Machine Learning for Physics and Astronomy

Juan Rojo

VU Amsterdam & Theory group, Nikhef

Natuur- en Sterrenkunde BSc (Joint Degree), Honours Track

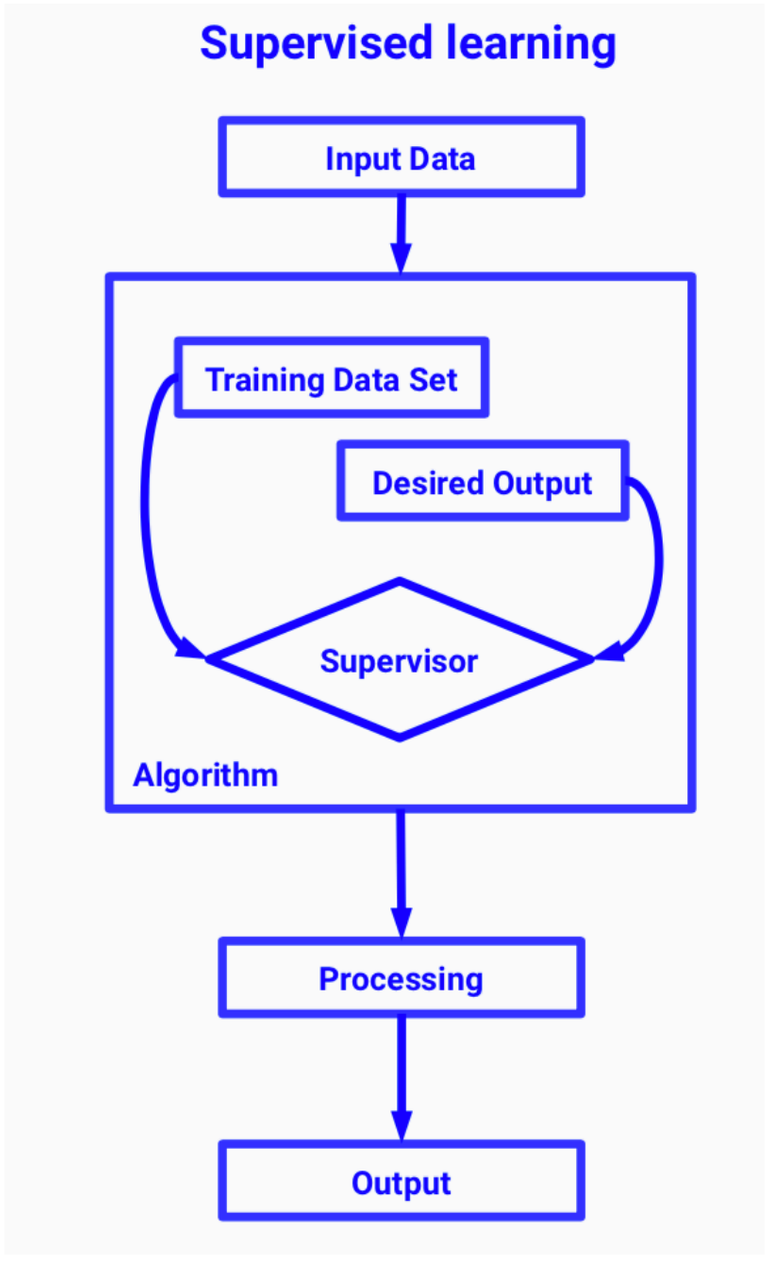
Lecture 5, 05/10/2021

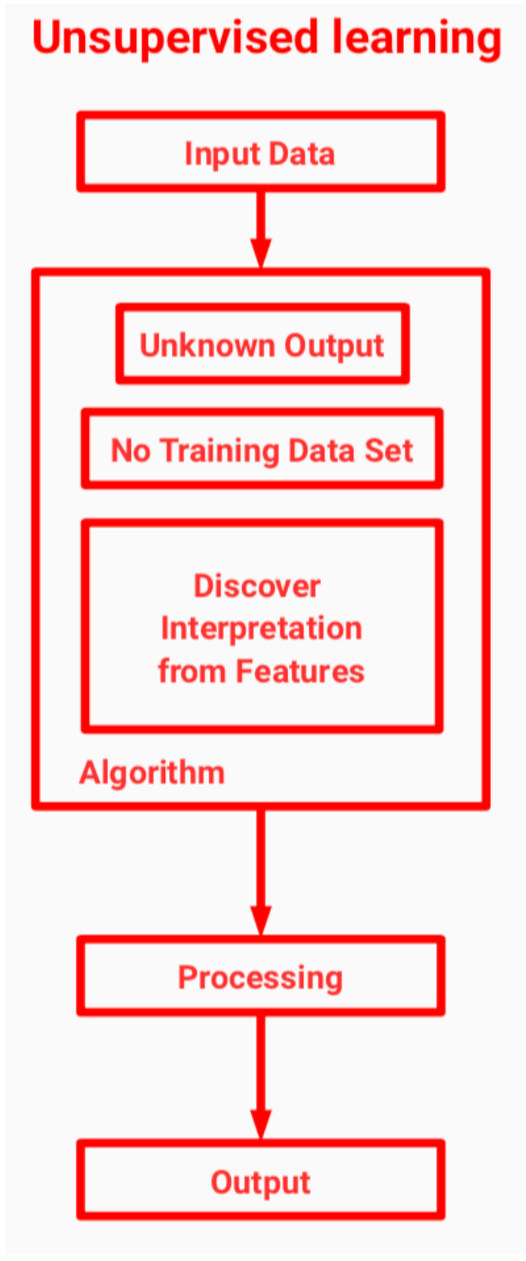
Today's lecture

- Classification problems in Machine Learning
- Classification with deep learning models
- Decision Theory
- Decision Trees and Random Forests
- Support Vector Machines

Classification problems in Machine Learning

Supervised Learning recap





supervised learning suitable for classification problems

Supervised Learning recap

problems in **Supervised Machine Learning** are defined by the following ingredients:

(1) Input dataset: $\mathscr{D} = (\boldsymbol{X}, \boldsymbol{Y})$

(2) Model: $f\left(\boldsymbol{X}, \boldsymbol{\theta}\right)$

(3) Cost function: $C\left(\boldsymbol{Y}; f(\boldsymbol{X}; \boldsymbol{\theta}\right)$

The cost function measures how well the model (for a specific choice of its parameters) is able to **describe the input dataset**

example of cost function for single dependent variable: sum of residuals squared

$$C\left(\boldsymbol{Y}; f(\boldsymbol{X}; \boldsymbol{\theta}\right) = \frac{1}{n} \sum \left(y_i - f(\boldsymbol{x}_i, \boldsymbol{\theta})\right)^2$$

Q: do you think this cost function is suitable / the best for classification problems?

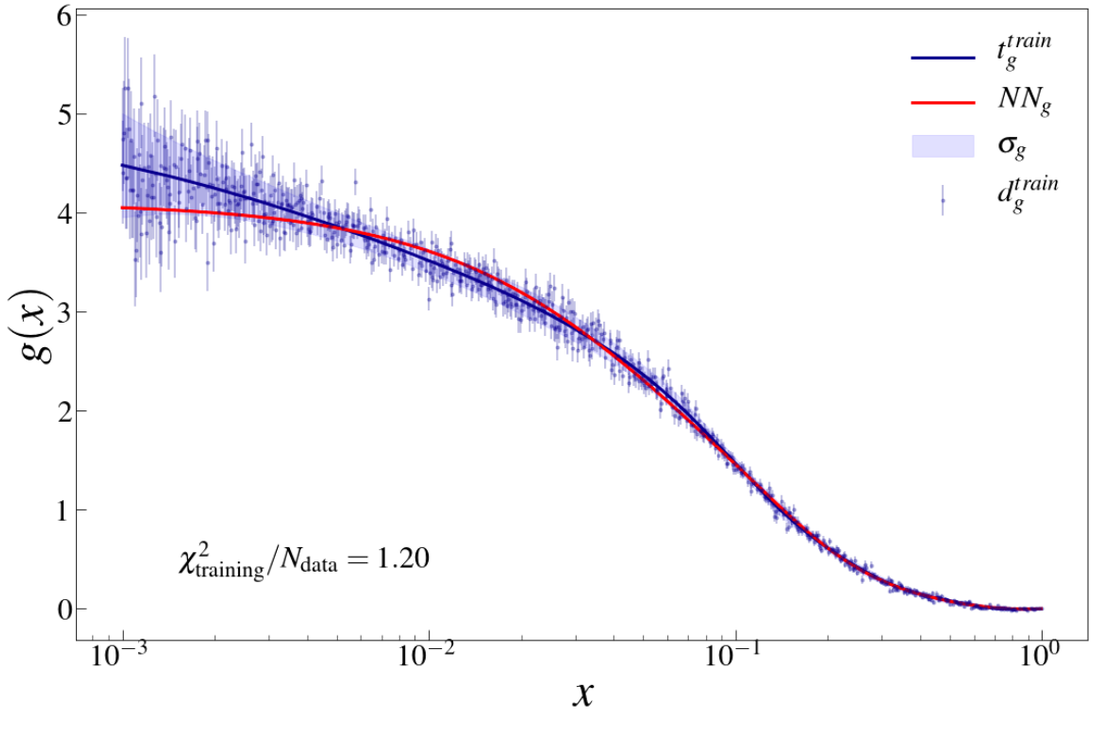
Supervised learning

We denote as **supervised learning** the ML task of **learning a function** that maps a **vector of inputs** to a **vector of outputs** from a finite set of training example

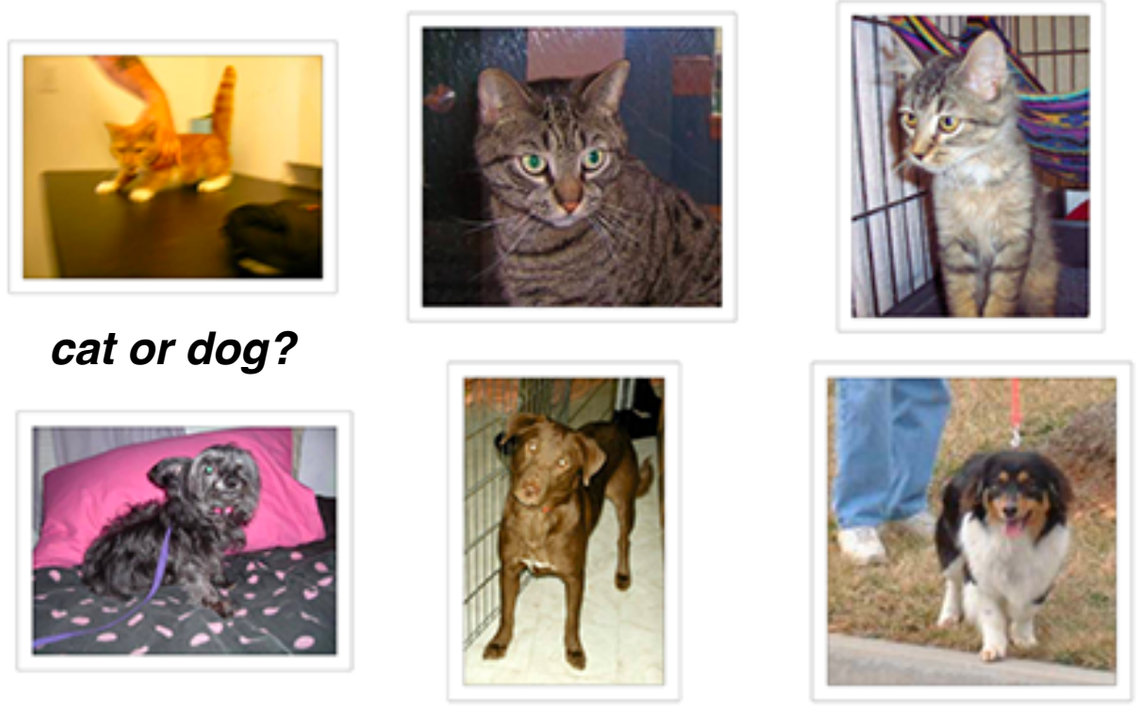
note that some assumptions will be needed: a function is an **infinite-dimensional object** but learning takes place from a **finite number of examples**

main property of supervised learning: the **training samples are labeled**

continuous outputs: regression

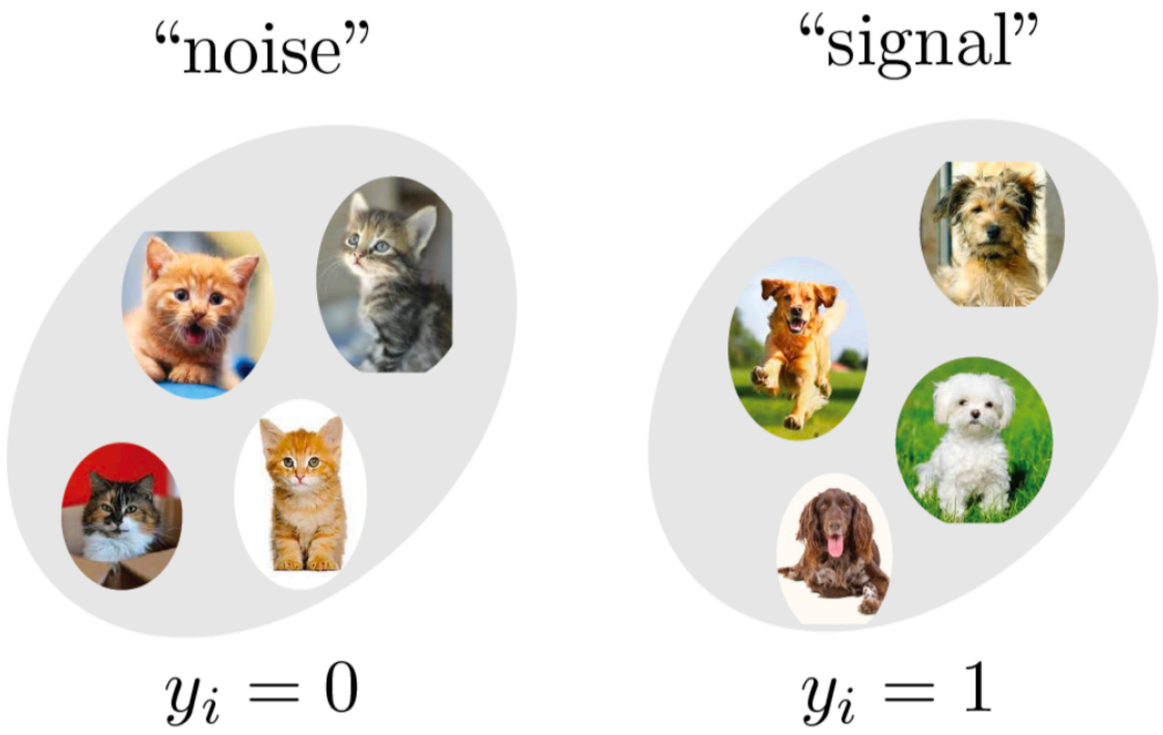


discrete outputs: classification

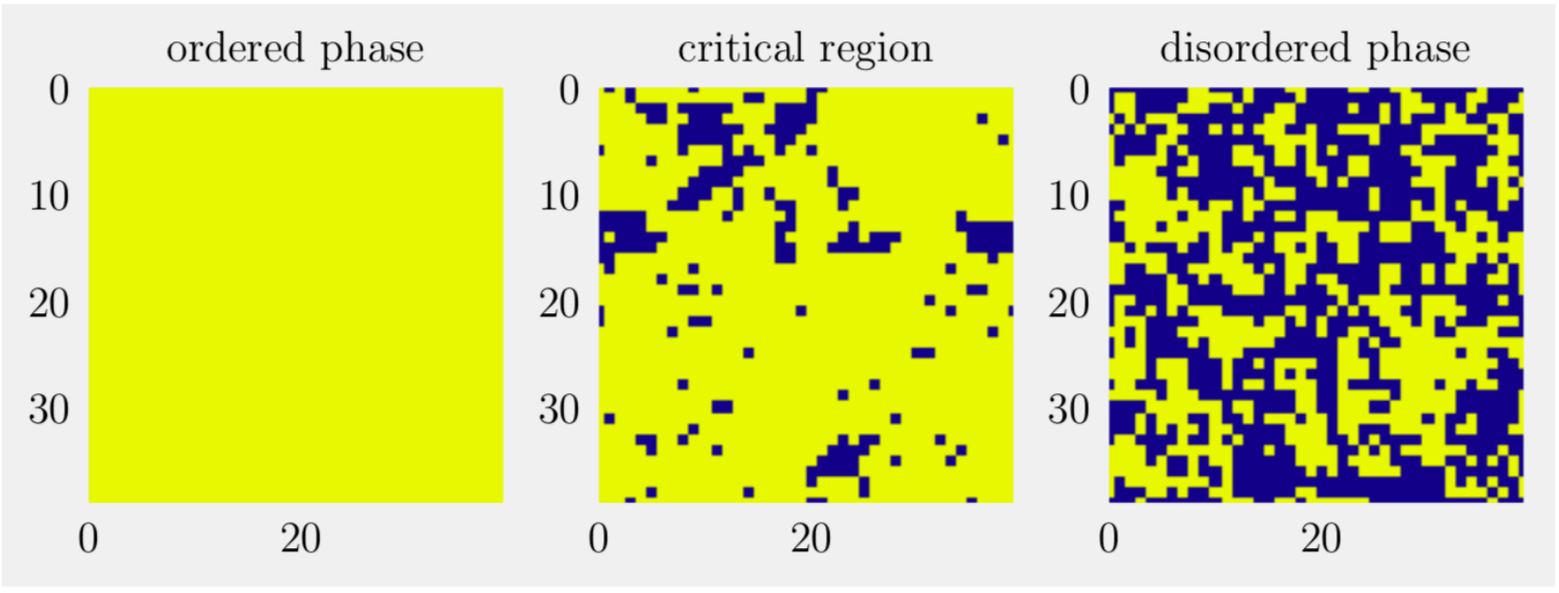


Classification tasks

relevant for Machine Learning applications where outcomes
are discrete variables, eg. **categories in classification problems**



