Machine Learning (CP322)

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Classification

The classification scenario, Logistic Regression, Linear Discriminant Analysis, Quadratic Discriminant Analysis

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Overview

- Classification versus Regression.
- Logistic Regression.
- Multiple logistic Regression.
- Linear Discriminant Analysis (LDA).
- Quadratic Discriminant Analysis (QDA).

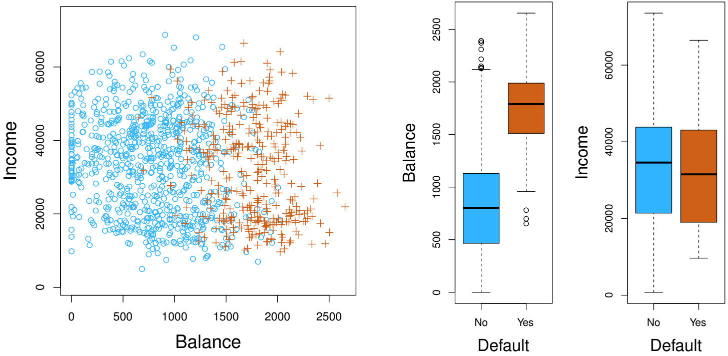
Many ideas from the regression scenario will carry over.

Examples

- Predicting a condition from symptoms in a hospital.
- Fraud detection in online payment systems.
- Predicting the probability of default on debt for credit card holders.

Classifications scenarios are very common.

Example: Default Data Set



Visualisation of the `Default` data set. The classes are color coded.

This is a simulated data set with an unusually high number of defaulters.

Example: Default Data Set

- In this example the response is *binary*:

$$y = \begin{cases} 1 & \text{if } \texttt{default} \text{ is } \texttt{Yes} \\ 0 & \text{if } \texttt{default} \text{ is } \texttt{No} \end{cases}$$

- We encode qualitative responses the same way we encode qualitative predictors.
- Linear regression would work but is not ideal.
- *Logistic regression* is the superior method.

Logistic regression predicts probabilities.

Example: Default Data Set

- For the `Default` data set we would like to predict the probability of $\texttt{default} = \texttt{Yes}$:

$$P(\texttt{default} = \texttt{Yes}|\texttt{balance})$$

- The probability is between 0 and 1.
- We can the *classify* based on P:

$$P(\texttt{default} = \texttt{Yes}|\texttt{balance}) > 0.5 \; : \; \texttt{default} = \texttt{Yes}$$

we can of course choose different *working points*.

The Logistic Model

- Out goal is to model the relationship

$$p(X) = P(Y = 1|X) \longleftrightarrow X$$

- We could use a linear regression model

$$p(X) = \beta_0 + \beta_1 X$$

- This does work but has some problems.
- In particular, the predicted probabilities can be < 0 or > 1.

We prefer a method that does not violate our axioms.

The Logistic Model

- We must model $p(X)$ such that

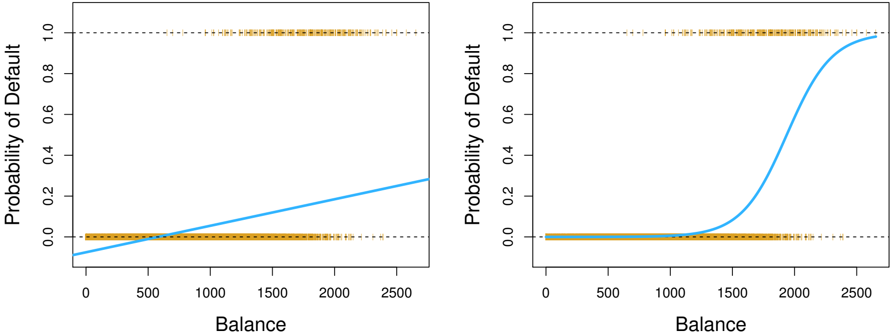
$$p(X) \in [0, 1] \quad \forall X$$

- There a many functions that guarantee that.
- We use the *logistic function*

$$p(X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$

We will need a new fitting method for this.

The Logistic Model



Left: Linear Regression, Right: Logistic Regression

The logistic model satisfies our axioms.

The Logistic Model

- The model looks complicated.
- How can we fit it?
- Some simple rearrangement yields the *odds*:

$$\frac{p(X)}{1 - p(X)} = e^{\beta_0 + \beta_1 X}$$

- For example:

$$p(0.2) \rightarrow \frac{1}{4} \quad \text{and} \quad p(0.9) \rightarrow 9$$

Odds originate from betting on horse races.

