Institute of Data

2023

Data Science and AI

Module 5

Supervised ML: Classification

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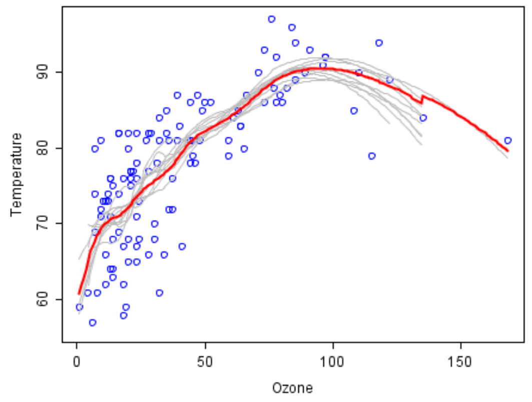
Agenda: Module 5

- Introduction to **Classification**
- **Logistic Regression**
- **Evaluating** Classification Results
- **Neural Networks**
- **Support Vector Machines**
- **Bayesian Inference**
- **Applications**

Classification

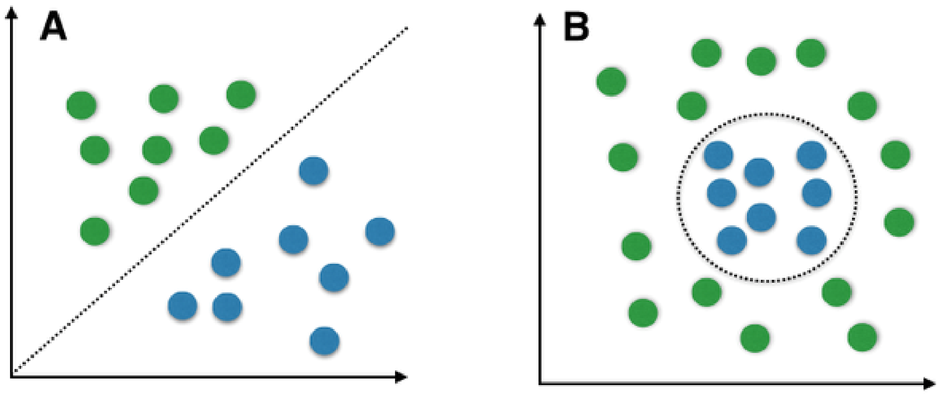
Regression

- train a model by fitting data to a **continuous** response
- *predict **continuous** numbers*



Classification

- train a model by fitting data to a **discrete** response
- predict **class membership**



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Logistic Regression

- Introduction to **classification**
- Logistic regression **algorithm**
- **Evaluating** classification results
- Measuring the **quality** of classification models
- **Dummy variables**

Classification

examples

- fraud detection
  - True / False

- customer segmentation:
  - frequent, high-value / regular, medium-value / occasional / transient

- credit risk
  - low / medium / high

- disease status
  - NYHA Class I / II / III / IV

Predicting Class Membership by Supervised Machine Learning

training data

- **features**
  - for now, assume these are continuous
- **response**
  - for now, assume this is binary (True/False)
  - Could be multiple classes in some case

