# Statistical learning - Vinciotti (2022)

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# Contents

# Part I

# Introduction

# Chapter 1

# General course information

## 1.1 Textbooks

- James et al (2021), Introduction to statistical learning in R, 2nd edition. (Book that is used as guidline for the course, but further concepts will be added during the lectures)
- Hastie et al (2001), Elements of statistical learning. (More advanced book for those who want to study the subject more in depth)

## 1.2 Assessment

- Three homework tasks during the course (Uploaded on moodle, two weeks of time for each, more practical and mainly focused on applying methods to some data. If done well they will add 2 points to the written exam score)
- Final written exam (More theoretical but still connected to the practical part, for instance by commenting on analysis output)

## 1.3 Topics

- Linear regression (Gauss, 1800) (Assumed to be already known from Statistical Learning 1)
- Linear discriminant analysis, LDA (Fisher, 1936) (Later extended to quadratic discriminant analysis, QDA)
- Logistic regression (1940s)
- Generalized linear models (Nelder and Wedderburn, 1972)
- Classification and regression trees (Breiman and Freidman, 1980s) (First introduction of computer intensive methods)
- Machine learning (1990s): support vector machines, neural networks/deep learning, unsupervised learning (clustering, PCA)
- Individual methods: theory, details, implementation ...

- General concept: model selection, inference, prediction ...

# Part II

# Statistical learning

Chapter 2

# What is statistical learning?

## 2.1 Definition of statistical learning

In general, a statistical learning problem can be formalized as follows:

- $Y$ : response/dependent/outcome variable
- $\underline{X} = (X_1, \ldots, X_p)$: vector of predictors/features/independent variables/covariates

We assume that there is a relationship between $Y$ and $\underline{X}$, which can be written as:

$$Y = f(\underline{X}) + \varepsilon$$

Where:

- $f(\underline{X})$ is the deterministic (but unknown) function of the vector $\underline{X} = (X_1, \ldots, X_p)$
- $\varepsilon$ is the error (stochastic part), for which we assume the following properties:
  - $E[\varepsilon] = 0$ (Its expected value is zero)
  - $\varepsilon \perp \underline{X}$ (It is independent from $\underline{X}$)

the $\epsilon$ value represents the stochastic error, which is the estimated error in a model that arises from the exclusion of an important explanatory variable or due to incorrect specification. Therefore, the expression **statistical learning** encompasses different methods to estimate $f(\underline{X})$.

## 2.2 Why estimate $f$?

There are two main reasons to estimate $f$, those two being **prediction** and **inference**.

### 2.2.1 Prediction

Predict $Y$ when we only have observations about $\underline{X}$. Since $E[\varepsilon] = 0$, we usually take:

$$\hat{Y} = \hat{f}(\underline{X})$$

With $\hat{f}$ being our estimate of $f$.

If this is the only reason to estimate $f$, then $\hat{f}$ can be a ***black-box*** method (deep learning). The accuracy of $\hat{Y}$ as a predictor of $Y$ can be described calculating the expected **MSE**, the test Mean Squared Error.

$$\begin{aligned}
&E[(Y - \hat{f}(\underline{X}))^2 \,|\, \underline{X} = \underline{x}\,] = && \text{where } \hat{f} \text{ is a fixed known function}\\
&\quad = E[(f(\underline{X}) + \varepsilon - \hat{f}(\underline{X}))^2] && \text{since } Y = f(\underline{X}) + \varepsilon\\
&\quad = E[(f(\underline{X}) - \hat{f}(\underline{X})) + \varepsilon)^2] && \text{rearranging}\\
&\quad = E[(f(\underline{X}) - \hat{f}(\underline{X}))^2 + \varepsilon^2 + 2\varepsilon(f(\underline{X}) - \hat{f}(\underline{X}))] && \text{solving the square}\\
&\quad = E[(f(\underline{X}) - \hat{f}(\underline{X}))^2] + E[\varepsilon^2] + 2E[\varepsilon(f(\underline{X}) - \hat{f}(\underline{X}))] && \text{separating the expectations}
\end{aligned}$$

Furthermore, since we know that:

$$\begin{aligned}
Var(\varepsilon) &= E[(\varepsilon - E(\varepsilon))^2] && \text{formal definition of variance}\\
&= E[\epsilon^2 + (E(\epsilon))^2 - 2E(\epsilon)\epsilon] && \text{solving the square}\\
&= E[\varepsilon^2] - (E[\varepsilon])^2 && \text{definition generally used during calculation}\\
&= E[\varepsilon^2] && \text{since } E[\varepsilon] = 0
\end{aligned}$$

Thus we get:

$$\begin{aligned}
&E[(Y - \hat{f}(\underline{X}))^2 \,|\, \underline{X} = \underline{x}\,] =\\
&\quad = E[(f(\underline{X}) - \hat{f}(\underline{X}))^2] + Var(\varepsilon) + 2E[\varepsilon(f(\underline{X}) - \hat{f}(\underline{X}))] && \text{substituting } E[\varepsilon^2] = Var(\varepsilon)\\
&\quad = (f(\underline{X}) - \hat{f}(\underline{X}))^2 + Var(\varepsilon) + 2(f(\underline{X}) - \hat{f}(\underline{X}))E[\varepsilon] && \text{since } f(\underline{X}) - \hat{f}(\underline{X}) \text{ is a constant}\\
&\quad = (f(\underline{X}) - \hat{f}(\underline{X}))^2 + Var(\varepsilon) && \text{since } E[\varepsilon] = 0
\end{aligned}$$

With:

- $(f(\underline{X}) - \hat{f}(\underline{X}))^2$ being the **reducible error**. The model choice can increase or reduce this value, hence it is mostly controllable.
- $Var(\varepsilon)$ being the **irreducible error**. This value depends on the innate randomness present in the data, hence you can only try and minimize it by deciding which variables to use in your prediction (but it will never be zero otherwise you would have a deterministic situation).

### 2.2.2 Inference

Inference is used when you want to understand the relation between $Y$ and $\underline{X}$ (and not just be able to make predictions). Namely, inference answers questions such as:

- *Which predictors/factors are most associated with the response?*
- *What is the relationship between $Y$ and $X_j$?*

## 2.3 How to extimate $f$?

Given some **training data** $(\underline{x}_i, y_i)$, $i = 1, \dots, n$, where $\underline{x}_i = (x_{i1}, \dots, x_{ip})^t$ is the vector of observations of unit $i$ while $y_i$ is the response for unit $i$, broadly speaking there are two types of methods to estimate $f$: **parametric methods** and **non-parametric methods**.

### 2.3.1 Parametric methods

In order to use parametric methods, we make an assumption about the functional form of $f(\underline{X})$, that assumption being that the form of the function depends on some *parameters* (which we can estimate). An example of parametric method is **linear regression**, which implies that $f(\underline{X})$ is in the form:

$$f(\underline{X}) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$$

Where the great $X$s represent the predictors. Given this assumption, statistical learning becomes **fitting** (or training) the model on the data, which means estimating the parameters $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p$ such that:

$$\hat{f}(\underline{X}) = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \cdots + \hat{\beta}_p X_p$$

The main disadvantage of these methods is that they may be **too restrictive**, as they would depend on a limited number of predictors.

Notice that linear models are <u>linear in the parameters</u>, not in the predictors, hence:

- $f(X_1) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_1^3 + \varepsilon$ (polynomial regression) is a linear model.
- $f(X_1) = \beta_0 X_1^{\beta_1}$ is <u>not</u> a linear model.

### 2.3.2 Non-parametric methods

Non-parametric methods do not make any explicit assumption on the function form of $f(\underline{X})$. These methods want to estimate $f$ by getting as close as possible to the data, without being too *rough or wiggly* (basically **overfitting**).

### 2.3.3 Parametric vs non-parametric methods

Despite parametric methods being more restrictive than non-parametric ones, we might still choose to adopt them for the sake of interpretability and generalizability outside of the training data.

## 2.4 Bias-variance trade-off

Assume you have some data pairs in the form $(x_i, y_i)$, $i = 1, \dots, n$; you can then define the estimate function $\hat{f}(x)$ as a linear model with up to $n - 1$ parameters (more parameters give the same result as $n-1$ parameters) and an intercept value. You could thus use, for instance, the models:

| | |
|---|---|
| 1 parameter | $f(x) = \beta_0 + \beta_1 x + \varepsilon$ |
| 2 parameters | $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon$ |
| $\vdots$ | $\vdots$ |
| $n-1$ parameters | $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_{n-1} x^{n-1} + \varepsilon$ |

You could choose the model with the highest number of parameters; this model would explain all the variance of the training data ($R^2 = 1$) yet it would be very complex and perform badly with new data points. On the other hand a model with a lower number of parameters would explain less of the variance of the training data, yet it could perform better with new data points.

Keeping in mind that $Y$ is random and that $\hat{f}$ is a random variable estimated from the data, when using the general formula to determine how well a model performs at generic $\underline{X}$, we notice:

$$\begin{aligned}
&E[(Y - \hat{f}(\underline{X}))^2 \,|\, \underline{X} = \underline{x}\,] = \\
&\quad = E[(f(\underline{X}) + \varepsilon - \hat{f}(\underline{X}))^2] && \text{since } Y = f(\underline{X}) + \varepsilon \\
&\quad = E[(f(\underline{X}) + \varepsilon - \hat{f}(\underline{X}) + E[\hat{f}(\underline{X})] - E[\hat{f}(\underline{X})])^2] && \text{since } E[\hat{f}(\underline{X})] - E[\hat{f}(\underline{X})] = 0 \\
&\quad = E[((f(\underline{X}) - E[\hat{f}(\underline{X})]) + \varepsilon + (E[\hat{f}(\underline{X})] - \hat{f}(\underline{X})))^2] && \text{grouping, square of three elements} \\
&\quad = E[(f(\underline{X}) - E[\hat{f}(\underline{X})])^2] + E[\varepsilon^2] + E[(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))^2] + \\
&\qquad + 2E[(f(\underline{X}) - E[\hat{f}(\underline{X})])\,\varepsilon] + \\
&\qquad + 2E[(f(\underline{X}) - E[\hat{f}(\underline{X})])(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))] + && \text{solving the square and} \\
&\qquad + 2E[(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))\,\varepsilon] && \text{dividing the expectations}
\end{aligned}$$

But notice that:

$$\begin{aligned}
E[(f(\underline{X}) - E[\hat{f}(\underline{X})])\,\varepsilon] &= E[\varepsilon](f(\underline{X}) - E[\hat{f}(\underline{X})]) && \text{since } f(\underline{X}) - E[\hat{f}(\underline{X})] \text{ is constant} \\
&= 0 && \text{since } E[\varepsilon] = 0
\end{aligned}$$

$$\begin{aligned}
&E[(f(\underline{X}) - E[\hat{f}(\underline{X})])(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))] = \\
&\qquad = (f(\underline{X}) - E[\hat{f}(\underline{X})])E[E[\hat{f}(\underline{X})] - \hat{f}(\underline{X})] && \text{since } f(\underline{X}) - E[\hat{f}(\underline{X})] \text{ is constant} \\
&\qquad = (f(\underline{X}) - E[\hat{f}(\underline{X})])E[\hat{f}(\underline{X}) - \hat{f}(\underline{X})] && \text{since } \hat{f}(\underline{X}) \text{ is a constant} \\
&\qquad = (f(\underline{X}) - E[\hat{f}(\underline{X})])E[0] \\
&\qquad = 0
\end{aligned}$$

$$\begin{aligned}
E[(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))\,\varepsilon] &= E[\varepsilon]E[E[\hat{f}(\underline{X})] - \hat{f}(\underline{X})] && \text{since } \varepsilon \perp \underline{X} \implies E[\varepsilon\underline{X}] = E[\varepsilon]E[\underline{X}] \\
&= 0 && \text{since } E[\varepsilon] = 0
\end{aligned}$$

Therefore we can simplify as:

$$\begin{aligned} E[(Y - \hat{f}(\underline{X}))^2 \mid \underline{X} = \underline{x}] &= E[(f(\underline{X}) - E[\hat{f}(\underline{X})])^2] \quad &+E[\varepsilon^2] \quad &+E[(E[\hat{f}(\underline{X})] - \hat{f}(\underline{X}))^2] \\ &= f(\underline{X}) - E[\hat{f}(\underline{X})])^2 \quad &+Var(\varepsilon) \quad &+Var(\hat{f}(\underline{X})) \end{aligned}$$

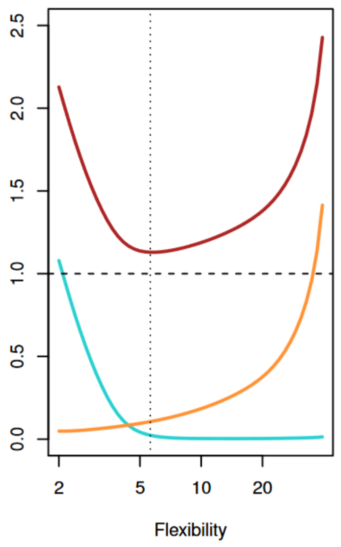
Where:

- $f(\underline{X}) - E[\hat{f}(\underline{X})])^2$ is the **bias**
- $Var(\varepsilon)$ is the **irreducible error**
- $Var(\hat{f}(\underline{X}))$ is the **variance** of the model

**Bias** is the amount that a model's prediction differs from the target value, compared to the training data. Generally bias is consequently results from simplifying the assumptions used in a model. If an estimated model performs well on multiple data sets, the estimated model has low bias. *High bias means that an estimated model is far from the real model.*

**Variance** refers instead to the amount by which $\hat{f}$ would change if we estimated it using a different training data set. Ideally, the $\hat{f}$ calculated through different datasets should be not significantly different, the model should be fitted equivalently using a different training dataset. The more flexible models, the more they are influenced by a changes of the training dataset.

