School of Electronic Engineering and Computer Science
Queen Mary University of London

ECS607/766 Data Mining
Week 3: Classification I

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Agenda

Recap (with some extras)

Formulation of classification problems

Linear classifiers

Logistic regression

Nearest neighbours

Final remarks

Flexibility, complexity and overfitting

The starting point of data science projects is to assume that data follow a **pattern** and any deviation from this pattern is considered to be **noise**.

Our models need to be **flexible enough to capture the complexity of the underlying pattern**, however we need to be careful not to learn irrelevant noise features, i.e. not to **overfit** our data.

By **testing** our model on a dataset different from the dataset used for **training**, we can assess how well we have been able to capture the pattern and discard the noise. **Validation** approaches use separate datasets as well.

Ventris' ultimate check

"... and a decisive check, preferably with the aid of **virgin material**, to ensure that the apparent results are not due to **fantasy**, **coincidence** or **circular reasoning**"

The curious case of the multiple inference

In inferential statistics, data are used during **hypothesis testing** to **retain** or **reject** the so-called **null hypothesis**.

You can think of it as asking a *YES-NO* question and being given the probability that the answer is *NO* when we say *YES*. This probability is **computed from our data** (different data give different values!).

If this probability is very low, we will happily say *YES* as we will think the probability of making an error is very low. However, if we ask multiple questions (i.e. if we conduct **multiple inference**), the probability of making an error in at least one question increases!

In Data Mining we have data plus computing power and are capable of asking many many questions after **snooping** our data. If we are not careful, **we might see something in our data when there is nothing**!

Don't fool yourself!

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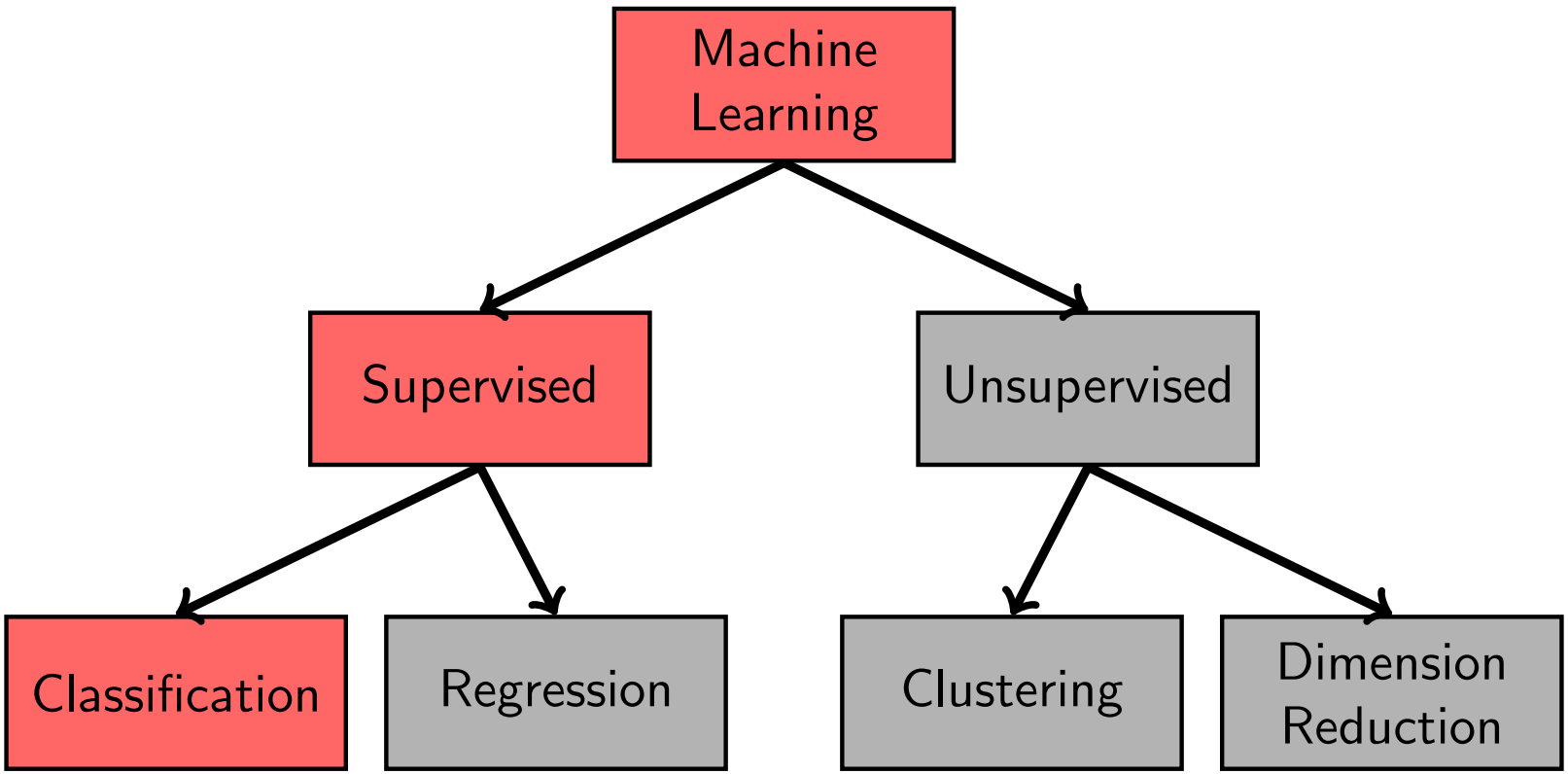
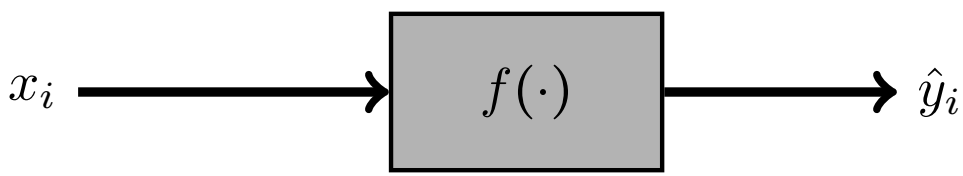
Data science taxonomy