goal

- predict $p(y = 1 \mid X)$

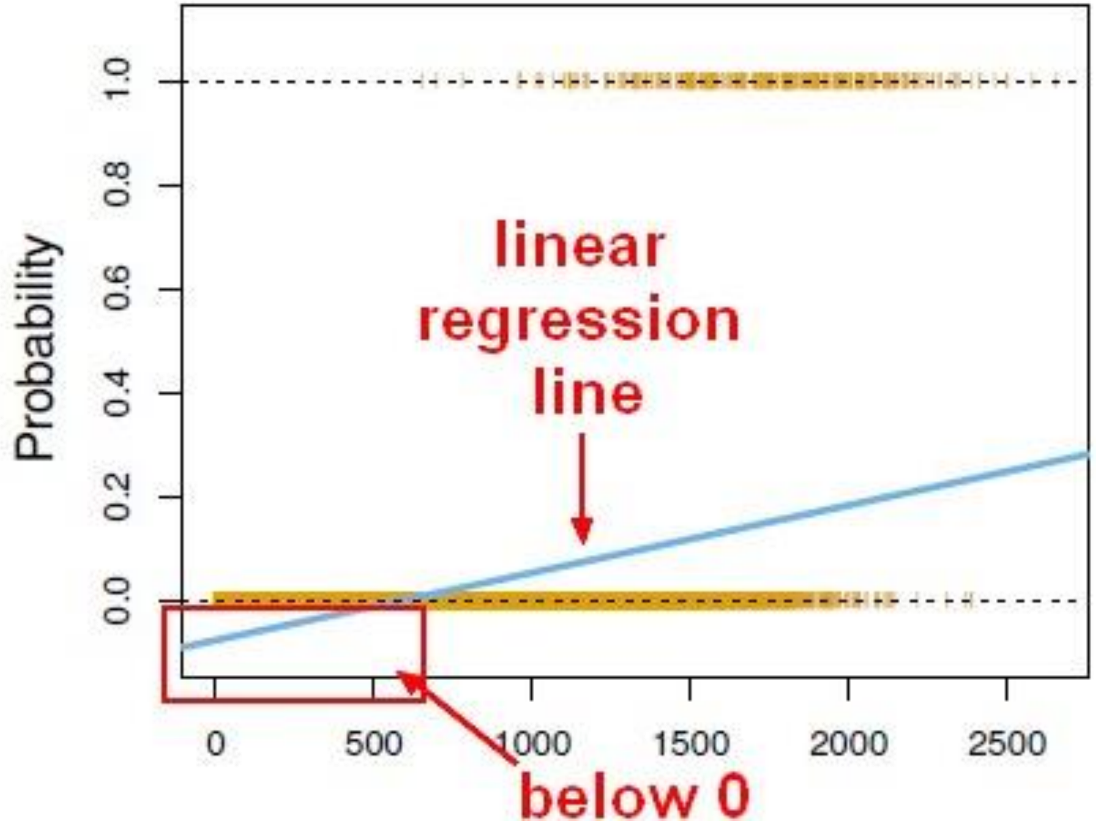
  the probability of ***y*** being True given the predictor(s) ***X***

Binary Class Prediction

- **can we use linear regression?**

$y \in \{\text{False, True}\}$ → $y = \beta X + \varepsilon$

  - binary response variable results in large residuals
  - predictions can be outside [0, 1]



Binary Class Prediction – cont’d

- need to transform the response so that ***y*** becomes discrete
  - model the ***probability*** of class membership!

- how about this:

$$\boldsymbol{p}\,(\boldsymbol{y} = 1 \mid \boldsymbol{X}) = \beta_0 + \beta_1 \boldsymbol{X}$$

