

# Statistical learning - Vinciotti (2022)

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# 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 guideline 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 Friedman, 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 ...

### 1.3. TOPICS

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- 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
- $\underline{X} = (X_1, \dots, X_p)$ : 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  $\underline{X} = (X_1, \dots, X_p)$
- $\varepsilon$  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  $\underline{X}$ )

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  $f$ .

### 2.3. HOW TO ESTIMATE $f$ ?

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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 (mean squared error):

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

Furthermore, since we know that:

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

Thus we get:

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

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 estimate $f$ ?

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:

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

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**.

Notice that linear models are linear in the parameters, 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 not 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 the former 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:

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

But notice that:

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

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

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

Therefore we can simplify as:

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

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** refers to the error that is introduced by approximating a problem, which may be extremely complicated, by a much simpler model. If an estimated model performs well on the training data but it does not perform well on new data, the estimated model has high bias. 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 more flexible models are generally more influenced by a change of dataset.

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 **simple 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.

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 polynomial) in order to choose the balance between bias and variance.

## Chapter 3

# Statistical decision theory

### 3.1 Definition of statistical decision theory

**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.

### 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).

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  $f(\underline{X})$ . Many loss functions can be used; the choice of a specific loss function determines which function is considered to be the true rule  $f(\underline{X})$ .

### 3.3 Regression setting

In a regression setting, the loss function which is generally used is the **squared error loss function**, which is defined as

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

### 3.3. REGRESSION SETTING

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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:

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

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  $g$ .

**Theorem 1** (Minimum of the expected prediction error).  *$\text{EPE}(f) = E_{Y,\underline{X}}[(Y - f(\underline{X}))^2]$  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, since the law of iterated expectations states that  $E[X] = E[E[X|Y]]$  (analogously to profile likelihood, you fix one variable and variate the other), 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

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

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

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

Since  $a = E[Y]$ , the function that minimizes the EPE is

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

□

### 3.4. CLASSIFICATION SETTING

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In a regression setting you could use other loss functions, such as

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

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

$$Y|\underline{X} = \underline{x} \sim N(\underline{x}^t \underline{\beta}, \sigma^2)$$

or focussing more on the conditional mean

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

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

#### 3.3.1 K nearest neighbour for regression

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

$$\hat{f}(\underline{x}) = \text{Average } (y_i | \underline{x}_i \in N_K(\underline{x}))$$

Where:

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

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.

### 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 classification 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

$$L(Y, \hat{Y}(\underline{X})) = \text{TODO Add punnet square}$$

Where:

### 3.4. CLASSIFICATION SETTING

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- $Y$  is the true class
- $\hat{Y}(\underline{X})$  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  $\hat{Y}$ , which is the function of  $\underline{X}$  such that it minimizes the **expected 0-1 loss**, defined as:

$$E[L(Y, \hat{Y}(\underline{X}))]$$

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

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

(Which is the weighted sum of  $\underline{x}$  belonging to each possible class). Then, considering the binary case, if the classifier predicts  $\underline{x}$  to belong to class 0 ( $\hat{y} = 0$ ), we have

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

On the other hand, if the classifier predicts  $\underline{x}$  to belong to class 1 ( $\hat{y} = 1$ ), 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 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

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

(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:

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

### 3.4. CLASSIFICATION SETTING

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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:

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

We talk about **perfect separation** of the classes 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. More often than not,  $\text{BER} > 0$ , 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

$$L(Y, \hat{Y}(\underline{x})) = \text{TODO add punnet square}$$

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; using a 0-1 loss function results in a model which always classifies patients as healthy, therefore it is 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 that takes into account different error weights.



### 3.5 Model accuracy

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

Therefore, a regression that uses MSE has for accuracy

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

Meanwhile, for a classification, you create a **confusion matrix**, estimate the probabilities via some method, substitute the values into the following formulas

$$\begin{aligned} \text{True positive rate (TPR)} &= \frac{\text{TP}}{\text{TP} + \text{TN}} &&= \text{sensitivity} \\ \text{False positive rate (FPR)} &= \frac{\text{FP}}{\text{FN} + \text{FP}} &&= 1 - \frac{\text{TN}}{\text{TN} + \text{FP}} = 1 - \text{specificity} \\ \text{Error rate} &= \frac{\text{FP} + \text{FN}}{m} \end{aligned}$$

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).

Different models have different ROC curves. The best possible curve would touch the top left corner, meaning that you never misclassify any observation and therefore the model is deterministic. The worst possible 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 highest in the region you are most interested in (based on sensibility and specificity).