Problem formulation

We will follow the same notation that we used for regression problems. In a classification problem:

- We assume the value of one of the attributes can be predicted based on the value of the remaining attributes (it is a **supervised** problem).
- The response y is a **discrete** (categorical/qualitative) **variable**, sometimes called the sample's **label**. Its values are called **classes** and we say sample x belongs to class y.
- As usual, our job is then to **find the** *best* **model** $f(\cdot)$ that relates the response attribute to the predictors, $\hat{y} = f(x)$ and we will use a **dataset** $\{(x_i, y_i) : 1 \leq i \leq N\}$ to infer the relationship between response and predictors.



A binary classification problem

There are many examples of classifiers that aim at predicting whether **individuals have or lack a specific characteristic or behavior** based on some data about them (for instance whether they have a certain disease based on medical data).

A popular dataset for binary classification in machine learning is the *Adult Data Set*, built from anonymised US census data:

- It contains nearly 50,000 instances (i.e. individuals)
- A total of **14 categorical and numerical attributes** (including age, workclass, education and gender) can be used as **predictors**
- A **binary label** denoting whether the instance's salary is greater or less than \$50K
- Downloadable from archive.ics.uci.edu/ml/datasets/Adult

Another binary classification problem

Sentiment analysis allows to identify human opinions expressed in fragments of text. Multiple opinions can be considered, but in it's simplest form two are defined, namely positive and negative.

The *Large Movie Review Dataset* was created to create models that recognise polar sentiments in fragments of text:

- It contains 2500 samples for training and 2500 samples for testing
- Each instance consists of a **fragment of text** (i.e. a vector of categorical variables) used as a **predictor** together with a **binary label** (0 being negative opinion, 1 positive opinion).
- Downloadable from ai.stanford.edu/~amaas/data/sentiment/

A multiclass classification problem

Recognising digits in images containing handwritten representations is a classic multiclass classification problem. The predictor is an array of values (image) and there are 10 classes, namely $0, 1, 2, \ldots 9$.

Machine learning approaches use datasets of **labelled images**, i.e. **images (predictors)** with the corresponding **digit (label)**, to build a model.

The MNIST dataset is a collection of handwritten digits:

- 60,000 images for training, 10,000 for testing
- Images are black and white, 28×28 pixels
- Downloadable from yann.lecun.com/exdb/mnist

The dataset as a table

We have already discussed that datasets can be represented as tables, where rows correspond to instances and columns to attributes. In classification problems, our datasets will share the same representation.

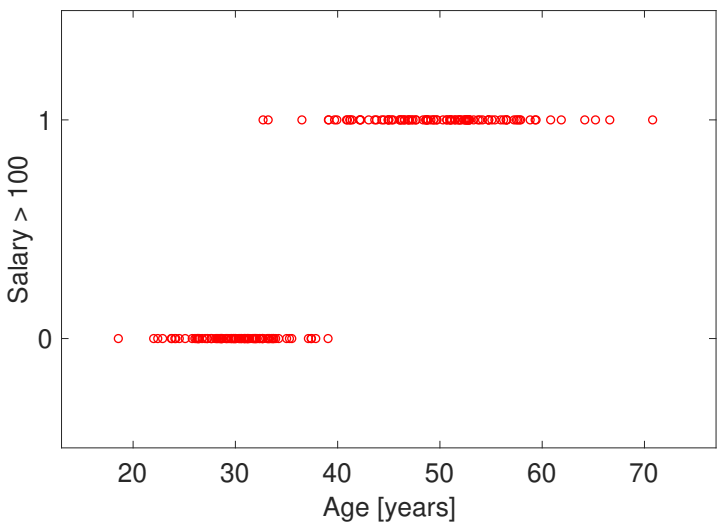
Data Science platforms offer different options to work with tabular datasets. For instance:

- Provided that **all attributes have the same type**, we can use **2D arrays** to represent the whole table (Matlab and Python/Numpy).
- We can store the values of numerical/categorical attributes in different **vectors** (**1D arrays** in Matlab and Python/Numpy). All such vectors must have the **same size** (the number of instances).
- When attributes are more complex (for instance an image or text), instead of 1D arrays we can use **2D or 3D arrays**.
- **Tables** in Matlab and **dataframes** in Python/pandas are similar to 2D arrays, but **columns can be of different types**.

The dataset as a graph

Labels can be represented as points on a vertical axis. However be careful: **the notions of ordering and distance do not apply to categorical variables**.