**Figure 2.1:** As the flexibility of a model increases, the Bias decreases, and the varaiance of the model increases



In order to minimize the expected error, we need to achieve low bias and low variance. In practice, one needs to find a good **trade-off** between bias and variance, since reducing one often involves increasing the other. In general:

- A **simpe model** has high bias (it is far from the real model) and low variance (when fitting using different training data you get similar estimated parameters).
- A **complex model** has low bias and high variance, as the complexity of the model has the aim of making it as near as possible to the real $f$.

Both in parametric and non-parametric methods, you generally have at least one **tuning parameter**, which is a parameter that can be tweaked (for instance the degree of the polinomial) in order to choose the balance between bias and variance.

# Chapter 3

# Statistical decision theory

## 3.1 Definition of statistical decision theory

The **statistical decision theory** is a set of quantitative methods for reaching optimal decisions for well posed problems. Statistical decision theory applies to supervised learning, while it does not apply to unsupervised learning. For most of the course we will focus on supervised learning (decision theory statistics from Britannica).

## 3.2 Supervised learning

**Supervised learning** is a set of methods whose objective is, given the observations $(\underline{x}_i, y_i)$ with $i = 1, \dots, n$, to **find a rule $\hat{f}$ that allows us to predict $Y$ from $\underline{X}$**, meaning that $\hat{Y} = \hat{f}(\underline{X})$. $\hat{f}(\underline{X})$ is thus an approximation of the true rule $f(\underline{X})$. Finding $\hat{f}$ corresponds to training (or fitting) a model using labelled data pairs (both predictors and response values are known). In this case, the term *fitting* refers to adjusting the parameters in the model to improve the accuracy. *Model fitting*, insted, is the measure of how well a machine learning model generalizes data similar to that with which it was trained. A good model fit refers to a model that accurately approximates the output when it is provided with unseen inputs.

Broadly, there are two main types of methods of supervised learning:

- **Regression methods**, in which the response $Y$ is quantitative (numerical). In this case $\hat{f}$ is called ***regression function***.
- **Classification methods**, in which the response $Y$ is qualitative (categorical). In this case $\hat{f}$ is called ***classifier***.

The predictors ($\underline{X}$) can take any form, numerical or categorical. In general there are no assumptions on the form of the predictors (but not always).

To evaluate a model you use **loss functions**, which are functions used to penalize the differences between $Y$ and $\hat{f}(\underline{X})$. Many loss functions can be used; the choice of a specific loss function determines which function is considered to be the true rule $f(\underline{X})$ (since this moment I will refer $\hat{f}(x)$ as $f(x)$).

## 3.3 Regression setting

In a regression setting, the loss function which is generally used is the **squared error loss function** (also referred as the risk of estimating $Y$ using $\hat{f}(\underline{X})$), which is defined as:

$$L(Y, f(\underline{X})) = (Y - f(\underline{X}))^2$$

When using this loss function, the criterion for choosing the model becomes finding $f$ such that it minimizes the **expected prediction error** (EPE), which is the expected value of the squared error loss function:

$$\begin{aligned}\text{EPE}(f) &= E_{Y,\underline{X}}[(Y - f(\underline{X}))^2] \\ &= \iint (y - f(\underline{x}))^2 g_{Y,\underline{X}}(y, \underline{x})\, dy\, d\underline{x} && \textbf{if } Y \textbf{ is continuous}\end{aligned}$$

This error is an expectation since you usually do not know the distribution of $Y$ and $\underline{X}$. If Y is continuous you can rewrite this expectation as the double integral times the joint density function $g_{Y,\underline{X}}(y, \underline{x})$.

**Theorem 1** (Minimum of the expected prediction error). *EPE($f$) $= E_{Y,\underline{X}}[(Y - f(\underline{X}))^2]$ has a* ***minimum*** *when $f(\underline{x}) = E[Y|\underline{X} = \underline{x}]$. $f(\underline{x})$ is called regression function.*

*Proof.* (Sketch) By definition we know that

$$\text{EPE}(f) = E_{Y,\underline{X}}[(Y - f(\underline{X}))^2]$$

Then, because of the law of *iterated expectations* we get

$$E_{Y,\underline{X}}[(Y - f(\underline{X}))^2] = E_{\underline{X}}[E_{Y|\underline{X}}[(Y - f(\underline{X}))^2]|\underline{X}]$$

If we then consider a specific value of $\underline{X}$, meaning $\underline{X} = \underline{x}$, the inner expectation becomes

$$E[(Y - f(\underline{x}))^2|\underline{X} = \underline{x}]$$

But since $\underline{x}$ is fixed, $f(\underline{x})$ is a constant, hence this expectation can be written as a function in some parameter $a$

$$g(a) = E_Y[(Y - a)^2]$$

Then we want to find the (constant) value of $a$ that minimizes $g(a)$

$$\begin{aligned}g(a) &= E_Y[(Y - a)^2] \\ &= E[Y^2 - 2aY + a^2] && \text{compute the square} \\ &= E[Y^2] - 2aE[Y] + E[a^2] && \text{separate expectations} \\ &= E[Y^2] - 2aE[Y] + a^2 && \text{pull out } a^2 \text{ since constant}\end{aligned}$$

Then, setting the derivative to zero we get

$$\frac{dg}{da} = -2E[Y] + 2a \overset{!}{=} 0 \implies \hat{a} = E[Y]$$

Notice that if you plug $\hat{a}$ into $g(a) = E_Y[(Y-a)^2]$ you get

$$g(\hat{a}) = E_Y[(Y - E[Y])^2] = Var(Y)$$

Since $a = E[Y]$, the function that minimizes the $g(a)$ function and consequently the EPE is

$$f(\underline{x}) = E[Y|\underline{X} = \underline{x}]$$

$\square$

In a regression setting you could use other loss functions, such as the ***absolute error loss*** function

$$L(Y|f(\underline{X})) = |Y - f(\underline{X})|$$

which is used in **least absolute deviation** (LAD) regression. In this case $f(\underline{x})$ **is the median of** $Y$ **given** $\underline{x}$, therefore you have a model which is more robust to outliers.

We will choose the squared error loss and this motivates how the methods are developed. For example:

- **Linear regression** (parametric regression) can be expressed as

  $$Y|\underline{X} = \underline{x} \sim N(\underline{x}^t\underline{\beta}, \sigma^2) \qquad \text{Meaning that } \underline{\text{x}} \text{ is composed of}$$

  or focusing more on the conditional mean

  $$E[Y|\underline{X} = \underline{x}] = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

- **K-nearest neighbours regression**: one of the most used non-parametric regression

### 3.3.1 K-nearest neighbours regression (KNN)

In the scope of regression, K-nearest neighbours method is defined as

$$\hat{f}(\underline{x}) = \text{Average}(y_i|\underline{x_i} \in N_K(\underline{x})) = \frac{1}{K}\sum_{x_i \in N_{\underline{x}}} y_i \tag{3.1}$$

Where:

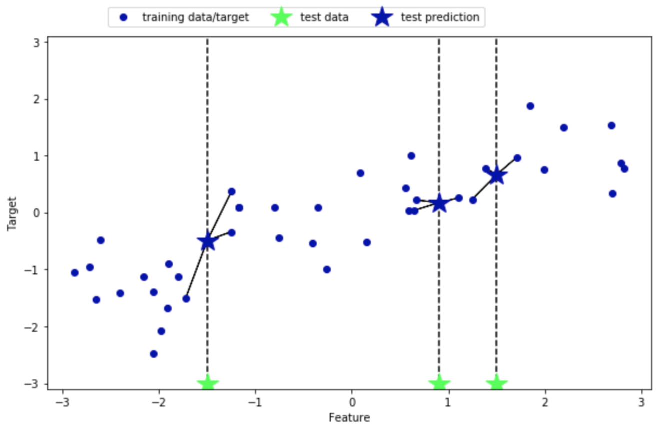
- Average is the sample mean
- $N_K(\underline{x})$ is the neighbourhood of $K$ points closest to $\underline{x}$
- $K$ is an integer

This method makes two approximations:

- It uses sample mean to approximate population mean
- It uses a neighbourhood of $\underline{x}$ rather than only $\underline{x}$

This method works well if you have a high amount of data and the number of parameters ($p$) is small. This simple method is rarely used, but it has inspired the development of more sophisticated kernel methods.

**Figure 3.1:** The training data are shown in blue dots, test data and predictions of test data are star-shaped. The predicted value on test data is given making the average of the neighbours' values



## 3.4 Classification setting

In a classification setting the response $Y$ *is categorical*, with $K$ categories. A **classifier** is deciding which class to assign to a new observation $\underline{x}$. In this case $\hat{Y}$ is the predicted class.

An example of loss function that can be used in classificiation setting is the 0-1 **loss function** which penalizes classifying a datapoint in the wrong class. Assume for instance the binary case, meaning $K = 2$ (but you could generalize for any number of classes); in that case the 0-1 loss function can be represented as:

| **True value, Prediction** | **0** | **1** |
|---|---|---|
| **0** | 0 | 1 |
| **1** | 1 | 0 |

**Table 3.1:** This is the table representing the possible values of the 0-1 loss function: $L(Y, \hat{Y}(\underline{X}))$. $Y$ is the true class, while instead $\hat{Y}(\underline{X})$ is the predicted class.

Notice that this function penalizes the same way all the misclassified observations (it assigns them the value 1).

Using the 0-1 loss function, the criterion for choosing the model becomes finding the classifying function $\hat{Y}$, dependent on $\underline{X}$, that **minimizes the expected 0-1 loss function** when applied to every possible value $\underline{x}$. In practice, we want to find the function $\hat{Y}$ so that the expected value $E[L(Y, \hat{Y}(\underline{X}))]$ is the minor.

To find $\hat{Y}$, let us consider just one $\underline{x}$, therefore the problem becomes minimizing

$$E[L(Y, \hat{Y}(\underline{x}))] = \sum_{k=1}^{k} L(k, \hat{Y}(\underline{x}))\ p(k|\underline{x})$$

[This equation means that $E[L(Y, \hat{Y}(\underline{x}))]$, is equal to the sum of all the possible values of the loss function (calculated for each class with respect to the predicted class) multiplied by the probability of that class given $\underline{x}$]. Then, considering the binary case (with two possible classes 0 and 1), if the classifier predicts $\underline{x}$ to belong to class 0 ($\hat{y} = 0$), we have

$$\begin{aligned} E[L(Y,0)] &= L(0,0)p(0|\underline{x}) + L(1,0)p(1|\underline{x}) \\ &= 0 \cdot p(0|\underline{x}) + 1 \cdot p(1|\underline{x}) \\ &= p(1|\underline{x}) \end{aligned}$$

Logically, $E[L(Y,0)]$ will be the loss value (1) multiplied by the probability of x belonging to class 1, Y = 1. On the other hand, if the classifier predicts $\underline{x}$ to belong to the class 1, $p(1|\underline{x})$, we have

$$\begin{aligned} E[L(Y,1)] &= L(0,1)p(0|\underline{x}) + L(1,1)p(1|\underline{x}) \\ &= 1 \cdot p(0|\underline{x}) + 0 \cdot p(1|\underline{x}) \\ &= p(0|\underline{x}) \end{aligned}$$

Predicting $\underline{x}$ to the class that minimizes the expected 1-0 loss results in classifying $\underline{x}$ to class 1 if $p(1|\underline{x}) > p(0|\underline{x})$. Since $p(0|\underline{x}) = 1 - p(1|\underline{x})$, we can write

$$p(1|\underline{x}) > 1 - p(1|\underline{x}) \implies 2p(1|\underline{x}) > 1 \implies p(1|\underline{x}) > 0.5$$

Therefore, in the binary case, $\underline{x}$ is predicted to belong to the class with more than 0.5 probability (which is intuitive).