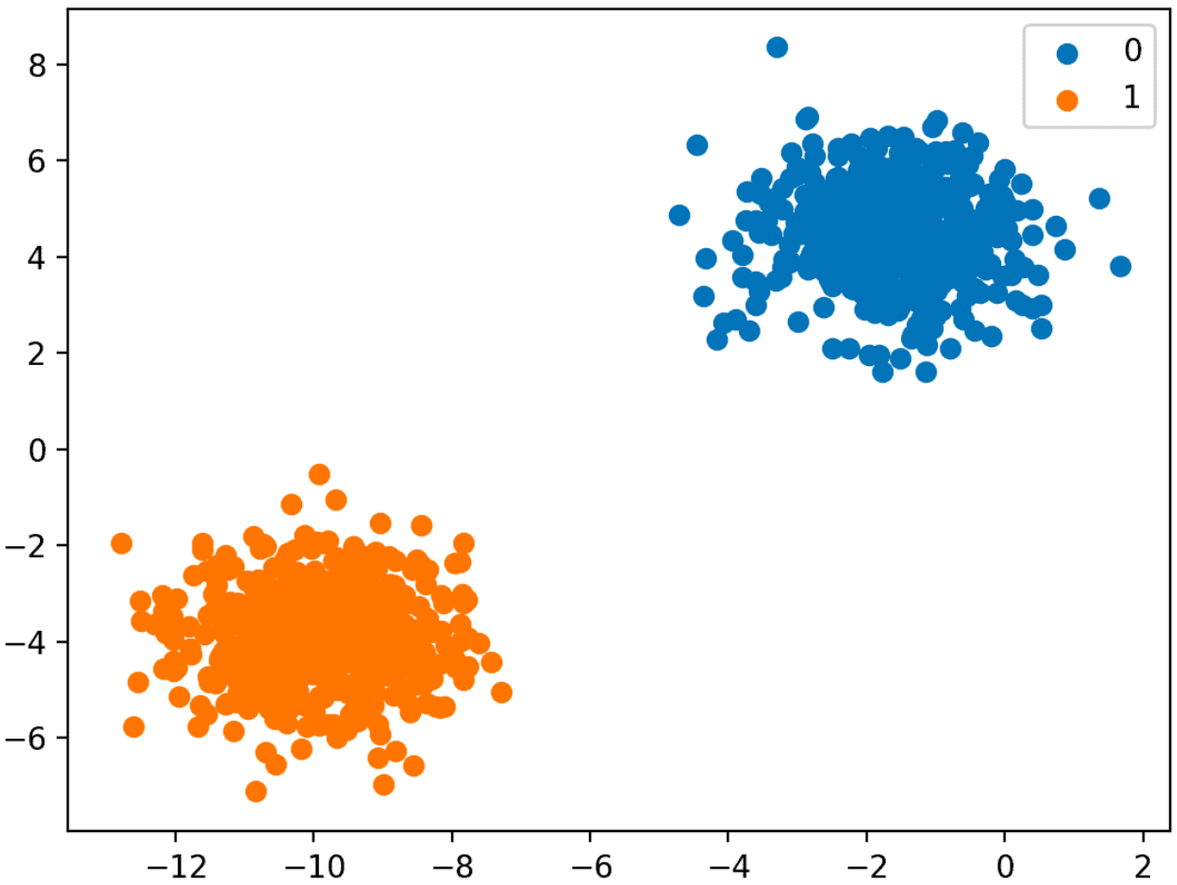
can we tell apart
cats from dogs?

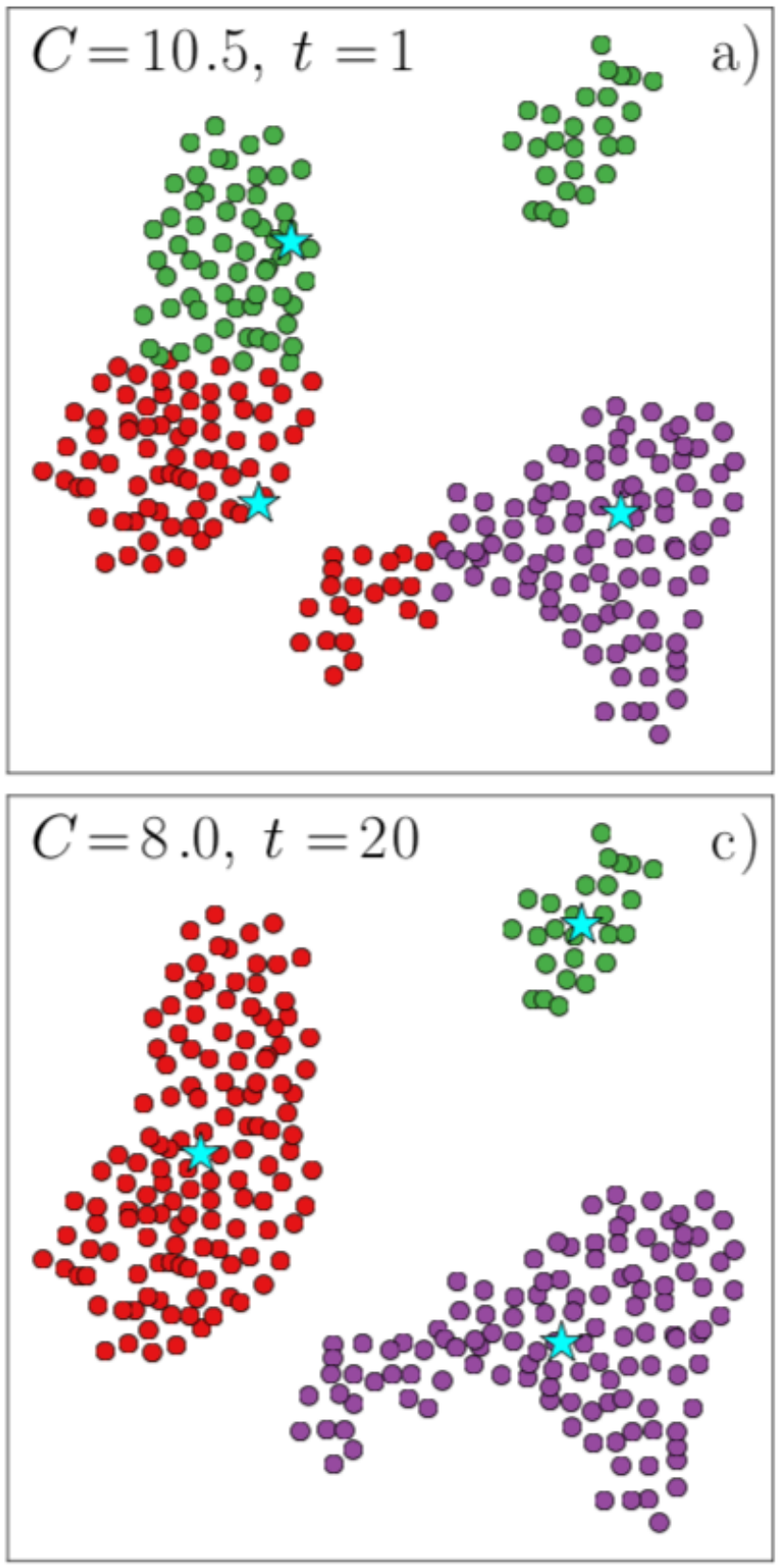


can we identify the phase
(ordered/disordered) of
spin configurations in 2D Ising?

supervised vs unsupervised learning

assume someone gives you this **dataset**
and tells you to categorise a new point to
either **“0” or “1”**



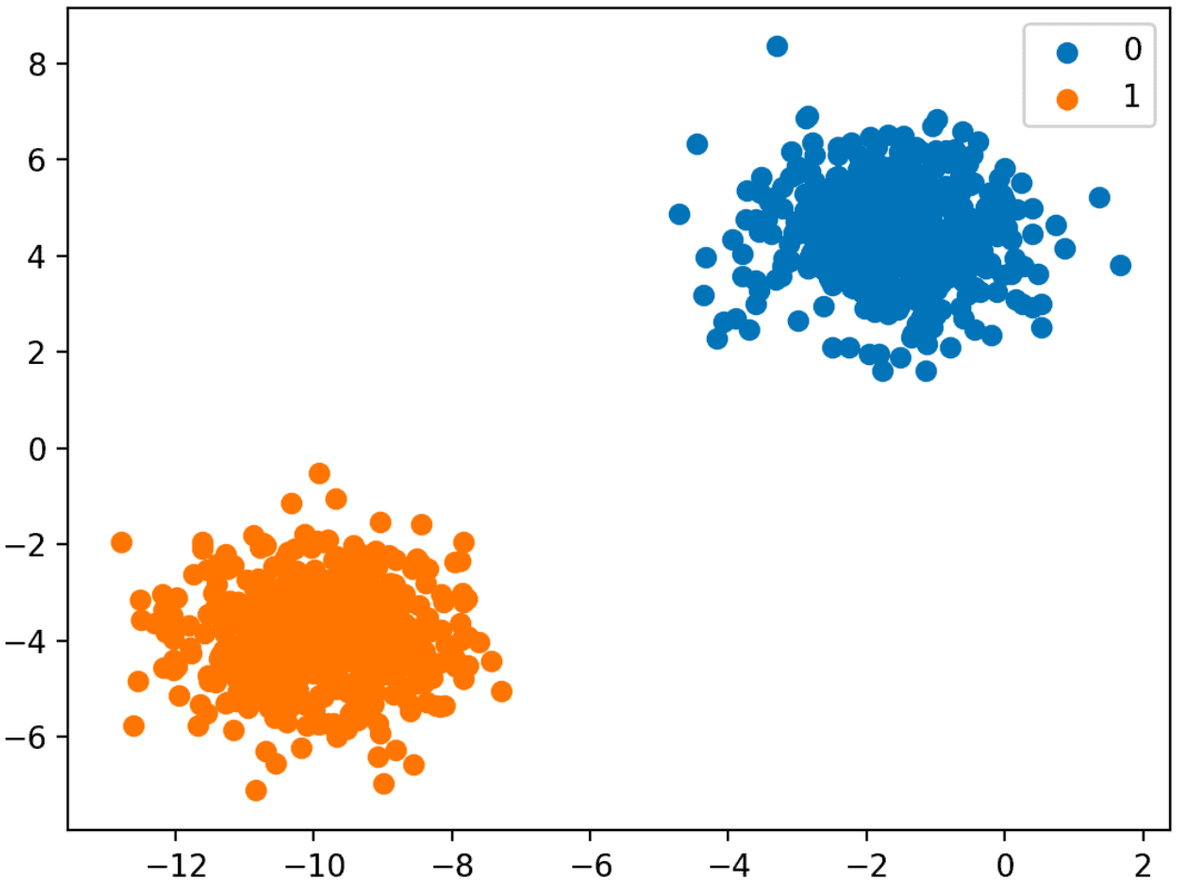


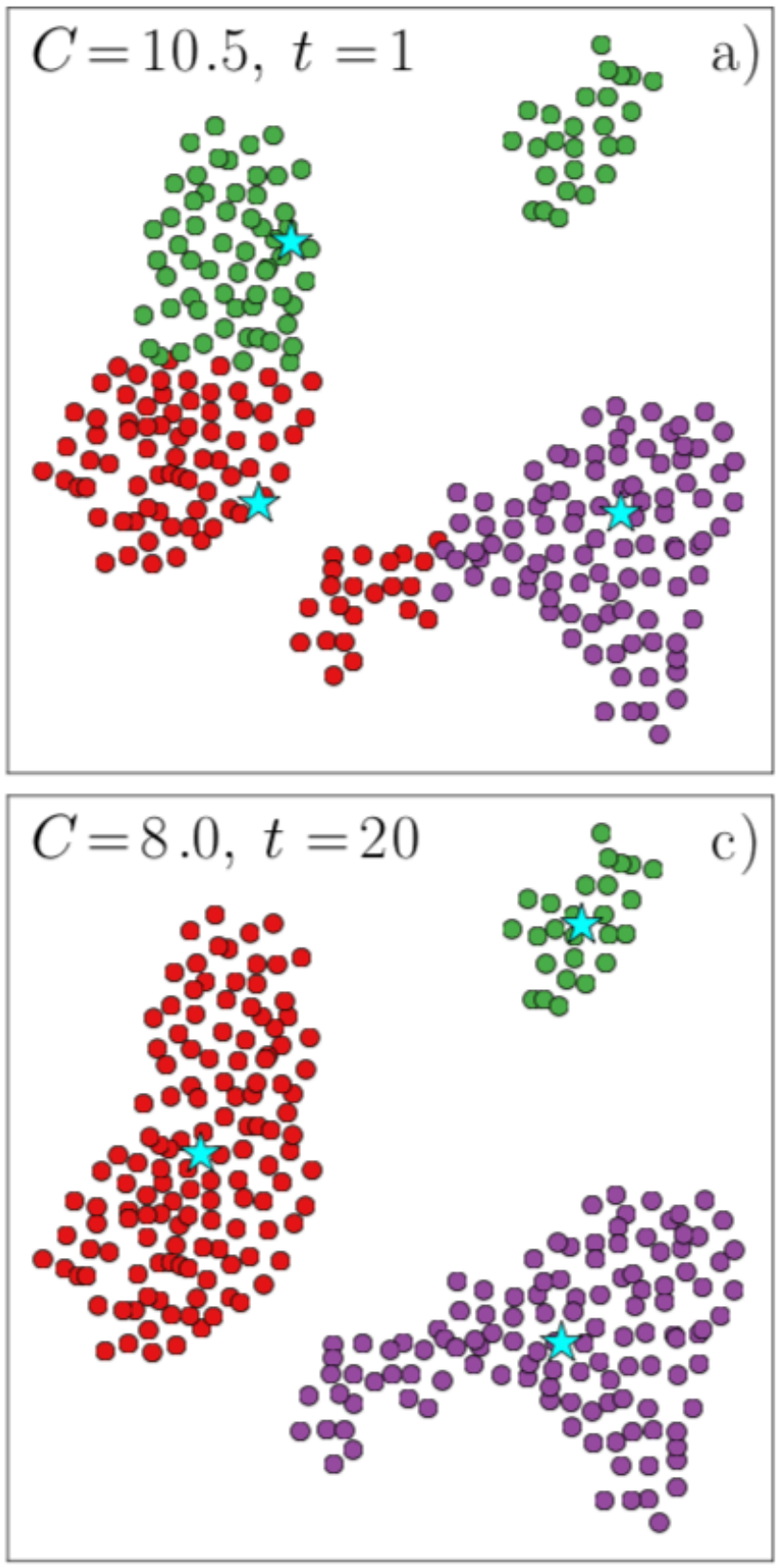
Q1: in which respect this problem is different from clustering?