One predictor, two classes

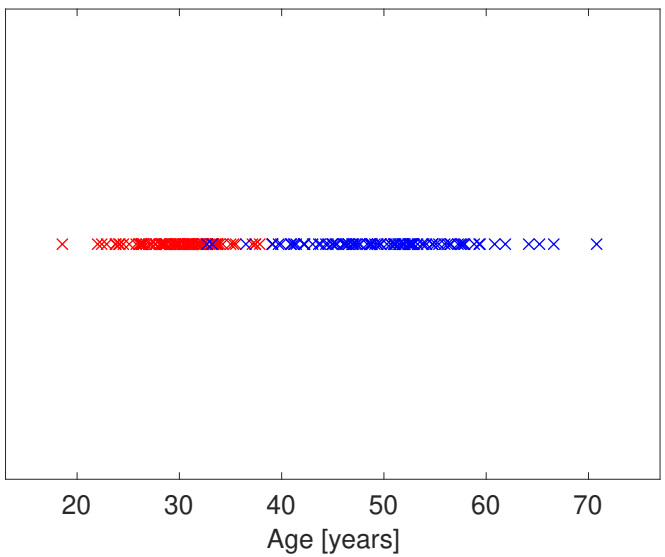


Two predictors, three classes

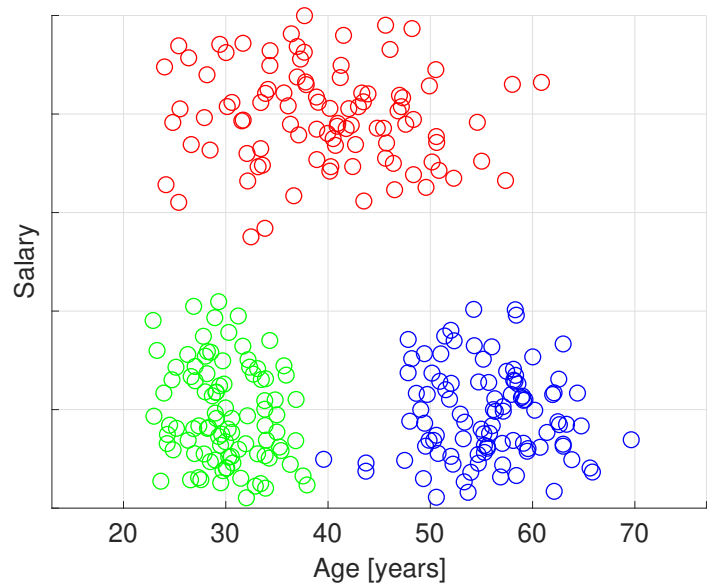
The dataset as a graph

Datasets can also be represented as collections of points in the **predictor space** that use **different symbols depending on the label**.

One predictor, two classes



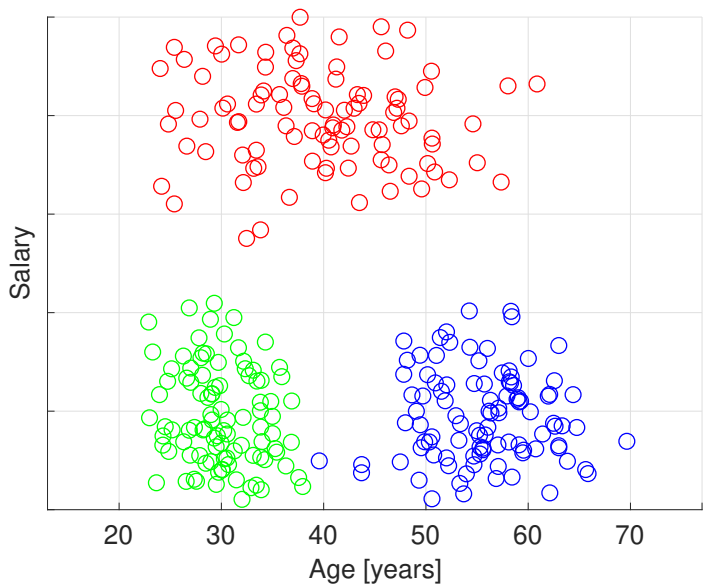
Two predictors, three classes



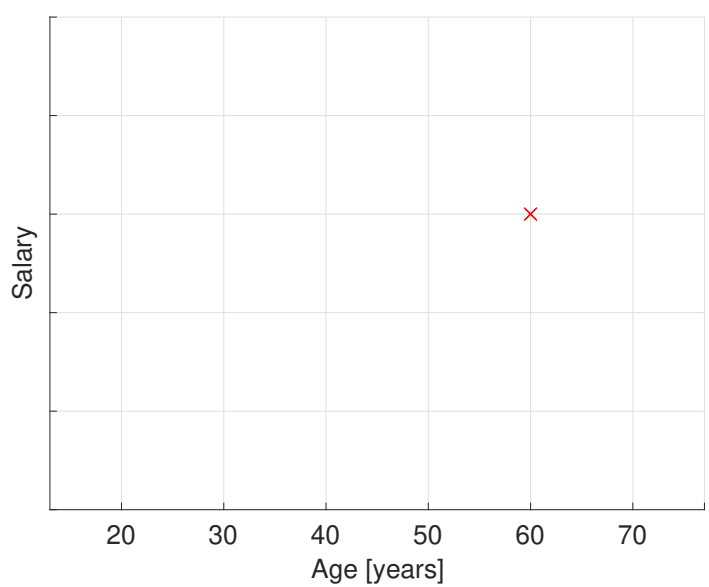
What does a solution look like?

A regression model can be represented as a curve (or as a surface, if we consider several predictors) such that for every predictor a single response is returned. How can we represent a classification model?

Training data



New data point



What does a solution look like?

In classification problems we use the notion of **decision regions** in the predictor space.

