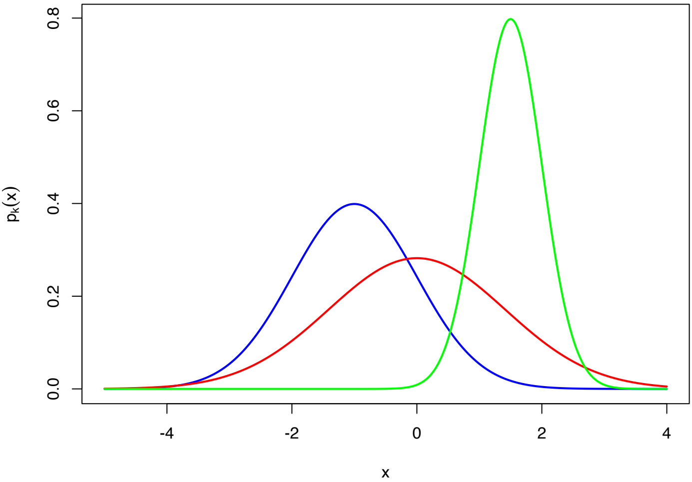
$$p_k(x) = \phi(x; \mu_k, \sigma_k)$$

where ϕ is the normal pdf, with

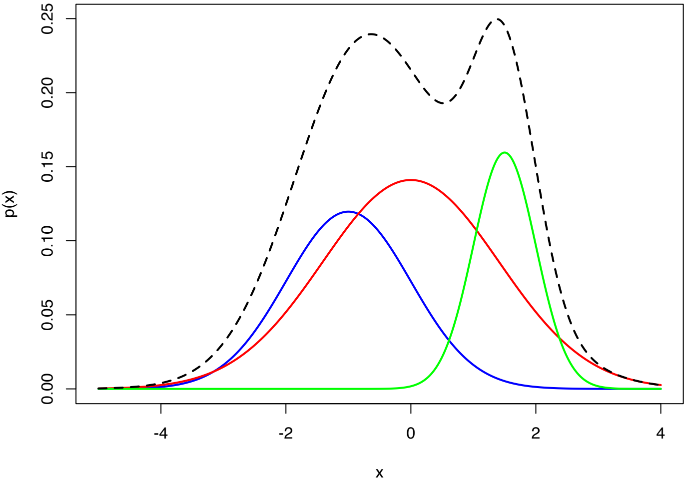
$$\mu_1 = -1, \quad \mu_2 = 0, \quad \mu_3 = 1.5$$

$$\sigma_1 = 1, \quad \sigma_2 = \sqrt{2}, \quad \sigma_3 = 0.5$$

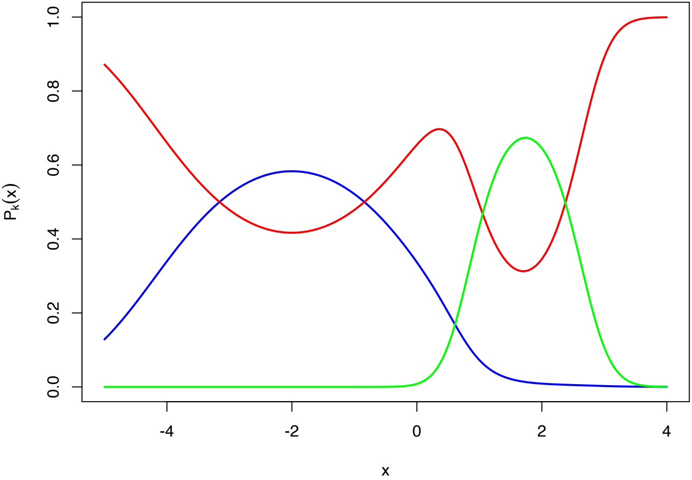
Example: conditional densities $p_k(x)$



Example: marginal density $p(x)$



Example: posterior probabilities $P_k(x)$



Overview

1. Introduction to classification
   - Basic notions
   - Bayes classifier
   - Voting K-NN rule
2. Linear and quadratic discriminant analysis
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4. Appendix

The Bayes classifier

- The conditional error probability for classifier $C(x)$ is

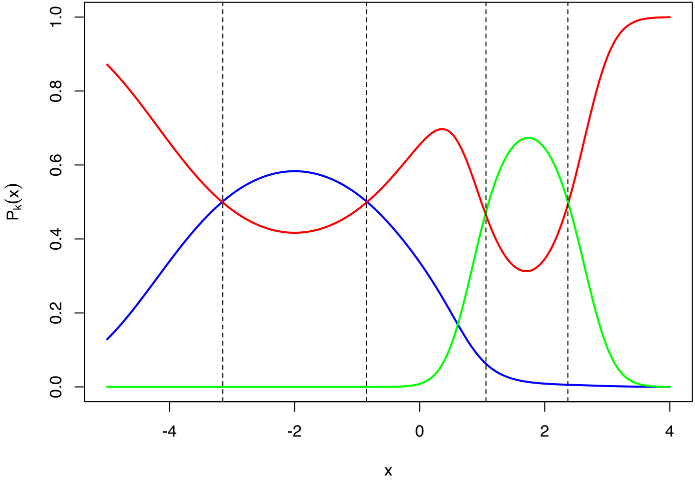
$$\begin{aligned}\mathbb{P}(\text{error} \mid X = x) &= \mathbb{P}(C(X) \neq Y \mid X = x)\\ &= 1 - \mathbb{P}(C(X) = Y \mid X = x)\end{aligned}$$

- If $C(x) = k$, then

$$\mathbb{P}(\text{error} \mid X = x) = 1 - \mathbb{P}(Y = k \mid X = x) = 1 - P_k(x)$$

- To minimize $\mathbb{P}(\text{error} \mid X = x)$, we must choose k such that $P_k(x)$ is maximum.
- The corresponding classifier $C^*(x)$ is called the Bayes classifier. It has the lowest error probability.

Example: decision regions of the Bayes classifier



Bayes error rate

- For $X = x$, the Bayes classifier predicts class k^* such that $P_{k^*}(x) = \max_k P_k(x)$, and the conditional error probability

$$1 - P_{k^*}(x) = 1 - \max_k P_k(x)$$

- The error probability of the Bayes classifier (averaged over all values of X) is

$$\text{Err}_B = \mathbb{E}_X \left[1 - \max_k P_k(X) \right] = \int \left[1 - \max_k P_k(x) \right] p(x) dx$$

- This probability is called the Bayes error rate. It is the lowest error probability that can be achieved by a classifier. It characterizes the difficulty of the classification task.

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2. Linear and quadratic discriminant analysis
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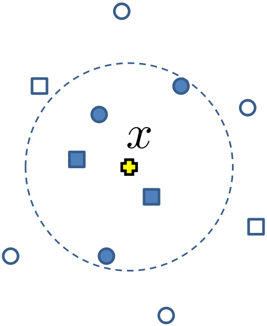
4. Appendix

K nearest neighbors



- Nearest-neighbor averaging can be used as in regression.
- Let $x_{(1)}, \ldots, x_{(K)}$ denote the K nearest neighbors of x in the learning set, and $y_{(1)}, \ldots, y_{(K)}$ the corresponding class labels.

Voting K-nearest-neighbor rule

- The posterior probability of class k can be estimated by the proportion of observations from that class among the K nearest neighbors of x:

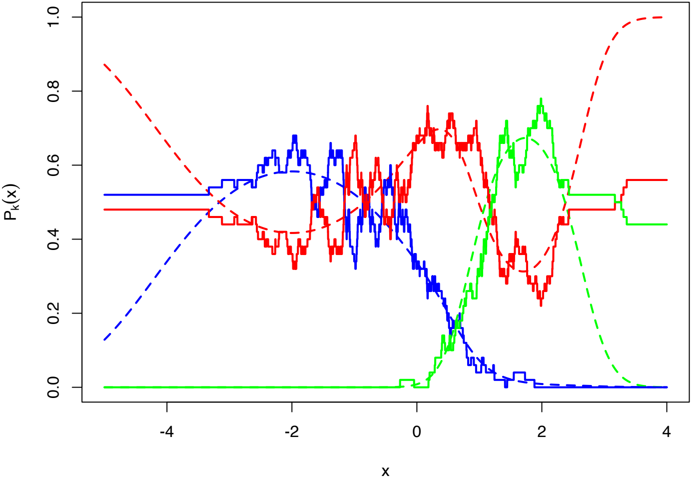
$$\widehat{P}_k(x) = \frac{1}{K} \#\{i \in \{1, \ldots, K\} : y_{(i)} = k\}$$

- Voting K-nearest neighbor (K-NN) rule: select the majority class among the K nearest neighbors:

$$C_K(x) = \arg\max_k \widehat{P}_k(x).$$

- As in regression, the K-NN rule breaks down as dimension grows. However, the impact on $C_K(x)$ is less than that on the probability estimates $\widehat{P}_k(x)$.