  - still gives $\boldsymbol{y} < 0$, $\boldsymbol{y} > 1$

  - need an approximating function that ensures $\boldsymbol{y} \in [0,1]$

Binary Class Prediction – cont'd

- $\frac{p}{1-p}$ = odds ratio

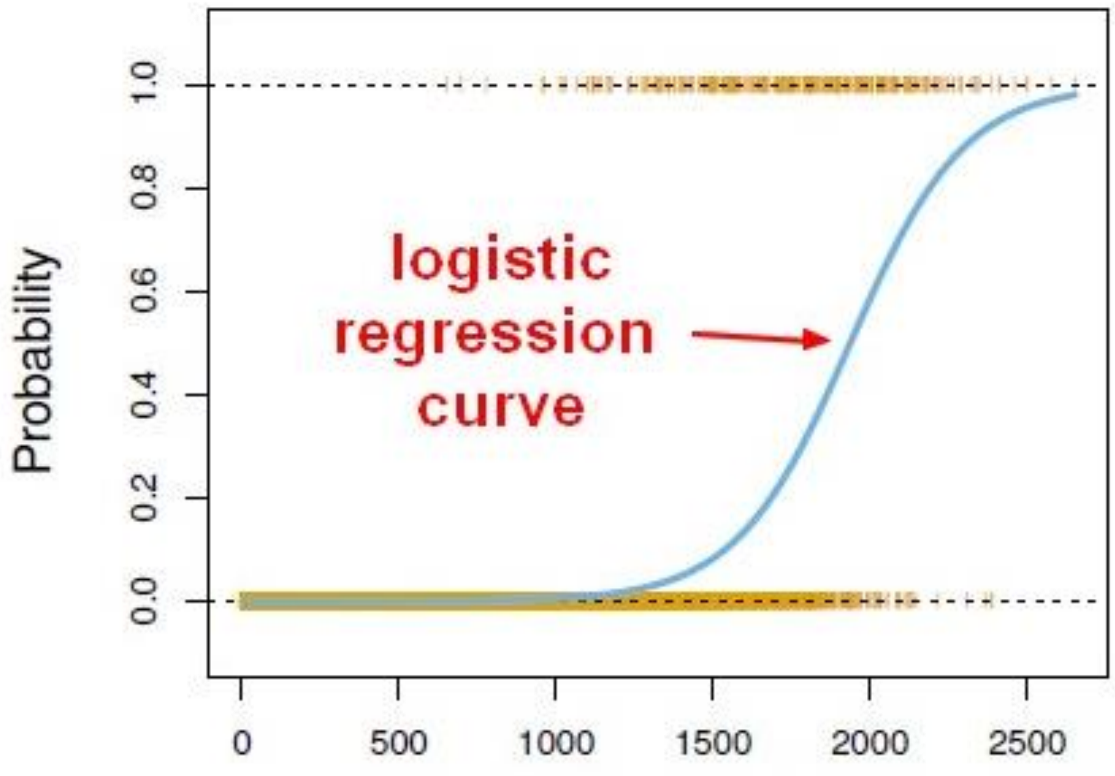
  (p = probability of True)

$\log\left(\frac{p}{1-p}\right)$ = logit (*aka* log odds)

solve:

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

logit function



Logistic Regression

- β_0, β_1 are known from regression results:

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

let $\boldsymbol{X}$ be a new data point for prediction,

calculate $\hat{y}$:

$$\hat{y} = \beta_0 + \beta_1 \boldsymbol{X}$$

then calculate p:

$$p = \frac{e^{\hat{y}}}{e^{\hat{y}} + 1} = \frac{1}{1 + e^{-\hat{y}}}$$

Conditions:

$p > 0$

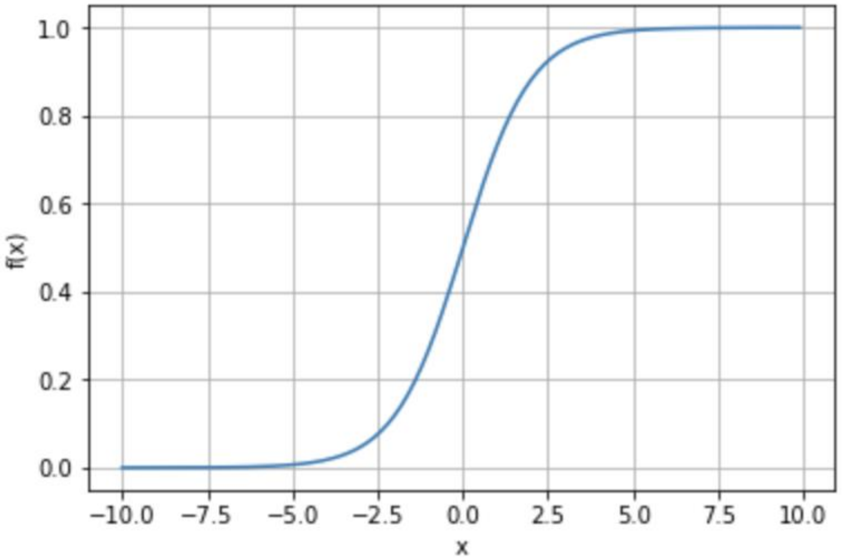
$p < 1$

Logistic Regression

Appropriate when predicting a **binary categorical** outcome variable from a set of predictor variables (features) that may be **continuous and/or categorical**

Features should be independent with no missing data.