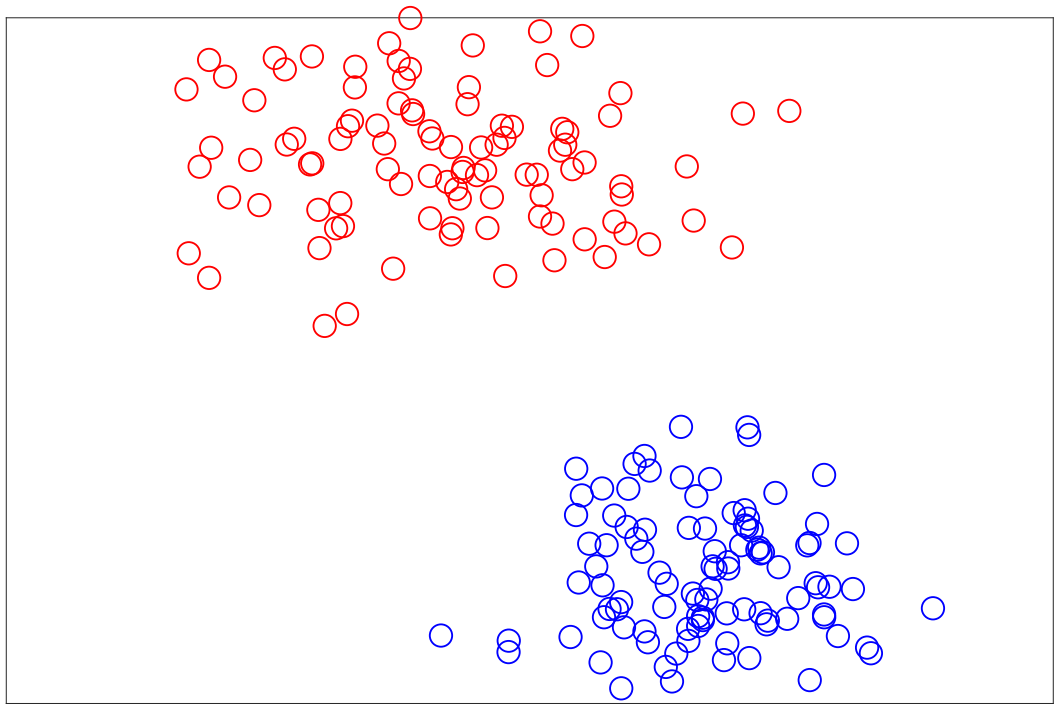
- A decision region in the predictor space corresponds to all the **points that are associated to the same label**.
- Regions can be defined by identifying their **boundaries**.
- Therefore, a solution model in classification is **defined by a set of regions or boundaries between regions**.

Now that we know what a solution looks like, we need to answer two questions"

- How do we define a sensible **goodness of fit** to identify the *best* mode?
- How can we express our solution as a **computation**?

Overfitting in classifiers

The notions of flexibility, complexity and overfitting can also be applied to classifiers and are best understood by looking at the boundaries defining the decision regions.



Model evaluation: Goodness of fit

In regression, we defined goodness of fit metrics (MSE, RMSE or MAE) based on the notion of **prediction error** $e_i = y_i - \hat{y}_i$ (the **distance** between the desired response y_i and the predicted response $\hat{y}_i$).

The MNIST dataset is a collection of images containing handwritten digits. Data scientists use the MNIST dataset to build models that can recognise the digits $0, 1, 2, \ldots 9$ from handwritten digits.

To build a model that recognises digits from their handwritten versions, the notion of distance between a desired response y_i and the predicted one $\hat{y}_i$:

(a) Can be defined as the subtraction $y_i - \hat{y}_i$

(b) Can be defined as the normalised subtraction $(y_i - \hat{y}_i)/10$

(c) Cannot be defined

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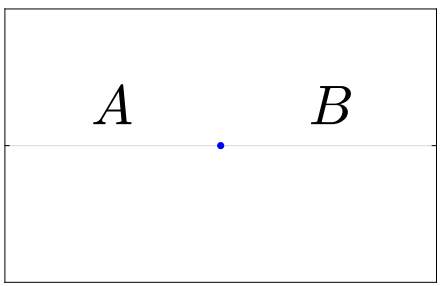
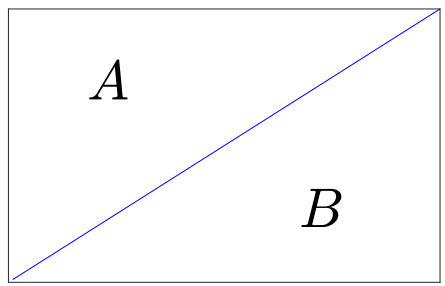
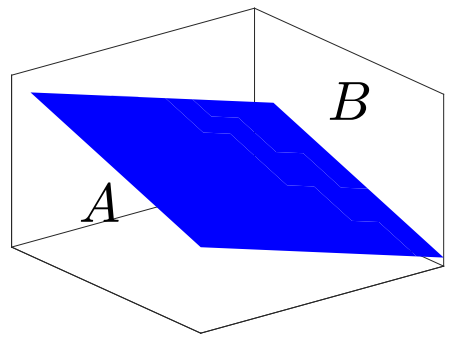
The simplest boundary

Let's consider a **binary** classification problem (i.e. two labels, for instance A and B). The simplest boundary between the two decision regions is:

- A point for one predictor.
- A straight line for 2 predictors.
- A plane surface for 3 predictors.







Definition of linear classifiers

Linear classifiers define straight lines, planes and hyperplanes as boundaries between decision regions:

- Linear boundaries are defined by the linear equation $\boldsymbol{w}^T\boldsymbol{x} = 0$. The extended vector $\boldsymbol{x} = [1, x_\alpha, x_\beta ...]^T$ contains the predictor variables
- The **idea** is to classify a sample based on whether it's on one side of the boundary or the other
- The **implementation** is simple. Given sample i's predictors, build the extended vector $\boldsymbol{x}_i$. Then carry out the operation $\boldsymbol{w}^T\boldsymbol{x}_i$. If the results is positive, you are on one side of the boundary. If it is negative, you are on the other
- The question we still need to answer is: What is the **best linear classifier** for a given dataset? In other words, what is the best $\boldsymbol{w}$?

Goodness of fit

The **only operation that we can perform with categorical variables is the logical comparison**, i.e. we can assess whether $y_i = \hat{y}_i$ is either true or false.