Example: voting K-NN rule with $n = 1000$ and $K = 50$



Error probability estimation

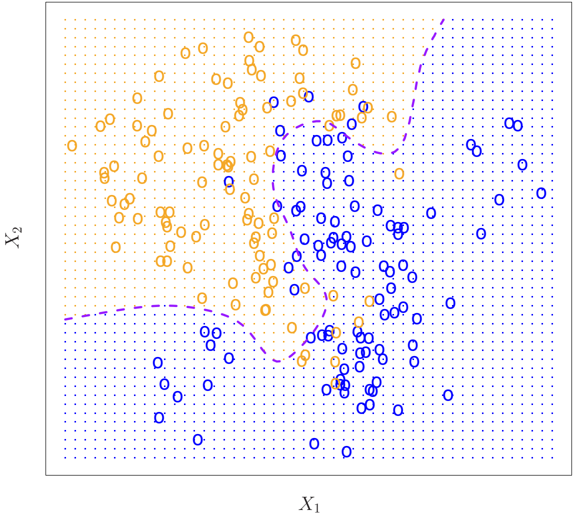
- Typically, we measure the performance of a classifier $C(X)$ using the test error rate:

$$\text{Err}_{\mathcal{T}} = \frac{1}{m} \# \left\{ i \in \{1, \ldots, m\} : y'_i \neq C(x'_i) \right\},$$

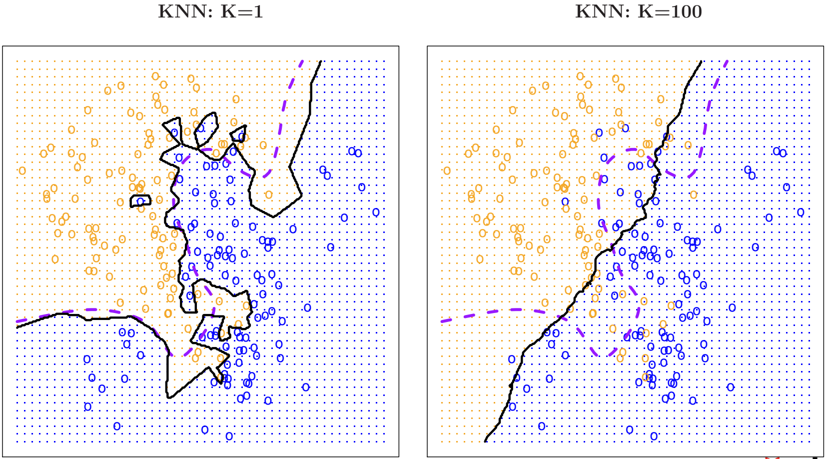
where $\mathcal{T}$ is a test dataset.

- The test error rate allows us to select the best model in a set of candidate models (more on this later).

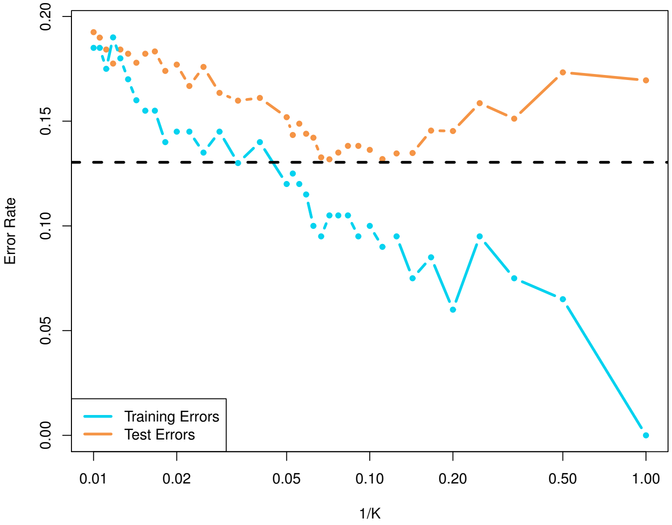
Example: simulated data and Bayes decision boundary



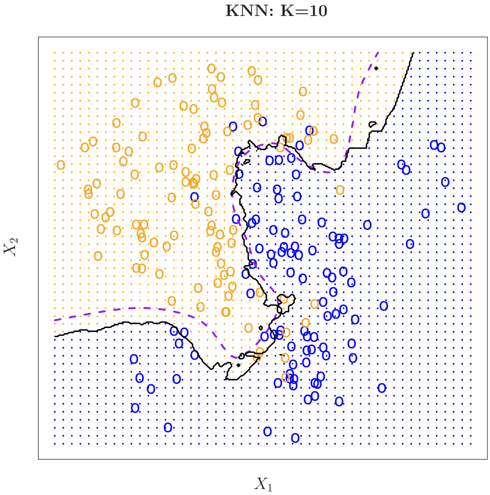
Decision boundaries for $K = 1$ and $K = 100$



Training and test error rates vs. $1/K$



Decision boundary for the best value of K



Overview

1. Introduction to classification
   - Basic notions
   - Bayes classifier
   - Voting K-NN rule
2. Linear and quadratic discriminant analysis
   - Model
   - Case of binary classification
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   - Binary logistic and probit regression
   - Multinomial logistic regression
   - Ordered probit and logit regression
4. Appendix

Linear/quadratic classification

- Since our classifier $C(X)$ takes values in a finite set $\mathcal{C}$, we can always divide the input space into a collection of decision regions:

$$\mathcal{R}_k = \{x \in \mathbb{R}^p : C(x) = k\}, \quad k = 1, \ldots, c.$$

- The boundaries of these regions can be rough or smooth, depending on the prediction function.
- For an important class of procedures, these decision boundaries are linear or quadratic, i.e., they have equations of the form

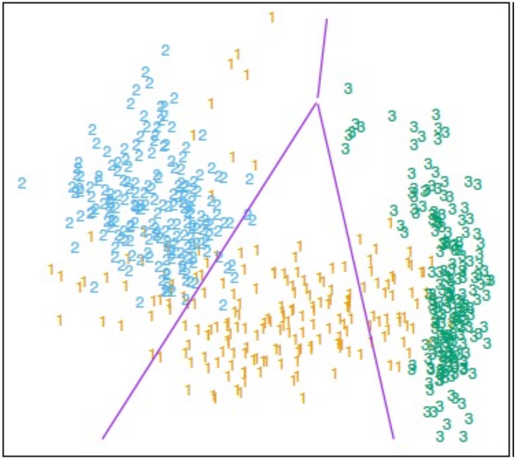
$$\beta^T x + \beta_0 = 0 \quad \text{(linear)}$$

or

$$x^T Q x + \beta^T x + \beta_0 = 0 \quad \text{(quadratic)}$$

- This is what we will mean by linear and quadratic methods for classification.

Example



Generative vs. discriminative models

- To approximate Bayes' rule, we need to estimate the posterior probabilities $P_k(x) = P(Y = k \mid X = x)$.
- We can distinguish two kinds of models for classification:

  Generative models represent the conditional pdf's $p_k(x)$ and the prior probabilities π_k. Using Bayes' theorem, we then get the posterior probabilities $P_k(x)$.

  Discriminative models represent the conditional probabilities $P_k(x)$ directly, or a direct map from inputs x to $\mathcal{C}$.
- In this chapter, we will focus on two families of classifiers:
  1. Linear and quadratic classifiers based on a generative model: Linear Discriminant Analysis (LDA) and Quadratic Discriminant Analysis (QDA).
  2. A linear classifier based on a discriminative model: Logistic regression.