In general ($k$ classes), the 0-1 loss is minimized by the **bayes classifier**, which states to assign $\underline{x}$ to class $j$ where

$$j = \underset{i \in classes}{\operatorname{argmax}}\, p(Y = j|\underline{X} = \underline{x})$$

(Which means assigning $\underline{x}$ to the class with the highest probability). This approach tells us how to set the problem, but it does not give any information on the probabilities, which have to be estimated by the single method.

To rewrite the binary case in another way:

$$\text{assign } \underline{x} \text{ to class} \begin{cases} 1 \text{ if } p(1|\underline{x}) > 0.5 \\ 0 \text{ if } p(1|\underline{x}) < 0.5 \end{cases}$$

The line formed by the points with probability $p(1|\underline{x}) = 0.5$ is called **bayes decision boundary** or **decision surface**.

The **bayes error rate** (BER) is the probability of committing an error when classifying observations. It is defined as:

$$\text{BER } = 1 - E_{\underline{X}}\left(\max_j p(j|\underline{x})\right)$$

(Since the class with the highest probability is the one considered by us to classify observations, the probability of getting an error is equal to the total probability subtracted with the probability used to assign the class).

**Figure 3.2:** Bayes decision boundary in green. In the simplest case, when we have two classes with equivalent probability, $p(1|\underline{x}) = p(0|\underline{x} = 0.5)$

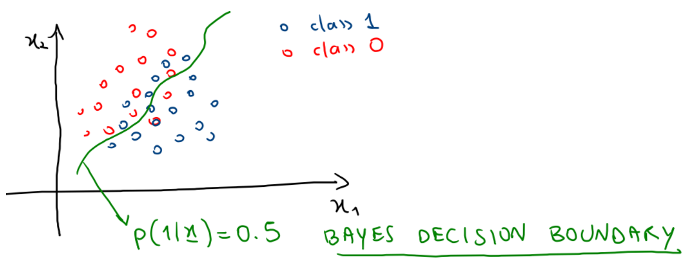
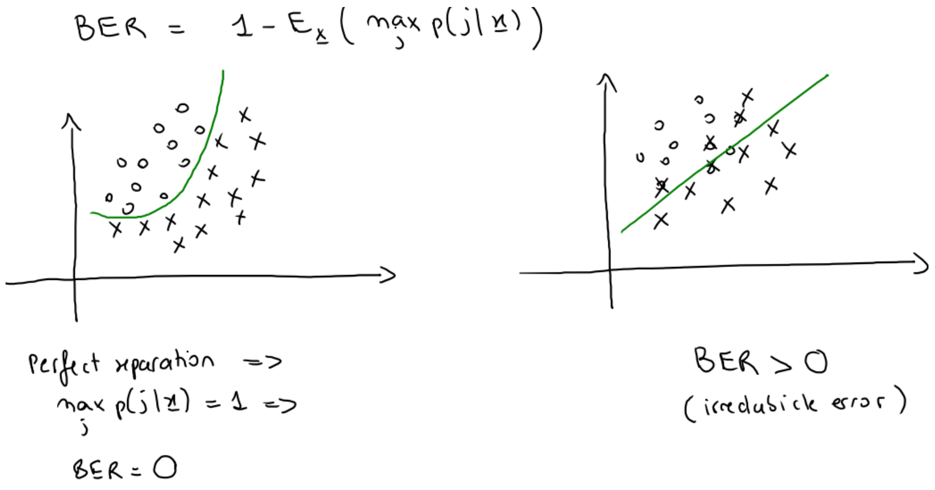


**Figure 3.3:** The figure on the left represents the best possible scenario, as the BES value is 0, and the decision surface separate completely the elements belonging to the two classes. The graph on the left instead shows an intermadiate situation, where $BER \neq 0$


$BER = 1 - E_{\underline{x}}(\max_j p(j|\underline{x}))$
Perfect separation =>
$\max_j p(j|\underline{x}) = 1$ =>
$BER = 0$
$BER > 0$
(irreducible error)

We talk about **perfect separation** of the classes (figure 3.3) when

$$\max_j p(j|\underline{x}) = 1 \implies \text{BER } = 0$$

In this case it is possible to classify any $\underline{x}$ without error. Generally, **BER** $> 0$, therefore you have some irreducible error due to a partial overlap of the classes.

It is possible to use a more generic loss function, called **misclassification loss function**, which can be represented (if $K = 2$) as:

**Table 3.2:** This is the table representing the possible values of $L(Y, \hat{Y}(\underline{X}))$. $c_0$ and $c_1$ represent two different cost values

| **True value, Predictions** | **0** | **1** |
|---|---|---|
| **0** | 0 | $c_0$ |
| **1** | $c_1$ | 0 |

This loss function is analogous to the 0-1 loss function, but it assigns **different weights to different errors**, therefore the misclassifications have different costs:

- $c_0$ is the misclassification cost of misclassifying a class 0 to 1
- $c_1$ is the misclassification cost of misclassifying a class 1 to 0

Just like the 0-1 loss function, misclassification loss function can be generalized for $K$ classes. This loss function is generally better than the 0-1 loss function since***in real situations it is likely for misclassifications to have different relevance*** (credit risk evaluation, medical context and others). Moreover, this loss function allows you to adjust for unbalanced classes. Consider for example a rare disease; consider the 1 value to be indicative of the ill state, and 0 of the healthy state. We would obtain in all the cases

$$\begin{aligned} E[L(Y,0)] = L(1,0)p(1|\underline{x}) & \qquad \text{prediction for the 0 (healthy) class} \\ <<< \; E[L(Y,1)] = L(0,1)p(0|\underline{x}) & \qquad \ldots \text{ for the 1 (ill) class} \end{aligned}$$

since $p(1|\underline{x})$ is really low, and consequently, using a 0-1 loss function results in a model which always classifies patients as healty. The model would be almost always correct, but it does not perform well when trying to determine which patients are affected by the disease. When using misclassification loss function, you can instead increase the weight of the misclassification "classify a patient as healthy when they are not", which may lead to worse results in terms of identifying healthy patients, but way better results in terms of identifying diseased patients.

Repeating the same steps used for 0-1 loss function, we can determine the threshold for the misclassification function (for $k = 2$ but it can be generalized)

$$E[L(Y,0)] = c_1 p(1|\underline{x}) \text{ and } E[L(Y,1)] = c_0 p(0|\underline{x})$$

Therefore we assign $\underline{x}$ to class 1 if

$$c_1 p(1|\underline{x}) > c_0 p(0|\underline{x})$$

But since $p(0|\underline{x}) = 1 - p(1|\underline{x})$, we can instead write

$$\begin{aligned} c_1 p(1|\underline{x}) &> c_0 - c_0 p(1|\underline{x})) \\ p(1|\underline{x}) &> \frac{c_0}{c_0 + c_1} \end{aligned}$$

which is the **classification threshold**.

## 3.5 Model accuracy

In practice, we would use our chosen method to estimate $f(\underline{x}) = E[Y|\underline{X} = \underline{x}]$ (regression) or $p(1|\underline{x})$ (classification) from training data $(\underline{x}_i, y_i)$, $i = 1, \ldots, n$. The **accuracy** of the model is typically measured on some **test data** $(\underline{x}_i^{(t)}, y_i^{(t)})$, $i = 1, \ldots, m$.

Therefore, a regression that uses MSE has for accuracy

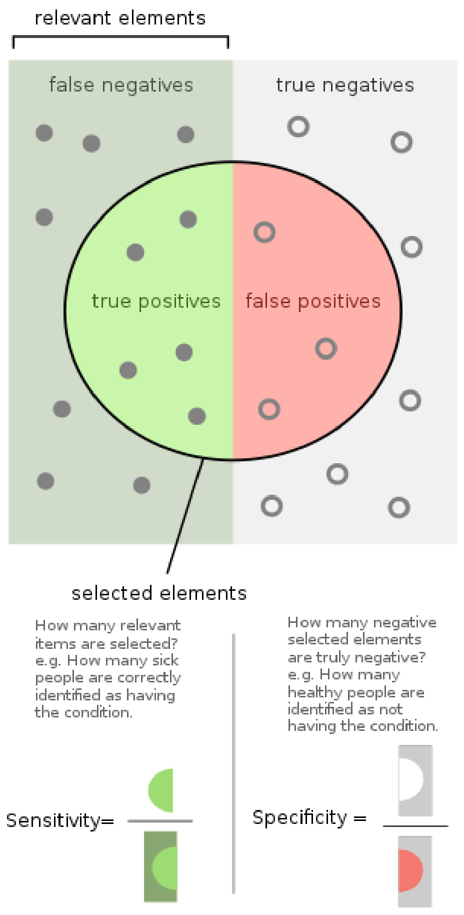
$$\text{MSE } = \frac{1}{m} \sum_{i=1}^{m} \left( y_i^{(t)} - \hat{f}\left(\underline{x}_i^{(t)}\right)\right)^2$$

| **True value, Predictions** | **0** | **1** |
|---|---|---|
| **0** | $TN$ | $FP$ |
| **1** | $FN$ | $TP$ |

**Table 3.3:** Confusion matrix

Meanwhile, for a classification, you create a **confusion matrix** (table 3.3), estimate the probabilities via some method, substitute the values into the following formulas to obtain

**Figure 3.4:** graphical explanation for dummy guys


relevant elements
false negatives
true negatives
true positives
false positives
selected elements
How many relevant items are selected? e.g. How many sick people are correctly identified as having the condition.
How many negative selected elements are truly negative? e.g. How many healthy people are identified as not having the condition.
Sensitivity=
Specificity =

**sensitivity and specificity** (figure 3.4).

$$\textbf{True positive rate (TPR)} = \frac{\text{TP}}{\text{TP} + \text{FN}} = \textbf{sensitivity}$$

$$\textbf{False positive rate (FPR)} = \frac{\text{FP}}{\text{FN} + \text{FP}} = 1 - \frac{\text{TN}}{\text{TN} + \text{FP}} = 1 - \textbf{specificity}$$

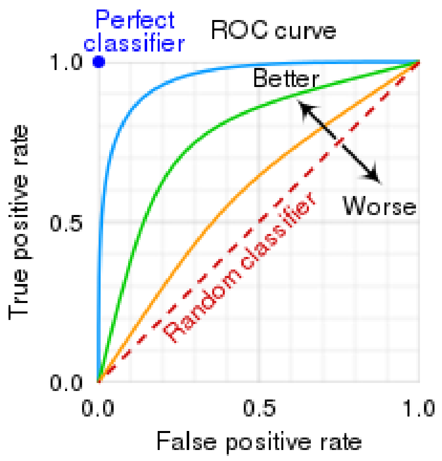
$$\textbf{Error rate} = \frac{\text{FP} + \text{FN}}{m}$$

Notice that this last formula only works when using a 1-0 loss function; if you are using a misclassification loss function, the formula is similar but weighted:

$$\text{Misclassification cost} = \frac{c_0 \text{ FP} + c_1 \text{ FN}}{m}$$

Since defining the exact costs of the misclassifications might prove difficult, a possible approach is using the **Receiver Operating Characteristic (ROC) curve**. Basically you plot all the pairs (FPR, TPR) you obtain by varying the classification threshold from 0 to 1; you will then obtain a curve from which you can decide which value to use as a threshold (the one you see fit for your needs of specificity and sensibility).

**Figure 3.5:** Image taken from Wikipedia. Receiver Operating Characteristic (ROC) curve.



Different models have different ROC curves. The best possible curve would touch the top left corner (figure 3.5), meaning that you never misclassify any observation and therefore the model is deterministic. The worst possibile curve corresponds to the diagonal (from bottom left to top right corner), meaning that you have a 1/2 chance of misclassifying the observation (the same as tossing a coin to decide). The **Area Under the Curve (AUC)** is the area between the curve and the main diagonal. Its value goes from 0 in the worst case to 0.5 in the best one. For these reasons, you want a curve that is as high as possible (and thus has the biggest possible AUC). When choosing between two models, if the ROC curve of one of the models is always above the ROC of the other model, the former one is the strictly better one; if the two ROC curves intersect, you choose the model whose curve is the highest in the region you are most interested in (based on sensibility and specificity).