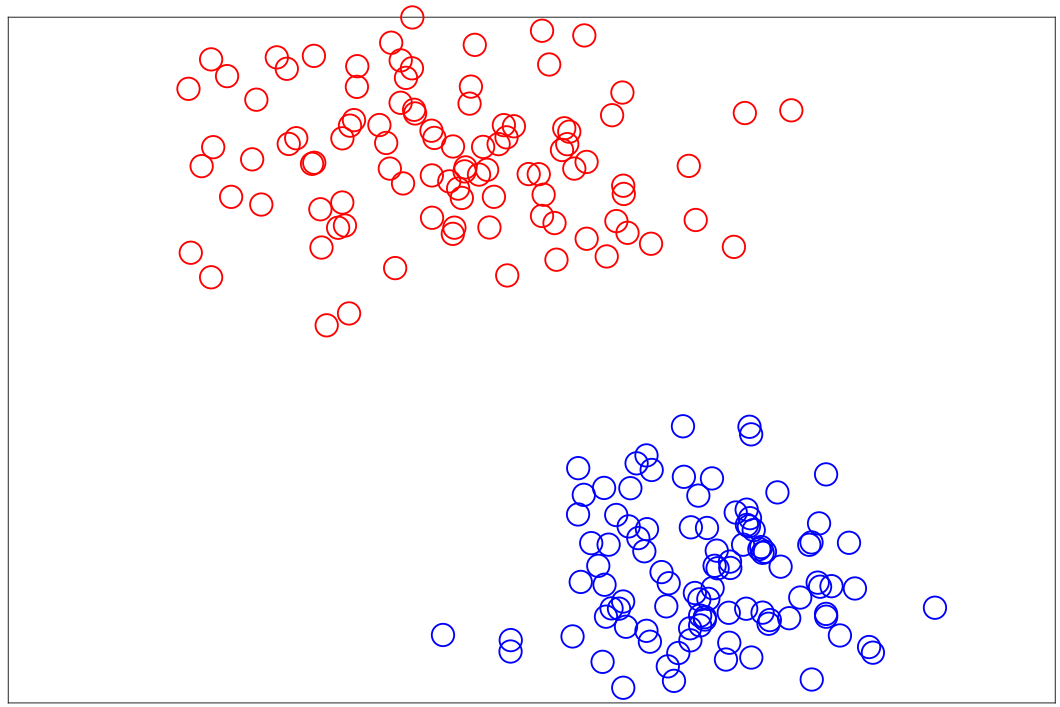
In a dataset with N_A instances labeled A and N_B instances labelled B:

- We can calculate the number of **true predictions** for a class (e.g. samples with label A that have been classified as A)
- We can calculate the number of **false predictions** for a class (e.g. samples with label B that have been classified as A)
- We can calculate the overall number of true and false predictions

A useful notion of goodness is the **accuracy** A, which is defined as the number correctly classified samples over the total number of samples. The **best linear classifier is the one with the highest accuracy**.

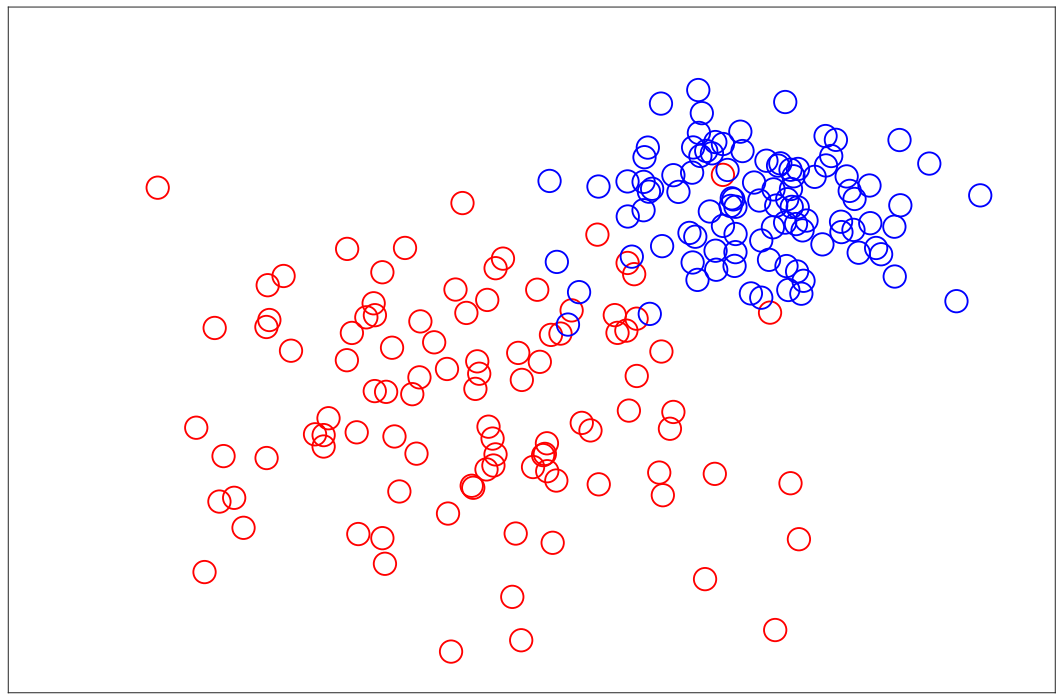
The best linear classifier: Separable case

When dealing with linearly separable datasets, we can achieve the maximum accuracy $A = 1$. Notice there can be multiple *best* solutions.



The best linear classifier: Non separable case

In the case of non linearly-separable datasets, the accuracy is always $A < 1$. The best solution will be the one(s) achieving the highest accuracy.