Overview

1. Introduction to classification
   - Basic notions
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2. Linear and quadratic discriminant analysis
   - Model
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   - Multinomial logistic regression
   - Ordered probit and logit regression
4. Appendix

Model

- Linear discriminant analysis (LDA) and quadratic discriminant analysis (QDA) both use multivariate normal densities for $p_k(x)$

$$p_k(x) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}_k|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu_k)^T\boldsymbol{\Sigma}_k^{-1}(x-\mu_k)\right\},$$

  where $\mu_k = \mathbb{E}(X \mid Y=k)$ and $\boldsymbol{\Sigma}_k = \mathrm{Var}(X \mid Y=k)$.
- LDA further assumes that the covariance matrices are equal:

$$\boldsymbol{\Sigma}_k = \boldsymbol{\Sigma}, \quad \text{for all } k.$$

- We start with a study of LDA.

Linear boundaries of the Bayes classifier

Proposition

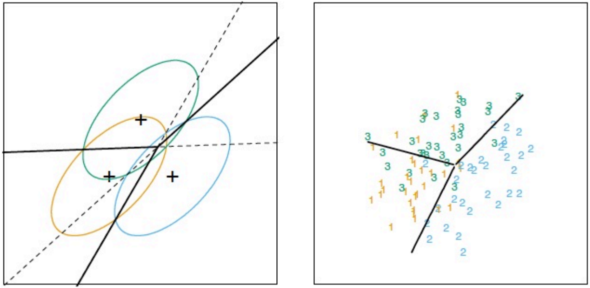
Under the assumptions of LDA, the boundary between any two decision regions $\mathcal{R}_k$ and $\mathcal{R}_\ell$ of the Bayes classifier is a hyperplane defined by the equation:

$$(\mu_k - \mu_\ell)^T \mathbf{\Sigma}^{-1} x - \frac{1}{2}(\mu_k + \mu_\ell)^T \mathbf{\Sigma}^{-1}(\mu_k - \mu_\ell) + \log \frac{\pi_k}{\pi_\ell} = 0 \qquad (1)$$

Proof.

See example on next slide.

Example



Left: contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and the Bayes decision boundaries separating all three classes are the thicker solid lines. Right: a sample of 30 drawn from each distribution, and the fitted LDA decision boundaries.

Plug-in LDA classifier

- The model parameters are π_k, μ_k $(k = 1, \ldots, c)$ and the common covariance matrix $\boldsymbol{\Sigma}$.
- To implement LDA, we compute the maximum likelihood estimates (MLEs) of these parameters and we "plug in" these estimates in the expressions of the conditional probabilities $P_k(x)$.
- From the consistency of the MLEs, the resulting plug-in classifier will tend to the Bayes classifier as the sample size n tends to infinity (assuming the model to be correct).

Maximum likelihood estimates

- The MLEs are

$$\widehat{\pi}_k = \frac{n_k}{n}, \quad \widehat{\mu}_k = \frac{1}{n_k}\sum_{i=1}^{n} y_{ik} x_i, \quad \text{and} \quad \widehat{\boldsymbol{\Sigma}} = \frac{1}{n}\sum_{k=1}^{c} n_k \widehat{\boldsymbol{\Sigma}}_k$$

where $\widehat{\boldsymbol{\Sigma}}_k$ is the sample covariance matrix in class k:

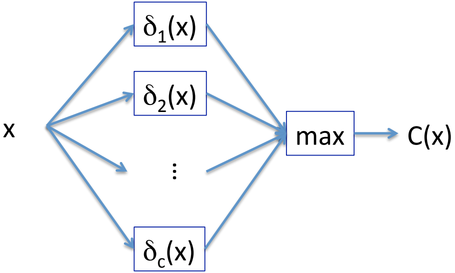
$$\widehat{\boldsymbol{\Sigma}}_k = \frac{1}{n_k}\sum_{i=1}^{n} y_{ik}(x_i - \widehat{\mu}_k)(x_i - \widehat{\mu}_k)^T,$$

with $y_{ik} = I(y_i = k)$ and $n_k = \sum_{i=1}^{n} y_{ik}$.

- It can be shown that $\widehat{\boldsymbol{\Sigma}}$ is biased. An unbiased estimator of $\boldsymbol{\Sigma}$ is

$$\mathbf{S} = \frac{n}{n-c}\widehat{\boldsymbol{\Sigma}}.$$

Discriminant functions



Discriminant functions (DF's) are functions $\delta_k(x)$ such that classifier C(x) can be written as

$$C(x) = \arg\max_k \delta_k(x).$$

- Simple DF's can be obtained by computing the log $\widehat{P}_k(x)$, and dropping the terms that are constant for all classes. Here, we get (Proof)

$$\delta_k(x) = \widehat{\mu}_k^T \widehat{\boldsymbol{\Sigma}}^{-1} x - \frac{1}{2} \widehat{\mu}_k^T \widehat{\boldsymbol{\Sigma}}^{-1} \widehat{\mu}_k + \log \widehat{\pi}_k.$$

- The LDA classifier can thus be implemented using linear discriminant functions.

Example: Letter recognition dataset

- Source: P. W. Frey and D. J. Slate, *Machine Learning*, Vol 6 #2, March 91.
- Objective: identify black-and-white rectangular pixel displays as one of the 26 capital letters in the English alphabet.
- The character images were based on 20 different fonts and each letter within these 20 fonts was randomly distorted to produce a file of 20,000 instances.
- Each instance was converted into 16 primitive numerical attributes (statistical moments and edge counts) which were scaled to fit into a range of integer values from 0 through 15.

LDA in R

```
letter <- read.table("letter-recognition.data",header=FALSE)
n<-nrow(letter)

library(MASS)

napp=15000
ntst=n-napp
train<-sample(1:n,napp)
letter.test<-letter[-train,]
letter.train<-letter[train,]

lda.letter<- lda(V1~.,data=letter.train)

pred.letters<-predict(lda.letter,newdata=letter.test)

perf <-table(letter.test$V1,pred.letters$class)
1-sum(diag(perf))/ntst
```

Confusion matrix and test error rate

```
Console ~/Documents/R/Scripts/teaching/sy19/
> table(letter.test$V1,pred.letters$class)

      A   B   C   D   E   F   G   H   I   J   K   L   M   N   O   P   Q   R   S   T   U   V   W   X   Y   Z
  A 155   0   0   0   0   0   0   2   0   1   1   0   2   0   2   0   0   0   6   0   0   0   2   0   4   0
  B   0 134   0   9   0   0   3   4   0   0   1   0   1   0   3   0   0  21  14   0   0   0   0   5   0   1
  C   0   0 151   0   9   2  16   2   0   0   9   0   0   0   1   0   0   0   3   2   1   1   1   0   0   0
  D   0  10   0 158   0   0   1   2   1   4   0   0   4   3   8   0   0   0   4   0   0   0   0  10   0   0
  E   0  12  19   1  90   1  23   0   2   0   5   0   0   0   0   0   2   6   5   2   2   0   0  23   0   6
  F   0  11   0   3   0 138   2   0   1   0   0   0   0   1   0  26   7   1   2   7   1   0   1   5   1   0
  G   1  10  25   1   6   0  95   5   0   0  10   1   1   1   3   0  14   7  12   0   0   0   2   2   0   0
  H   0   5   0   7   0   2   2  82   0   0  13   0   1  13  18   2   6   6   0   0   6   0   1  13   0   0
  I   0   3   0   2   1   3   1   0 153   1   0   0   0   0   0   1   4   1   6   0   0   0   0   2   3   0
  J   1   1   0   3   0  10   0   1  28 128   0   0   0   0   4   4   3   0  20   0   0   0   0   7   0   0
  K   0   3   1   3   4   0   4   1   0   0 124   0   2   0   1   0   0  19   0   0   1   2   0  10   0   0
  L   3   6   1   0   6   0  10   0   4   4   3 143   0   0   0   0   1   1   3   0   0   0   0   3   0   0
  M   1   0   0   0   0   0   0   5   0   2   1   0 189   6   3   0   0   3   0   0   0   0   3   0   0   0
  N   0   0   0   5   0   0   0   8   0   0   3   0   1 158   3   0   0   1   0   0   1   0   6   2   0   0
  O   5   0   0  18   0   0   5  21   0   0   2   0   0   3 116   0   1   0   0   0   0   0   5   1   0   0
  P   0   5   0   2   0  18   1   0   0   0   2   0   0   1   1 165   8   0   0   0   0   1   4   0   8   0
  Q   2  11   0   1   1   0  14   2   0   0   1   2   1   0  19   0 123   1   6   0   0   1   3   5   1   0
  R   0  16   0  11   0   0   1   7   0   0   7   0   1   1   0   0   0 136   0   0   0   0   0   5   0   0
  S   8  15   0   2   1   5   8   1   2   1   0   3   0   0   1   0   1   8  72   0   0   0   0  15   3  29
  T   0   1   0   1   2  16   4   2   1   0   2   0   0   0   1   1   0   1   4 142   0   2   0   1   1   6
  U   0   0   1   0   0   0   0  14   0   0   3   0  11   7  11   0   0   0   0   0 158   0   3   0   0   0
  V   0   1   0   0   0   0   2   4   0   0   2   0   1   0   3   1   0   1   0   2   1 156   5   0   2   0
  W   0   0   0   0   0   0   0   9   0   0   1   0   4   4   0   0   0   0   0   0   0   1 175   0   0   0
  X   0   6   0   2   0   0   2   0   0   0   5   0   0   0   1   0   9   3  18   0   5   0   0 143   3   1
  Y   0   0   0   1   0  18   0   0   0   0   0   0   0   0   1   0  24   0   6   8   3  47   0   0 101   0
  Z   0   0   0   0  14   2   2   0   0   6   0   0   0   0   0   0   4   1  21   0   0   0   0   2   0 115
> 1-sum(diag(perf))/ntst
[1] 0.3
>
```