Q2: what is the main output of solving this problem?

supervised vs unsupervised learning

assume someone gives you this **dataset**
and tells you to categorise a new point to
either **“0” or “1”**





A1: we have labelled samples to begin with

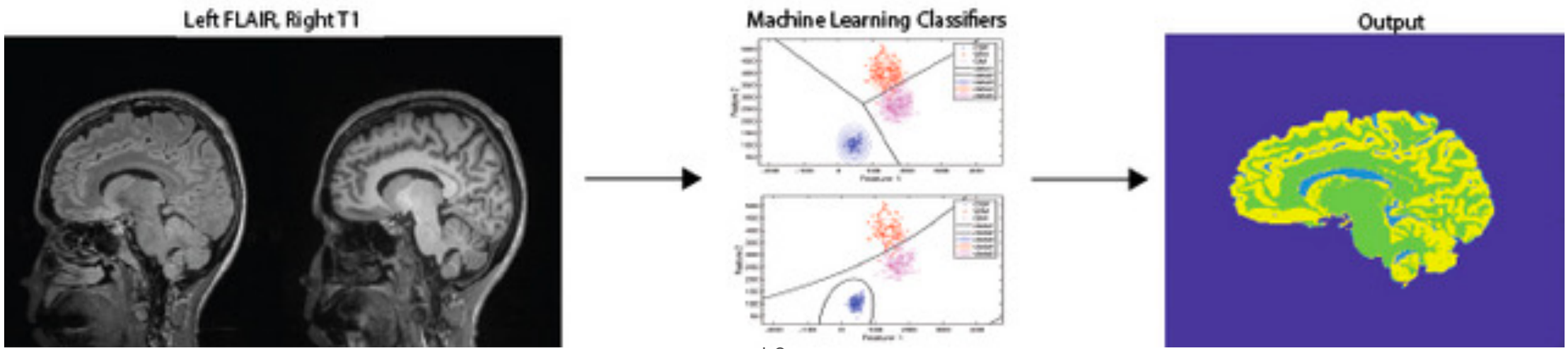
A2: a rule to classify a new data point to belong to either of the two classes

Classification in ML

The goal is to **predict a class label** from a pre-defined list of possibilities

- Is this email spam?
- Should I sell these stocks now?
- Which handwritten number/letter/character is this one?
- Is the animal in the photo a car or a dog?
- Given a user profile, should I offer them specific products?
- Given a MRI scan, is this person awake or dreaming?
- Given this sample tissue, is this person healthy or sick?

can you think of other user cases?



Classification tasks

The goal is to **predict a class label** from a pre-defined list of possibilities

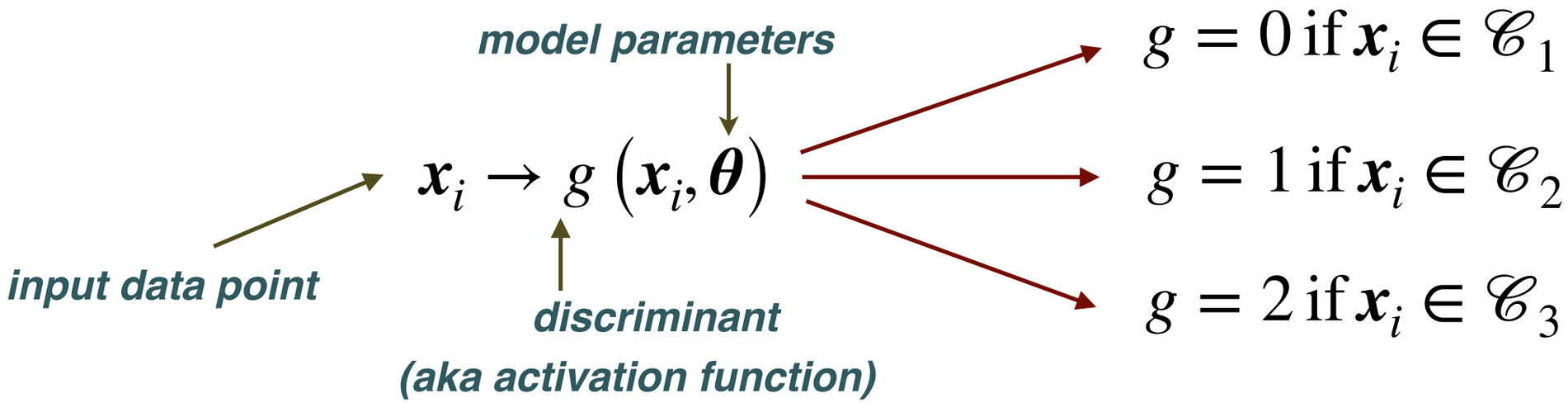
the simplest type of problem is **binary classification** (yes/no problems)

e.g. should I put this email in the spam folder?

but in general one considers **multiclass classification** (> 2 categories)

e.g. which type of bird is the one I just photographed?

In the context of ML applications there exist a large number of approaches to classifications tasks. The most basic one is based on assembling a **discriminant function** that maps each input data point to its specific class



Linear classifiers

In this class of problems, the **dependent variables y_i** are discrete and take values *m=0, …, M-1*, so the index *m* also labels the *M* categories

The goal is to **classify the *n* input samples**, each composed by ***p*** **features,** intro the ***M*** **possible categories** of the problem

A simple classifier is the **perceptron:** a **linear classifier** that categorises examples from a linear combination of the features

$$\sigma(s_i) = \text{sign}(s_i) = \text{sign}\left(\boldsymbol{x}_i^T \boldsymbol{\theta} + b_0\right)$$

p features of the samples

model parameters

a perceptron is a **hard classifier** where each sample is assigned to a category with 100% probability

more complex models can be used as classifiers!

Linear classifiers

In this class of problems, the **dependent variables y_i** are discrete and take values *m=0, …, M-1*, so the index *m* also labels the *M* categories

The goal is to **classify the *n* input samples**, each composed by ***p*** **features,** intro the ***M*** **possible categories** of the problem

A simple classifier is the **perceptron:** a **linear classifier** that categorises examples from a linear combination of the features

$$\sigma(s_i) = \text{sign}(s_i) = \text{sign}\left(\boldsymbol{x}_i^T \boldsymbol{\theta} + b_0\right)$$

p features of the samples

model parameters

a perceptron is a **hard classifier** where each sample is assigned to a category with 100% probability

more complex models can be used as classifiers, including NNs

simple linear models are great to gain physical intuition about how ML algorithms work

Linear classifiers

the perceptron (linear classifier) only has **two possible outcomes**

$$\boldsymbol{x}_i \rightarrow g\left(\boldsymbol{x}_i, \boldsymbol{\theta}\right) \begin{cases} g = 1 \text{ if } \boldsymbol{x}_i \in \mathscr{C}_1 \text{ , } \left(\boldsymbol{x}_i^T \boldsymbol{\theta} + b_0\right) \geq 0 \\ g = -1 \text{ if } \boldsymbol{x}_i \in \mathscr{C}_1 \text{ , } \left(\boldsymbol{x}_i^T \boldsymbol{\theta} + b_0\right) < 0 \end{cases}$$

the **decision boundary** of the classifier is then defined by the condition

$$\left(\boldsymbol{x}_i^T \boldsymbol{\theta} + b_0\right) = 0$$

the properties of the decision boundary of this problem can be easily evaluated

For two points that belong to this boundary one has

$$\begin{cases} \left(\boldsymbol{x}_1^T \boldsymbol{\theta} + b_0\right) = 0 \\ \left(\boldsymbol{x}_2^T \boldsymbol{\theta} + b_0\right) = 0 \end{cases} \rightarrow \left(\boldsymbol{x}_1^T - \boldsymbol{x}_2^T\right) \boldsymbol{\theta}$$

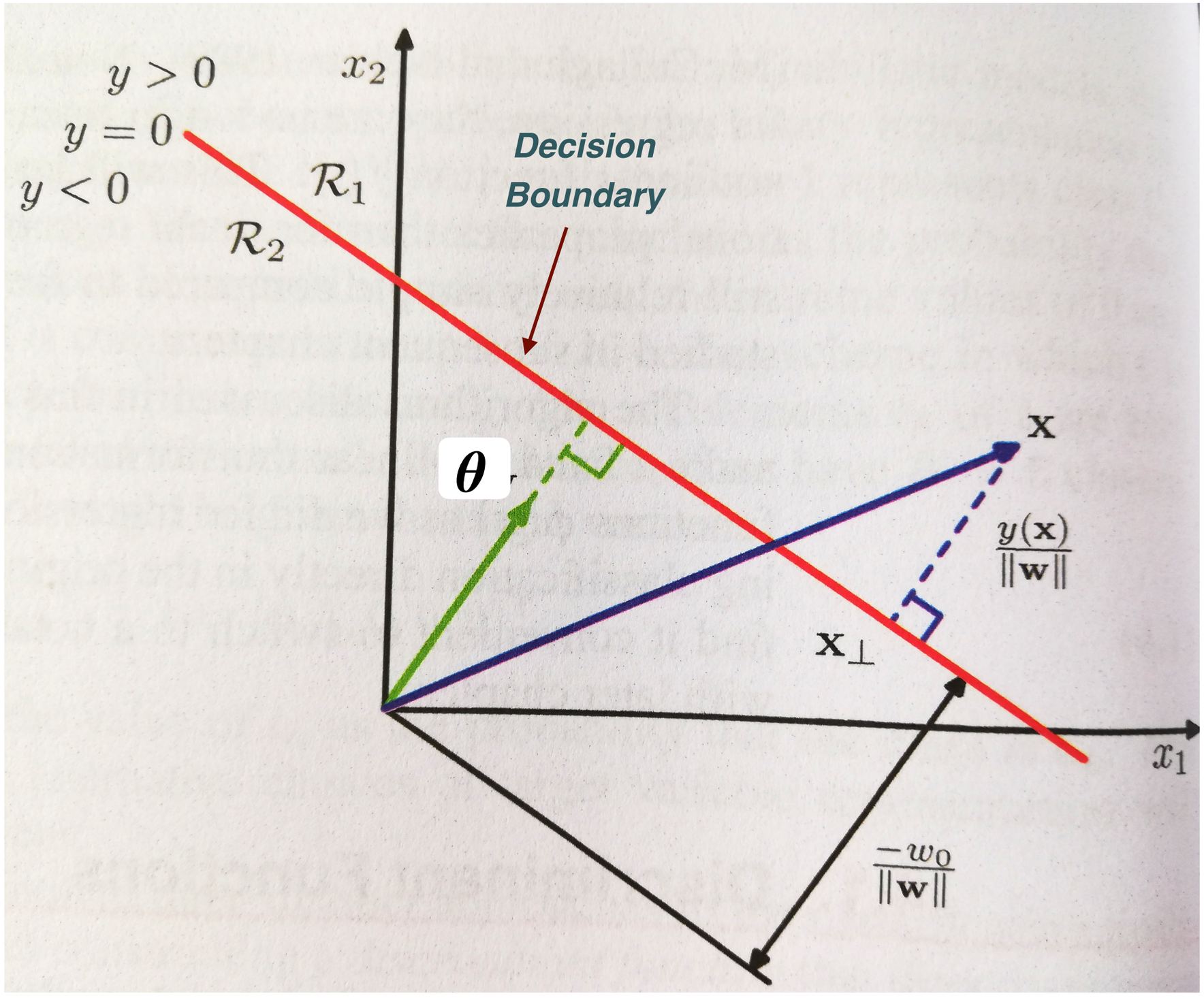
the model parameter vector is perpendicular to the decision boundary!

several other geometric properties can be evaluated

recall that both x and θ live in the p-dimensional feature space

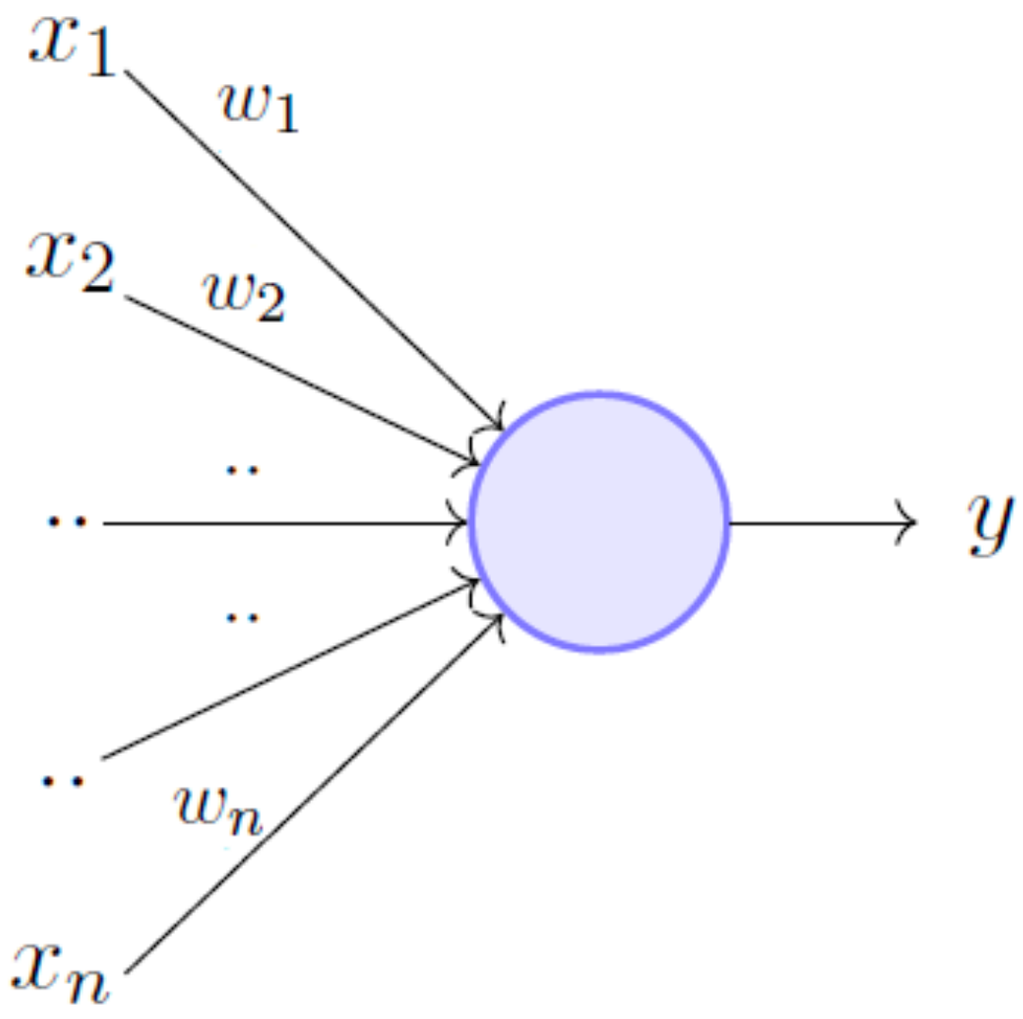
Linear classifiers

example of linear classification for 2d datasets



Perceptrons

You can think of a perceptron as a very simple, linear neural network

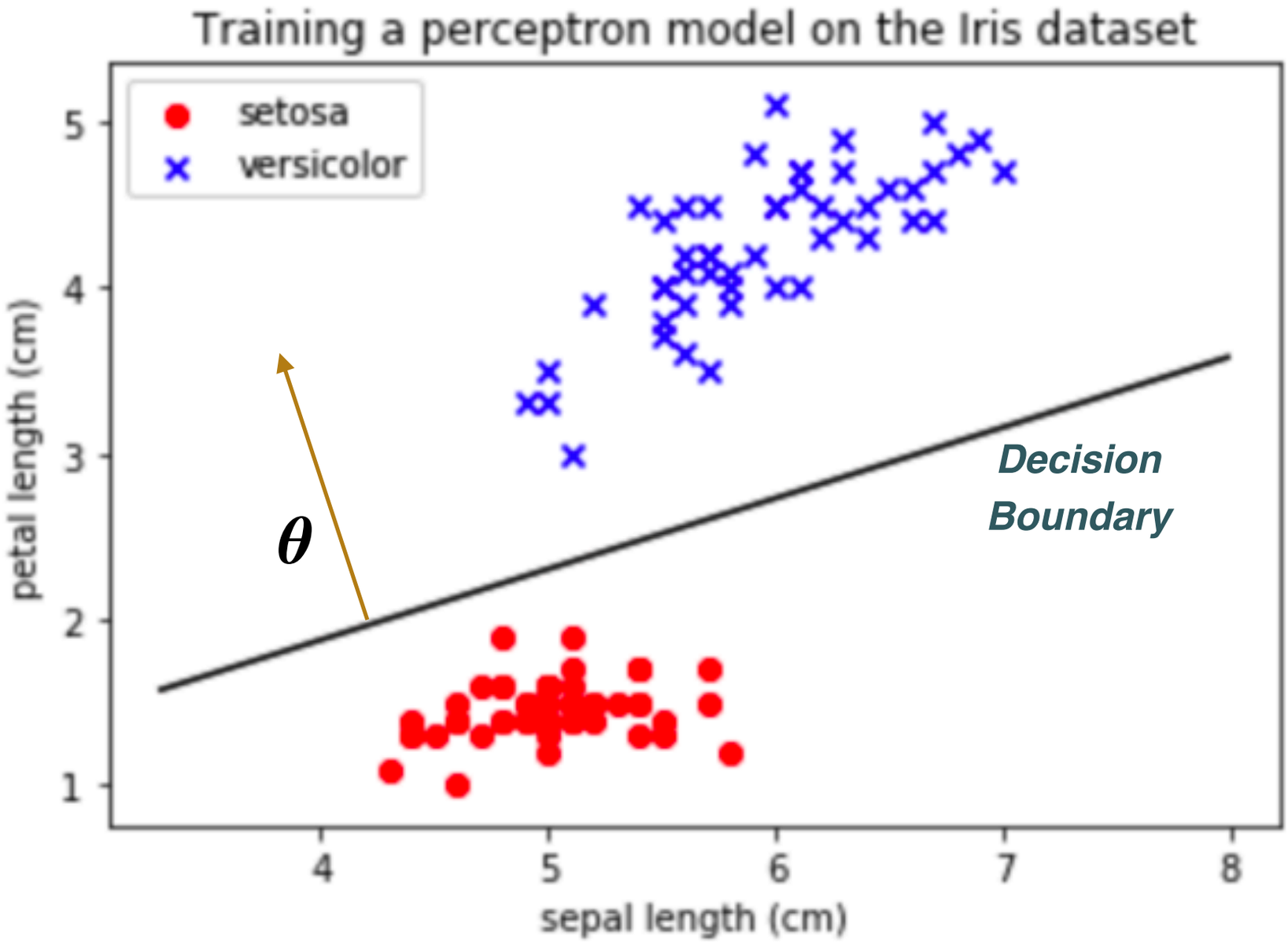


$$y = 1 \text{ if } \left(\boldsymbol{x}_i^T \boldsymbol{\omega} + b_0\right) \geq 0$$

$$y = -1 \text{ if } \left(\boldsymbol{x}_i^T \boldsymbol{\omega} + b_0\right) < 0$$

Perceptrons

You can think of a perceptron as a very simple, linear neural network



Looking at this example, which feature is typical for the decision boundary of a perceptron?
And for which problems do you expect the perceptron to fail?