The Logistic Model

- How can the expression for the odds help us?
- How can we fit it?
- We take the logarithm of both sides to obtain

$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X$$

- The left-hand side is called the *log odds* or *logit*.

The model for the logit is linear in X.

The Logistic Model

- Recall that in linear regression β_1 describes the increase of Y for a one-unit change in X.
- Here the interpretation is slightly more complicated.
- Changing X by one unit changes the *logit* by β_1.
- Or equivalently, it multiplies the odds bt e^{β_1}.
- This does *not* imply a change of β_1 of $p(X)$!
- However, any *tendency* is preserved.

The logistic model has a nice interpretation.

Maximum Likelihood

- Given
$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X$$
we could fit the logistic model with a linear lest square fit.
- Instead, we will use a maximum likelihood fit.
- We have done this before without mentioning it.

Least Squares is just a special case of maximum likelihood.

Maximum Likelihood & Bayes' Theorem

$$P(Y|X, I) = \frac{P(X|Y, I) \times P(Y|I)}{P(X|I)}$$

Term	***Name***
$P(Y\|X, I)$	posterior probability
$P(X\|Y, I)$	likelihood
$P(Y\|I)$	prior probability
$P(X\|I)$	evidence

We are going to derive the maximum likelihood method.

Maximum Likelihood & Bayes' Theorem

- We aim to produce the best estimate of $\boldsymbol{\beta}$.
- These are the *most probable* values of β_0 and β_1 given the training data.
- That is, we seek to maximise
$$P(\boldsymbol{\beta}|X, I)$$
- A priori, we do not know how to construct this probability.

And here comes the power of Bayes' theorem...

Maximum Likelihood & Bayes' Theorem

- Given the training data *and* a model description we *can* construct the likelihood

$$P(X|\boldsymbol{\beta}, I)$$

- We can then use Bayes' theorem to obtain the posterior probability

$$P(\boldsymbol{\beta}|X, I) = \frac{P(X|\boldsymbol{\beta}, I)P(\boldsymbol{\beta}|I)}{P(X|I)}$$

- Or, up to a normalisation factor

$$P(\boldsymbol{\beta}|X, I) \propto P(X|\boldsymbol{\beta}, I)P(\boldsymbol{\beta}|I)$$

All we need is a prior and we are all set.

Maximum Likelihood & Bayes' Theorem

- We choose the prior to reflect our knowledge (or rather lack thereof) *without* taking the training data into account.
- A good start is to assume complete ignorance.
- In many cases a good ignorant prior is a flat distribution:

$$P(\boldsymbol{\beta}|I) = \text{const.}$$

The influence of the prior quickly becomes negligible for large data sets.

Maximum Likelihood & Bayes' Theorem

- The uniform (constant) prior can be absorbed in the normalisation and we obtain

$$P(\boldsymbol{\beta}|X,I) \propto \underbrace{P(X|\boldsymbol{\beta},I)}_{\text{likelihood}}$$

- In practice we often use the logarithm of the likelihood

$$\log\left(P(X|\boldsymbol{\beta},I)\right)$$

- Sometimes this allows for nice & easy analytical solutions.
- More importantly in practice it is numerically much more stable.

Now maximising the likelihood does maximise the posterior!

Maximum Likelihood & Bayes' Theorem

- Under the assumption that the x_i are independent we have

$$P(X|\boldsymbol{\beta}, I) = \prod_{i=1}^{n} P(x_i|\boldsymbol{\beta}, I)$$

- This follows from the product rule

$$P(x_i, x_k|\boldsymbol{\beta}, I) = P(x_i|x_k, \boldsymbol{\beta}, I)P(x_k|\boldsymbol{\beta}, I)$$

  and the independence assumption

$$P(x_i|x_k, \boldsymbol{\beta}, I) = P(x_i|\boldsymbol{\beta}, I)$$

We still need a model, though.

The Binomial Distribution

- We need a model to describe a qualitative response variable with two classes (levels).
- The binomial distribution describes this situation

$$P(r|n, I) = \frac{n!}{n!(n-r)!} p^r (1-p)^{n-r}$$

This is the probability to observe *r* "successes".