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1. Introduction to classification
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4. Appendix

Case $c = 2$: fixing the threshold

- From (1), in the case of $c = 2$ classes, LDA assigns x to class 2 if

$$(\widehat{\mu}_2 - \widehat{\mu}_1)^T \widehat{\mathbf{\Sigma}}^{-1} x > s,$$

  where the threshold s depends on the estimated parameters, including the estimated prior probabilities $\widehat{\pi}_1$ and $\widehat{\pi}_2$.
- If the prior probabilities cannot be estimated, or if the model assumptions are not verified, a different threshold may give better results.
- The Receiver Operating Characteristic (ROC) curve describes the performance of the classifier for any value of s.

Confusion matrix ($c = 2$)

- Assuming $c = 2$, call one class "positive" and the other one "negative".
- For a given threshold s, we get a confusion matrix such as

	predicted	
true	P	N
P	true positive (TP)	false negative (FN)
N	false positive (FP)	true negative (TN)

- The true positive rate (sensitivity) and false positive rate (1-specificity) are defined, respectively, as

$$TPR = \frac{TP}{TP + FN}, \quad FPR = \frac{FP}{FP + TN}$$

- If we decrease s, we increase both the TPR and the FPR.
- The ROC curve is a plot of the TPR as a function of the FPR, for different values of s.

Example: Pima diabetes dataset

- Data about diabetes in the population of Pima Indians leaving near Phoenix, Arizona, USA.
- All 768 patients were females and at least 21 years old.
- Variables:
  1. Number of times pregnant
  2. Plasma glucose concentration a 2 hours in an oral glucose tolerance test
  3. Diastolic blood pressure (mm Hg)
  4. Triceps skin fold thickness (mm)
  5. 2-Hour serum insulin (mu U/ml)
  6. Body mass index (weight in kg/(height in m)^2)
  7. Diabetes pedigree function
  8. Age (years)
  9. Tested positive (1) or negative (0) for diabetes
- Problem: predict the test result for the 8 predictors.

LDA of the Pima dataset

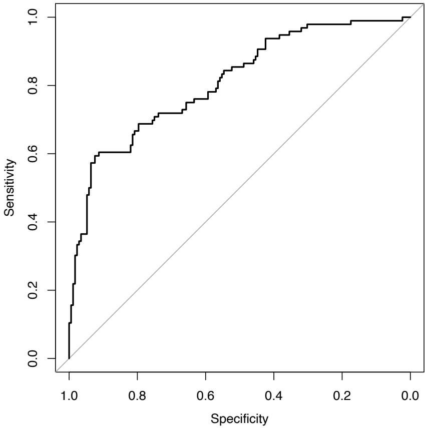
```
pima<-read.csv('pima-indians-diabetes.data',header=FALSE)
names(pima)<-c("pregnant","glucose","BP","skin","insulin","bmi","diabetes",
"age","class")
n<-nrow(pima)
napp=500
ntst=n-napp
train<-sample(1:n,napp)
pima.test<-pima[-train,]
pima.train<-pima[train,]
lda.pima<- lda(class~.,data=pima.train)
pred.pima<-predict(lda.pima,newdata=pima.test)
table(pima.test$class,pred.pima$class)
> perf

       0    1
 0   152   15
 1    45   56
```

Here, the TPR is 56/(45+56)=0.55, and the FPR is 15/(152+15)=0.089. The error rate is $(15+45)/268 \approx 0.22$.

ROC curve for the LDA classifier (Pima dataset)

```
library(pROC)
roc_curve<-roc(pima.test$V9,as.vector(pred.pima$x))
plot(roc_curve)
```



Overview

1. Introduction to classification
   - Basic notions
   - Bayes classifier
   - Voting K-NN rule
2. Linear and quadratic discriminant analysis
   - Model
   - Case of binary classification
   - Related models
3. Logistic regression and related models
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   - Multinomial logistic regression
   - Ordered probit and logit regression
4. Appendix

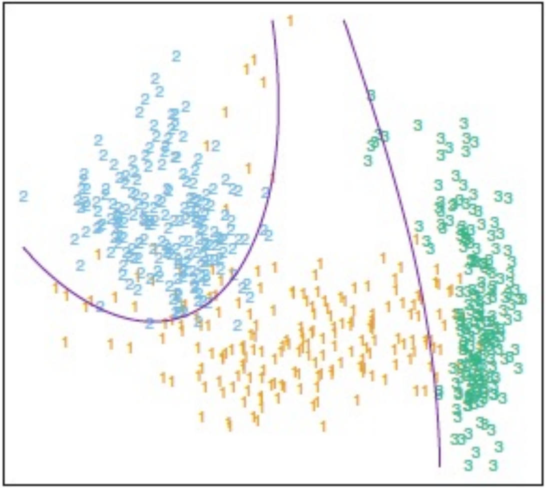
Quadratic Discriminant Analysis (QDA)

- We have seen that obtain discriminant functions by computing the $\log \widehat{P}_k(x)$ from Bayes' rule, and dropping the terms that are constant for all classes.
- If the $\mathbf{\Sigma}_k$ are not assumed to be equal, then the quadratic terms now depend on k, and we get quadratic discriminant functions:

$$\begin{aligned}\delta_k^*(x) &= \log \widehat{p}_k(x) + \log \widehat{\pi}_k \\ &= -\frac{1}{2}(x-\widehat{\mu}_k)^T \widehat{\mathbf{\Sigma}}_k^{-1}(x-\widehat{\mu}_k) - \frac{1}{2}\log|\widehat{\mathbf{\Sigma}}_k| + \log \widehat{\pi}_k\end{aligned}$$

Proof

Example



Application of QDA to the letter recognition data

```
qda.letter<- qda(V1~.,data=letter.train)
pred.letters<-predict(qda.letter,newdata=letter.test)

perf <-table(letter.test$V1,pred.letters$class)
1-sum(diag(perf))/ntst

0.1218
```

Naive Bayes classifiers

- Starting from the QDA model, we get a simpler model by assuming that the covariance matrices $\mathbf{\Sigma}_k$ are diagonal:

$$\mathbf{\Sigma}_k = \mathrm{diag}(\sigma^2_{k1}, \ldots, \sigma^2_{kp}),$$

where $\sigma^2_{kj} = \mathrm{Var}(X_j \mid Y = k)$.
- This assumption means that the predictors are conditionally independent given the class variable Y, i.e., for all $k \in \{1, \ldots, c\}$,

$$p_k(x_1, \ldots, x_p) = \prod_{j=1}^{p} p_{kj}(x_j)$$

- Remark: conditional independence does not imply independence. (Example: Height and vocabulary of kids are not independent; but they are conditionally independent given age).