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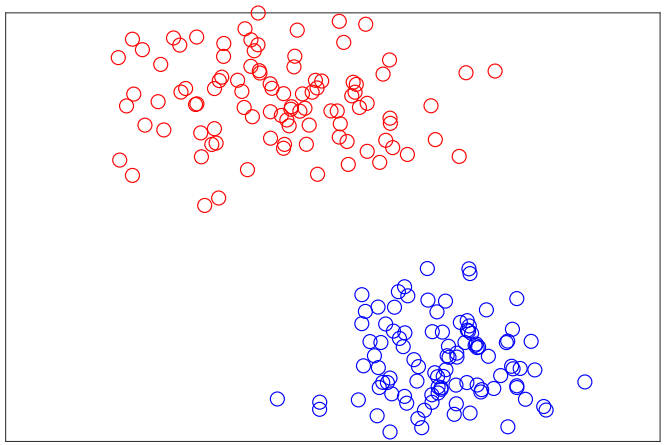
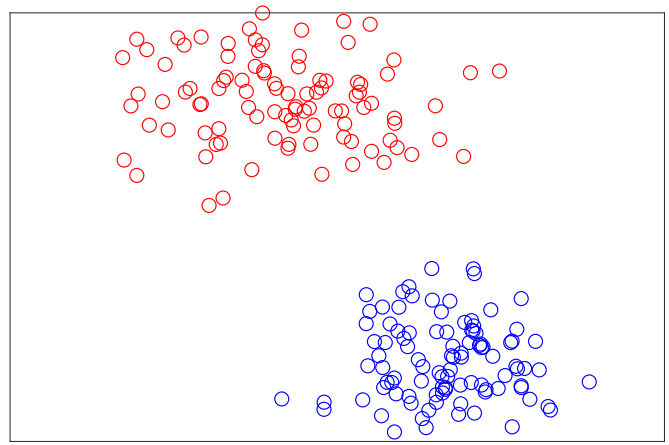
Best, but risky, linear solutions

Draw two linear classifiers (i.e. two linear boundaries) for the same dataset that achieve an accuracy $A = 1$. Which one would you choose? Why?

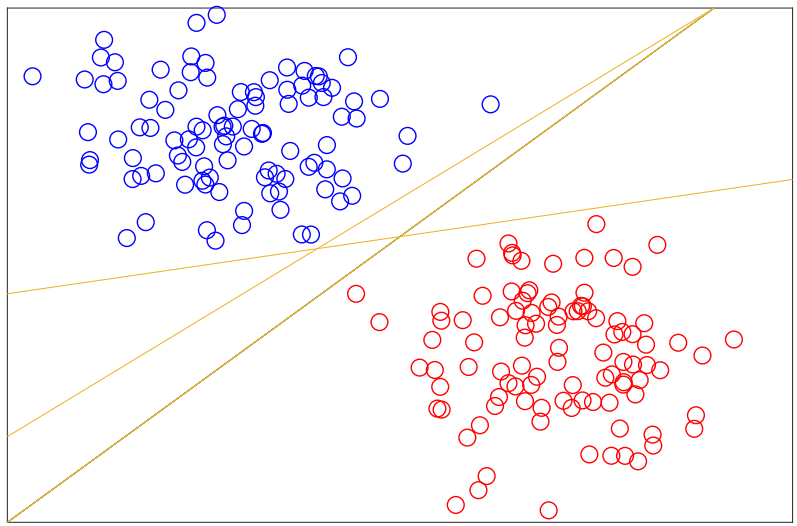




If you prefer one over the other, you might be inadvertently assessing their generalisation ability.

Keep that boundary away from me!

As we get closer to the boundary between two decision regions, life gets harder for a classifier: it is noise territory. Our uncertainty about the true identity of a sample there would be greater than far from the boundary.



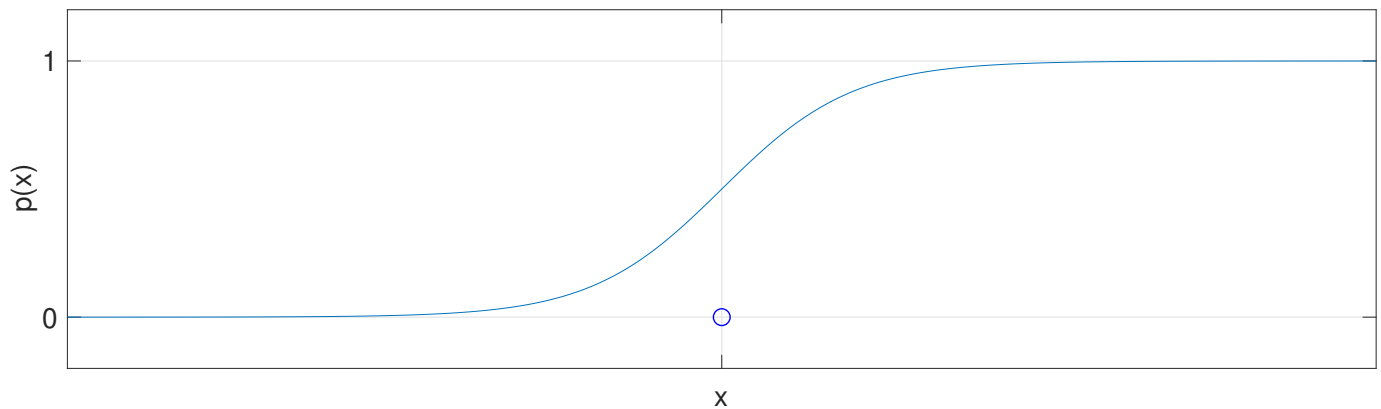
In other words, **the further we are from the boundary, the higher the chances we will be classifying our samples correctly**.