The Likelihood Function

- We can now construct the *likelihood function* for the logistic regression:

$$
\begin{aligned}
P(X|\boldsymbol{\beta}, I) &= \prod_{i=1}^{n} P(x_i|\boldsymbol{\beta}, I) \\
&= \prod_{y_i=1} p(x_i) \prod_{y_i \neq 1} (1 - p(x_i))
\end{aligned}
$$

with

$$
p(x_i) = \frac{e^{\beta_0+\beta_1 x_i}}{1 + e^{\beta_0+\beta_1 x_i}}
$$

Different problems require different likelihood functions.

Maximum Likelihood Estimate

- In practice we often us the logarithm of the likelihood function.
- The logarithm is a strictly monotonic function, so the extrema a preserved.
- Sometimes we minimise the negative logarithm.
- This is simply because of the abundance of minimisation libraries.

Wo do not care whether there is an analytical solution.

Logistic Regression Results

	Coefficient	Std. Error	Z-statistic	p-value
`Intercept`	-10.6513	0.3612	-29.5	< 0.0001
`balance`	0.0055	0.0002	24.9	< 0.0001

- Where the Z-statistic associated with β_1 is

$$Z = \frac{\hat{\beta}_1}{\mathrm{SE}(\hat{\beta}_1)}$$

- For large samples the Z-statistic approaches the t-statistic.

In logistic regression we use the Z-statistic and the associated p-value.

Hypothesis Testing

- The logistic null hypothesis is

$$H_0 : \beta_1 = 0 \implies p(X) = \frac{e^{\beta_0}}{1 + e^{\beta_0}}$$

- And the alternative hypothesis is

$$H_a : \beta_1 \neq 0 \implies p(X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$

We reject the null hypothesis based on a cut on the p-value of the Z-statistic.

A Word of Warning

- The term “maximum likelihood” suggests that we have found the most probable values of the parameters.
- This is in general *not* the case!
- We just determined the $\boldsymbol{\beta}$ that makes the *training data* most probable.
- It is important to keep this in mind.
- Consider the probability of rain given there are clouds versus the probability of clouds given it is raining.

In general $\boldsymbol{P(A|B) \neq P(B|A)}$.

Multiple Logistic Regression

- We can generalise the logistic approach using the logit:

$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_P$$

where

$$X = (X_1, \ldots, X_p)$$

are the p predictors as ususal.

We start from the logit to stress the similarity to OLS.

Multiple Logistic Regression

- We can easily translate this back to the logistic function:

$$p(x) = \frac{e^{\beta_0+\beta_1 X_1+\cdots+\beta_p Xp}}{1 + e^{\beta_0+\beta_1 X_1+\cdots+\beta_p Xp}}$$

As in the simple case we use maximum likelihood.

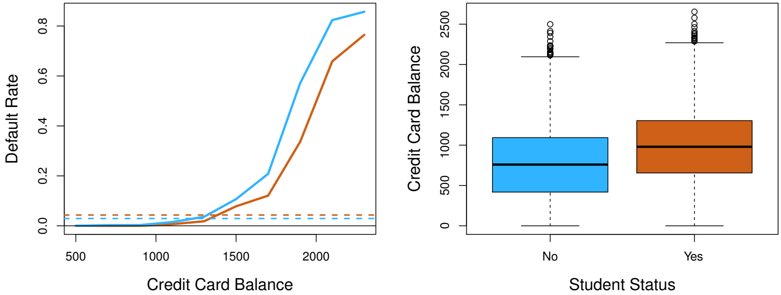
Multiple Logistic Regression

	Coefficient	Std. Error	Z-statistic	p-value
`Intercept`	−10.8690	0.4923	−22.08	< 0.0001
`balance`	0.0057	0.0002	24.75	< 0.0001
`income`	0.0030	0.0082	0.37	0.7115
`student[Yes]`	−0.6468	0.2362	−2.74	0.0062

- The negative coefficient for `student[Yes]` indicates that students are *less* likely to default.
- This holds fir *fixed values* of `balance` and `income`.

We should investigate this a bit further.

Multiple Logistic Regression



- Students (orange) and non-students (blue).
- Solid lines: `default` $= f($`balance`$)$.
- Dashed: overall default rate.
- Students have a higher `balance`.

There is a correlation!

The Bayes Classifier

- Suppose we have K classes with $K \geq 2$.
- The we can specify the posterior probability as

$$P(Y = k | X = x) = \frac{\pi_k f_k(x)}{\sum_{l=1}^{K} \pi_l f_l(x)}$$

where π_k is the prior and

$$f_k(x) = P(X = x | Y = k)$$

- The problem now is the specification of f_k.

The Bayes classifier is the gold standard.