Training the model

as in the case of regression problems, also for classifications we need to introduce a **figure of merit** (error function) to be optimised

the simplest option is based again on **least squares.** Let's consider a binary linear classifier

the sign function is added back after the training

$$g\left(\boldsymbol{x}_i\right) = \left(\boldsymbol{x}_i^T\boldsymbol{\theta} + b_0\right)$$

recall that x_i and θ have p features each

and one is given a **training dataset** with *N* instances

$$\left\{\boldsymbol{x}_i^T, t_i\right\}, \quad i = 1,\ldots,N, \quad t_i \in (-1,1)$$

in this case the error function depending on the **model parameters** is

$$E_{\text{tr}}(\boldsymbol{\theta}, b_0) = \frac{1}{N}\sum_{i=1}^{N}\left(\left(\boldsymbol{x}_i^T\boldsymbol{\theta} + b_0\right) - t_i\right)^2$$

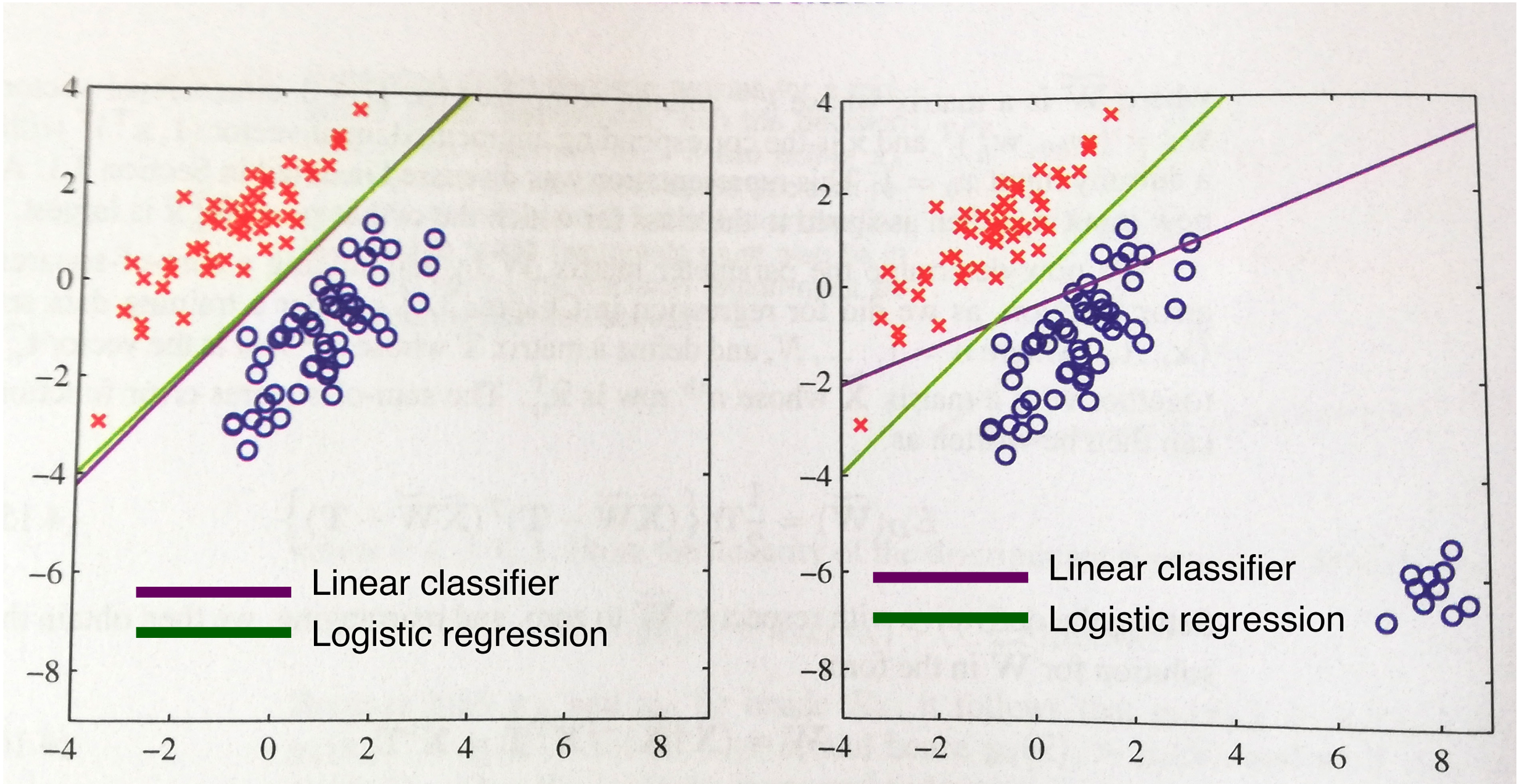
Which is amenable to analytic optimisation, for example

linear system of equations for the model params

$$\frac{\partial}{\partial b_0}E_{\text{tr}} = \frac{1}{N}\sum_{i=1}^{N}\left(\left(\boldsymbol{x}_i^T\boldsymbol{\theta} + b_0\right) - t_i\right) = 0 \rightarrow b_0 = \frac{1}{N}\sum_{i=1}^{N}\left(t_i - \boldsymbol{x}_i^T\boldsymbol{\theta}\right) = 0$$

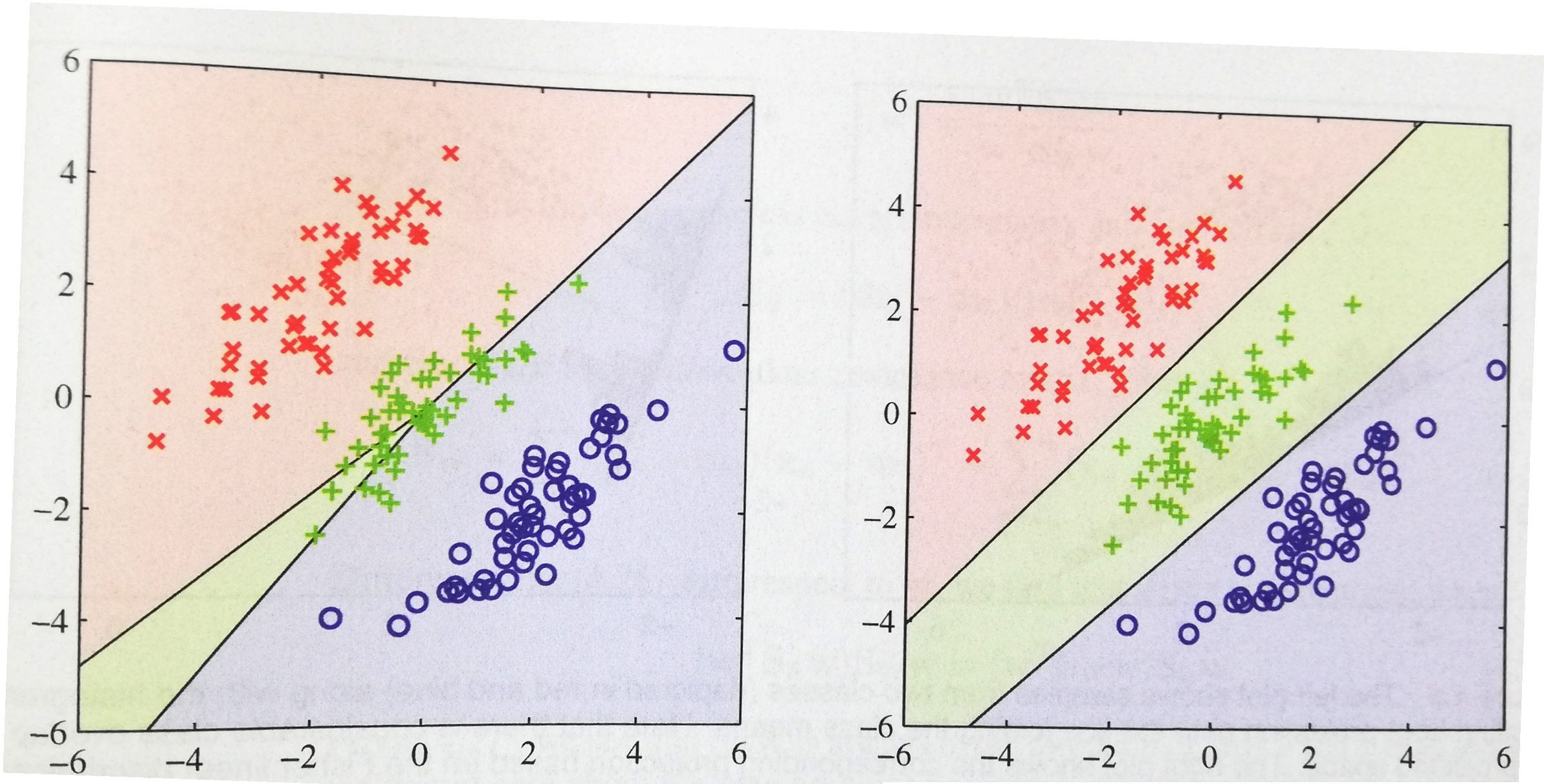
Limitations of the linear classifier

☑ As in regression problems, a linear classifier trained with least squares lacks **robustness with respect to the presence of outliers**



Limitations of the linear classifier

☑ Also the categorisation for multiclass problems can be problematic even when the **decision boundaries** should be easy to find



Linear classifier

Logistic regression

Logistic Regression

Logistic regression

in many cases a **soft classifier,** that **outputs the probability** of a given category, is advantageous over a **hard classifier**. Also, non-linear models exhibit many positive features for classification problems

In **logistic regression** the probability that a data point $\boldsymbol{x}_i$ belongs to a category y_i is given by

$$P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \frac{1}{1 + e^{-\boldsymbol{x}_i^T \boldsymbol{\theta}}} = \sigma(\boldsymbol{x}_i^T \boldsymbol{\theta})$$

non-linear sigmoid function

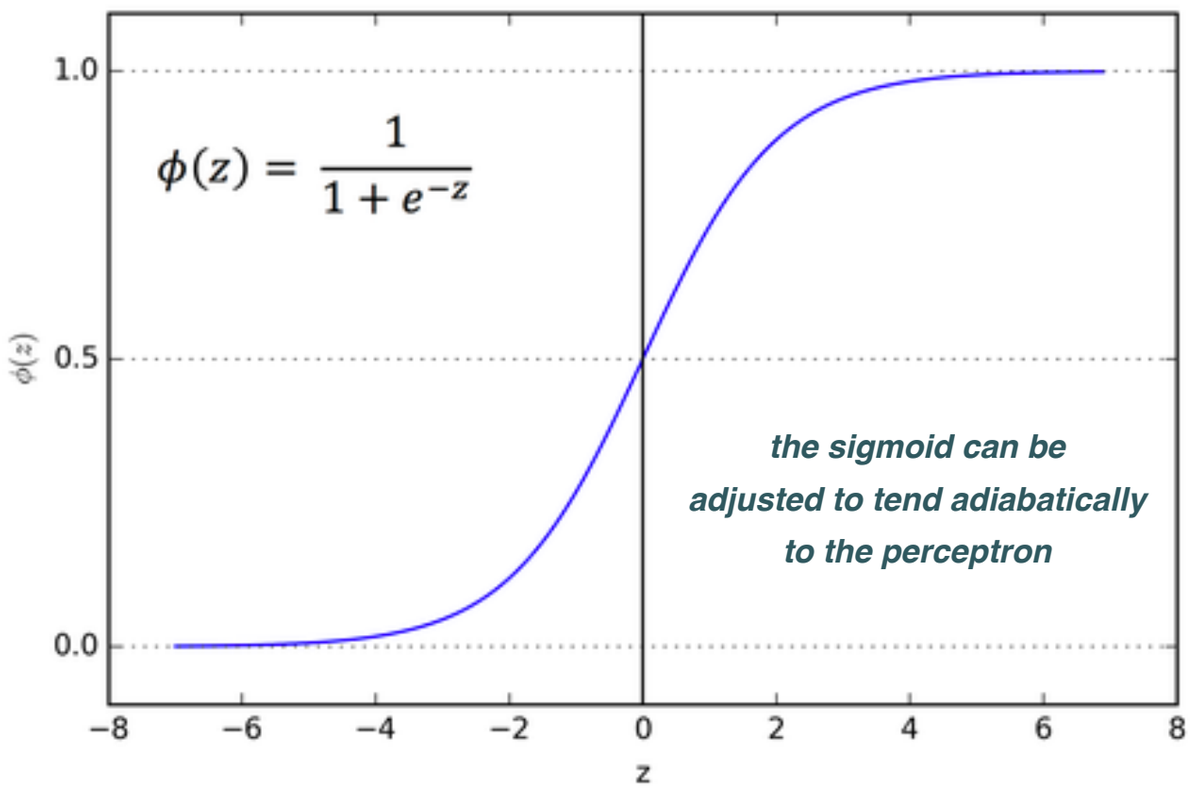
$$P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - \sigma(\boldsymbol{x}_i^T \boldsymbol{\theta}) = \sigma(-\boldsymbol{x}_i^T \boldsymbol{\theta})$$

where we have used the logistic (or sigmoid) function:

$$\sigma(s) = \frac{1}{1 + e^{-s}}$$

$$\sigma(-s) = 1 - \sigma(s)$$

Q: could one use other models for this probability?



Logistic regression

cost function for logistic regression from **Maximum Likelihood Estimation** (MLE):
choose parameters that maximise the probability of seeing the observed data

$$P(y_i \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \Big(P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{y_i} \times \Big(P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{1-y_i}$$

``probability generalisation': recovers limits when y_i=0, y_i=1

$$P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \Big(P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{1} \times \Big(P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{0} = P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})$$

$$P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \Big(P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{0} \times \Big(P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{1} = P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})$$

Logistic regression

cost function for logistic regression from **Maximum Likelihood Estimation** (MLE):
choose parameters that maximise the probability of seeing the observed data

$$P(y_i \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \Big(P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{y_i} \times \Big(P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta})\Big)^{1-y_i}$$

now use that we are modelling the probability with a sigmoid function:

$$P(y_i \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \Big(\sigma(\boldsymbol{x}_i^T \boldsymbol{\theta})\Big)^{y_i} \times \Big(1 - \sigma(\boldsymbol{x}_i^T \boldsymbol{\theta})\Big)^{1-y_i}$$

assuming that all observations are Bernoulli **independent**, the total likelihood is

$$\mathscr{L}(\boldsymbol{\theta} \,|\, \mathscr{D}) = \prod_{i=1}^{n} P(y_i \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \prod_{i=1}^{n} \Big(\sigma(\boldsymbol{x}_i^T \boldsymbol{\theta})\Big)^{y_i} \times \Big(1 - \sigma(\boldsymbol{x}_i^T \boldsymbol{\theta})\Big)^{1-y_i}$$

probability distribution of the model parameters θ given the observed data D

note that this is soft classification: the probability is not only 0 or 1 but any value in between is possible

Logistic regression

probability distribution of the model parameters θ given the observed data D

$$\mathscr{L}(\boldsymbol{\theta}\,|\,\mathscr{D}) = \prod_{i=1}^{n} P(y_i\,|\,\boldsymbol{x}_i,\boldsymbol{\theta}) = \prod_{i=1}^{n} \left(\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}\right)^{y_i} \times \left(1-\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}\right)^{1-y_i}$$

Since the cost function is the **negative log-likelihood**, we find that for logistic regression

$$E(\boldsymbol{\theta}) = -\log\mathscr{L} = \sum_{i=1}^{n} -\left(y_i \log\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}) + (1-y_i)\log(1-\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}))\right)$$

which is known as the cross-entropy function

The parameters of the model are determined by minimising the cross-entropy

$$\hat{\theta} = \arg\,\min_{\theta}\left\{ \sum_{i=1}^{n} \left(-y_i \log\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}) - (1-y_i)\log(1-\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}))\right) \right\}$$

note that no analytic solution is possible, and numerical methods are required, e.g. Gradient Descent

Q: how do you think that one can use Neural Networks in this context?