# Chapter 4

# Statistical decision theory II

Just like in the regression setting, there are parametric and non-parametric methods in a classification setting too, these methods being:

- **Logistic regression** (parametric classification)
- **K nearest neighbour** (non-parametric classification)

## 4.1 K nearest neighbour for classification

K-nearest neighbour is a non-parametric method for classification, meaning it allows to estimate the probability of a testing observation belonging to each of the classes. Formally this can be written as:

$$P(Y = j|\underline{X} = \underline{x}_0), \quad \text{for } j = 1, \ldots, C$$

Where:

- $\underline{x}_0$ is the test observation
- $j$ is a specific class
- $C$ is the number of classes

$K$ is a positive integer and represents the number of training data points closest to the observation data point to consider when classifying. $K$ is called **tuning parameter**, meaning that it can be tweaked in order to change how the model works; notice that the model is still non-parametric since $K$ does not depend on the training data points.

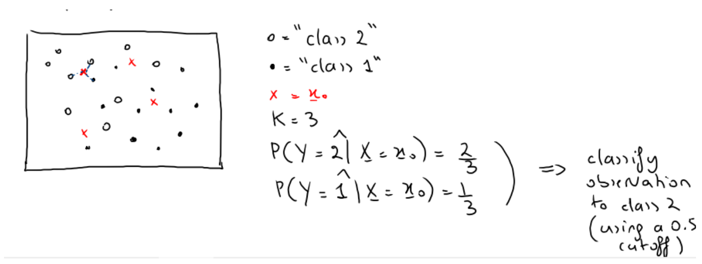
In order to use this method you have to:

1. **Identify the K training observations** that are closest (according to some distance, typically we consider the Eucledian distance) to $\underline{x}_0$. These observations are then indexed with $\underline{N}_0$.
2. **Compute the probability of the observation to belong to each of the classes** using the following formula:

$$P(Y = \hat{j|}\underline{X} = \underline{x}_0) = \frac{1}{k} \sum_{i \in \underline{N}_0} I(\hat{y}_i = j), \quad \text{where } j = 1, \ldots, C$$

Put into words, the equation above means: compute the probability that, given a test observation $\underline{x}_0$, it belongs to a specific class $j$ by dividing the number of neighbours belonging to that class by the number of neighbours ($K$). The $I$ is an indicator variable that equals 1 if $y_i \neq \hat{y}_i$, while instead it is equal to 0 if $y_i = \hat{y}_i$. The indicator is used for each $i \in \underline{N_0}$ observation. Repeat for each class.

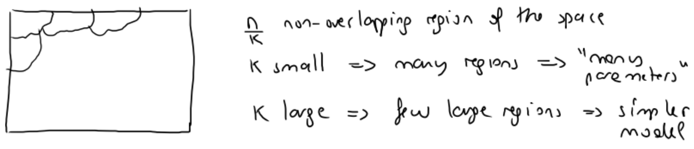
**Figure 4.1:** Classification process with K-neighbour method



o = "class 2"
• = "class 1"
x = $\underline{x}_0$
K = 3
$P(Y = \hat{2} \mid \underline{X} = \underline{x}_0) = \frac{2}{3}$
$P(Y = \hat{1} \mid \underline{X} = \underline{x}_0) = \frac{1}{3}$
=> classify observation to class 2 (using a 0.5 cutoff)

### 4.1.1 Bias-Variance trade off in K nearest neighbour classification

**Figure 4.2:** Tuning the $K$ parameter



$\frac{n}{K}$ non-overlapping region of the space
K small => many regions => "many parameters"
K large => few large regions => simpler model

The tuning parameter $K$ relates to the complexity of the model and it is the determinant to balance the bias and the variance of the model. Usually the value of $K$ is chosen using some training data. Intuitively (NOT formally), the model space could be considered as an area of dimension $n$ which is divided in regions containing $k$ training points, therefore you have $\frac{n}{k}$ regions, hence:

- if **K is small**, then there are many small regions in the space and the model is complex. For this reason, if we change $\underline{x}_0$ with another value, the decision surface position changes quite a lot; if K is too small, the model could be overfitting and thus perform poorly with new test data points (low bias, high variance).
- if **K is large**, then there are few big regions in the space and the model is simple. For this reason, if we change $\underline{x}_0$ with another value, the decision surface position will barely change; if K is too big, the model will give similar results for many different values of $\underline{x}_0$ (high bias, low variance).

The graph shown in figure 4.4 represents the behaviour of different error rates (on test data, the constant error, and on training data) depending on the complexity of the model. As it can be seen ...

*An increase in model complexity is always associated with a lowering of the error rate on the training data, while it is not generally associated with a decrease of the error rate performed on the*

**Figure 4.3:** Complex and smooth decision surfaces, that respectively belong to complex models and simpler models

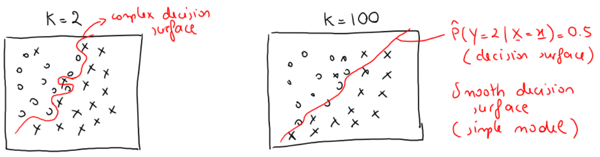
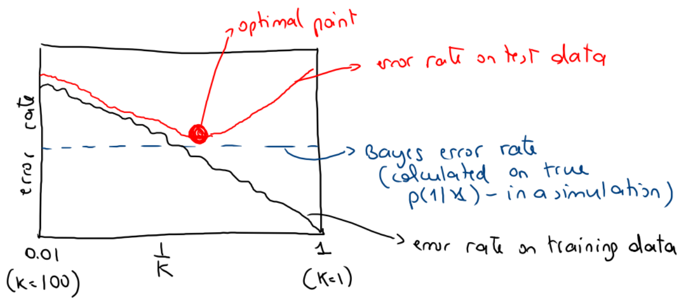


**Figure 4.4:** Error rate on test data (red), error rate on training data (black), Bayes|constant error rate



*test data. The latter in fact decreases until a certain moment, when it starts to increase making a U-shaped curvature. The best case scenario would be the model where both the error rates are at their minimum.*

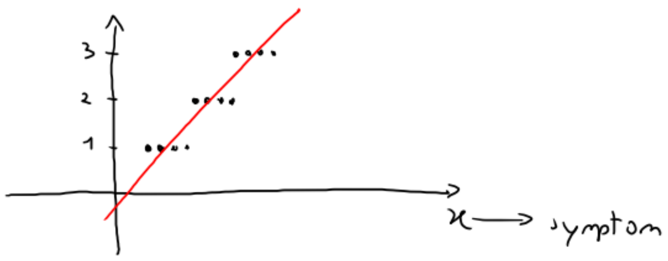
## 4.2 Logistic regression

### 4.2.1 Why we cannot use linear regression in classification setting

**Example 1:** We want to predict the medical condition of a patient in the emergency room based on their symptoms. Assume that $Y$ takes only 3 possible values:

$$Y = \begin{cases} 1 \text{ if stroke} \\ 2 \text{ if overdose} \\ 3 \text{ if seizures} \end{cases}$$

**Figure 4.5:** Image representing a possible linear regression model for distinguishing classes



A linear regression may seem to work, but you have some **problems**:

- If the order of the data points changes, the model changes.
- We are arbitrarely assigning an order to not necessarely ordered classes.
- We are imposing an arbitrary distance between the categories.

**Example 2:** Assume that $Y$ from the previous example only takes 2 values:

$$Y = \begin{cases} 0 \text{ if stroke} \\ 1 \text{ if overdose} \end{cases}$$

In this case $Y$ is a random variable described by a Bernoulli distribution with some probability $p$ of taking the value 1, only two possible values are admitted; therefore

$$Y = \begin{cases} 1 & p \\ 0 & 1-p \end{cases}$$

The Bernoulli random variable, that can assume either 0 or 1 value, has this particular expected value:

$$E[Y] = 0 \cdot (1-p) + 1 \cdot p = p \qquad \text{where } p \text{ represents the probability of getting a 1}$$

Given these premises, you can write:

$$E[Y|\underline{X} = \underline{x}] = p(1|\underline{x}) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

Or considering just the Bernoulli case:

$$E[Y|\hat{\underline{X}} = \underline{x}] = \hat{\beta}_0 + \hat{\beta}_1 x_1$$

But notice that:

- $p(1|\underline{x}) \in (0,1)$, so the probability should span between 0 to 1
- $\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p \in (-\infty, +\infty)$, yet using linear regression the probability spans over the entirety of $\mathbb{R}$.

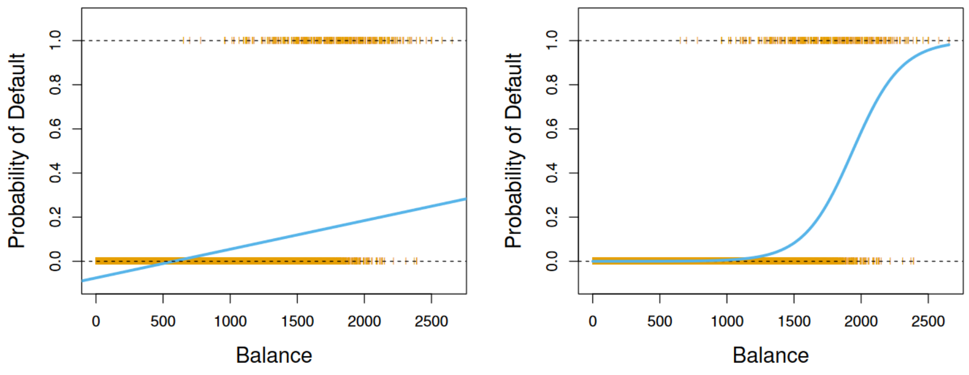
Any time a straight line is fit to a binary response that is coded as 0 or 1, in principle we can always predict $p(1|\underline{x}) < 0$ for some values of $X$ and $p(1|\underline{x})) > 1$ for others. Therefore we must find a way to normalize the regression in the range $(0,1)$.

### 4.2.2 Characteristics of the logistic regression

We have to model $p(1|\underline{x})$ using a function that gives outputs between 0 and 1 for each value of $X$. **Logistic regression** solves the problem by utilizing a function of the probability $p(1|\underline{x})$, namely $g$, such that

$$g(p(1|\underline{x})) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = \underline{\beta}^t \underline{x}$$

**Figure 4.6:** Linear regression (left) **vs** Logistic regression (right) for classification problems. Notice on the left the fact that values under 0 for certain values of $\underline{x}$ are possible.



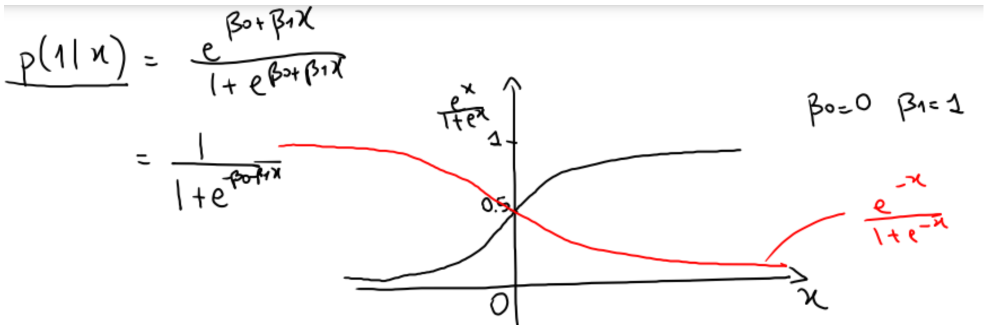
Logistic regression uses the **logistic function** (also named sigmoid function or activation function), which is defined as

$$p(1|\underline{x}) = \frac{e^{\beta_0+\beta_1 x_1+\cdots+\beta_p x_p}}{1+e^{\beta_0+\beta_1 x_1+\cdots+\beta_p x_p}}$$

and it has the following properties (figure 4.6):

- Its codomain corresponds to the interval $(0,1)$
- Taken any $\underline{x}$, the logistic function classifies it to the "1" class if $p(1|\underline{x}) > 0.5$, otherwise to the "0" class.

**Figure 4.7:** Linear regression (left) **vs** Logistic regression (right) for classification problems. Notice on the left the fact that values under 0 for certain values of $\underline{x}$ are possible.


$p(1|x) = \frac{e^{\beta_0+\beta_1 x}}{1+e^{\beta_0+\beta_1 x}}$
$= \frac{1}{1+e^{-\beta_0+\beta_1 x}}$
$\frac{e^x}{1+e^x}$
1
0.5
0
$x$
$\beta_0=0 \quad \beta_1=1$
$\frac{e^{-x}}{1+e^{-x}}$

Considering the ***binomial*** case ($p(1|\underline{x}) = \frac{e^{\beta_0+\beta_1 x_1}}{1+e^{\beta_0+\beta_1 x_1}}$) with $\beta_0 = 0$ and $\beta_1 = 1$, as shown in figure 4.7, the curve is sigmoid shape with intercept in $y = 0.5$. It increases when the value of $\beta_1 > 0$.

The $g$ function is the inverse of the conversion from linear regression to logistic function.