Logistic Regression typically requires **a relatively large sample size.** A general rule of thumb is that you need at least 10 cases of the least frequent outcome for each independent variable in your model.



Sigmoid or logistic curve

Logistic Regression – Scikit-learn

from **sklearn.linear_model** import LogisticRegression

- Can deal with any number of features
- **Features must be numeric**
    - Categorical features should be converted to dummy features
- Can perform **multi-class classification**

Evaluating Classification Results

There are a number of metrics that can be used to evaluate a classification model. Many of these metrics revolve around values drawn from the Confusion Matrix.

The **Confusion Matrix** is a table that contains counts of the predictions of the model versus the actuals.

Note that if we are interested in predicting the opposite class, the entries would be reversed (the positive becomes negative and vice versa).

Actual	Positive	Negative
Prediction		
Positive	True Positive (TP)	False Positive (FP)
Negative	False Negative (FN)	True Negative (TN)

Confusion Matrix

It is useful to develop an intuition of the meaning of each row and column and key combinations of the counts in the Confusion Matrix

Actual	Positive	Negative	
Prediction			
Positive	True Positive (TP)	False Positive (FP)	Total predicted positive
Negative	False Negative (FN)	True Negative (TN)	Total predicted negative
	Total actual positive	Total actual negative	Total Sample count