Naive Bayes classifiers (continued)

- To estimate $\mathbf{\Sigma}_k$ under the conditional independence assumption, we simply set the off-diagonal terms in $\widehat{\mathbf{\Sigma}}_k$ to 0. The variance σ_{kj}^2 of X_j conditionally on $Y = k$ is estimated by

$$\widehat{\sigma}_{kj}^2 = \frac{1}{n_k} \sum_{i=1}^{n} y_{ik} (x_{ij} - \widehat{\mu}_{kj})^2.$$

- A further simplification is achieved by assuming that the covariance matrices are diagonal and equal:

$$\mathbf{\Sigma}_1 = \cdots = \mathbf{\Sigma}_c = \mathbf{\Sigma} = \mathrm{diag}(\sigma_1^2, \ldots, \sigma_p^2).$$

This model can be called "Naive LDA".

Advantages of Naive Bayes classifiers

- In spite of their simplicity, naive Bayes classifiers often (but not always) have very good performances.
- They can accommodate mixed feature vectors (qualitative and quantitative). If X_j is qualitative, estimate the probability mass functions $p_{kj}(x_j)$ using histograms over discrete categories.

Naive Bayes classifier in R

```
library(naivebayes)
naive.letter<- naive_bayes(V1~.,data=letter.train)
pred.letters.naive<-predict(naive.letter,newdata=letter.test)

perf.naive <-table(letter.test$V1,pred.letters.naive)
1-sum(diag(perf.naive))/ntst

0.3474
```

Comparison of the different models

- QDA is the most general model. However, it does not always yield the best performances, because it has the largest number of parameters.
- Although LDA also has a number of parameters proportional to p^2, it is usually much more stable than QDA. This method is recommended when n is small.
- Naive Bayes classifiers have a number of parameters proportional to p. They usually outperform other methods when p is very large.

Model	Number of parameters
QDA	$c\left(p+\frac{p(p+1)}{2}\right)+c-1$
naive QDA	$2cp+c-1$
LDA	$cp+\frac{p(p+1)}{2}+c-1$
naive LDA	$cp+p+c-1$

Example

- We consider $c = 2$ classes with $p = 3$ normally distributed input variables, with the following parameters

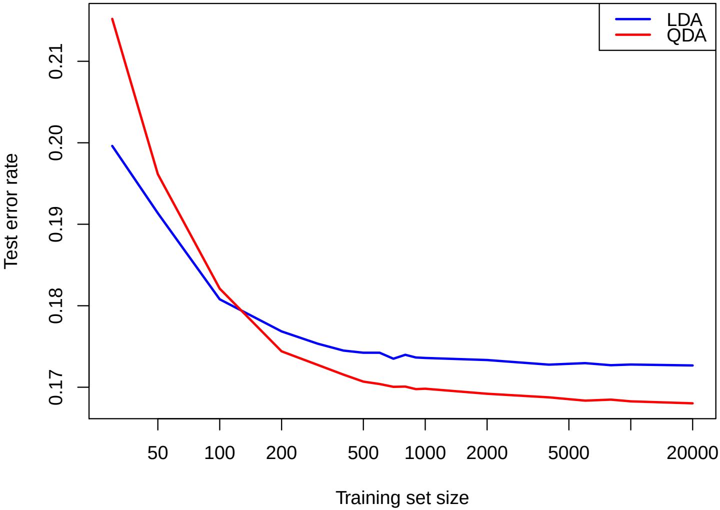
$$\pi_1 = \pi_2 = 0.5$$

$$\mu_1 = (0, 0, 0)^T, \quad \mu_2 = (1, 1, 1)^T$$

$$\Sigma_1 = \mathbf{I}_3, \quad \Sigma_2 = 0.7\mathbf{I}_3.$$

- LDA and QDA classifiers were trained using training sets of different sizes between 30 and 20,000, and their error rate was estimated using a test set of size 20,000.
- For each training set size, the experiment was repeated 20 times. The next figure shows error rates over the 20 replications.

Result


LDA
QDA
Test error rate
0.17
0.18
0.19
0.20
0.21
50
100
200
500
1000
2000
5000
20000
Training set size

Overview

1. Introduction to classification
   - Basic notions
   - Bayes classifier
   - Voting K-NN rule
2. Linear and quadratic discriminant analysis
   - Model
   - Case of binary classification
   - Related models
3. Logistic regression and related models
   - Binary logistic and probit regression
   - Multinomial logistic regression
   - Ordered probit and logit regression
4. Appendix

Overview

1. Introduction to classification
   - Basic notions
   - Bayes classifier
   - Voting K-NN rule
2. Linear and quadratic discriminant analysis
   - Model
   - Case of binary classification
   - Related models
3. Logistic regression and related models
   - Binary logistic and probit regression
   - Multinomial logistic regression
   - Ordered probit and logit regression
4. Appendix

Searching for a linear discriminative model

- Consider a binary classification problem with $c = 2$ classes, $Y \in \{0, 1\}$. Let $P(x) = \mathbb{P}(Y = 1 \mid X = x)$ be the conditional probability of class $Y = 1$.
- We want to find a simple model for $P(x)$. An idea could be to use a linear model of the form

$$P(x) = \beta_0 x_0 + \beta_1 x_1 + \ldots + \beta_p x_p = \beta^T x,$$

  where by convention $x_0 = 0$. However, this is not suitable because $\beta^T x$ can take any value in $\mathbb{R}$, whereas $P(x) \in [0, 1]$.
- A better idea is to assume that Y depends on a latent (unobserved) continuous variable Y^*, which is linearly related to x.

Model

- Assume that

$$Y^* = \beta^T x + \epsilon,$$

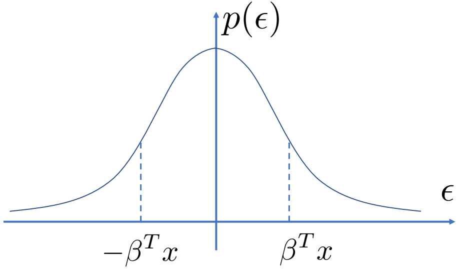
where ϵ is a random error term with 0 mean and cumulative distribution function (cdf) F, and

$$Y = I(Y^* > 0).$$

- We then have

$$P(x) = \mathbb{P}(Y = 1 \mid x) = \mathbb{P}(Y^* > 0 \mid x) = \mathbb{P}(\epsilon > -\beta^T x).$$

Model (continued)



- If we assume the distribution of ϵ to be symmetric, then

$$\mathbb{P}(\epsilon > -\beta^T x) = \mathbb{P}(\epsilon \leq \beta^T x) \quad \text{and} \quad \boxed{P(x) = F(\beta^T x)}$$

- Different choices of F give us different models. Whatever the choice of F we get a linear classifier, as the equation of the decision boundary is

$$P(x) = \frac{1}{2} \Leftrightarrow \beta^T x = F^{-1}(0.5) = 0$$

Logit model

- In the logit model, we assume that ϵ has a standard logistic distribution with cdf

$$F(u) = \Lambda(u) = \frac{\exp(u)}{1+\exp(u)}.$$

- We then have

$$P(x) = \frac{\exp(\beta^T x)}{1+\exp(\beta^T x)} \quad \text{and} \quad 1 - P(x) = \frac{1}{1+\exp(\beta^T x)}$$

- The log-odds ratio is linear in x:

$$\boxed{\log \frac{P(x)}{1-P(x)} = \beta^T x}$$

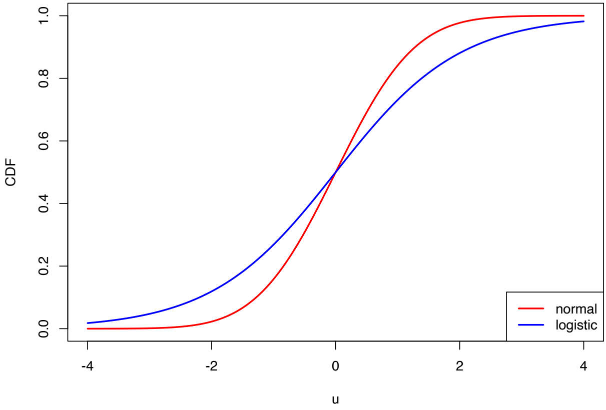
Probit model

- In the probit model, we assume that ϵ has a standard normal distribution with cdf Φ. We then have

$$P(x) = \Phi(\beta^T x).$$

- In practice, the two models usually give very similar results.
- Logistic regression based on the logit model is more popular in ML.