Linear Discriminant Analysis

- For now we assume one predictor, that is $p = 1$
- We want to find $f_k(x)$ in order to find $p_k(x)$.
- Once we have that, we can classify observations by choosing the class with the greatest $p_k(x)$.

We need to make some further assumptions about f_k.

Linear Discriminant Analysis

- We now also assume that $f_k(x)$ is *normal* (*Gaussian*).
- In the case of $p = 1$ this means

$$f_k(x) = \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right)$$

where μ_k and σ_l may vary by class.

Even more assumptions follow…

Linear Discriminant Analysis

- For now we further assume that

$$\sigma_1 = \sigma_2 = \cdots = \sigma_K = \sigma$$

- This yields

$$p_k(x) = \frac{\pi_k \exp\left(-\frac{1}{2\sigma^2}(x-\mu_k)^2\right)}{\sum_{l=1}^{K} \pi_l \exp\left(-\frac{1}{2\sigma^2}(x-\mu_l)^2\right)}$$

We assign the observation $X = x$ to the class with the largest $p_k(x)$.

Linear Discriminant Analysis

- By taking the logarithm, this is equivalent to choosing the class k for which

$$\delta_k(x) = x\frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k)$$

  is largest.
- For example, if $K = 2$ and $\pi_1 = \pi_2$, the Bayes classifier assigns:

$$\text{class} = \begin{cases} 1 & \text{if } 2x(\mu_1 - \mu_2) > \mu_1^2 - \mu_2^2 \\ 0 & \text{otherwise} \end{cases}$$

In practice we don't have access to the true parameters.

Linear Discriminant Analysis

- We have to *estimate* the parameters taking into account our assumptions.
- LDA does just that and yields

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{y_i = k} x_i$$

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{y_i = k} (x_i - \hat{\mu}_k)^2$$

Let's talk about the interpretation.

Linear Discriminant Analysis

- The estimate $\hat{\mu}_k$ is the average of all training observations of the kth class.
- The estimate $\hat{\sigma}^2$ is the weighted average of the sample variances of the K classes.
- If we don't know the $\pi_!, \ldots, \pi_K$ we estimate them from their frequencies in the training sample:

$$\hat{\pi}_k = \frac{n_k}{n}$$

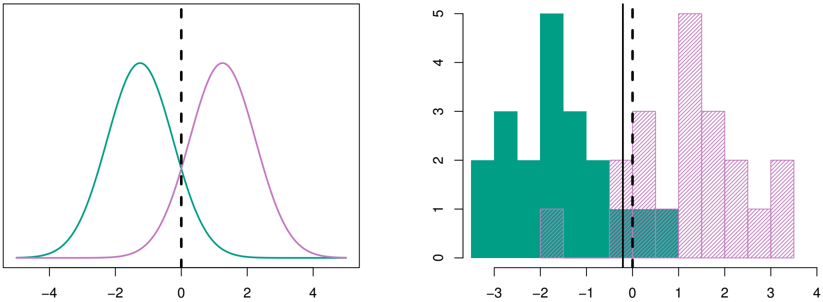
- We can now construct $\hat{\delta}(x)$:

$$\hat{\delta}_k(x) = x\frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log(\hat{\pi}_k)$$

LDA is linear in the sense that $\hat{\delta}_k$ is linear in x

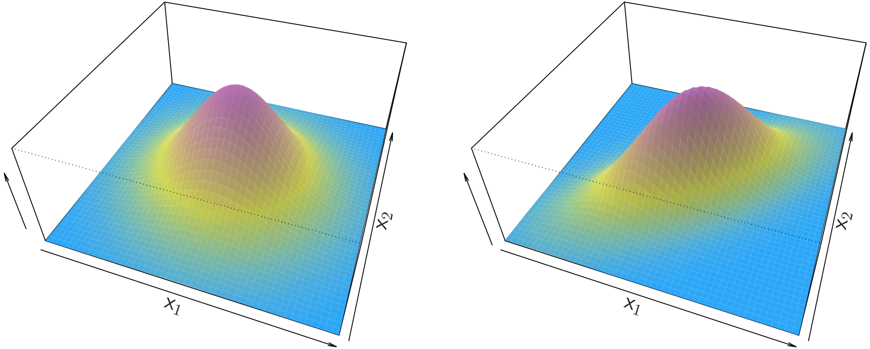
.

Linear Discriminant Analysis



The error rate is only 0.5%. LDA is doing well on this simulation.