Logistic regression

probability distribution of the model parameters θ given the observed data D

$$\mathscr{L}(\boldsymbol{\theta}\,|\,\mathscr{D}) = \prod_{i=1}^{n} P(y_i\,|\,\boldsymbol{x}_i,\boldsymbol{\theta}) = \prod_{i=1}^{n} \left(\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}\right)^{y_i} \times \left(1-\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}\right)^{1-y_i}$$

Since the cost function is the **negative log-likelihood**, we find that for logistic regression

$$E(\boldsymbol{\theta}) = -\log\mathscr{L} = \sum_{i=1}^{n} -\left(y_i \log\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}) + (1-y_i)\log(1-\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}))\right)$$

which is known as the cross-entropy function

The parameters of the model are determined by minimising the cross-entropy

$$\hat{\theta} = \arg\,\min_{\theta}\left\{ \sum_{i=1}^{n} \left(-y_i \log\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}) - (1-y_i)\log(1-\sigma(\boldsymbol{x}_i^T\boldsymbol{\theta}))\right) \right\}$$

note that no analytic solution is possible, and numerical methods are required, e.g. Gradient Descent

A: by replacing the sigmoid by a deep learning model

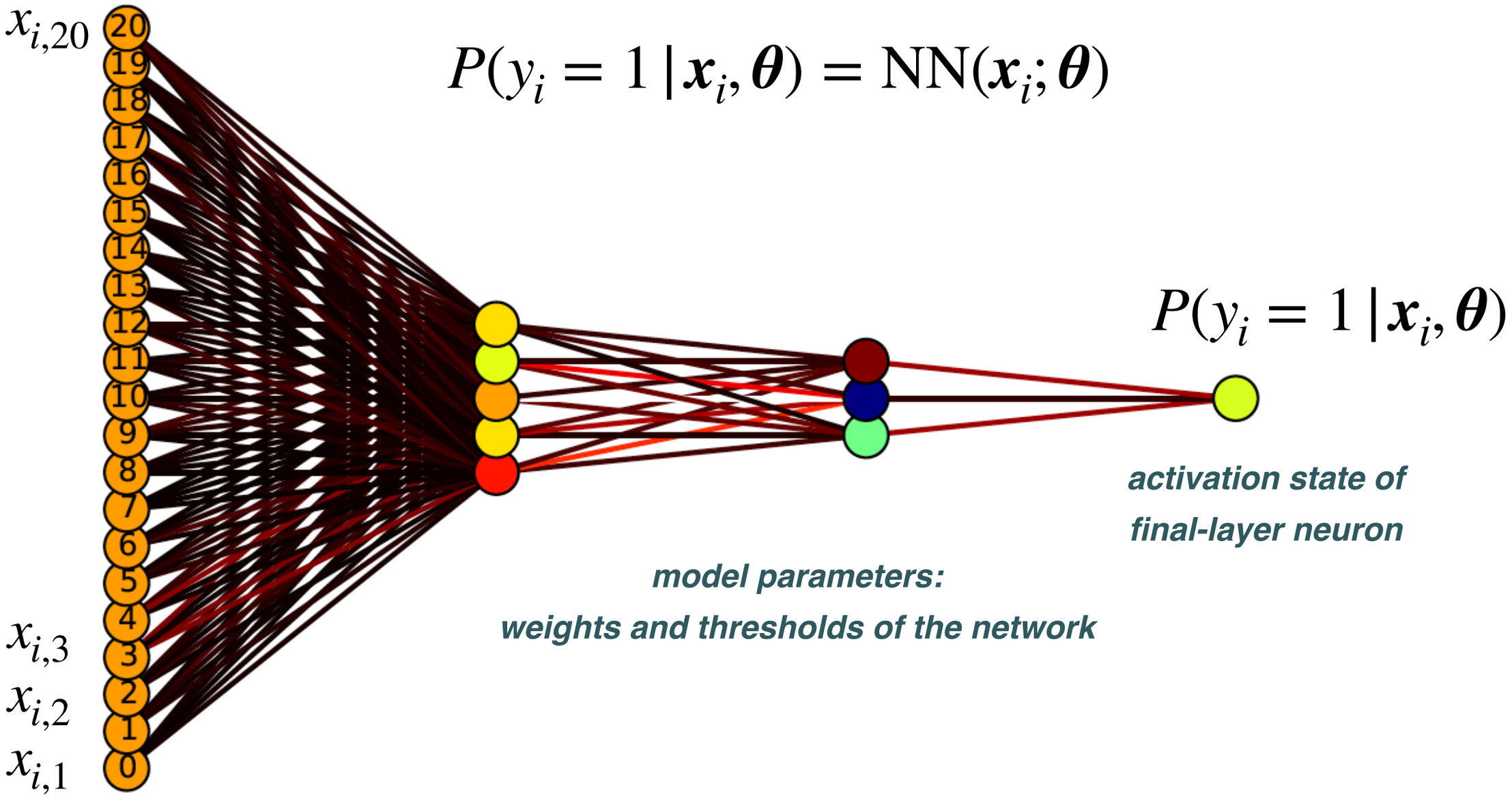
Neural Networks for Classification

instead of modelling the classification probability by a **simple logistic function**

$$P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \frac{1}{1 + e^{-\boldsymbol{x}_i^T \boldsymbol{\theta}}}$$

one can adopt more complex models, such as deep neural networks

$$P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta})$$



Decision Theory

Hence assume that we have constructed a model for the **classification probability** in some classification problem,

$$P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta})$$

$$P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta})$$

and that using the input labelled data we have **determined the model parameters** from minimising the cross-entropy cost function using e.g. backpropagation

$$\hat{\theta} = \arg\,\min_{\theta}\left\{ \sum_{i=1}^{n} \left(-y_i \log \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta}) - (1 - y_i) \log(1 - \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta})) \right) \right\}$$

are we done?

Q: think of a typical classification problem, what extra piece of information is missing?

Decision Theory

Hence assume that we have constructed a model for the **classification probability** in some classification problem,

$$P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta})$$

$$P(y_i = 0 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - P(y_i = 1 \,|\, \boldsymbol{x}_i, \boldsymbol{\theta}) = 1 - \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta})$$

and that using the input labelled data we have **determined the model parameters** from minimising the cross-entropy cost function using e.g. backpropagation

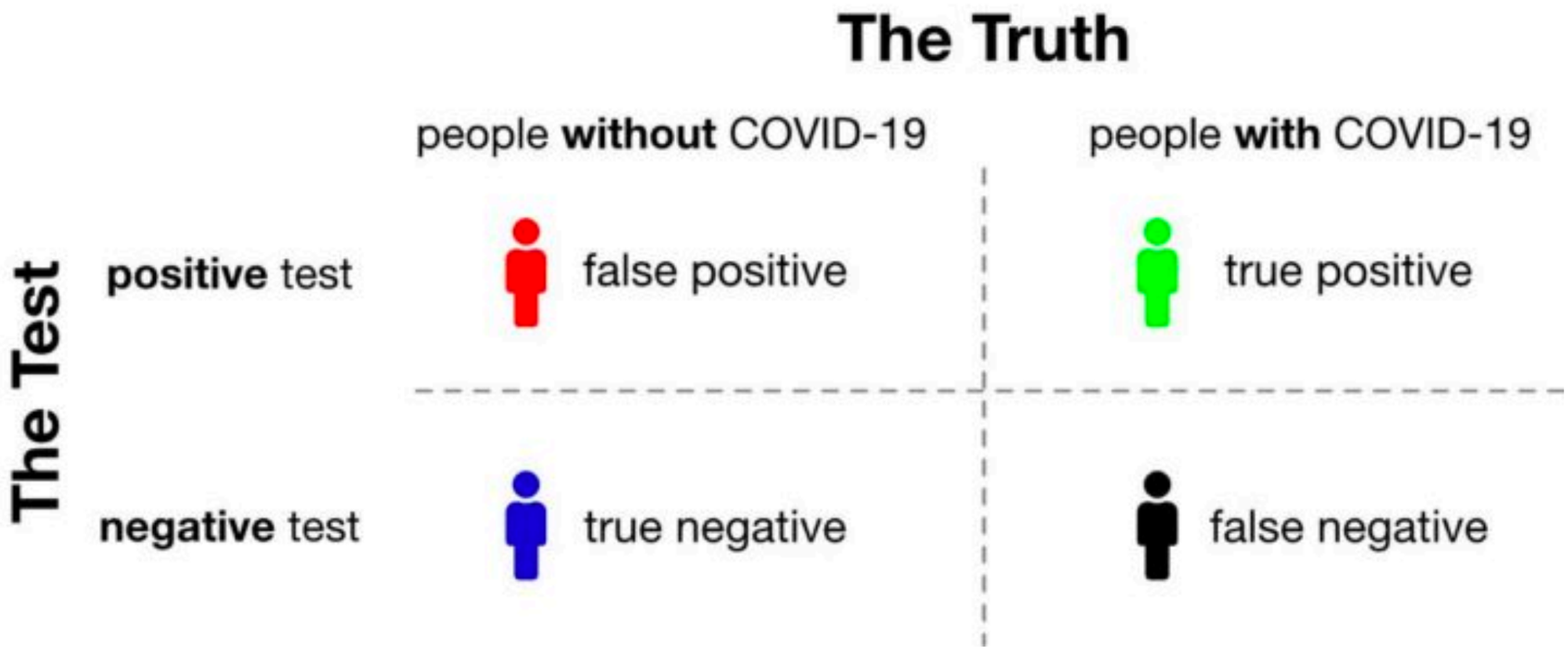
$$\hat{\theta} = \arg\,\min_{\theta}\left\{ \sum_{i=1}^{n} \left(-y_i \log \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta}) - (1 - y_i) \log(1 - \mathrm{NN}(\boldsymbol{x}_i; \boldsymbol{\theta})) \right) \right\}$$

are we done?

Q: think of a typical classification problem, what extra piece of information is missing?

A: we have a classification probability, but unclear how to use it!

Decision Theory

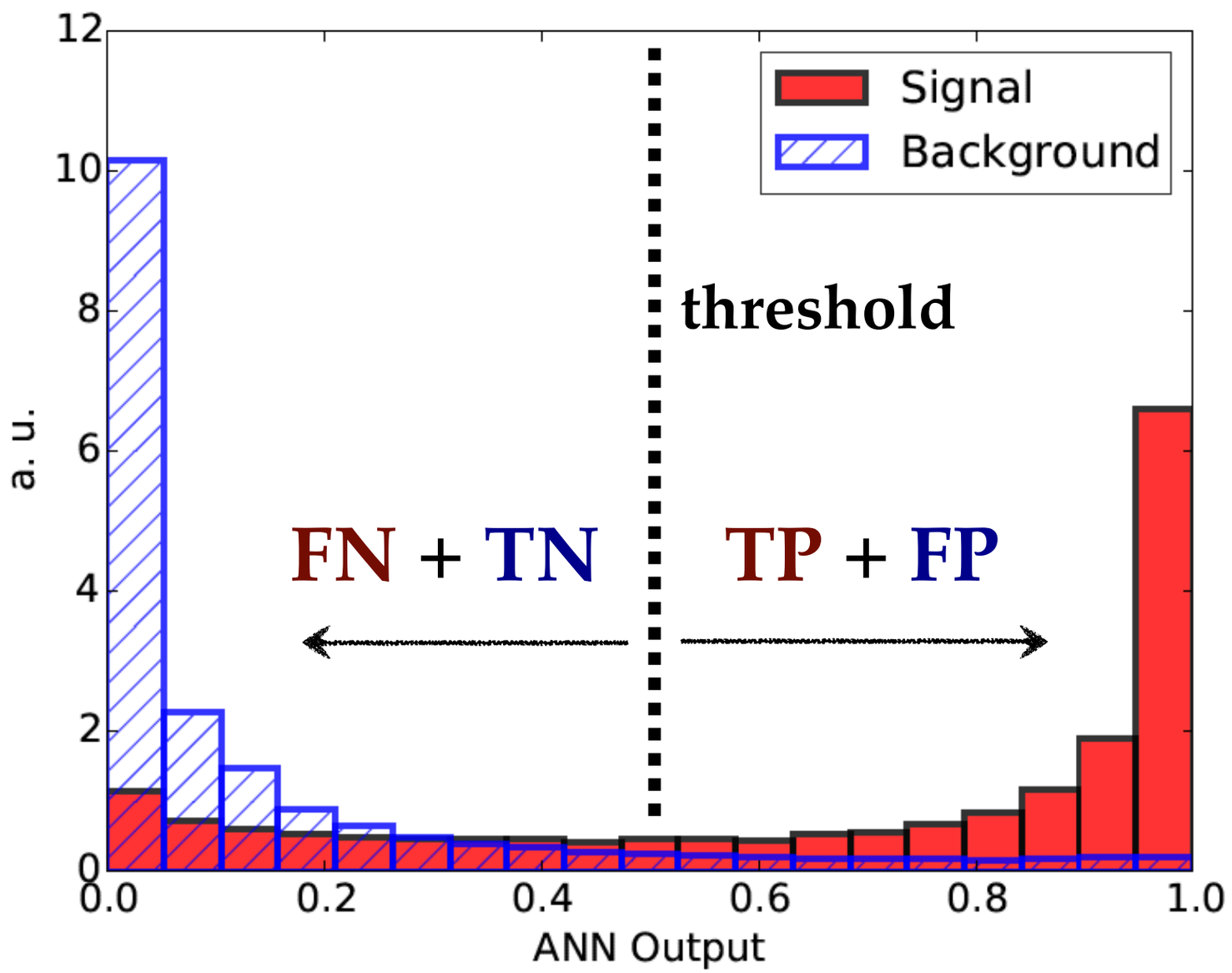


in many cases even a small probability of false positives can be very harmful, e.g. in breast cancer screenings

Decision Theory

In most ML classification problems there is a **threshold** that can be varied to decide at what output of the model a given data point is assigned to each category:

- ☑ conservative threshold: **maximise True Positives**, but also **False Positives** might be large
- ☑ aggressive threshold **reduces False Positives** but then **False Negatives** might be large.