In the binomial case, the logistic function can be written as:

$$\begin{aligned}
p(1|\underline{x}) &= \frac{e^{\beta_0+\beta_1 x_1}}{1+e^{\beta_0+\beta_1 x_1}} && \text{binomial case for simplicity}\\
&= \frac{e^{\beta_0+\beta_1 x_1}}{e^0+e^{\beta_0+\beta_1 x_1}} && \text{reorganizing for clarity}\\
&= \frac{1}{e^{\beta_0+\beta_1 x_1}} \cdot \frac{e^{\beta_0+\beta_1 x_1}}{\frac{e^0}{e^{\beta_0+\beta_1 x_1}}+1} && \text{by collecting } e^{\beta_0+\beta_1 x_1} \text{ from the denominator}\\
&= \frac{1}{\frac{e^0}{e^{\beta_0+\beta_1 x_1}}+1} && \text{simplifying}\\
&= \frac{1}{1+e^{-\beta_0-\beta_1 x_1}} && \text{since } \frac{a^x}{a^y} = a^{x-y}
\end{aligned}$$

Let us define a quantity called **odds**, which is the ratio between positive and negative outcomes.

$$\begin{aligned}
\text{Odds } &= \frac{p(1|\underline{x})}{1-p(1|\underline{x})} && \text{by definition}\\
&= \frac{\frac{e^{\underline{\beta}^t \underline{x}}}{1+e^{\underline{\beta}^t \underline{x}}}}{1-\frac{e^{\underline{\beta}^t \underline{x}}}{1+e^{\underline{\beta}^t \underline{x}}}} && \text{since } p(1|\underline{x}) = \underline{\beta}^t\underline{x}\\
&= \frac{\frac{e^{\underline{\beta}^t \underline{x}}}{1+e^{\underline{\beta}^t \underline{x}}}}{\frac{1+e^{\underline{\beta}^t \underline{x}}-e^{\underline{\beta}^t \underline{x}}}{1+e^{\underline{\beta}^t \underline{x}}}} && \text{minimum common denominator}\\
&= \frac{\frac{e^{\underline{\beta}^t \underline{x}}}{1+e^{\underline{\beta}^t \underline{x}}}}{\frac{1}{1+e^{\underline{\beta}^t \underline{x}}}} && \text{simplifying}\\
&= \frac{e^{\underline{\beta}^t \underline{x}}}{1+e^{\underline{\beta}^t \underline{x}}} \cdot \frac{1+e^{\underline{\beta}^t \underline{x}}}{1} && \text{reorganizing}\\
&= e^{\underline{\beta}^t \underline{x}} && \text{simplifying}
\end{aligned}$$

As it can be seen from the formula, $Odds = \frac{p(1|\underline{x})}{1-p(1|\underline{x})} = e^{\underline{\beta}^t \underline{x}}$ can take any value between $[0, +\inf]$, indicating very low and high probabilities of positive outcome respectively. The predictor for this measure is called **log-odds** or **logit** (it is the $g$ function from before) is obtained applying a logarithmic tranformation, hence:

$$\log\left(\frac{p(1|\underline{x})}{1-p(1|\underline{x})}\right) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p = \underline{\beta}^t \underline{x}$$

The formal definition of a logistic regression model (assuming the random variable to be Bernoulli distributed) then becomes:

$$\begin{gathered}
Y|\underline{X} = \underline{x} \sim Bernoulli(p(1|\underline{x}))\\
\log\left(\frac{p(1|\underline{x})}{1-p(1|\underline{x})}\right) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p
\end{gathered}$$

The coefficients can be interpeted as follows: a one-unit increase in $X_j$ (while everithing else is kept constant) induces a change in the log-odds of $\beta_j$ (while it induces a multiple factor of $e^{\beta_j}$ for the odds).

### 4.2.3 Example of logistic regression

**Example**: Logistic regression for a single predictor $X$ which is binary.

To compute the change of the log-odds for a one-unit change of $X$ we compute

$$\begin{aligned}
\log(\text{odds ratio}) &= \log\left(\frac{p(1|X=x_1+1)}{1-p(1|X=x_1+1)}\right) - \log\left(\frac{p(1|X=x_1)}{1-p(1|X=x_1)}\right) && \text{log odds in 1 minus log odds in 0}\\
&= \beta_0 + \beta_1(x_1+1) - \beta_0 - \beta_1 x_1 && \text{by definition of logistic regression}\\
&= \beta_1 && \text{simplifying}
\end{aligned}$$

This quantity is called **log(odds ratio)** since the subtraction of two logarithms in the same base is equal to the logarithm of the ratio of the arguments. Notice that, as expected, a one unit increase of the value of $x_1$ results in an increment of $\beta_1$.

If we instead consider the same increment for the **odds ratio**, we get:

$$\begin{aligned}
\text{odds ratio} &= \frac{\frac{p(1|X=x_0+1)}{1-p(1|X=x_0+1)}}{\frac{p(1|X=x_0)}{1-p(1|X=x_0)}} && \text{odds in 1 divided by odds in 0}\\
&= \frac{e^{\beta_0+\beta_1(x_0+1)}}{e^{\beta_0+\beta_1 x_0}} && \text{using the fact that } \log\left(\frac{p(1|\underline{x})}{1-p(1|\underline{x})}\right) = \underline{\beta}^t\underline{x}\\
&= \frac{e^{\beta_0+\beta_1 x_0+\beta_1}}{e^{\beta_0+\beta_1 x_0}} && \text{rearranging}\\
&= e^{\beta_1} && \text{since } \frac{x^a}{x^b} = x^{a-b}
\end{aligned}$$

Therefore we have an increase of $e^{\beta_1}$ as expected.

### 4.2.4 Parameter estimation in logistic regression

When estimating parameters for non-linear regressions you often get non-closed form expressions, therefore the maximum likelihood(s) for the parameter(s) must be maximised numerically. Notice that, contrarely to linear regression, you cannot use the least square method.

For instance, give some training data $(\underline{x}_i, y_i)$, $i = 1, \ldots, n$, we want to estimate $\beta_0, \beta_1, \ldots, \beta_p$. To do so we need to compute the maximum likelihood given that $Y$ is binary, thus

$$Y|\underline{X} = \underline{x} \sim \mathit{Bernoulli}(p(1|\underline{x})),\ f(y|\underline{x}) = p(1|\underline{x})^y(1-p(1|\underline{x}))^{1-y}$$

The likelihood conditional to the observations hence is:

$$L(\underline{\beta}) = \prod_{i=1}^n f(y_i|\underline{x}_i) = \prod_{i=1}^n p(1|\underline{x}_i)^{y_i}(1-p(1|\underline{x}_i))^{1-y_i}$$

We then compute the log-likelihood and reorganize it in order to make evident its dependence from $\underline{\beta}$:

$$
\begin{aligned}
l(\underline{\beta}) &= \sum_{i=1}^{n} [y_i \log(p(1|\underline{x}_i)) + (1-y_i)\log(1-p(1|\underline{x}_i))] && \text{applying logarithm}\\
&= \sum_{i=1}^{n} [y_i \log(p(1|\underline{x}_i)) - y_i \log(1-p(1|\underline{x}_i)) + \log(1-p(1|\underline{x}_i))] && \text{multiplying}\\
&= \sum_{i=1}^{n} \left[ y_i \log\left(\frac{p(1|\underline{x}_i))}{1-p(1|\underline{x}_i))}\right) + \log(1-p(1|\underline{x}_i))\right] && \log(a)-\log(b) = \log\left(\frac{a}{b}\right)\\
&\text{but since } \log\left(\frac{p(1|\underline{x})}{1-p(1|\underline{x})}\right) = \underline{\beta}^t\underline{x} \text{ and } p(1|\underline{x}) = \frac{e^{\beta_0+\beta_1 x_1}}{1+e^{\beta_0+\beta_1 x_1}}\\
&= \sum_{i=1}^{n} \left[ y_i \underline{\beta}^t \underline{x}_i + \log\left(1 - \frac{e^{\underline{\beta}^t\underline{x}_i}}{1+e^{\underline{\beta}^t\underline{x}_i}}\right)\right]\\
&= \sum_{i=1}^{n} \left[ y_i \underline{\beta}^t \underline{x}_i + \log\left(\frac{1}{1+e^{\underline{\beta}^t\underline{x}_i}}\right)\right] && \text{using mcm and simplifying}\\
&= \sum_{i=1}^{n} \left[ y_i \underline{\beta}^t \underline{x}_i + \log(1) - \log\left(1+e^{\underline{\beta}^t\underline{x}_i}\right)\right] && \text{dividing the logarithms}\\
&= \sum_{i=1}^{n} \left[ y_i \underline{\beta}^t \underline{x}_i - \log\left(1+e^{\underline{\beta}^t\underline{x}_i}\right)\right] && \text{since } \log((1) = 0
\end{aligned}
$$

We then compute the first derivative in $\underline{\beta}$ (notice that since you want to derive in a vector, you need to take the partial derivatives in each of the elements of the vector):

$$
\begin{aligned}
\frac{\partial l(\beta)}{\partial \beta_j} &= \frac{\partial}{\partial \beta_j}\left(\sum_{i=1}^{n} \left[ y_i \underline{\beta}^t \underline{x}_i - \log\left(1+e^{\underline{\beta}^t\underline{x}_i}\right)\right]\right) \quad j = 0, \dots, p\\
&\text{but } \frac{\partial \underline{\beta}^t \underline{x}}{\partial \beta_j} = \frac{\partial}{\partial \beta_j}(\beta_0 x_{i0} + \dots + \beta_p x_{ip}) = x_{ij} \text{ since the other terms simplify}\\
&= \sum_{i=1}^{n}\left[ y_i x_{ij} - \frac{e^{\underline{\beta}^t\underline{x}_i}}{1+e^{\underline{\beta}^t\underline{x}_i}} x_{ij}\right]\\
&\text{but } \frac{e^{\underline{\beta}^t\underline{x}_i}}{1+e^{\underline{\beta}^t\underline{x}_i}} = p(1|\underline{x}) \text{ therefore}\\
&= \sum_{i=1}^{n} [y_i x_{ij} - p(1|\underline{x}_i) x_{ij}]
\end{aligned}
$$

By setting this derivative to zero you obtain $p+1$ equations in $p+1$ parameters, therefore to optimize numerically the function (by solving the equations) you must use an optimization method like **Newton-Raphson**; the *gml* function in R uses an iterative reweighted least-squares algorithm, which is a variation of the Newton-Raphson method).

From the optimization you get $\hat{\underline{\beta}} = \hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p$, which can be used to estimate $p(1|\underline{x})$, since

$$
p(\hat{1}|\underline{x}) = \frac{e^{\hat{\underline{\beta}}^t \underline{x}}}{1+e^{\hat{\underline{\beta}}^t \underline{x}}}
$$

# Chapter 5

# Generalized linear models

**Generalized linear models (GLMs)** are a broad family of regression models which includes, for instance, linear, logistic and poisson regressions (and many more). The concept was created by Nelder and Wedderburn in 1972, in order to map into a single framework all regressions models. In general regression models are characterized by:

- $Y$: the random **response variable** you want to predict
- $\underline{X} = (X_1, \dots, X_p)$: a **vector of random predictors** (generally known)

Notice that, since these models describe the value of $Y$ with respect to the vector $\underline{X}$ $(Y|\underline{X} = \underline{x})$, they do not give information on the actual distribution of $Y$, but rather on the values that it takes conditionally to the values taken by the predictors, which can be written as

$$Y_i = (Y|\underline{X} = \underline{x}_i)$$

Therefore, if you have $n$ vectors of random predictors, $Y_1, \dots, Y_n$ are independent random variables but not identically distributed.