The logistic model

Given a linear boundary defined by $\boldsymbol{w}^T\boldsymbol{x} = 0$ and a sample's predictor vector $\boldsymbol{x}_i$, the logistic function defined as

$$p(\boldsymbol{x}_i) = \frac{e^{\boldsymbol{w}^T\boldsymbol{x}_i}}{1 + e^{\boldsymbol{w}^T\boldsymbol{x}_i}}$$

In the case of one single predictor variable and a boundary at 0, the logistic function looks like this



The logistic model

Remember $\boldsymbol{w}^T\boldsymbol{x}_i$ can be interpreted as a distance from a point in the predictor space to the boundary. This distance is negative if $\boldsymbol{x}_i$ is in one region (say A), positive if it's in the other region (say B).

Notice that:

- If $\boldsymbol{x}_i$ is on the boundary, $p(\boldsymbol{x}_i) = 0.5$.
- If $\boldsymbol{w}^T\boldsymbol{x}_i > 0$ (we are in region B), as we move away from the boundary $p(\boldsymbol{x}_i) \to 1$.
- If $\boldsymbol{w}^T\boldsymbol{x}_i < 0$ (we are in region A)as we move away from the boundary, $p(\boldsymbol{x}_i) \to 0$

Here is the tricky point, so use **all your neurons**:

- If $y_i = B$, then $p(\boldsymbol{x}_i)$ is the **classifier's certainty** that $y_i = B$.
- If $y_i = A$, then $1 - p(\boldsymbol{x}_i)$ is the **classifier's certainty** that $y_i = A$.

The logistic model

Given a linear boundary defined by $\boldsymbol{w}$ and a labelled sample $(\boldsymbol{x}_i, y_i)$, we know how to calculate the classifier's certainty. This certainty is a quantity between 0 and 1, and the maximum uncertainty is 0.5.

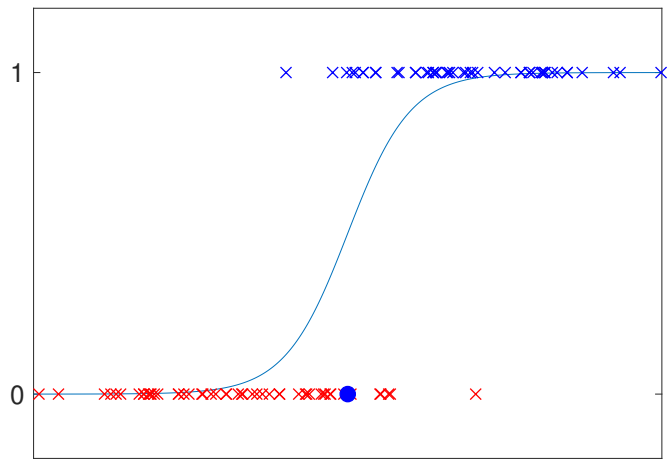
Can we calculate the classifier's certainty for a whole dataset of N labelled samples $\{(\boldsymbol{x}_i, y_i) : 1 \leq i \leq N\}$? The answer is yes, by simply **multiplying** the individual certainties:

$$L(\boldsymbol{w}) = \prod_{y_i=A} (1 - p(\boldsymbol{x}_i)) \prod_{y_i=B} p(\boldsymbol{x}_i)$$

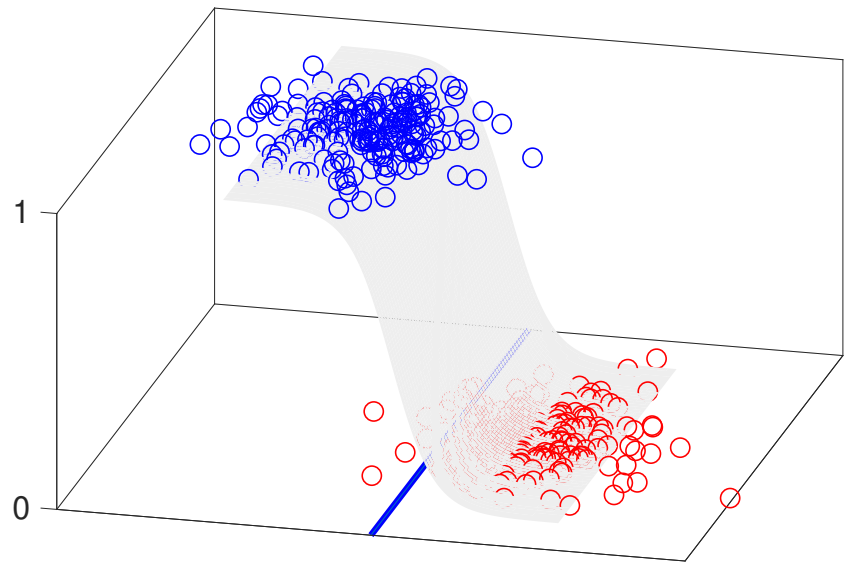
We can define a goodness of fit based on $L(\boldsymbol{w})$. We call the classifier $\boldsymbol{w}$ that maximises $L(\boldsymbol{w})$ **MaxEnt classifier**, **Maximum Likelihood** or simply **Logistic Regression**. Did I say regression?

Visualising logistic regression

One predictor



Two predictors



Final thoughts about linear logistic regression

- What should we do if our classes are not linearly separable?
- How do we generalise to multiclass classification?
- What is the effect of outliers?
- What is the meaning of the weights $\boldsymbol{w}$?
- What if one of our predictors is a categorical variable?

Agenda

Parametric and non-parametric approaches

Linear classifiers belong to the family of **parametric** approaches : we assume a type of boundary (in this case linear) and use our dataset to identify the best boundary (defined by the vector $\boldsymbol{w}$) within the assumed type of boundaries.