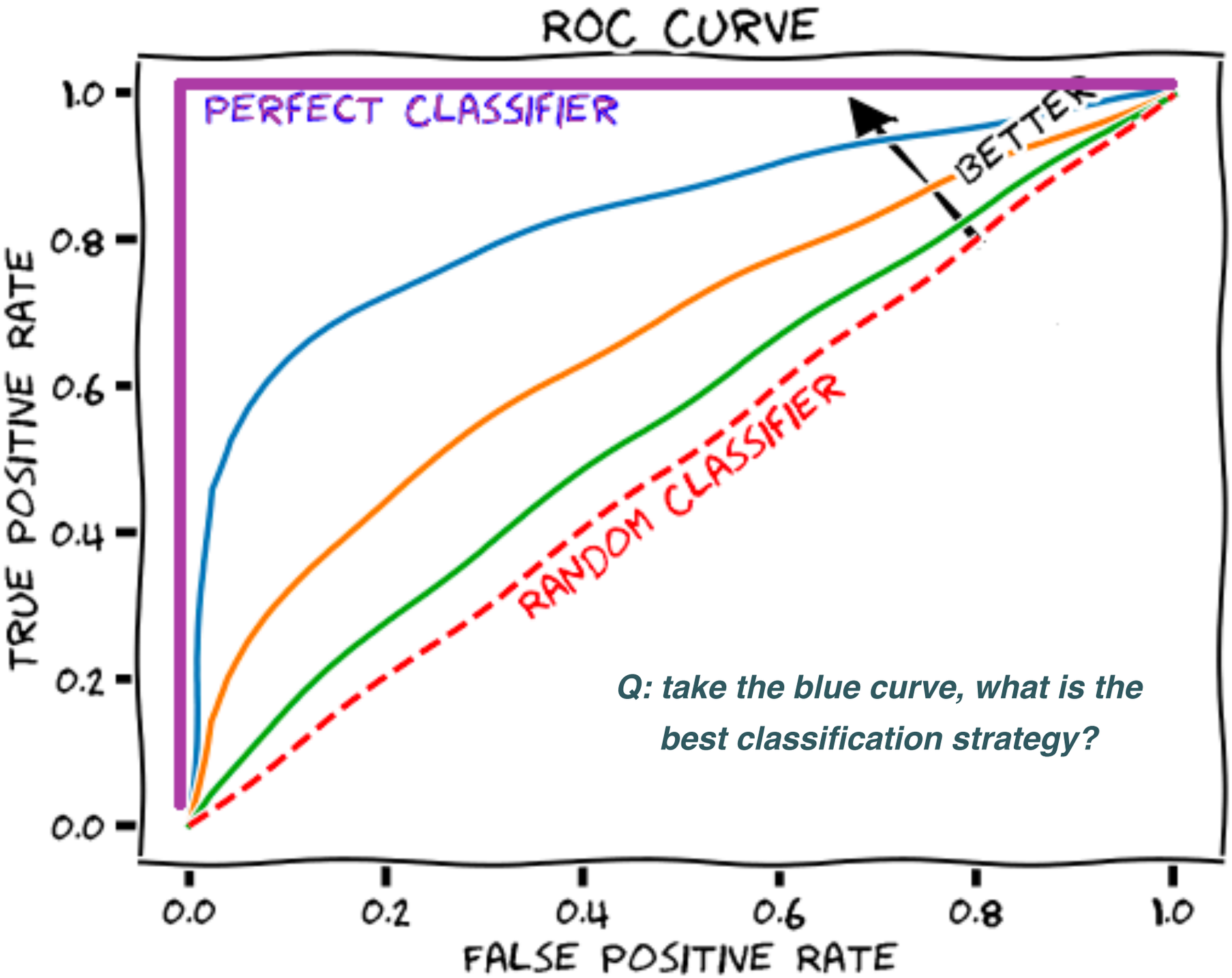
$\mathrm{NN}(\boldsymbol{x}_i \in \mathscr{C}_1; \boldsymbol{\theta})$

$\mathrm{NN}(\boldsymbol{x}_i \in \mathscr{C}_2; \boldsymbol{\theta})$

histogram composed by feeding to the NN all training examples belonging to the two classes

Decision Theory

$P(y_i = 1 \mid \boldsymbol{x}_i \in \mathscr{C}_1, \boldsymbol{\theta})$



$P(y_i = 1 \mid \boldsymbol{x}_i \in \mathscr{C}_2, \boldsymbol{\theta})$

Decision Theory

Decision Theory

we have discussed several ML models that provide a **probability distribution** for a given outcome given some inputs. However, we still need to **take decisions** based on this info

assume that we have the usual **training dataset**, either for regression or classification

$$\left(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\right) \ , \qquad \boldsymbol{t} = \left(t_1, \ldots, t_N\right)$$

depending on our application, we can try to achieve different goals

- Given a new input vector ***x,*** make a prediction for *t*
- Given a new input vector ***x,*** **make a decision** based on the expectations for *t*
- Construct the joint probability distribution *p(**x**,t)* associated to the training dataset: this is known as the **inference problem**

the goal of Decision Theory is to help us making **optimal decisions** given our knowledge of the involved probabilities

Decision Theory

for example, our goal could be to **minimise the misclassification rate**

e.g. in clinical diagnosis that require an invasive treatment

we will have trained our classifier on the input examples, and end up with a map of the input space into **decision regions** (assigned to an specific class) separated by **decision boundaries**

the probability of incurring in a **classification mistake** will be given by

$$p(\text{mistake}) = p(\boldsymbol{x} \in \mathscr{R}_1, \mathscr{C}_2) + p(\boldsymbol{x} \in \mathscr{R}_2, \mathscr{C}_1) = \int_{\mathscr{R}_1} p(\boldsymbol{x}, \mathscr{C}_2) d\boldsymbol{x} + \int_{\mathscr{R}_2} p(\boldsymbol{x}, \mathscr{C}_1) d\boldsymbol{x}$$

probability that an input in decision region R_1 is classified as class C_2

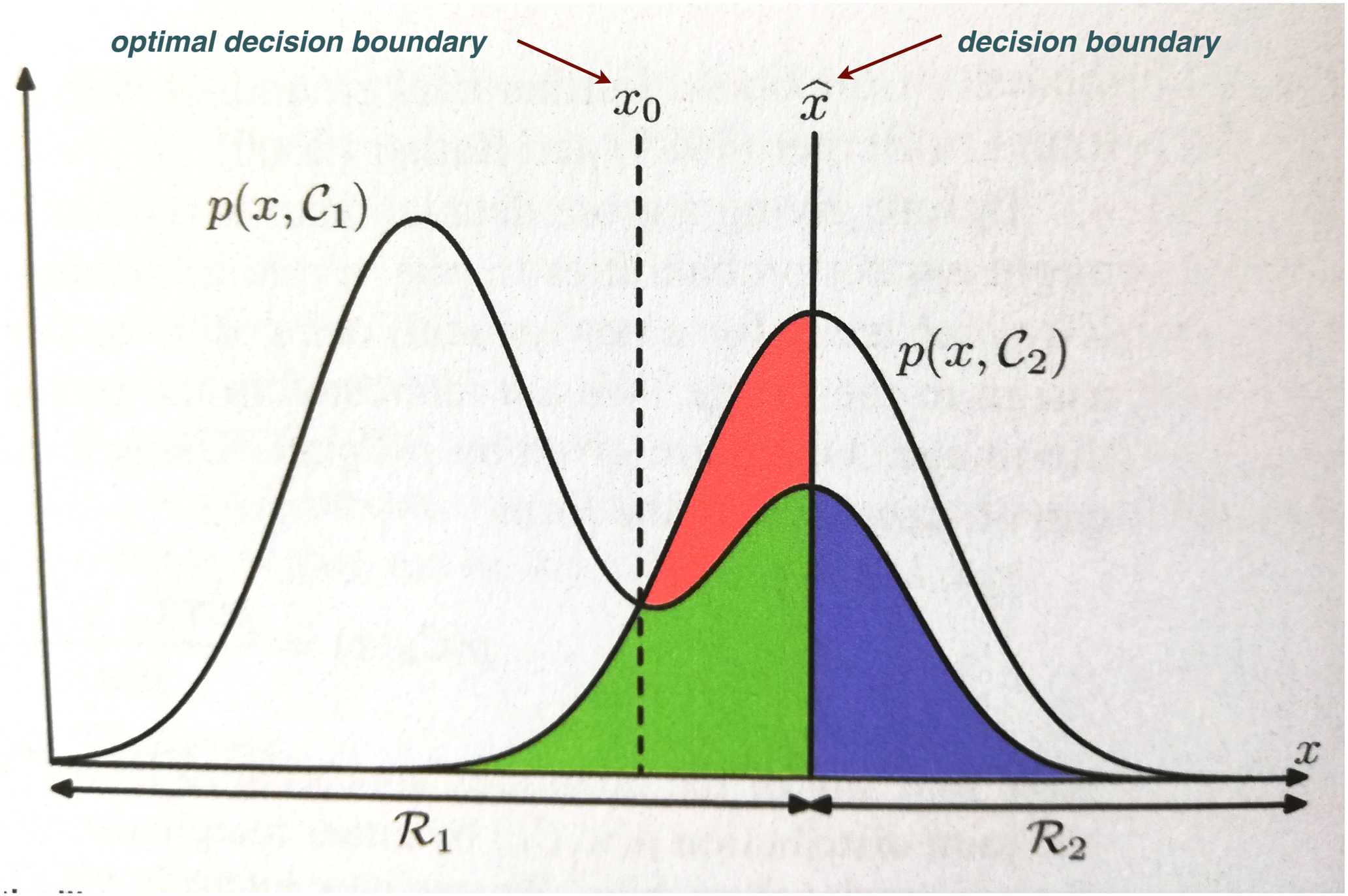
note that we still need to decide the **rule** that assigns a given point ***x*** to each category.

From the product rule of probabilities we have that

$$p(\boldsymbol{x}, \mathscr{C}_k) = p(\mathscr{C}_k | \boldsymbol{x}) p(\boldsymbol{x})$$

The misclassification rate is minimised by the decision boundary defined when each point ***x*** is assigned to the class for which its posterior probability $p(\mathscr{C}_k | \boldsymbol{x})$ is the largest

Decision Theory



red, green, blue regions: **misclassification probability**

green+blue constant as decision boundary varied: optimal choice is that one that minimises red region

Metrics for binary classification

there are many **useful metrics** that are used in ML binary classification problems

example classification problem: 34 training samples, of which

True Positives (TP) e.g. 8	False Positives (FP) e.g. 2
False Negatives (FN) e.g. 4	True Negatives (TN) e.g. 20

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} = \frac{8 + 20}{8 + 20 + 2 + 4} = 0.823$$

however accuracy is not the right metric for classification problems

defined by a large disparity between classes, e.g. when TN >> TP

$$\text{Accuracy} \simeq \frac{\text{TN}}{\text{TN} + \text{FN}} + \ldots$$

Metrics for binary classification

there are other **useful metrics** that are used in ML binary classification problems

example classification problem: 34 training samples, of which

True Positives (TP) e.g. 8	False Positives (FP) e.g. 2
False Negatives (FN) e.g. 4	True Negatives (TN) e.g. 20

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN} = \frac{8 + 20}{8 + 20 + 2 + 4} = 0.823$$

$$\text{Precision} = \frac{TP}{TP + FP} = 0.80$$

proportion of correct positive classifications

$$\text{Recall} = \frac{TP}{TP + FN} = 0.67$$

proportion of correct actual positive classifications

ROC curve

In most ML classification problems there is a **threshold** that can be varied to decide at what output of the model a given data point is assigned to each category:

- ☑ A conservative threshold will **maximise TP**, but also FP might be large
- ☑ An aggressive threshold **reduces FP** but then FN might be large.

effect of threshold is quantified by the **Receiver Operating Characteristic** (ROC) curve

$$\text{Recall} = \text{True Positive Rate} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$ ← *proportion of correctly classified positives*

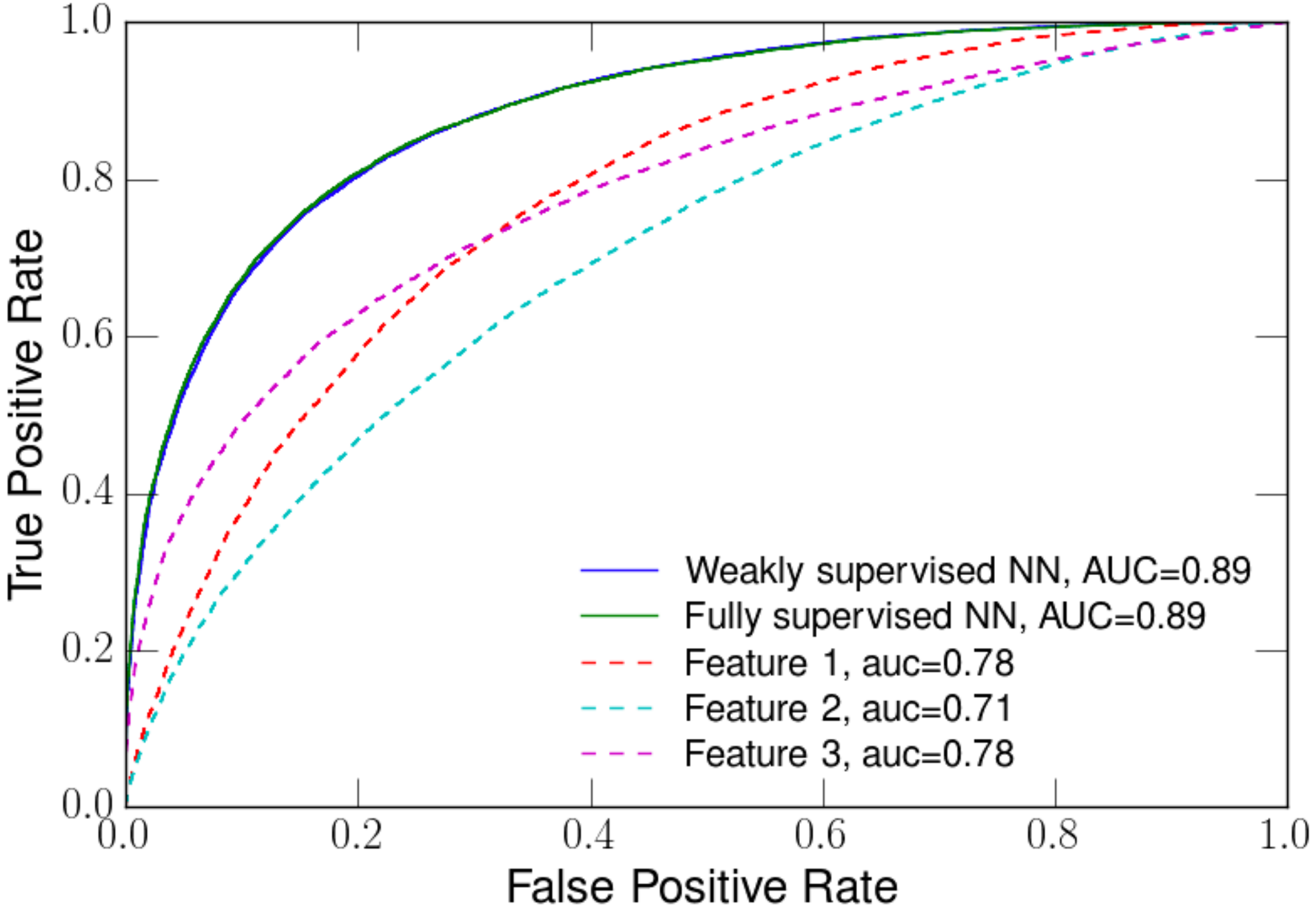
vs

$$\text{False Positive Rate} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$ ← *incorrectly classified negatives*

a good classifier should maximise TPR while minimising FPR

ROC curve

$$\text{Recall} = \text{True Positive Rate} = \frac{\text{TP}}{\text{TP} + \text{FN}} \qquad \text{False Positive Rate} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$



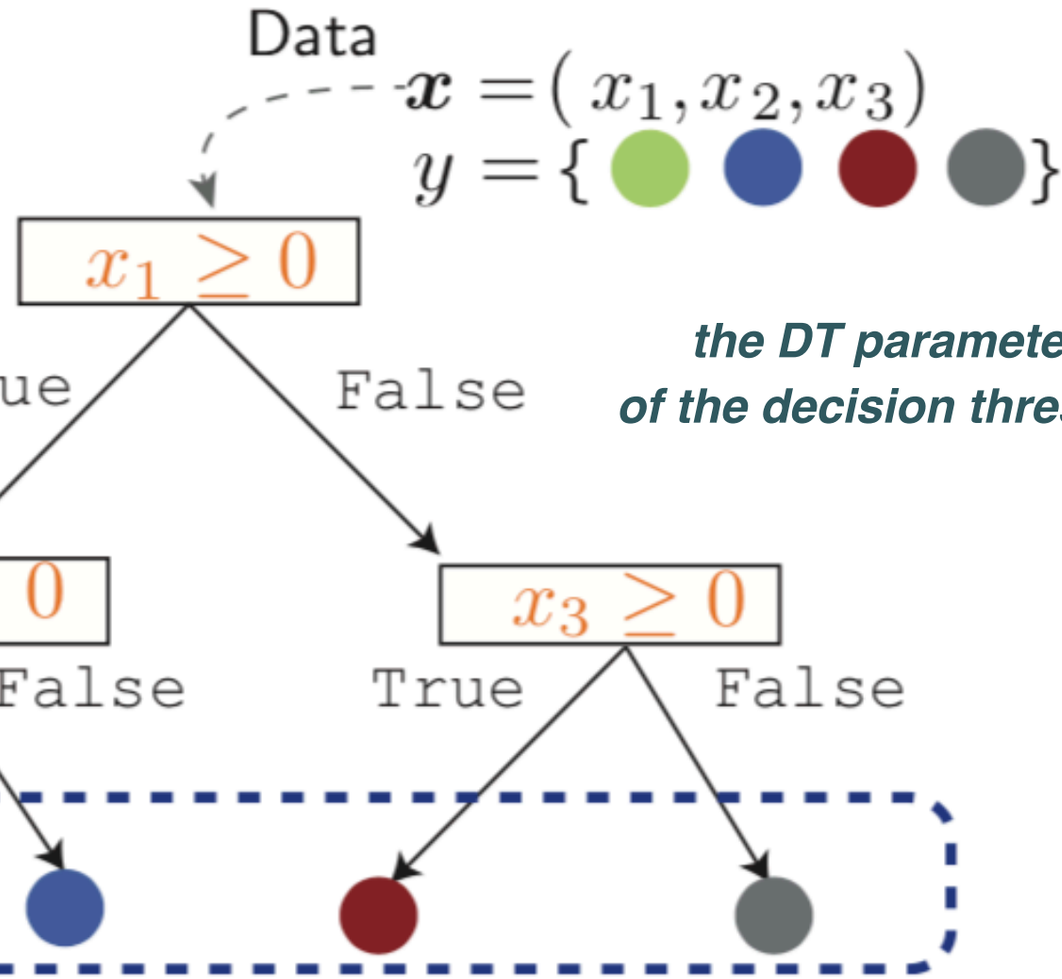
Decision Trees and Random Forests

aka another family of Machine Learning **Classification algorithms**

Decision Trees

Decision Trees are classifiers that work by partitioning the input space into **hypercubes** and then assign a model (e.g. a constant) to each region