Plot of the logistic and normal cdfs



Conditional likelihood function

- Logit and probit models are usually fit by maximizing the conditional likelihood, which is the likelihood function, assuming the x_i are fixed.
- Assuming $Y_1, \ldots, Y_n$ to be independent conditionally on $X_1 = x_1, \ldots, X_n = x_n$, the conditional likelihood is

$$\begin{aligned} L(\beta) &= \mathbb{P}(Y_1 = y_1, \ldots, Y_n = y_n \mid X_1 = x_1, \ldots, X_n = x_n) \\ &= \prod_{i=1}^{n} \mathbb{P}(Y_i = y_i \mid X_i = x_i; \beta) \\ &= \prod_{i=1}^{n} P(x_i; \beta)^{y_i} \left[1 - P(x_i; \beta)\right]^{1-y_i} \end{aligned}$$

where $y_i \in \{0, 1\}$ and $P(x_i; \beta) = \mathbb{P}(Y = 1 | X = x_i; \beta)$.

Conditional log-likelihood (logit model)

- The conditional log-likelihood for the logit model is

$$\ell(\beta) = \sum_{i=1}^{n} \{y_i \log P(x_i;\beta) + (1-y_i)\log(1-P(x_i;\beta))\}$$
$$= \sum_{i=1}^{n} \left\{ y_i \beta^T x_i - \log(1+\exp(\beta^T x_i)) \right\},$$

Proof

- This function is non linear and the score equation $\frac{\partial \ell}{\partial \beta} = 0$ does not have a closed-form expression: we need to use an iterative nonlinear optimization procedure such as the Newton-Raphson algorithm.

Update equation (logit model)

- Let $\mathbf{y}$ denote the vector of y_i values, $\mathbf{X}$ the $n \times (p+1)$ matrix of x_i values, $\mathbf{p}$ the vector of fitted probabilities with i-th element $P(x_i;\beta)$.
- The gradient and Hessian of $\ell(\beta)$ can be written as

$$\frac{\partial \ell}{\partial \beta} = \mathbf{X}^T(\mathbf{y}-\mathbf{p}) \quad \text{and} \quad \frac{\partial^2 \ell(\beta)}{\partial\beta\partial\beta^T} = -\mathbf{X}^T\mathbf{W}\mathbf{X},$$

  where $\mathbf{W}$ an $n \times n$ diagonal matrix of weights with i-th diagonal element $P(x_i;\beta)\{1-P(x_i;\beta)\}$. Proof
- The update equation is, thus,

$$\boxed{\beta^{(t+1)} = \beta^{(t)} + (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{y}-\mathbf{p})}$$

Asymptotic distribution of $\widehat{\beta}$

- A central limit theorem shows that the distribution of $\widehat{\beta}$ converges to

$$\mathcal{N}(\beta, (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}).$$

  when $n \to +\infty$.
- This results makes it possible to compute confidence intervals and to test the significance of the coefficients β_j.
- Similar results hold for probit regression.

Binomial logistic regression in R

```
glm.fit<- glm(class~.,data=pima.train,family=binomial)
```

```
> summary(glm.fit)

Call:
glm(formula = class ~ ., family = binomial, data = pima.train)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.5516  -0.7228  -0.3801   0.7290   2.8209

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -8.733508   0.923597  -9.456  < 2e-16 ***
pregnant     0.110968   0.042667   2.601   0.0093 **
glucose      0.034018   0.004535   7.501 6.35e-14 ***
BP          -0.017566   0.007367  -2.384   0.0171 *
skin         0.004783   0.008659   0.552   0.5807
insulin     -0.001856   0.001197  -1.551   0.1209
bmi          0.109417   0.019992   5.473 4.43e-08 ***
diabetes     1.006970   0.379084   2.656   0.0079 **
age          0.017200   0.012145   1.416   0.1567
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 643.65  on 499  degrees of freedom
Residual deviance: 462.01  on 491  degrees of freedom
AIC: 480.01
```

Prediction (logit model)

```
pred.pima.glm<-predict(glm.fit,newdata=pima.test,type='response')

table(pima.test$class,pred.pima.glm>0.5)

    FALSE  TRUE
 0    158    14
 1     41    55
```

The error rate is $(14+41)/268 \approx 0.21$.

Binomial probit regression in R

```
probit.fit<- glm(class~.,data=pima.train,family=binomial("probit"))
```

```
> summary(probit.fit)

Call:
glm(formula = class ~ ., family = binomial("probit"), data = pima.train)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.5488  -0.7291  -0.3691   0.7558   2.9030

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept) -5.0692691  0.5018665 -10.101  < 2e-16 ***
pregnant     0.0674591  0.0247598   2.725  0.00644 **
glucose      0.0189866  0.0025196   7.536 4.86e-14 ***
BP          -0.0107108  0.0042744  -2.506  0.01222 *
skin         0.0038887  0.0050731   0.767  0.44336
insulin     -0.0011300  0.0006979  -1.619  0.10545
bmi          0.0658705  0.0113925   5.782 7.38e-09 ***
diabetes     0.5366801  0.2167489   2.476  0.01328 *
age          0.0108750  0.0071087   1.530  0.12606
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 643.65  on 499  degrees of freedom
Residual deviance: 462.67  on 491  degrees of freedom
AIC: 480.67
```

Comparison logit vs. probit

```
> summary(glm.fit)

Call:
glm(formula = class ~ ., family = binomial, data = pima.train)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.5516  -0.7228  -0.3801   0.7290   2.8209

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -8.733508   0.923597  -9.456  < 2e-16 ***
pregnant     0.110968   0.042667   2.601   0.0093 **
glucose      0.034018   0.004535   7.501 6.35e-14 ***
BP          -0.017566   0.007367  -2.384   0.0171 *
skin         0.004783   0.008659   0.552   0.5807
insulin     -0.001856   0.001197  -1.551   0.1209
bmi          0.109417   0.019992   5.473 4.43e-08 ***
diabetes     1.006970   0.379084   2.656   0.0079 **
age          0.017200   0.012145   1.416   0.1567
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 643.65  on 499  degrees of freedom
Residual deviance: 462.01  on 491  degrees of freedom
AIC: 480.01
```

```
> summary(probit.fit)

Call:
glm(formula = class ~ ., family = binomial("probit"), data = pima.train)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-2.5488  -0.7291  -0.3691   0.7558   2.9030

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
(Intercept) -5.0692691  0.5018665 -10.101  < 2e-16 ***
pregnant     0.0674591  0.0247598   2.725  0.00644 **
glucose      0.0189866  0.0025196   7.536 4.86e-14 ***
BP          -0.0107108  0.0042744  -2.506  0.01222 *
skin         0.0038887  0.0050731   0.767  0.44336
insulin     -0.0011300  0.0006979  -1.619  0.10545
bmi          0.0658705  0.0113925   5.782 7.38e-09 ***
diabetes     0.5366801  0.2167489   2.476  0.01328 *
age          0.0108750  0.0071087   1.530  0.12606
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 643.65  on 499  degrees of freedom
Residual deviance: 462.67  on 491  degrees of freedom
AIC: 480.67
```

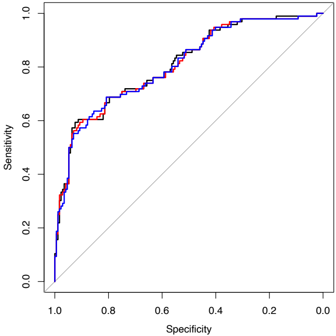
Prediction (probit model)

```
pred.pima.probit<-predict(probit.fit,newdata=pima.test,
type='response')

table(pima.test$class,pred.pima.probit>0.5)

    FALSE  TRUE
 0    158    14
 1     43    53
```

The error rate is $(14 + 43)/268 \approx 0.21$.