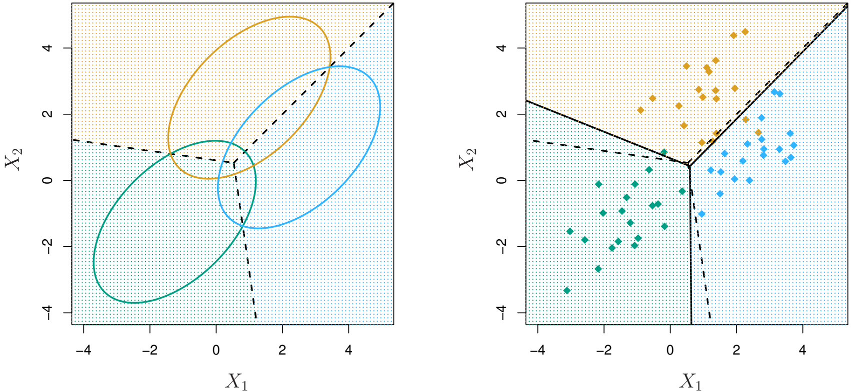
LDA with $p > 1$



- We now have a multivariate Gaussian distribution.
- We now have to estimate the covariance matrix $\boldsymbol{\Sigma}$.

Note that the variances can now be different.

LDA with $p > 1$



- Dashed: Bayes decision boundary.
- Solid: LDA estimate.

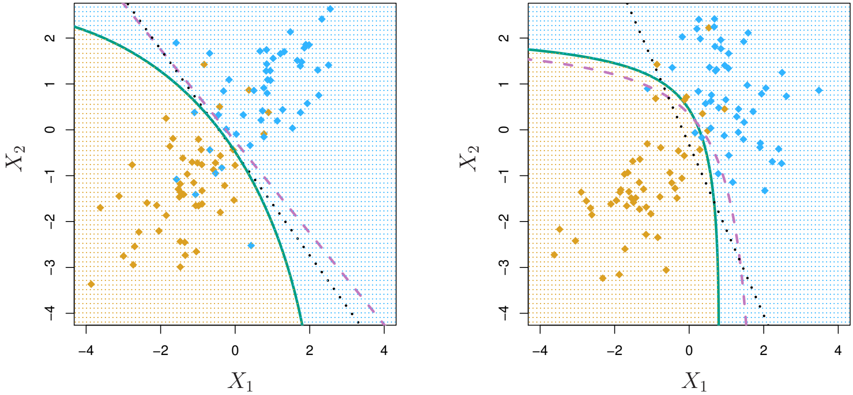
This is a simulated example with three classes.

Quadratic Discriminant Analysis

- QDA is an alternative approach to LDA that allows for curved boundaries.
- We drop the assumption that $\boldsymbol{\Sigma}$ is common to all classes.
- That means QDA provides an estimate $\hat{\boldsymbol{\Sigma}}_k$ in addition to $\hat{\mu}_k$ and $\hat{\pi}_k$.

The resulting $\hat{\boldsymbol{\delta}}_{\boldsymbol{k}}$ is now quadratic in $\boldsymbol{x}$.

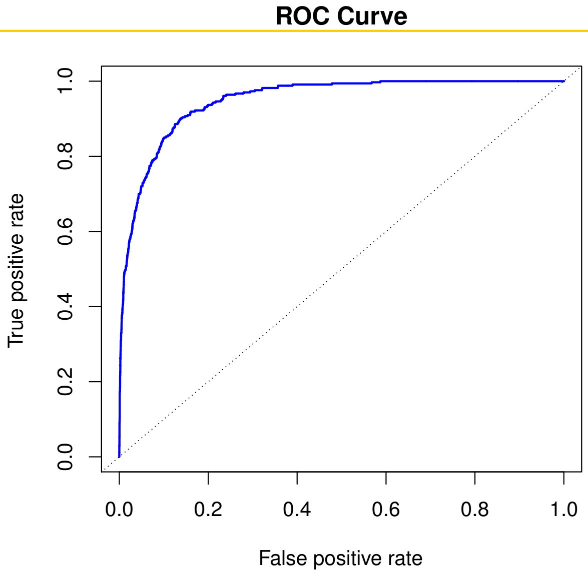
Quadratic Discriminant Analysis



- Left: $\mathbf{\Sigma}_1 = \mathbf{\Sigma}_2$
- Right: $\mathbf{\Sigma}_1 \neq \mathbf{\Sigma}_2$

The QDA performs better when the boundary is curved.

Classifier Performance



we can use this tho choose a *working point*

Questions?

Thank you!