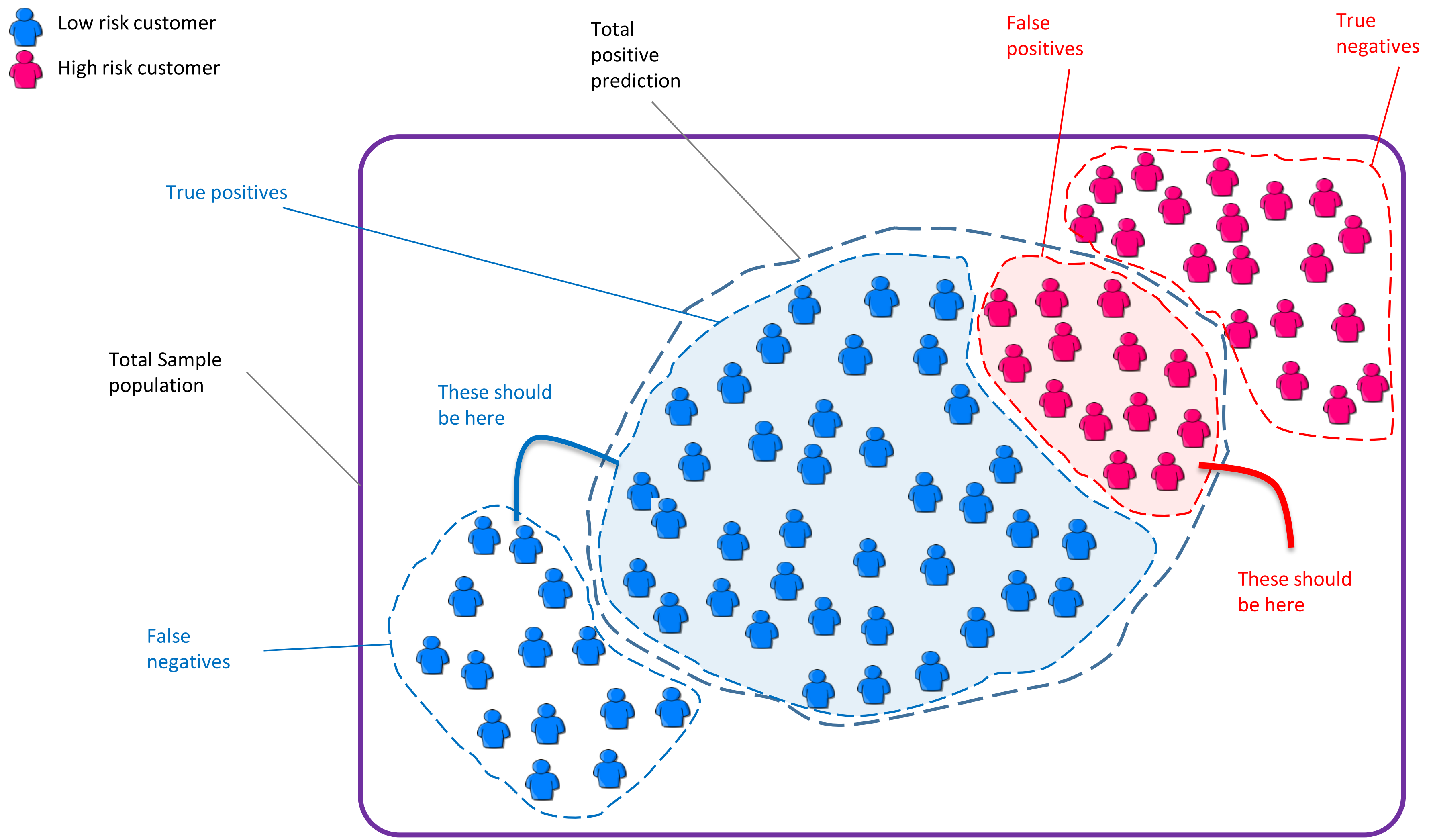
Total true prediction

Evaluating Classification Results – cont’d

- **Accuracy**: the fraction of predictions that the model got right. i.e. Number of correct prediction / total prediction
  - Accuracy = Total true prediction / Total sample count
- **Precision**: how many of the prediction were correct. It is a measure of **exactness**.
  - Precision = TP / Total positive prediction (TP + FP)
- **Recall**: how many of the actual positive did the model predict. It is a measure of **completeness**.
  - Recall = TP / Total actual positive (TP + FN)

Actual	Positive	Negative	
Prediction			
Positive	True Positive (TP)	False Positive (FP)	Total predicted positive
Negative	False Negative (FN)	True Negative (TN)	Total predicted negative
	Total actual positive	Total actual negative	Total Sample count

Total true prediction



Actual	Positive	Negative	
Prediction			
Positive	True Positive (TP)	False Positive (FP)	Total predicted positive
Negative	False Negative (FN)	True Negative (TN)	Total predicted negative
	Total actual positive	Total actual negative	Total Sample count

Total true prediction

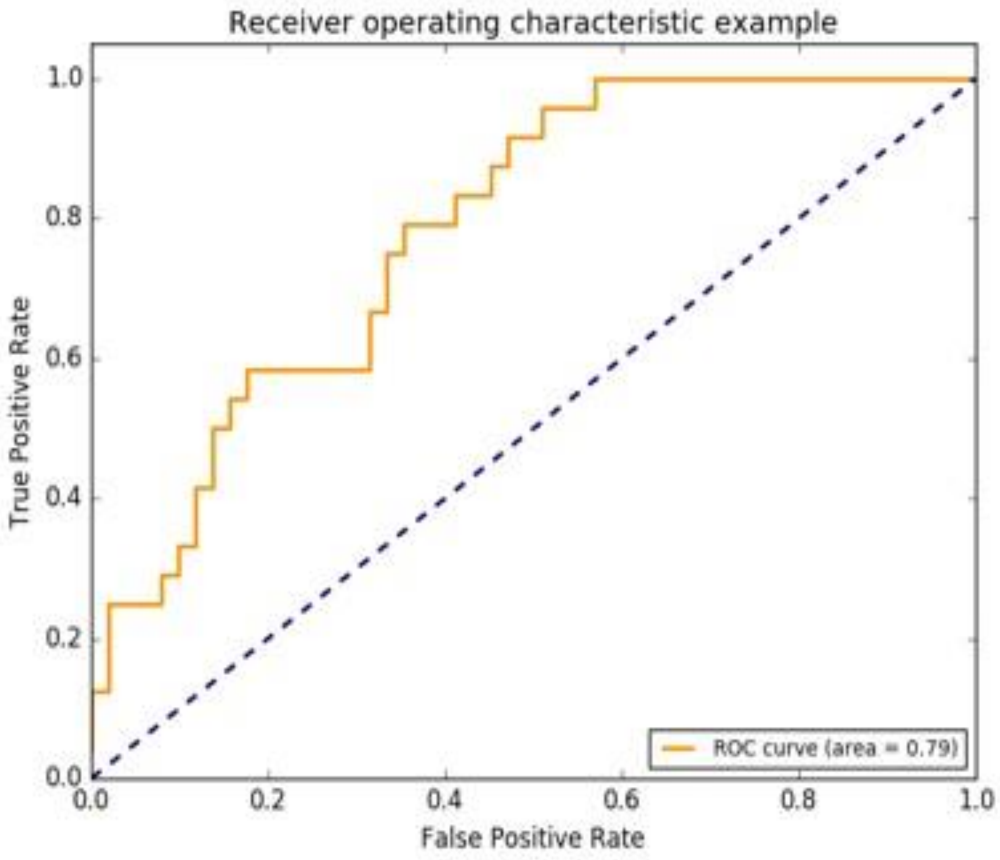
Note: icons are positioned where they are for illustration purpose only.