ROC curve: comparison with LDA

```
logit<-predict(glm.fit,newdata=pima.test,type='link')
probit<-predict(probit.fit,newdata=pima.test,type='link')
roc_curve<-roc(pima.test$class,as.vector(pred.pima$x)) # LDA plot(roc_curve)
roc_glm<-roc(pima.test$class,logit)
roc_probit<-roc(pima.test$class,probit)
plot(roc_glm,add=TRUE,col='red')
plot(roc_probit,add=TRUE,col='blue')
```



Overview

1. Introduction to classification
   - Basic notions
   - Bayes classifier
   - Voting K-NN rule
2. Linear and quadratic discriminant analysis
   - Model
   - Case of binary classification
   - Related models
3. Logistic regression and related models
   - Binary logistic and probit regression
   - Multinomial logistic regression
   - Ordered probit and logit regression
4. Appendix

Model

- Multinomial logistic regression extends binomial logistic regression to $c > 2$ by assuming the following model for the posterior probabilities $P_k(x) = \mathbb{P}(Y = k \mid X = x)$:

$$\boxed{P_k(x) = \frac{\exp(\beta_k^T x)}{\sum_{l=1}^{c} \exp(\beta_l^T x)}}$$

- However, there is indeterminacy in the model, because the probabilities are unchanged if we add a constant vector α to all β_k's:

$$\frac{\exp((\beta_k + \alpha)^T x)}{\sum_{l=1}^{c} \exp((\beta_l + \alpha)^T x)} = \frac{\exp(\beta_k^T x)}{\sum_{l=1}^{c} \exp(\beta_l^T x)}$$

- To remove this indeterminacy, we set $\beta_1 = 0$.

Model (continued)

- We then have

$$P_1(x) = \frac{1}{1 + \sum_{l=2}^{c} \exp(\beta_l^T x)}$$

and

$$P_k(x) = \frac{\exp(\beta_k^T x)}{1 + \sum_{l=2}^{c} \exp(\beta_l^T x)}, \quad k = 2, \ldots, c.$$

- The log-odds ratios for class k vs. class 1 are still linear in x:

$$\boxed{\log \frac{P_k(x)}{P_1(x)} = \beta_k^T x}$$

Learning

- The conditional likelihood for the multinomial model is

$$L(\beta) = \prod_{i=1}^{n} \mathbb{P}(Y_i = y_i \mid X_i = x_i; \beta)$$
$$= \prod_{i=1}^{n} \prod_{k=1}^{c} [P_k(x_i; \beta)]^{y_{ik}}$$

- The conditional log-likelihood is

$$\ell(\beta) = \sum_{i=1}^{n} \sum_{k=1}^{c} y_{ik} \log P_k(x_i; \beta),$$

- It can be maximized by the Newton-Raphson algorithm as in the binary case.

Multinomial logistic regression in R

```
library(nnet)
fit<-multinom(V1~.,data=letter.train)
pred.letters<-predict(fit,newdata=letter.test)

perf <-table(letter.test$V1,pred.letters)
1-sum(diag(perf))/ntst

0.2726
```

Overview

1. Introduction to classification
   - Basic notions
   - Bayes classifier
   - Voting K-NN rule
2. Linear and quadratic discriminant analysis
   - Model
   - Case of binary classification
   - Related models
3. Logistic regression and related models
   - Binary logistic and probit regression
   - Multinomial logistic regression
   - Ordered probit and logit regression
4. Appendix

Ordinal classification/regression

- In ordinal regression/classification, the response Y is an ordinal variable, i.e., it takes values in a finite ordered set.
- For instance, a variable "Customer satisfaction" may take values in the set $\{\text{High}, \text{Medium}, \text{Low}\}$.
- To solve ordinal regression problems, we can still use classification methods, but the results will often not be optimal because the ordering relation between the values of Y is ignored.
- A much better option to use a specific method such as ordered probit or logit regression.

Ordinal logit and probit models

- As in the binary logit and probit model, we assume the existence of a latent variable Y^* linearly related to x:

$$Y^* = \beta^T x + \epsilon$$

- We now assume that Y is determined by Y^* as follows:

$$Y = \begin{cases} 1 & \mu_0 \leq Y^* \leq \mu_1 \\ 2 & \mu_1 \leq Y^* \leq \mu_2 \\ \vdots & \\ c & \mu_{c-1} \leq Y^* \leq \mu_c \end{cases}$$

where $-\infty = \mu_0 \leq \mu_1 \leq \ldots \leq \mu_{c-1} \leq \mu_c = +\infty$ are unknown parameters.

Ordinal logit and probit models (continued)

- The logit and probit models correspond to different assumptions about the distribution of ϵ: respectively, logistic ($F = \Lambda$) or normal ($F = \Phi$).
- The conditional log-likelihood function is

$$\begin{aligned}\ell(\theta) &= \sum_{i=1}^{n}\sum_{k=1}^{c} y_{ik} \log P_k(x)\\ &= \sum_{i=1}^{n}\sum_{k=1}^{c} y_{ik} \log \left[F(\mu_k - \beta^T x) - F(\mu_{k-1} - \beta^T x)\right],\end{aligned}$$

  with $\theta = (\beta, \mu_1, \ldots, \mu_{c-1})$.
- The MLE of θ can be found by an iterative nonlinear optimization algorithm.

Example: Housing dataset

- Package `MASS`, 72 rows and 5 variables.
- Variables:

  Sat: Satisfaction of householders with their present housing circumstances, (High, Medium or Low, ordered factor).

  Infl: Perceived degree of influence householders have on the management of the property (High, Medium, Low).

  Type: Type of rental accommodation, (Tower, Atrium, Apartment, Terrace).

  Cont: Contact residents are afforded with other residents, (Low, High).

  Freq: Frequencies: the numbers of residents in each class.

Ordered logit regression in R

```
library("MASS")
house.logit <- polr(Sat ~ Infl + Type + Cont, weights = Freq,
data = housing, method = "logistic")
```

```
> summary(house.logit, digits = 3)

Re-fitting to get Hessian

Call:
polr(formula = Sat ~ Infl + Type + Cont, data = housing, weights = Freq,
    method = "logistic")

Coefficients:
               Value Std. Error t value
InflMedium     0.566     0.1047    5.41
InflHigh       1.289     0.1272   10.14
TypeApartment -0.572     0.1192   -4.80
TypeAtrium    -0.366     0.1552   -2.36
TypeTerrace   -1.091     0.1515   -7.20
ContHigh       0.360     0.0955    3.77

Intercepts:
            Value  Std. Error t value
Low|Medium  -0.496  0.125     -3.974
Medium|High  0.691  0.125      5.505

Residual Deviance: 3479.149
AIC: 3495.149
```

Ordered probit regression in R

```
house.probit <- polr(Sat ~ Infl + Type + Cont, weights = Freq,
data = housing, method = "probit")
```

```
> summary(house.probit, digits = 3)

Re-fitting to get Hessian

Call:
polr(formula = Sat ~ Infl + Type + Cont, data = housing, weights = Freq,
    method = "probit")

Coefficients:
               Value Std. Error t value
InflMedium     0.346     0.0641    5.40
InflHigh       0.783     0.0764   10.24
TypeApartment -0.348     0.0723   -4.81
TypeAtrium    -0.218     0.0948   -2.30
TypeTerrace   -0.664     0.0918   -7.24
ContHigh       0.222     0.0581    3.83

Intercepts:
            Value  Std. Error t value
Low|Medium  -0.300  0.076     -3.937
Medium|High  0.427  0.076      5.585

Residual Deviance: 3479.689
AIC: 3495.689
```

Overview

1. Introduction to classification
   - Basic notions
   - Bayes classifier
   - Voting K-NN rule
2. Linear and quadratic discriminant analysis
   - Model
   - Case of binary classification
   - Related models
3. Logistic regression and related models
   - Binary logistic and probit regression
   - Multinomial logistic regression
   - Ordered probit and logit regression
4. Appendix

Decision boundaries of LDA I

- The decision boundary between regions $\mathcal{R}_k$ and $\mathcal{R}_\ell$ is defined by the equation $P_k(x) = P_\ell(x)$, which can be written as

$$\log \frac{P_k(x)}{P_\ell(x)} = \log \frac{p_k(x)\pi_k}{p_\ell(x)\pi_\ell} = \log p_k(x) - \log p_\ell(x) + \log \frac{\pi_k}{\pi_\ell} = 0$$

- Now,

$$p_k(x) = \frac{1}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)\right\},$$

so

$$\begin{aligned}\log p_k(x) &= -\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k) + \text{cst} \\ &= -\frac{1}{2}x^T\mathbf{\Sigma}^{-1}x + \mu_k^T\mathbf{\Sigma}^{-1}x - \frac{1}{2}\mu_k^T\mathbf{\Sigma}^{-1}\mu_k + \text{cst}\end{aligned}$$