Non-parametric approaches offer a more flexible alternative, as they do not assume any type of boundary. In this section, we will study two popular approaches:

- Nearest Neighbours (NN)
- K Nearest Neighbours (kNN)

Nearest Neighbours

A classifier is essentially a partition of the predictor space into decision regions separated by boundaries:

- Given a new sample x_i, its label y_i is determined by identifying the decision region where it is.

In nearest neighbours, boundaries in binary classifiers are defined as points that are half-way between two samples from different classes:

- To classify a new sample, we just need use the **label of the closest (*most similar*) training sample**.
- We need to **memorise the whole training dataset** (linear classifiers only needed to memorise the vector $\boldsymbol{w}$). That's why sometimes we call them **instance-based methods**.

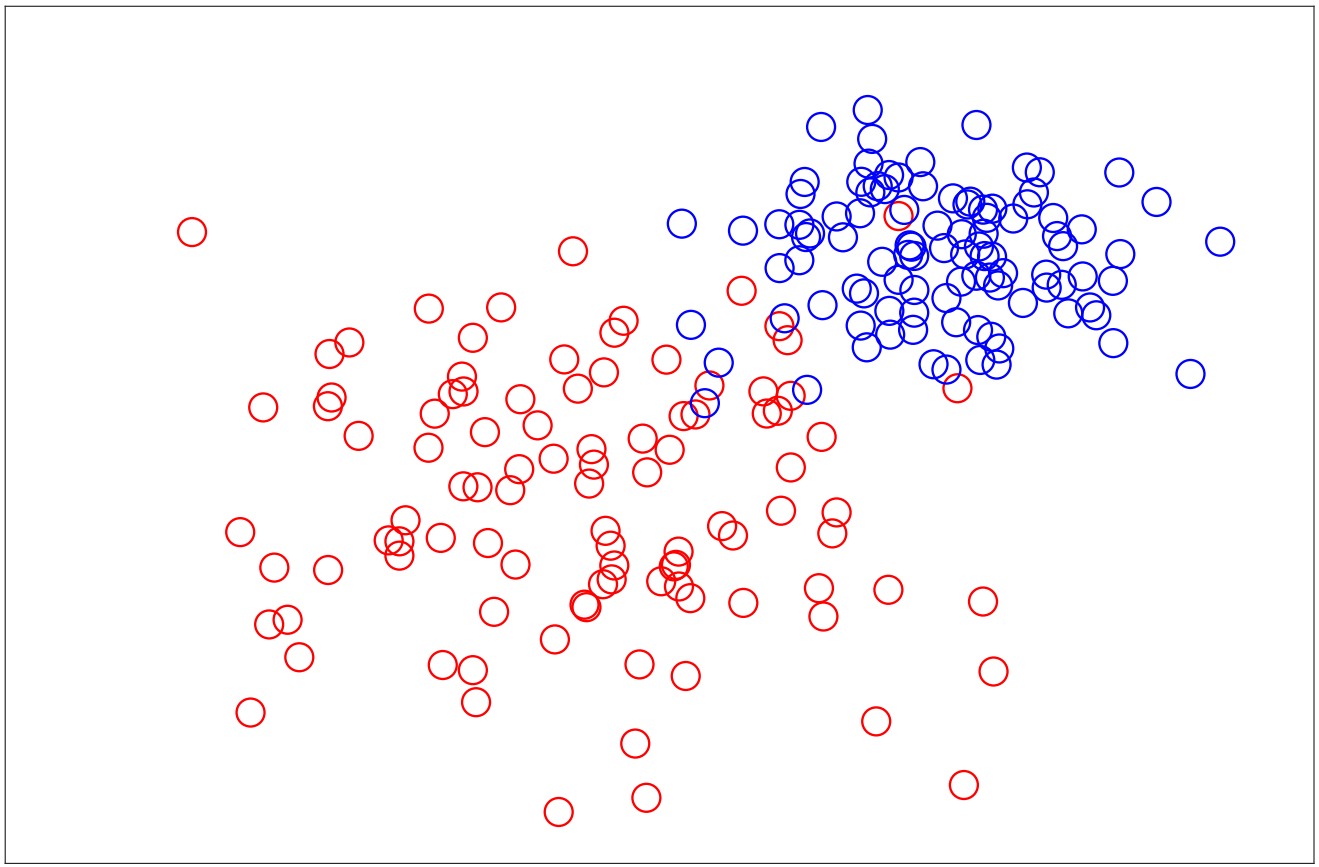
The notion of distance

Mathematically, we can use different *distances*:

- Euclidean
$$D_E(\boldsymbol{a}, \boldsymbol{b}) = \sum_k (a_k - b_k)^2$$
- Manhattan
$$D_M(\boldsymbol{a}, \boldsymbol{b}) = |a_k - b_k|$$
- Hamming
$$D_H(\boldsymbol{a}, \boldsymbol{b}) = \sum_k (a_k \neq b_k)$$

The shape of the final boundary depends on the definition of distance.
When is each distance appropriate?

Boundaries in Nearest Neighbours classifiers



k Nearest Neighbours

Boundaries in nearest neighbours classifiers can be too complicated, noisy and hard to interpret. How could we smooth them? K Nearest neighbours proceeds as follows. Given a new sample x:

- We calculate the distance to all the training samples.
- Choose the K closest points
- Note the class of each of the K points
- Assign a label based on the most popular class among those k points.

k Nearest neighbours: Example

Final thoughts about Nearest Neighbors

- How do we choose K?
- A predictor could have different units (for instance cm, m, km). Which one should we use?
- Different predictors have different units. What is the meaning of a distance in the predictor space?

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Do we always need data-driven approaches?

Inside a MoDem