classify 3D instances into four possible categories

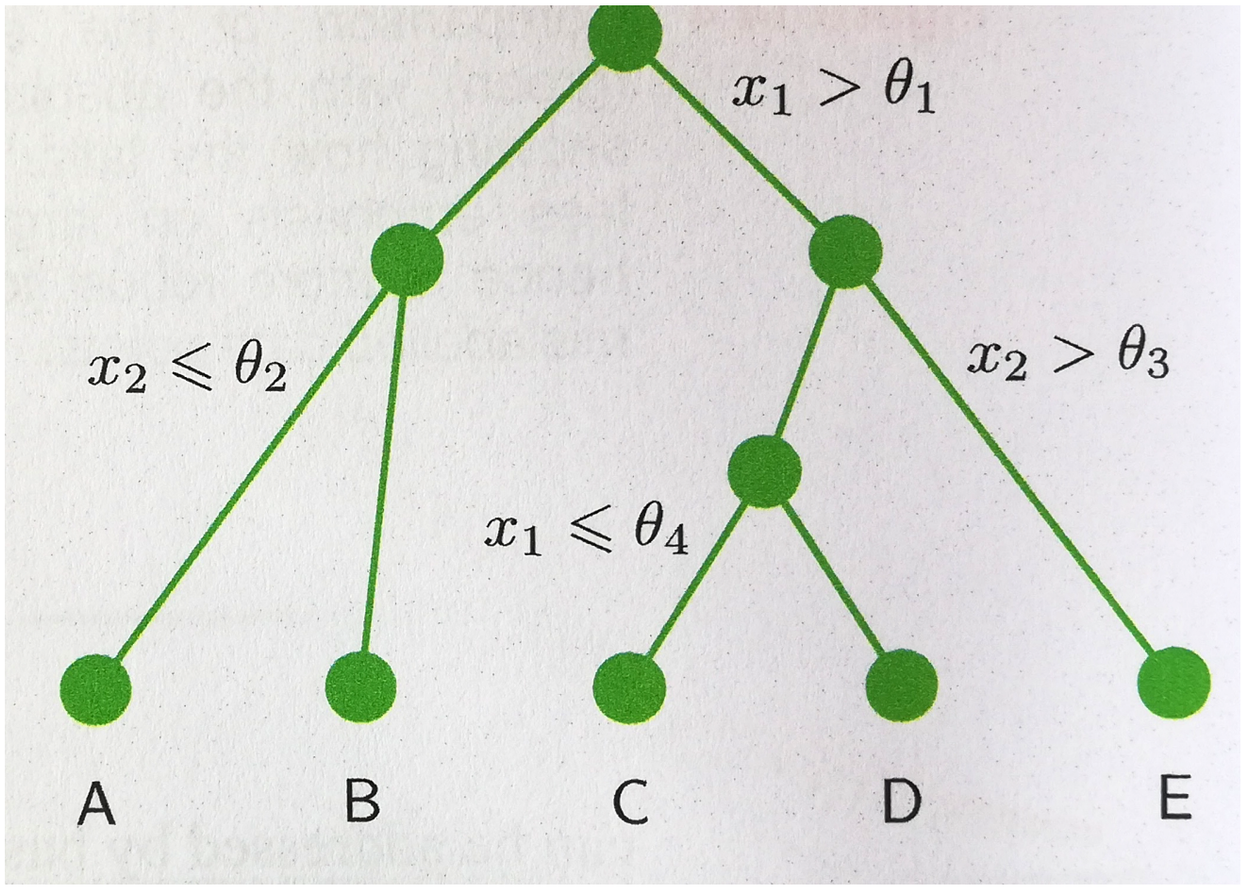


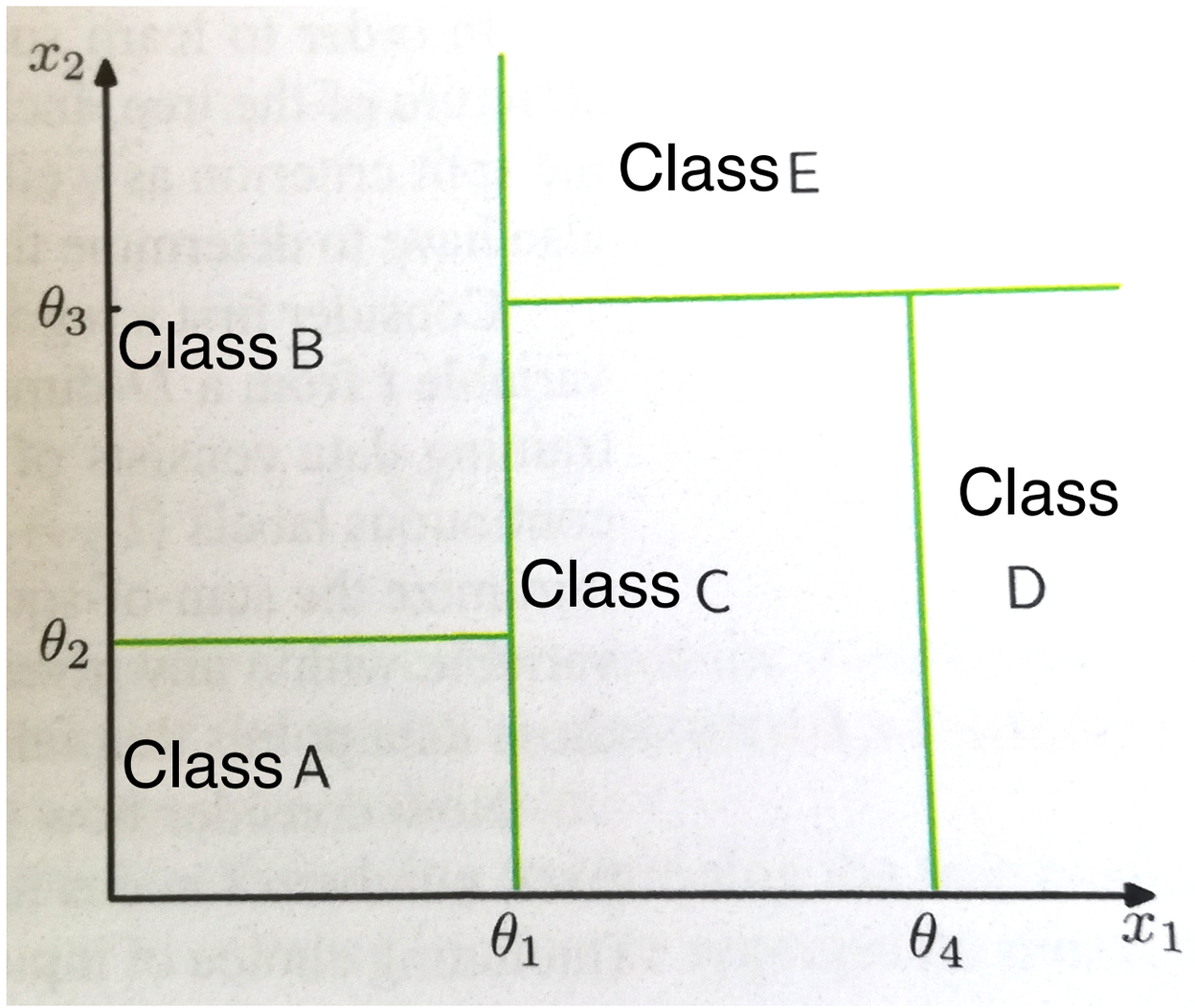
the DT parameters are the values of the decision thresholds at each node

In ML, a **decision tree** is an algorithm which uses a series of questions to hierarchically partition the data, where each branch of the tree splits the data into smaller subsets

Decision Trees

Decision trees have the key property that their output is **human-interpretable:** sequence of binary decisions applied to individual input variables

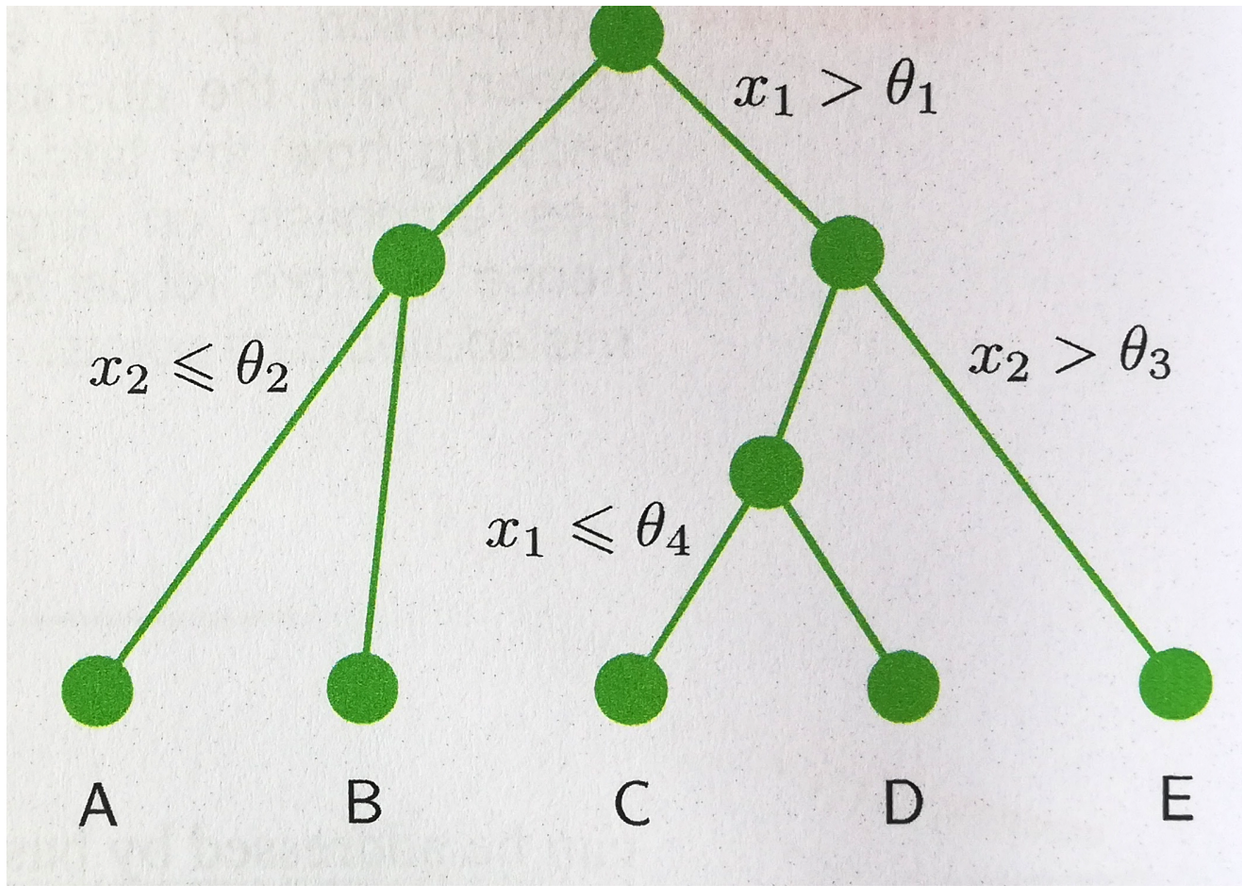




to train a decision tree we need to determine which **variable is chosen at each node** for the split criterion and the value of the **threshold for the split**

Decision Trees

Decision trees have the key property that their output is **human-interpretable:** sequence of binary decisions applied to individual input variables



Q: what are the model parameters of a decision tree?

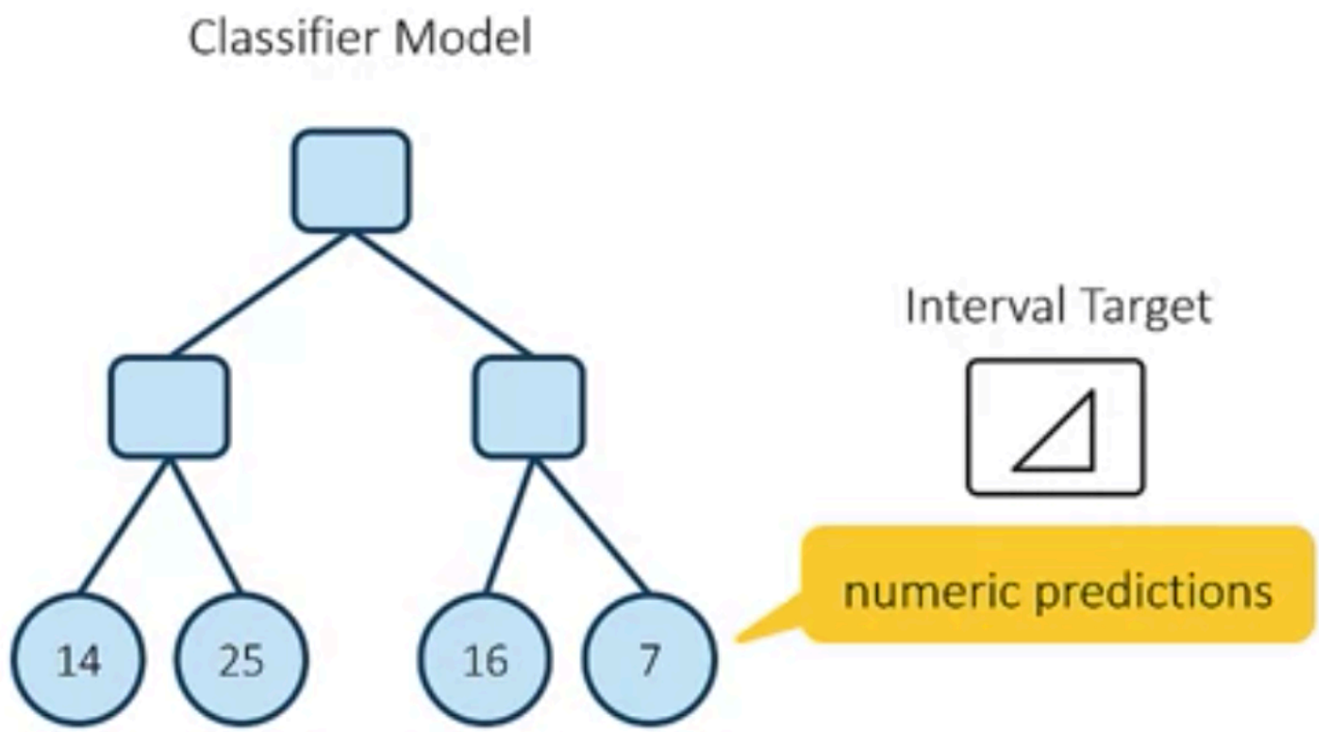
Which parameters we can vary to improve classification?