## 5.1 From linear models to generalized linear models

Linear models make some implicit assumptions that must be removed in order to generalize.

| **Linear models** | **Generalized linear models** |
|---|---|
| $Y_i \sim N(\mu_i, \sigma^2)$ | $Y_i \sim f(y_i; \mu_i, \phi)$ |
| $\mu_i = E[Y_i] = E[Y|\underline{X} = \underline{x}_i] = \eta_i$ | $g(\mu_i) = \eta_i$ |
| $\eta_i = \underline{x}_i^t \underline{\beta} = \beta_0 x_{i0} + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}$ | $\eta_i = \underline{x}_i^t \underline{\beta}$ |

First of all, linear models assume that the random variable $Y_i$ is normal distributed, with mean $\mu_i$, meaning that $E[Y|\underline{X} = \underline{x}_i] = \mu_i$, and $\sigma^2 = Var(Y_i) = Var(Y|\underline{X} = \underline{x}_i)$. Notice that the variance is constant, therefore *homoskedasticity* is assumed. On the other hand, generalized linear models do not make any assumptions on the shape of the distribution of $Y_i$; $Y_i$ is distributed according to some function $f(y_i)$ with the parameters $\mu_i$ and $\phi$. $\phi$ is called **special parameter** and it may or may not be present in the model. The **linear predictor** is the function used to predict the outcome of the random variable $Y_i$ knowing some values for the predictor $\underline{X}_i$; in both cases the linear predictor is defined as $\eta_i = \underline{x}_i^t\underline{\beta} = \beta_0 x_{i0} + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}$, where $p$ is the number of parameters and the coefficients $\beta_0, \dots, \beta_p$ are the weights for the predictors (therefore the linear predictor is a linear combination in $\underline{\beta}$ of the predictors). The difference is in the relation between $\mu_i$ and $\eta_i$. In linear models $\mu_i$ coincides with $\eta_i$, because assuming a normal distribution $\mu_i = E[Y_i] = E[Y|\underline{X} = \underline{x}_i] = \eta_i$; in generalized linear models $\mu_i$ and $\eta_i$ are related by a **link function**, which is a function $g$ of $\mu_i$ such that $g(\mu_i) = \eta_i$. A generalized linear model is then a choice of a distribution function $f$ and a link function $g$; for instance, if $f$ is a normal distribution (with $\sigma^2 = \phi$) and $g$ is the identity function (therefore $\mu_i = \eta_i$), we get the linear model.

## 5.2 Exponential dispersion family

The function $f$, describing the distribution of the random variable $Y_i$, needs to be a member of the **exponential dispersion family (EDF)**. A density belonging to the EDF can be written as

$$f(y_i; \theta_i, \phi) = \exp\left\{\frac{y_i\theta_i - b(\theta_i)}{a_i(\phi)} + c(y_i; \phi)\right\}$$

With:

- $f(y_i)$ is a generic density function
- $\theta_i$ and $\phi$ are some parameters. The values of $\theta_i$ are called *canonical parameters.*
- $a_i$, $b$ and $c$ are some functions.

It is obvious that, if a density function could be related to this family, it is possible to derive from its fundamental parameters the functions $a_i$, $b$ and $c$, and $\theta_i$. Now we'll try to understand if some major density functions belong to the EDF family.

### 5.2.1 Example: normal distribution is a member of the EDF

We want to demonstrate that the normal distribution is a member of the EDF.

$$\begin{aligned}
f(y_i; \mu_i, \sigma^2) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2}\frac{(y_i - \mu_i)^2}{\sigma^2}\right\} && \text{definition of normal distribution} \\
&= \exp\left\{-\frac{1}{2}\frac{(y_i - \mu_i)^2}{\sigma^2} + \log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)\right\} && \text{pull coefficient inside the exponential} \\
&= \exp\left\{-\frac{1}{2}\frac{(y_i - \mu_i)^2}{\sigma^2} - \frac{1}{2}\log\left(2\pi\sigma^2\right)\right\} && \text{rearrange using log properties} \\
&= \exp\left\{-\frac{1}{2}\frac{y_i^2 - 2y_i\mu_i + \mu_i^2}{\sigma^2} - \frac{1}{2}\log\left(2\pi\sigma^2\right)\right\} && \text{compute the square} \\
&= \exp\left\{\frac{y_i\mu_i + \mu_i^2/2}{\sigma^2} - \frac{1}{2\sigma^2}y_i^2 - \frac{1}{2}\log\left(2\pi\sigma^2\right)\right\} && \text{group terms containing } \mu_i
\end{aligned}$$

The normal distribution therefore belongs to the EDF by setting:

$$\begin{aligned}
\theta_i &= \mu_i, \\
\phi &= \sigma^2, \\
b(\theta_i) &= \theta_i^2/2, \\
a_i(\phi) &= \phi, \\
c(y_i;\phi) &= -\frac{1}{2\phi}y_i^2 - \frac{1}{2}\log(2\pi\phi)
\end{aligned}$$

### 5.2.2 Example: binomial distribution is a member of the EDF

We want to demonstrate that the binomial distribution is a member of the EDF.

$$\begin{aligned}
f(y_i;n_i,\pi_i) &= \binom{\pi_i}{y_i}\pi_i^{y_i}(1-\pi_i)^{n_i-y_i} && \text{definition of binomial distribution} \\
&= \exp\left\{\log\left(\binom{\pi_i}{y_i}\pi_i^{y_i}(1-\pi_i)^{n_i-y_i}\right)\right\} && \text{exponentiate to compare with EDF} \\
&= \exp\left\{y_i\log\pi_i + (n_i-y_i)\log(1-\pi_i) + \log\binom{n_i}{y_i}\right\} && \text{split log and simplify} \\
&= \exp\left\{\frac{y_i\log\left(\frac{\pi_i}{1-\pi_i}\right) + n_i\log(1-\pi_i)}{1} + \log\binom{n_i}{y_i}\right\} && \text{group terms containing } \pi_i
\end{aligned}$$

The binomial distribution therefore belongs to the EDF by setting:

$$\begin{aligned}
\theta_i &= \log\left(\frac{\pi}{1-\pi}\right)(\textbf{logit}) \\
\phi &= 1 \\
b(\theta_i) &= -n_i\log(1-\pi_i) \\
&= -n_i\log(1-\frac{e^{\theta_i}}{1+e^{\theta_i}}) \\
&= n_i\log(1+e^{\theta_i}) \\
a_i(\phi) &= \phi \\
c(y_i;\phi) &= \log\binom{n_i}{y_i}
\end{aligned}$$

We replaced $\pi_i = \frac{e^{\theta_i}}{1+e^{\theta_i}}$ as:

$$\begin{aligned}
e^{\theta_i} = \frac{\pi_i}{1-\pi_i} &\Rightarrow (1-\pi_i)e^{\theta_i} = \pi_i \\
&\Rightarrow e^{\theta_i} - \pi_i e^{\theta_i} = \pi_i \Rightarrow \pi_i = \frac{e^{\theta_i}}{1+e^{\theta_i}}
\end{aligned}$$

For the binomial distribution ($Y_i \sim Bin(n_i, \pi_i)$) it is possble to write the relation between old and new parameters explicitely Link from $\theta_i$ to $\mu_i$.

$$E[Y_i] = \mu_i = n_i\pi_i = n_i\frac{e^{\theta_i}}{1+e^{\theta_i}}$$

Link from $\mu_i$ to $\theta_i$.

$$\pi_i = \frac{\mu_i}{n_i} \implies \theta_i = \log\left(\frac{\pi_i}{1-\pi_i}\right) = \log\left(\frac{\mu_i/n_i}{1-\mu_i/n_i}\right) = \log\left(\frac{\mu_i}{n_i-\mu_i}\right)$$

Notice that **heteroskedasticity** in naturally embedded in the model since the variance depends on $\mu_i$:

$$Var(Y_i) = n_i\pi_i(1-\pi_i) = n_i\frac{\mu_i}{n_i}\left(1-\frac{\mu_i}{n_i}\right) = \mu_i\left(\frac{n_i-\mu_i}{n_i}\right)$$

This hold true for all GLMs but linear models which is the only homoskedastic model of the group. The fact that heteroskedasticity is mandatory is not a big problem since most datasets are not homoskedastic anyway.

## 5.3 Connection between $\theta_i$ and $\mu_i$, $Var(Y_i)$

In general, one can show that, for any function in the EDF,

$$\mu_i = E[Y_i] = b'(\theta_i)$$

Where $b'$ is the first derivative of the function $b$.

$$\begin{aligned} Var(Y_i) &= b''(\theta_i)\cdot a_i(\phi) \\ &= V(\mu_i)\cdot a_i(\phi) \end{aligned}$$

Where $b''$ is the second derivative of $b$ and $V(\mu_i)$ is the *variance function* (basically just a way to rewrite underlining the dependence on $\mu$).

### 5.3.1 Example: connection of $\theta_i$ , $\mu_i$ and $Var(Y_i)$ for the binomial model

We know, for the binomial function, that

$$b(\theta_i) = n_i\log(1+e^{\theta_i})$$

The first derivative in $\theta_i$ then becomes

$$b'(\theta_i) = \frac{n_ie^{\theta_i}}{1+e^{\theta_i}} = n_i\pi_i$$

But it is also known that

$$\mu_i = n_i\pi_i$$

Therefore, as expected from the general formula

$$\mu_i = b'(\theta_i)$$

We know that, for the binomial model

$$a_i(\phi) = 1$$

We then compute the second derivative of $b(\theta_i)$ in $\theta_i$:

$$\begin{aligned}
b''(\theta_i) &= n_i e^{\theta_i}\left[-\left(\frac{1}{1+e^{\theta_i}}\right)^2 e^{\theta_i}\right] + n_i\frac{e^{\theta_i}}{1+e^{\theta_i}} && \text{by deriving } b'(\theta_i)\\
&= -n_i\left(\frac{e^{\theta_i}}{1+e^{\theta_i}}\right)^2 + n_i\frac{e^{\theta_i}}{1+e^{\theta_i}} && \text{pulling both } e^{\theta_i} \text{ inside the square}\\
&= -n_i\pi_i^2 + n_i\pi_i && \text{since } \frac{e^{\theta_i}}{1+e^{\theta_i}} = \pi_i\\
&= n_i\pi_i(1-\pi_i) && \text{collecting } n_i\pi_i
\end{aligned}$$

Therefore, as expected, we get

$$Var(Y_i) = b''(\theta_i)a_i(\phi) = n_i\pi_i(1-\pi_i)$$

## 5.4 Choice of link function

The choice of link function is not unique and can depend on the function $f$ which was chosen.

### 5.4.1 Example: link function for a Bernoulli function

Assume that $Y_i$ is Bernoulli distributed with probability $\pi_i$ ($Y_i \sim Ber(\pi_i)$). Then:

- $\mu_i = \pi_i \in (0,1)$ (since $n_i = 1$)
- $Var(Y_i) = \pi_i(1-\pi_i) = \mu_i(1-\mu_i)$
- $\eta_i = \underline{x}_i^t\underline{\beta}$ with $\eta_i \in (-\infty, +\infty)$

We must find a function $g$ such that $g(\mu_i) = \eta_i$ which, taking into account that $\mu_i \in (0,1)$ and $\eta_i \in (-\infty,+\infty)$, means:

$$g : (0,1) \to (-\infty,+\infty)$$
$$g^{-1} : (-\infty,+\infty) \to (0,1)$$

These conditions are satisfied by any cumulative density functions (CDF), as long as it is continuous (since it must be invertible). We therefore have infinitely many functions $g$ that satify these conditions, but the three most common choices are:

1. **Standard normal CDF**: Choose $g^{-1} = \Phi$, with $\Phi \sim N(1,0)$, hence

$$g = \Phi^{-1} : (0,1) \to (-\infty,+\infty)$$

   This type of regression ($f \sim$ Bernoulli $, g = \Phi^{-1}$) is called **probit regression**.

2. **Logistic CDF**: Consider the logistic distribution, which has density

$$f(y;\mu,\sigma^2) = \frac{\exp({}^{(y-\mu)}/{}_{\sigma})}{\sigma^2(1+\exp\left({}^{(y-\mu)}/{}_{\sigma}\right)^2}\ , \quad \text{with } -\infty < y < +\infty$$

   Setting $\mu = 0$, $\sigma^2 = 1$ we get the sigmoid function

$$g^{-1} = F(y;0,1) = \frac{e^y}{1+e^y}$$

   The link function then becomes the logit link

$$\frac{e^\eta}{1+e^\eta} = \mu \implies \eta = \log\left(\frac{\mu}{1-\mu}\right)$$

   This regression ($f \sim$ Bernoulli $, g =$ logit ) is the **logistic regression**.