Decision boundaries of LDA II

- Consequently,

$$
\begin{aligned}
\log p_k(x) - \log p_\ell(x) &= \mu_k^T \boldsymbol{\Sigma}^{-1} x - \frac{1}{2}\mu_k^T \boldsymbol{\Sigma}^{-1}\mu_k \\
&\quad - \mu_\ell^T \boldsymbol{\Sigma}^{-1} x + \frac{1}{2}\mu_\ell^T \boldsymbol{\Sigma}^{-1}\mu_\ell \\
&= (\mu_k - \mu_\ell)^T \boldsymbol{\Sigma}^{-1} x - \frac{1}{2} \underbrace{\left[\mu_k^T \boldsymbol{\Sigma}^{-1}\mu_k - \mu_\ell^T \boldsymbol{\Sigma}^{-1}\mu_\ell\right]}_{(\mu_k+\mu_\ell)^T \boldsymbol{\Sigma}^{-1}(\mu_k-\mu_\ell)}
\end{aligned}
$$

Back

Discriminant functions of LDA

From

$$\widehat{P}_k(x) = \frac{\widehat{p}_k(x)\widehat{\pi}_k}{\widehat{p}(x)}$$

we get

$$\begin{aligned}
\log \widehat{P}_k(x) &= \log \widehat{p}_k(x) + \log \widehat{\pi}_k + \text{cst} \\
&= -\frac{1}{2}(x - \widehat{\mu}_k)^T \widehat{\boldsymbol{\Sigma}}^{-1}(x - \widehat{\mu}_k) + \log \widehat{\pi}_k + \text{cst} \\
&= \widehat{\mu}_k^T \widehat{\boldsymbol{\Sigma}}^{-1} x - \frac{1}{2}\widehat{\mu}_k^T \widehat{\boldsymbol{\Sigma}}^{-1}\widehat{\mu}_k + \log \widehat{\pi}_k + \text{cst}
\end{aligned}$$

(The quadratic term $x^T \widehat{\boldsymbol{\Sigma}}^{-1} x$ goes into the constant because if does not depend on k).

Back

Discriminant functions of QDA

From

$$\widehat{P}_k(x) = \frac{\widehat{p}_k(x)\widehat{\pi}_k}{\widehat{p}(x)}$$

we get

$$\begin{aligned}
\log \widehat{P}_k(x) &= \log \widehat{p}_k(x) + \log \widehat{\pi}_k + \text{cst} \\
&= -\frac{1}{2}(x - \widehat{\mu}_k)^T \widehat{\boldsymbol{\Sigma}}_k^{-1}(x - \widehat{\mu}_k) - \frac{1}{2}\log|\widehat{\boldsymbol{\Sigma}}_k| + \log \widehat{\pi}_k + \text{cst} \\
&= -\frac{1}{2}x^T \widehat{\boldsymbol{\Sigma}}_k^{-1} x + \widehat{\mu}_k^T \widehat{\boldsymbol{\Sigma}}_k^{-1} x - \frac{1}{2}\widehat{\mu}_k^T \widehat{\boldsymbol{\Sigma}}_k^{-1} \widehat{\mu}_k - \frac{1}{2}\log|\widehat{\boldsymbol{\Sigma}}_k| + \\
&\quad \log \widehat{\pi}_k + \text{cst}
\end{aligned}$$

(The quadratic terms $x^T \widehat{\boldsymbol{\Sigma}}_k^{-1} x$ now depend on k).

Back

Log-likelihood of binary logistic regression

From

$$P(x_i) = \frac{1}{1+\exp(-\beta^T x_i)} \quad \text{and} \quad 1 - P(x_i) = \frac{\exp(-\beta^T x_i)}{1+\exp(-\beta^T x_i)}$$

we get

$$\ell(\beta) = \sum_{i=1}^{n} \Bigg\{ -y_i \log[1+\exp(-\beta^T x)] \underbrace{-\beta^T x_i - \log[1+\exp(-\beta^T x_i)]}_{-\log[1+\exp(\beta^T x)]}$$

$$+ y_i \beta^T x_i + y_i \log[1+\exp(-\beta^T x)] \Bigg\}$$

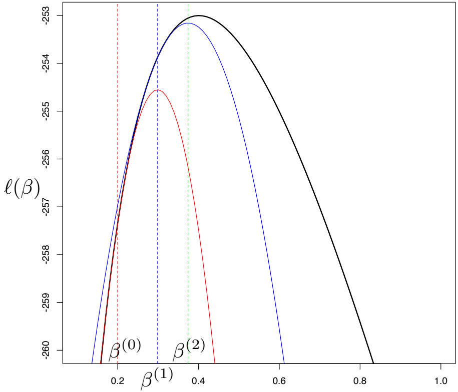
$$\ell(\beta) = \sum_{i=1}^{n} \left\{ y_i \beta^T x_i - \log[1+\exp(\beta^T x)] \right\}$$

Back

The Newton-Raphson algorithm

Main ideas

- An iterative optimization algorithm.
- Basic idea: at each time step, approximate $\ell(\beta)$ around the current estimate $\beta^{(t)}$ by the second-order Taylor series expansion.



The Newton-Raphson algorithm

- We have

$$\ell(\beta) \approx \ell(\beta^{(t)}) + (\beta - \beta^{(t)})^T \frac{\partial \ell(\beta^{(t)})}{\partial \beta} + \frac{1}{2}(\beta - \beta^{(t)})^T \frac{\partial^2 \ell(\beta^{(t)})}{\partial \beta \partial \beta^T}(\beta - \beta^{(t)}).$$

- Differentiating both sides w.r.t. β, we get

$$\frac{\partial \ell(\beta)}{\partial \beta} \approx \frac{\partial \ell(\beta^{(t)})}{\partial \beta} + \frac{\partial^2 \ell(\beta^{(t)})}{\partial \beta \partial \beta^T}(\beta - \beta^{(t)}).$$

- Setting $\frac{\partial \ell}{\partial \beta}(\beta) = 0$, we get the update equation

$$\boxed{\beta^{(t+1)} = \beta^{(t)} - \left(\frac{\partial^2 \ell(\beta^{(t)})}{\partial \beta \partial \beta^T}\right)^{-1} \frac{\partial \ell(\beta^{(t)})}{\partial \beta}}$$

Back

Gradient of $\ell(\beta)$

From

$$\ell(\beta) = \sum_{i=1}^{n} \left\{ y_i \beta^T x_i - \log(1 + \exp(\beta^T x_i)) \right\}$$

the gradient is

$$\frac{\partial \ell}{\partial \beta} = \sum_{i=1}^{n} y_i x_i - \underbrace{\frac{\exp(\beta^T x_i)}{1 + \exp(\beta^T x_i)}}_{P(x_i;\beta)} x_i$$

$$= \sum_{i=1}^{n} x_i \left(y_i - P(x_i;\beta)\right) = \mathbf{X}^T(\mathbf{y} - \mathbf{p})$$

where **y** denote the vector of y_i values, **X** the $n \times (p+1)$ matrix of x_i values, **p** the vector of fitted probabilities with i-th element $P(x_i;\beta)$.

Hessian of $\ell(\beta)$ I

- From

$$\frac{\partial \ell}{\partial \beta_j} = \sum_{i=1}^{n} x_{ij} \left(y_i - \underbrace{P(x_i;\beta)}_{\Lambda(\beta^T x)} \right)$$

and $\Lambda'(u) = \Lambda(u)[1 - \Lambda(u)]$, we have

$$\frac{\partial^2 \ell}{\partial \beta_j \partial \beta_k} = -\sum_{i=1}^{n} x_{ij} x_{ik} P(x_i;\beta)\,[1 - P(x_i;\beta)]$$

Hessian of $\ell(\beta)$ II

- The Hessian matrix can, thus, be written as

$$
\begin{aligned}
\frac{\partial^2 \ell(\beta)}{\partial\beta\partial\beta^T} &= -\sum_{i=1}^{n} x_i x_i^T P(x_i;\beta)\,[1 - P(x_i;\beta)] \\
&= -\mathbf{X}^T\mathbf{W}\mathbf{X},
\end{aligned}
$$

where $\mathbf{W}$ an $n \times n$ diagonal matrix of weights with i-th diagonal element $P(x_i;\beta)\,[1 - P(x_i;\beta)]$.

Back