Decision Trees

Example of decision tree

Decision Trees for Categorical Targets: Classification Trees

Compartir



Random Forests

individual trees have often **high variance** and are weak classifiers:

we can improve by incorporating them in an ensemble method

→ We need an ensemble of **randomised decision trees** (minimised correlations)

- ***(1)*** train each decision tree on a different bootstrapped dataset: **bagged decision tree**
- ***(2)*** use different random subset of features at each split: **random forest**

reduces correlations between trees that arise when only few features are strongly predictive

as other ML learning classifiers also Random Forests require some **regularisation**, for example a maximum depth of the tree, to control complexity and prevent overfitting

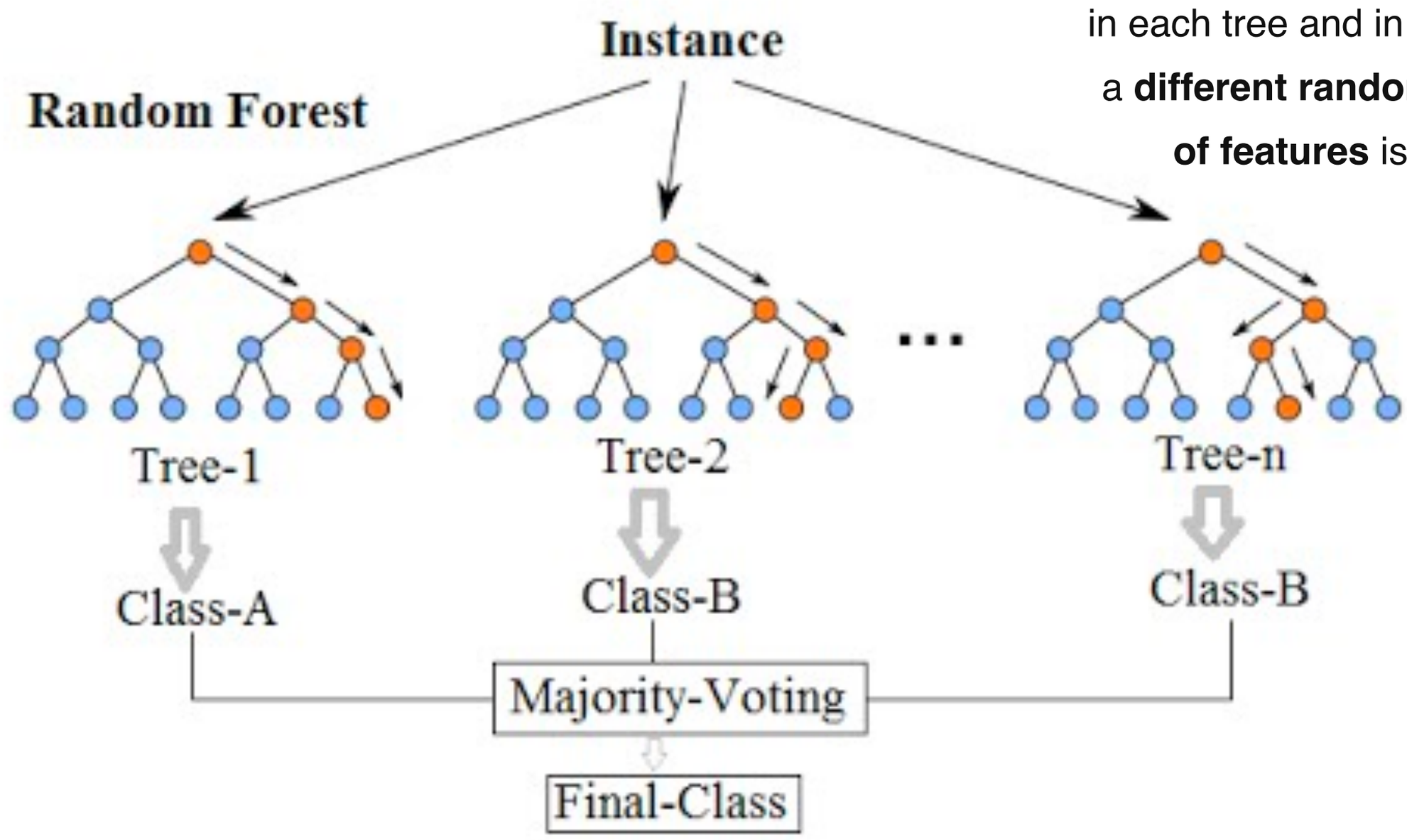
typically, a classification problem with p features, in RFs only $p^{1/2}$ features are used in each split

Random forests have other attractive features, for example, they can be used to **rank the importance of variables** in a regression or classification problem in a natural way

Random Forests

each decision tree in the ensemble is built upon a **random bootstrap sample** of the original data

in each tree and in each split, a **different random subset of features** is used



the final categorisation is assigned *e.g.* from **majority voting**

Support Vector Machines

Support Vector Machines

SVM are **kernel methods** popular for classification, regression, and novelty detection

A peculiar feature of SVM is that the model parameters are found by a solution of a convex optimisation problem: any local solution is also a **global optimum**

The advantages of support vector machines include:

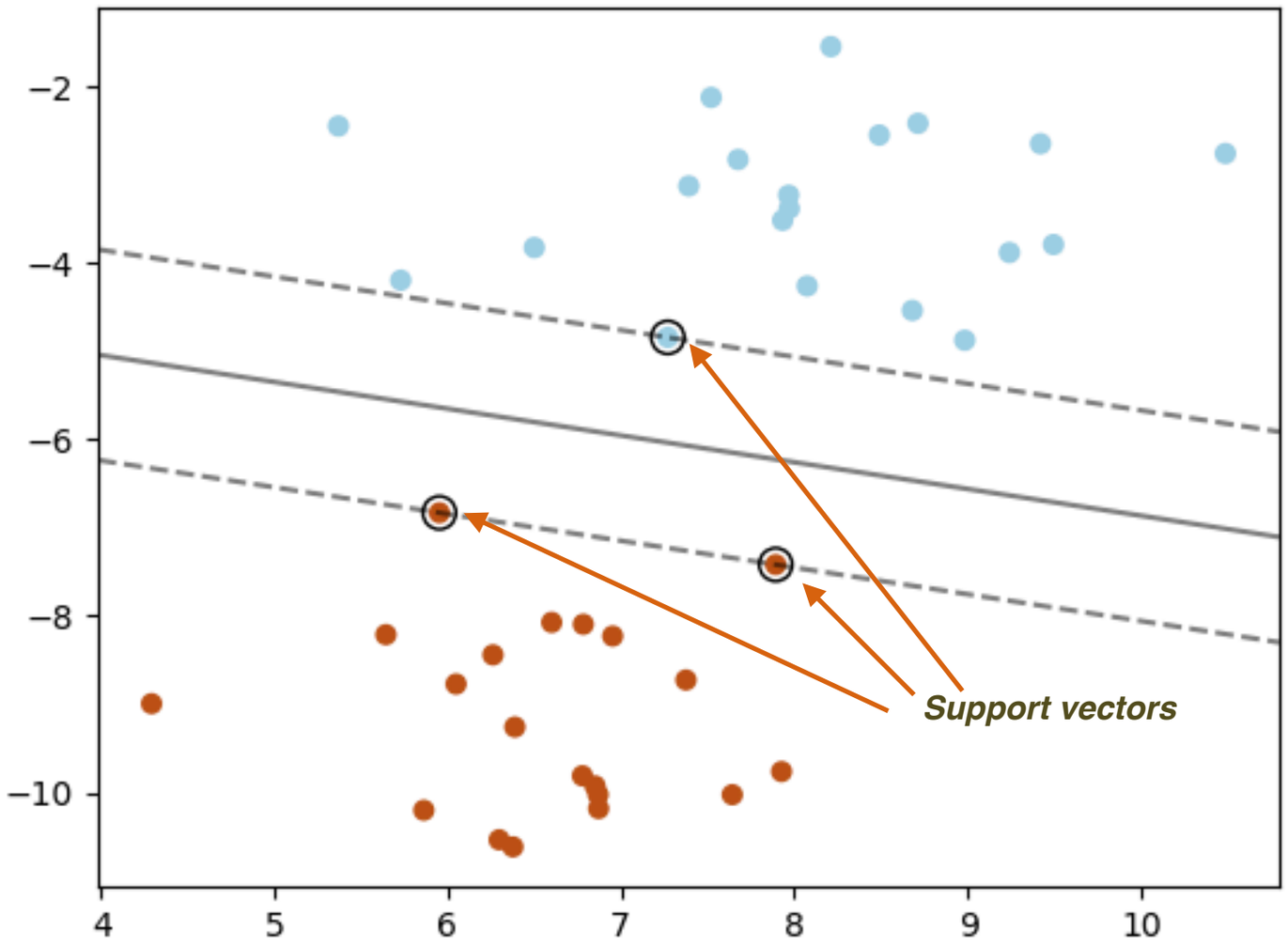
- Effective in **high dimensions.**
- Effective when number of dimensions is greater than number of samples.
- Includes on a **subset of training points** in the decision function (**support vectors**)
- Different **kernels functions** can be used for the figure of merit

kernel methods operate in a high-dimensional,
implicit feature space without computing the coordinates in data space

Support Vector Machines

SVM are ML algorithms popular for classification, regression, and novelty detection

A peculiar feature of SVM is that the model parameters are found by a solution of a convex optimisation problem: any local solution is also a **global optimum**



In SVM classification, the support vectors are samples that lie in the margin boundaries (at least for linearly separable problems)

Support Vector Machines

As other **classification algorithms**, the problem that SVM try to solve is the following. Starting from a training dataset

$$\{\boldsymbol{x}_i^T, t_i\}, \quad i = 1,\ldots,N, \quad t_i \in (-1,1)$$

binary classification

our goal is to find the **model parameters** such that the prediction from

$$\text{sign}(\boldsymbol{\theta}^T \boldsymbol{\phi}(\boldsymbol{x}) + b)$$

linear in model parameters, but non-linear in feature space

is correct for most of the samples. Here $\boldsymbol{\phi}$ is the **feature-space transformation**, where the *feature space* is where our data lives

Example of a feature-space transformation

$\boldsymbol{x}$	$\boldsymbol{\phi}(\boldsymbol{x})$
Height	***Height/Weight***
Weight	***Weight+Height***
Age	***Age * Weight***

Support Vector Machines

the problem then that SVM are aiming to solve is

inverse of margin between the two categories

$$\min_{\theta,b,\xi}\left(\frac{1}{2}\boldsymbol{\theta}^T\boldsymbol{\theta}+C\sum_{i=1}^{n}\xi_i\right)$$

subject to the **additional constraint** that

Class label of sample i → $t_i \times \left(\boldsymbol{\theta}^T\boldsymbol{\phi}(\boldsymbol{x}_i)+b\right) \geq 1-\xi_i$ ← *tolerance (regulator)*

which essentially aims to **maximise the margin between the two categories** while including a penalty when when a sample is misclassified or within the margin boundary, where the team proportional to *C* plays the role of a **regulator**

> SVM are an example of a **constrained optimisation problem,** where one tries to minimise a quadratic function subject to **linear constraints.** They are most efficiently solved by means of the Lagrange multiplier method

Support Vector Machines

In which respect SVD is a **kernel method**? So far it seems to work only in **feature space …**

we can reformulate the problem such that the feature space disappears completely!

many ML models for regression and classification can be reformulated in a **dual representation** where the kernel functions arise naturally

in doing so, we will also show in which respect kernel methods are special in that they **explicitly include the training examples** in the final decision model

Dual representations

many ML models for regression and classification can be reformulated in a **dual representation** where the kernel functions arise naturally

consider a linear regression model with a regularised least-squares error function

$$E_{\mathrm{tr}}(\boldsymbol{\theta}) = \frac{1}{2}\sum_{n=1}^{N}\left(\boldsymbol{\theta}^T\boldsymbol{\phi}(\boldsymbol{x_n}) - t_n\right)^2 + \frac{\lambda}{2}\boldsymbol{\theta}^T\boldsymbol{\theta}$$

regulator

inner product in feature space

sum over training samples

output from training examples

same structure as SVD!

the model parameters are determined **analytically** by requiring the vanishing of the gradient

$$\boldsymbol{\theta} = \sum_{n=1}^{N} a_n\boldsymbol{\phi}(\boldsymbol{x_n}), \quad a_n = -\frac{1}{\lambda}\left(\boldsymbol{\theta}^T\boldsymbol{\phi}(\boldsymbol{x_n}) - t_n\right)$$

recall that inner products take place in feature space

one can formulate a dual representation of the problem in terms of the **parameter vector**

$$\boldsymbol{a} = \left(a_1, a_2, \ldots, a_N\right)^T \qquad \boldsymbol{t} = \left(t_1, t_2, \ldots, t_N\right)^T$$

Dual representations

with some algebra one can show that the original figure of merit of the model

$$E_{\text{tr}}(\boldsymbol{\theta}) = \frac{1}{2}\sum_{n=1}^{N}\left(\boldsymbol{\theta}^T\boldsymbol{\phi}(\boldsymbol{x}_n) - t_n\right)^2 + \frac{\lambda}{2}\boldsymbol{\theta}^T\boldsymbol{\theta}$$

admits a **dual representation** in terms of **kernel function**

model params nor feature space maps do not appear in this formulation

$$E_{\text{tr}}(\boldsymbol{a}) = \frac{1}{2}\boldsymbol{a}^T\boldsymbol{K}\boldsymbol{K}\boldsymbol{a} - \boldsymbol{a}^T\boldsymbol{K}\boldsymbol{t} + \frac{1}{2}\boldsymbol{t}^T\boldsymbol{t} + \frac{\lambda}{2}\boldsymbol{a}^T\boldsymbol{K}\boldsymbol{a}$$

where ***K*** is known as the **Gram matrix**, an *N x N* symmetric matrix with entries

$$K_{nm} = k\left(\boldsymbol{x}_n, \boldsymbol{x}_m\right) = \boldsymbol{\phi}(\boldsymbol{x}_n)^T\boldsymbol{\phi}(\boldsymbol{x}_m)$$

matrix in space of input data

given by the **kernel function** evaluated over two of the **input training examples**

the crucial property of this dual representation is that now the predictions for new inputs will explicitly **depend on the training examples**

SVD can be expressed entirely in terms of kernels

Dual representations

the crucial property of this dual representation is that now the predictions for new inputs will explicitly **depend on the training examples**

$$y(\boldsymbol{x}) = \boldsymbol{k}(\boldsymbol{x})^T \left(\boldsymbol{K} + \lambda \boldsymbol{I}_N\right)^{-1} \boldsymbol{t}$$

output of trained model

new input

depends on the N original inputs

$$\boldsymbol{k}(\boldsymbol{x}) = \left(k(\boldsymbol{x}_1, \boldsymbol{x}), k(\boldsymbol{x}_2, \boldsymbol{x}), \ldots\right)$$

in the dual formulation we invert a *N x N* matrix (data space) rather than a *M x M* one (feature space), so this does not appear to be advantageous …

the main benefit is being able to **work directly with kernel functions** and bypass a choice of feature map

this allows one to work in feature spaces of **very high (even infinite) dimensionality**

Support Vector Machines

https://www.youtube.com/watch?v=5zRmhOUjjGY

The kernel trick

recall that the kernel function is constructed from a **feature space mapping**

$$k\left(\boldsymbol{x}_n, \boldsymbol{x}_m\right) = \boldsymbol{\phi}(\boldsymbol{x}_n)^T \boldsymbol{\phi}(\boldsymbol{x}_m) = \sum_{i=1}^{M} \phi_i(\boldsymbol{x}_n)\phi_i(\boldsymbol{x}_m)$$

one can also construct kernel functions directly, provided they can be expressed as above

e.g., for a 2D input space

$$k\left(\boldsymbol{x}, \boldsymbol{z}\right) = \left(\boldsymbol{x}^T \boldsymbol{z}\right)^2 = \left(x_1 z_1 + x_2 z_2\right)^2 = \boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{\phi}(\boldsymbol{z})$$

$$\boldsymbol{\phi}(\boldsymbol{x}) = \left(x_1^2, \sqrt{2} x_1 x_2, x_2^2\right)$$

note that feature space dimension (M=3) is bigger than input space dimensionality (d=2)

there exist more general methods to construct acceptable kernels e.g. using **basis functions**

a popular choice is Gaussian kernel, built from an **infinite-dimensional feature map**

$$k\left(\boldsymbol{x}, \boldsymbol{z}\right) = \exp\left(-||\boldsymbol{x} - \boldsymbol{z}||^2 / 2\sigma^2\right)$$

The kernel trick

a popular choice is Gaussian kernel, built from an **infinite-dimensional feature map**

$$k(\boldsymbol{x}, \boldsymbol{z}) = \exp\left(-||\boldsymbol{x} - \boldsymbol{z}||^2 / 2\sigma^2\right)$$

we can demonstrate that this is a **valid kernel** as follows: given two valid kernels

$$k_1(\boldsymbol{x}, \boldsymbol{z}) \ , \quad k_2(\boldsymbol{x}, \boldsymbol{z})$$

we can construct **new valid kernels** from them using the following rules

$$k(\boldsymbol{x}, \boldsymbol{z}) = f(\boldsymbol{x}) k_1(\boldsymbol{x}, \boldsymbol{z}) f(\boldsymbol{z}) \qquad k(\boldsymbol{x}, \boldsymbol{z}) = \exp(k(\boldsymbol{x}, \boldsymbol{z}))$$

so now we can check that the Gaussian kernel is indeed a *bona-fide* kernel by expanding

$$k(\boldsymbol{x}, \boldsymbol{z}) = \exp\left(-\boldsymbol{x}^T \boldsymbol{x} / 2\sigma^2\right) \exp\left(-\boldsymbol{x}^T \boldsymbol{z} / 2\sigma^2\right) \exp\left(-\boldsymbol{z}^T \boldsymbol{z} / 2\sigma^2\right)$$

linear kernel

the feature map associated to this kernel has infinite dimensionality!

Summary

- Classification problems in are everywhere in Machine Learning applications, from improving medical procedures to ensuring a spam-free inbox

- Linear classification models are intuitive but **restricted** to very specific problems

- Non-linear classifiers, from sigmoid-based to neural networks, are suitable for more complicated classification problems and allow for a **probabilistic interpretation**.

- Training a ML classifier is not enough to take decisions: we need to deploy the tools of **decision theory**

- **Random forests** represent useful alternative for many classification problems