3. **Poisson CDF**: This link function is rarely used since it performs well in niche cases, such as with a binomial distributions with $\pi \sim$ Bernoulli (e.g. the number of bacteria on a plate in a dilution bioassay, in which you do not measure the number of bacteria, just whether there are or not). Assume that $Z_i$ is a possion distributed random variable with parameter $\lambda_i$ ($Z_i \sim$ Poisson $(\lambda_i)$). Then assume that we measure

$$y_i = \begin{cases} 0 & \text{if } z_i = 0 \text{ (absent)} \\ 1 & \text{if } z_i > 0 \text{ (present)} \end{cases}$$

   We would like to describe how $y_i$ changes with time ($x = 0, 1, 2, \dots$), therefore we need a function that links $\mu_i$ and $\eta_i$. Since we know that

$$\eta_i = \log(\lambda_i)$$

   and that

$$\begin{aligned} \mu_i &= E[Y_i] \\ &= 0 \cdot P(Y_i = 0) + 1 \cdot P(Y_i = 1) \\ &= P(z_i > 0) \\ &= 1 - P(z_i = 0) \\ &= 1 - e^{-\lambda_i} \end{aligned}$$

   we can link $\mu_i$ and $\eta_i$ passing through $\lambda_i$ ($\mu_i \leftrightarrow \lambda_i \leftrightarrow \eta_i$). Firstly we rearrange the link between $\mu_i$ and $\lambda_i$:

$$\mu_i = 1 - e^{-\lambda_i} \implies e^{-\lambda_i} = 1 - \mu_i \implies \lambda_i = -\log(1-\mu_i)$$

   Then, plugging in the link between $\lambda_i$ and $\eta_i$ ($\log(\lambda_i) = \eta_i$) we get

$$\eta_i = \log(-\log(1-\mu_i))$$

   This link is called **complementary log-log link**

### 5.4.2 Canonical link

The logit link is also called **canonical link** since

$$\eta_i = \log\left(\frac{\mu_i}{1-\mu_i}\right) = \theta_i$$

In general a canonical link is a function g such that

$$\eta_i = g(\mu_i) = \theta_i$$

These link functions have some advantages:

- Clear interpretation of the parameters ($\underline{\beta}$)
- Some theoretical reasons (Fisher scoring and iteratively reweighted least squares algorithms are equivalent, zero sum residuals)
- It follows directly from the EDF formulation of the distribution (just derive), in fact $\mu_i = b'(\theta_i), \theta_i = (b')^{-1}(\mu_i)$

Despite these advantages the logit link is not always the correct one to use.

## 5.5 Residuals in generalized linear models

As already seen, a linear model can be express either as:

$$y_i = \eta_i + \varepsilon_i \text{ (signal + noise representation)}$$

Or as:

$$Y \sim N(\eta_i, \sigma^2)$$

From the first expression we get the usual definition or residuals (estimates of the errors) in linear models:

$$e_i = y_i - \hat{\eta}_i$$

Since for generalized linear models we can only use the formulation $Y \sim N(\eta_i, \sigma^2)$ (meaning that we cannot simply write the model as value plus noise), we need a new way to define the residuals. There are many options, but the most commonly used ones are **Pearson residuals** and **deviance residuals**.

### 5.5.1 Pearson residuals

Pearson residuals are defined as follows:

$$r_i^p = \frac{y_i - \hat{\mu}_i}{\sqrt{{}^{V\hat{ar}(y_i)}/_{\hat{\phi}}}}$$

If we apply this definition, for instance, to a poisson distribution ($\phi = 1$), we get

$$r_i^p = \frac{y_i - \hat{\mu}_i}{\sqrt{\hat{\mu}_i}} \text{ with } y_i \in (0, +\infty)$$

Beacause of the interval on which the values of $y_i$ are defined, the residuals may not be symmetric, but the assumption of gaussianity is usually satisfied with $\mu$ big.

### 5.5.2 Deviance residuals

The **deviance** of an observation $i$ is defined as:

$$d_i = 2[l_i(y_i; y_i) - l_i(\hat{\mu}_i; y_i)]$$

Where:

- $\hat{\mu}_i = e^{\underline{x}_i^t \underline{\hat{\beta}}}$
- $l_i(y_i; y_i)$ is the log-likeihood of the saturated model (most fitting non parametric model, therefore the highest possible likelihood)
- $l_i(\hat{\mu}_i; y_i)$ is the log-likelihood of the model using the estimated parameters
- $d_i \geq 0$

The overall deviance of the model is defined as the sum of the deviance of each observation

$$\text{deviance} := \sum_{i=1}^{n} d_i$$

The lower the deviance, the closer the model to a perfect fit.

The **deviance residuals** can be then defined as:

$$r_i^D = \sqrt{d_i} \cdot \text{sign}(y_i - \hat{\mu}_i) \quad \text{where } \text{sign}(y_i - \hat{\mu}_i) = \begin{cases} 1 & y_i > \hat{\mu}_i \\ -1 & y_i < \hat{\mu}_i \\ 0 & y_i = \hat{\mu}_i \end{cases}$$

Chapter 6

# Simulating data from a GLM in R

Simulating data is often used to test the performance of your model.

## 6.1 Example: simulating Poisson data

In general, in a Possion regression you have:

$$Y_i = (Y|\underline{X} = \underline{x}_i) \sim \text{Poisson}(\mu_i)$$

$$\mu = E[Y_i] \in (0, +\infty)$$

$$\eta_i = \underline{x}_i^t \underline{\beta} \in (-\infty, \infty)$$

If you then decide to use the canonical link:

$$\eta_i = \log(\mu_i) \implies \mu_i = e^{\eta_i}$$

Therefore you can generalize this Poisson regression as

$$Y_i \sim \text{Poisson}(e^{\underline{x}_i^t \underline{\beta}})$$

To then simulate data to test this model you must:

- Assume a number of predictors $p$(in our case $p = 1$ for plotting convenience)
- Fix some values for $\beta$ (in our case notice that $\eta_i = \beta_0 + \beta_i x_i$)
- Generate $n$ random values of $x_i$ (in this case $n = 100$) and compute the corresponding $y_i$ values.

In R this translates to:

```
# Simulate the data
set.seed(123)  # In order to get repeatable results
x <- rnorm(100, 0, 2)  # Does not matter, just to get random values following a normal distributio
beta0 <- 1  # Fixed
beta1 <- 2  # Fixed
eta <- beta0 + beta1 * x  # Vector of values, linear predictor calculated for each x value
```

```
mu <- exp(eta)  # Because we chose the canonical link
y <- rpois(100, lambda=mu)  # Y values corresponding to random X values

#I put myself in a situation where I know data (x, y) but I don't know where they come from. I use

plot(x, y)  # See that is not linear, could be log(y)?
plot(x, log(y))  # Since we obtain a line, we expect eta = beta0 + beta1x

# Try fitting linear model (not the best approach)
z <- log(y)  # Not good since you have many zeros and infinites, typical Poisson data contain seve
summary(z)
z <- log(y+1)  # Sudo-count transformation (commonly used)
summary(z)
modA <- lm(formula=z~x)  # Fit model
summary(modA)  # Estimated parameters are far from chosen ones
plot(modA)  # Notice systematic trends in residual analysis: it is suggested the presence of a qua
modB <- lm(z~x+I(x^2))  # Try adding quadratic term to match residual analysis
# Note: I(math_exp) is used to interpret the content as a mathematic expression
summary(modB)  # Not that far from starting data
plot(modB)  # Not the best but seems decent

# Proper way to try and fit data
y[1:100]  # Inspect the data and notice that the response in positive discrete
# You could then try fitting different distributions based on that, ...
# ... Poisson seems reasonable, which is the simplest to fit this kind of data. Negative binomiala
modC <- glm(formula=y~x, family="poisson")  # Canonical link by default
summary(modC)  # Estimates are rather close
# Note: Because of how glm works, you need decently big values for n. In linear regression models
# Note: Fisher Scoring gives info on optimization attempts number
plot(modC)  # Seems decent
# Note: Some regular-ish patterns may be seen when working with discrete data

# Use model to make predictions
p1<-predict(modC)  # ! Estimates linear predictors, not values of y
# coefficients(modC)[1] + coefficients(modC)[2] * x == predict(modC)
summary(p1)
# we compare the estimated values of eta with those obtained through log(y)
plot(p1, log(y))

p2<-predict(modC,type="response")  # Estimates values of y
summary(p2)
plot(p2,y)  # Plot predicted vs simulated values of y
abline(0,1)  # Line that should be approximated by the datapoints
```

## 6.2 Example: simulating exponential data

You can do the same with other distributions. This is the example for an exponential distribution.

```r
x <- rnorm(100, 0, 2)  # Does not matter, just to get random values
beta0 <- 1  # Fixed
beta1 <- 2  # Fixed
eta <- beta0 + beta1 * x  # Vector of values
mu <- exp(eta) / (1 + exp(eta))  # Use logit as link
y <- rbinom(100, size=1, prob=mu)  # Compute corresponding y values
plot(x, y)

modD <- glm(y~x, family="binomial")  # Create the model
# modD <- glm(y~x, family=binomial(link="logit"))  # Equivalent formulation

p4<-predict(modD) # Compute linear predictors
summary(p4)
p5<-predict(modD,type="response") # Compute fitted probabilities
summary(p5)
```

# Chapter 7

# Discriminant analysis

In a classification setting, the $Y$ response variable is a categorical variable that can belong to any class $j$ of the $k$ possible classes. The aim of classification is estimating the probability of $Y$ belonging to any class $j$, namely

$$P(Y = j|\underline{X} = \underline{x}),\ j = 1, \ldots, k$$

In discriminant analysis methods (LDA, QDA, naive Bayes...) the focus is on estimating:

$$f(\underline{x}|Y = j) = f_j(\underline{x})$$

which basically corresponds to the opposite conditional probability. With discriminant analysis methods, first you need to assume a distribution of $x$, then you estimate the conditional probability mentioned above, finally you use Bayes theorem to get the opposite conditional probability which is the one you are interested in.

$$\begin{aligned} P(Y = j|\underline{X} = \underline{x}) &= \frac{f(\underline{x}|Y = j)P(Y = j)}{f(\underline{x})} && \text{since } P(A|B) = \frac{P(B|A)P(A)}{P(B)} \\ &= \frac{f(\underline{x}|Y = j)p(Y = j)}{\sum_{i=1}^{k} f(\underline{x}|Y = i)P(Y = i)} && \text{since you have a discrete number of classes} \\ &= \frac{f_j(\underline{x})\pi_j}{\sum_{i=1}^{k} f_i(\underline{x})\pi_i} && \text{just rewriting in a clearer manner} \end{aligned}$$

Remember that $\pi_j$ is usually referred to as *a priori* probability, while $P(Y = j|\underline{X} = \underline{x})$ is usually called *a posteriori* probability. According to Bayes classifier, we choose $j$ that maximises $P(Y = j|\underline{X} = \underline{x})$, but since the denominator does not depend on $j$, we can just consider the numerator; the problem then becomes assigning $\underline{x}$ to the class $j$ which maximises $f_i(\underline{x})\pi_j$

Compared to other methods, discriminant analysis methods are usually flexible to any nymber of classes.

## 7.1 Estimating the *a priori* probability

In order to estimate $\pi_j,\ j = 1, \ldots, k$, there are two options:

- $\hat{\pi}_j = {}^{1}/_{k}$, meaning that all $k$ classes are equally likely.
- $\hat{\pi}_j = {}^{n_j}/_{n}$ with $n_j$ being the number of observations belonging to class $j$ and with $n = n_i + \cdots + n_k$, which means assigning to each class a weight dependent on its empirical frequence.

## 7.2 Discriminant analysis methods

$f_j(\underline{x})$ is a p-dimensional density which requires some assumptions; the chosen assumptions define which method is used, LDA, QDA or naive Bayes

## 7.3 Linear discriminant analysis

### 7.3.1 LDA with one predictor variable

LDA (assuming $p = 1$) makes two assumptions:

- **Gaussianity**, meaning that all classes are gaussian (without specifying anything about mean and variance), hence:

  $$f_j(x) = \frac{1}{\sqrt{2\pi\sigma_j^2}} e^{-\frac{1}{2}\left(\frac{x-\mu_i}{\sigma_j}\right)^2},\ x \in \mathbb{R}$$

  Where:

  - $\mu_j$ is the mean
  - $\sigma_j^2$ is the variance of $X$ conditional on $Y = j$

  This assumption does not work if the predictor is discrete.

- **Constant variance**, meaning that different groups can have different means but the same variance:

  $$\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_k^2 = \sigma^2$$

Writing these two assumptions with a single expression we get:

$$X|Y = j \sim N(\mu_j, \sigma^2)$$

### 7.3.2 Linear decision boundary (one predictor)

Assume we want to classify an observation $x$ using the LDA method. Starting from Bayes formula we have:

$$\begin{aligned}
P(Y=j|\underline{X}=\underline{x}) &= \frac{f_j(\underline{x})\pi_j}{\sum_{i=1}^k f_i(\underline{x})\pi_i} && \text{rearranged for discriminant analysis}\\
&= \frac{\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}\left(\frac{x-\mu_i}{\sigma}\right)^2}\pi_j}{\sum_{i=1}^k \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}\left(\frac{x-\mu_i}{\sigma}\right)^2}\pi_i} && \text{because of the assumptions}\\
&= \frac{e^{-\frac{1}{2}\left(\frac{x-\mu_i}{\sigma}\right)^2}\pi_j}{\sum_{i=1}^k e^{-\frac{1}{2}\left(\frac{x-\mu_i}{\sigma}\right)^2}\pi_i} && \text{simplifying}
\end{aligned}$$

We then assign $x$ to the class $j$ which maximises this function, but since the denominator does not depend on $j$, it corresponds to maximising the numerator, namely

$$e^{-\frac{1}{2}\left(\frac{x-\mu_i}{\sigma}\right)^2}\pi_j$$

or equivalently the logarithm of it

$$\log(\pi_j) - \frac{1}{2}\left(\frac{x-\mu_i}{\sigma}\right)^2 = \log(\pi_j) - \frac{x^2}{2\sigma^2} + \frac{x\mu_j}{\sigma} - \frac{\mu_j^2}{2\sigma^2}$$

But since $-\frac{x^2}{2\sigma^2}$ does not depend on $j$ we can simplify to

$$\log(\pi_j) + \frac{x\mu_j}{\sigma} - \frac{\mu_j^2}{2\sigma^2}$$

We thus assign $x$ to class $j$ that maximises

$$\delta_j(x) = \left(\log(\pi_j) - \frac{\mu_j^2}{2\sigma^2}\right) + x\left(\frac{\mu_j}{\sigma}\right)$$

and if we define:

$$\begin{aligned}
(\beta_0)_j &= \left(\log(\pi_j) - \frac{\mu_j^2}{2\sigma^2}\right)\\
(\beta_1)_j &= \left(\frac{\mu_j}{\sigma}\right)
\end{aligned}$$

We notice that the expression is in linear form:

$$\delta_j(x) = (\beta_0)_j + x(\beta_1)_j$$

In the case of two classes, the decision boundary is given by:

$$\delta_1(x) = \delta_2(x)$$

Which is a linear decision boundary.

### 7.3.3 Estimating parameters (one predictor)

The parameters to use in the LDA method (namely $\pi_1, \dots, \pi_k$, $\mu_1, \dots, \mu_k$ and $\sigma^2$) must be estimated. The estimators for these parameters are:

$$\hat{\pi}_j = \frac{n_j}{n} \qquad \text{empirical frequency of class } j$$

$$\hat{\mu}_j = \sum_{i:y=j} \frac{x_i}{n_j} \qquad \text{sample mean in class } j$$

$$\hat{\sigma^2} = \frac{\sum_{j=1}^{k}(n_j-1)S_j^2}{\sum_{j=1}^{k}(n_j-1)} = \frac{\sum_{j=1}^{k}\sum_{i:y=j}(x_i-\hat{\mu}_j)^2}{n-k} \qquad \text{pooled variance}$$

The method assumes homoskedasticity; for this reason, rather than using the empirical variance of the individual group, a weighted average of the variances of all groups is used. This measure in called pooled variance.

Having defined these estimators, $x$ is classified according to

$$\delta_j\hat{(x)} = \log(\hat{\pi}_j) - \frac{\hat{\mu}_j^2}{2\hat{\sigma^2}} + x\frac{\hat{\mu}_j}{\hat{\sigma}},\ j = 1, \dots, k$$

### 7.3.4 Multivariate LDA

We talk about multivariate LDA when $p \geq 1$, meaning that you do not have a single predictor variable, but rather a vector of predictors $\underline{X} = (X_1, \dots, X_p)$. In this model, the probability of an observation belonging to a certain class $j$ is **multivariate normal** distributed, meaning

$$\underline{X}|Y = j \sim N_p(\underline{\mu_j}, \Sigma)$$

Where:

- $\underline{\mu_j} = \begin{pmatrix} \mu_{1j} \\ \vdots \\ \mu_{pj} \end{pmatrix}$ is a vector of mean values (which is class dependent)
- $\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{1,2} & \cdots & \sigma_{1,p} \\ \sigma_{2,1} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \sigma_{p,1} & \cdots & \cdots & \sigma_p^2 \end{pmatrix}$ is the covariance matrix

Remember that:

- $\sigma_{i,e} = Cov(X_i, X_e)$
- $\sigma_e^2 = Cov(X_e, X_e) = Var(X_e)$

This model assumes that each of the predictors is normal distributed and that the covariance matrix is the same for all groups (meaning $\Sigma_1 = \Sigma_2 = \cdots = \Sigma_k = \Sigma$).

### 7.3.5 Linear decision boundary (multiple predictors)

The fact that the decision boundary for LDA is linear can be demonstrated.

$$\begin{aligned}
P(Y = j|\underline{X} = \underline{x}) &= \frac{\pi_j f_j(\underline{x})}{\sum_{i=1}^k \pi_i f_i(\underline{x})} && \text{from Bayes formula}\\
&= \frac{\pi_j \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(\underline{x}-\underline{\mu_j})^t\Sigma^{-1}(\underline{x}-\underline{\mu_j})\right\}}{\sum_{i=1}^k \pi_i \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(\underline{x}-\underline{\mu_j})^t\Sigma^{-1}(\underline{x}-\underline{\mu_j})\right\}} && f_j(\underline{x}) \sim \text{ multiv. normal}\\
&= \frac{\pi_j \exp\left\{-\frac{1}{2}(\underline{x}-\underline{\mu_j})^t\Sigma^{-1}(\underline{x}-\underline{\mu_j})\right\}}{\sum_{i=1}^k \pi_i \exp\left\{-\frac{1}{2}(\underline{x}-\underline{\mu_j})^t\Sigma^{-1}(\underline{x}-\underline{\mu_j})\right\}} && \text{simplifying}
\end{aligned}$$

We then assign observation $\underline{x}$ to class $j$ which maximises the logarithm of the numerator (since the denominator does not depend on $j$)

$$\begin{aligned}
\delta_j(\underline{x}) &= \log(\pi_j) - \frac{1}{2}(\underline{x}-\underline{\mu_j})^t\Sigma^{-1}(\underline{x}-\underline{\mu_j}) && \text{function to maximise}\\
&= \log(\pi_j) - \frac{1}{2}\underline{x}^t\Sigma^{-1}\underline{x} + \underline{x}^t\Sigma^{-1}\underline{\mu_j} - \frac{1}{2}\underline{\mu_j}^t\Sigma^{-1}\underline{\mu_j} && \text{multiplying}\\
&\propto \left(\log(\pi_j) - \frac{1}{2}\underline{\mu_j}^t\Sigma^{-1}\underline{\mu_j}\right) + \underline{x}^t\left(\Sigma^{-1}\underline{\mu_j}\right) && \text{ignoring terms not depending on } j\\
&\propto (\beta_0)_j + \underline{x}^t(\underline{\beta})_j && \text{with } (\underline{\beta})_j = (\beta_{1j} \ \cdots \ \beta_{pj})^t\\
&= \beta_{0j} + x_i\beta_{1j} + x_2\beta_{2j} + \cdots + x_p\beta_{pj} && \text{which is linear}
\end{aligned}$$

### 7.3.6 Estimating parameters (multiple predictors)

The estimated parameters are analogous to the single predictor case:

$$\begin{aligned}
\hat{\pi}_j &= \frac{n_j}{n} && \text{empirical frequency of class } j\\
\underline{\hat{\mu}_j} &= \frac{1}{n}\sum_{i:y=j} \underline{x_i} && \text{vector of sample means in class } j\\
\hat{\Sigma} &= \frac{1}{n-k}\sum_{j=1}^k \sum_{i:y=j} (\underline{x_i} - \underline{\hat{\mu}_j})(\underline{x_i} - \underline{\hat{\mu}_j})^t && \text{pooled covariance matrix}
\end{aligned}$$

The class probabilities are obtained when these estimates go into $\delta_j(\underline{x})$ leading to

$$P(Y = \hat{j}|\underline{X} = \underline{x}) = \frac{e^{\hat{\delta_j}(\underline{x})}}{\sum_{i=1}^k e^{\hat{\delta_i}(\underline{x})}}$$

With:

$$\hat{\delta_j}(\underline{x}) = \log(\hat{\pi}_j) - \frac{1}{2}\underline{\hat{\mu}_j}^t\hat{\Sigma}^{-1}\underline{\hat{\mu}_j} + \underline{x}^t\Sigma^{-1}\underline{\hat{\mu}_j}$$

### 7.3.7 LDA vs logistic regression

Assume you want to compare LDA and logistic regression. Take $k = 2$; you can then write the log odds as:

$$\begin{aligned}
\text{log-odds}_{LR} &= \log\left(\frac{p(1|x)}{1-p(1|x)}\right) &&= \log\left(\frac{p(1|x)}{p(0|x)}\right) = \delta_1(x) - \delta_0(x) &&= \beta_0 + \beta_1 x \\
\text{log-odds}_{LDA} &= \log\left(\frac{p(1|x)}{1-p(1|x)}\right) &&= \log\left(\frac{p(1|x)}{p(0|x)}\right) = \delta_1(x) - \delta_0(x) &&= \alpha_0 + \alpha_1 x
\end{aligned}$$

The main difference, assuming that $f_i(\underline{x})$ can be approximated by a multivariate normal, is the estimation of parameters:

- LR: $\underline{\hat{\beta}}$ is estimated directly by maximum likelihood
- LDA: $\underline{\hat{\alpha}}$ are estimated indirectly via $\underline{\hat{\mu_j}}$, $\hat{\Sigma}$

Logistic regression optimization procedure is more unstable when the classes are well separated (probability close to 0 and 1).

## 7.4 Quadratic discriminant analysis

Quadratic discriminant analysis (QDA) is similar to LDA in the sense that it is still defined as a multinormal distribution, but the assumption of homoskedasticity falls; this means that you assume all predictor variables to be normal distributed but each of them can have its own expected value and covariance matrix. Therefore we can write QDA as

$$\underline{X}|Y = j \sim N_p(\underline{\mu_j}, \Sigma_j)$$

### 7.4.1 Quadratic boundary

For QDA it can be shown that the decision boundary is quadratic.

$$\begin{aligned}
P(Y = j|\underline{X} = \underline{x}) &= \frac{\pi_j f_j(\underline{x})}{\sum_{i=1}^k \pi_i f_i(\underline{x})} && \text{from Bayes formula} \\
&= \frac{\pi_j \frac{1}{(2\pi)^{p/2}|\Sigma_j|^{1/2}} \exp\left\{-\frac{1}{2}(\underline{x}-\underline{\mu_j})^t\Sigma_j^{-1}(\underline{x}-\underline{\mu_j})\right\}}{\sum_{i=1}^k \pi_i \frac{1}{(2\pi)^{p/2}|\Sigma_i|^{1/2}} \exp\left\{-\frac{1}{2}(\underline{x}-\underline{\mu_j})^t\Sigma_i^{-1}(\underline{x}-\underline{\mu_j})\right\}} && \text{from the assumptions} \\
&= \frac{\pi_j |\Sigma_j|^{-1/2} \exp\left\{-\frac{1}{2}(\underline{x}-\underline{\mu_j})^t\Sigma_j^{-1}(\underline{x}-\underline{\mu_j})\right\}}{\sum_{i=1}^k \pi_i |\Sigma_i|^{-1/2} \exp\Big\{-\frac{1}{2}(\underline{x}-\underline{\mu_j})^t\Sigma_i^{-1}(\underline{x}-\underline{\mu_j})\Big)\}} && \text{simplifying}
\end{aligned}$$

Then assign observation $\underline{x}$ to class $j$ which maximises the logarithm of the numerator (since the denominator does not depend on $j$)

$$\begin{aligned}
\delta_i(\underline{x}) &= \log(\pi_j) - \frac{1}{2}\log(|\Sigma_j|) - \frac{1}{2}(\underline{x} - \underline{\mu_j})^t\Sigma_j^{-1}(\underline{x} - \underline{\mu_j}) && \text{function to maximise} \\
&= \log(\pi_j) - \frac{1}{2}\log(|\Sigma_j|) - \frac{1}{2}\underline{x}^t\Sigma_j^{-1}\underline{x} + \underline{x}^t\Sigma_j^{-1}\underline{\mu_j} - \frac{1}{2}\underline{\mu_j}^t\Sigma_j^{-1}\underline{\mu_j} && \text{multiplying} \\
&= -\frac{1}{2}\underline{x}^t\Sigma_j^{-1}\underline{x} + \underline{x}^t\Sigma_j^{-1}\underline{\mu_j} + \log(\pi_j) - \frac{1}{2}\log(|\Sigma_j|) && \text{which is quadratic in } \underline{x}
\end{aligned}$$

### 7.4.2 LDA vs QDA

QDA has more parameters than LDA, namely

$$\begin{aligned}
&\text{QDA: } pk + k\frac{p(p+1)}{2} && \underline{\mu_1}, \ldots, \underline{\mu_k}, \Sigma_1, \ldots, \Sigma_k \\
&\text{LDA: } pk + \frac{p(p+1)}{2} && \underline{\mu_1}, \ldots, \underline{\mu_k}, \Sigma_{p\times p}
\end{aligned}$$

For example, if we take $k = 2$ and $p = 50$, then LDA has 1375 parameters, while QDA has 2650.