Accuracy = Total true prediction / Total sample count
Precision = TP / Total positive prediction (TP + FP)
Recall = TP / Total actual positive (TP + FN)

Evaluating Classification Results – cont'd

Receiver operating characteristics (ROC) curve

- Compares True Positive Rate and False Positive Rate
- **True Positive Rate (TPR)** = Recall
- **False Positive Rate (FPR)** is FP/ Total negative count (FP+ TN)
- ROC plots **TPR** vs **FPR** by varying threshold over the entire range of threshold settings. It depicts relative **trade-offs between true positive (benefits) and false positive (costs)**
- **Area Under Curve (AUC)** is equal to the probability that the model will rank a randomly chosen positive instance higher than a randomly chosen negative one.



Evaluating Classification Results – cont'd

- There are many other metrics and many other names for the same metrics
- It is better to stick with a small number of metrics that make sense in your domain before using other metrics
- **Accuracy, precision, recall** and **AUC** are the most common metrics

Dummy Variables

How can we use categorical variables in an algorithm that requires numerical predictors?

- ***ordinal categoricals***
  - can be converted to a sequence of integers, if it makes sense to do so

cold	cool	moderate	warm	hot
1	2	3	4	5

√

- the above implies hot < warm < moderate < cool < cold
  ... which makes sense

Dummy Variables

How can we use categorical variables in an algorithm that requires numerical predictors?

- ***cardinal categoricals***

apples	bananas	peaches	oranges	pears
1	2	3	4	5

> *this implies pears > oranges > peaches > bananas > apples ... does not make sense!*

> must convert to dummy variables instead

Cardinal Dummy Variables

- full definition (number of variables = number of categories):
  - fruit_apples: 1 = apples, 0 = no apples
  - fruit_bananas: 1 = bananas, 0 = no bananas
  - fruit_peaches: 1 = peaches, 0 = no peaches
  - fruit_oranges; 1 = oranges, 0 = no oranges
  - fruit_pears; 1 = pears, 0 = no pears
- compact definition (number of variables is one less than number of categories):
  - fruit_bananas: 1 = bananas, 0 = apples
  - fruit_peaches: 1 = peaches, 0 = no peaches
  - fruit_oranges; 1 = oranges, 0 = no oranges
  - fruit_pears; 1 = pears, 0 = no pears

Python:

pandas.get_dummies

Lab 5.1: Logistic Regression

- Purpose:
  - To predict survival amongst Titanic passengers using the LogisticRegression() method of Scikit-Learn

- Materials:
  - ‘Lab 5.1.ipynb’

Discussion

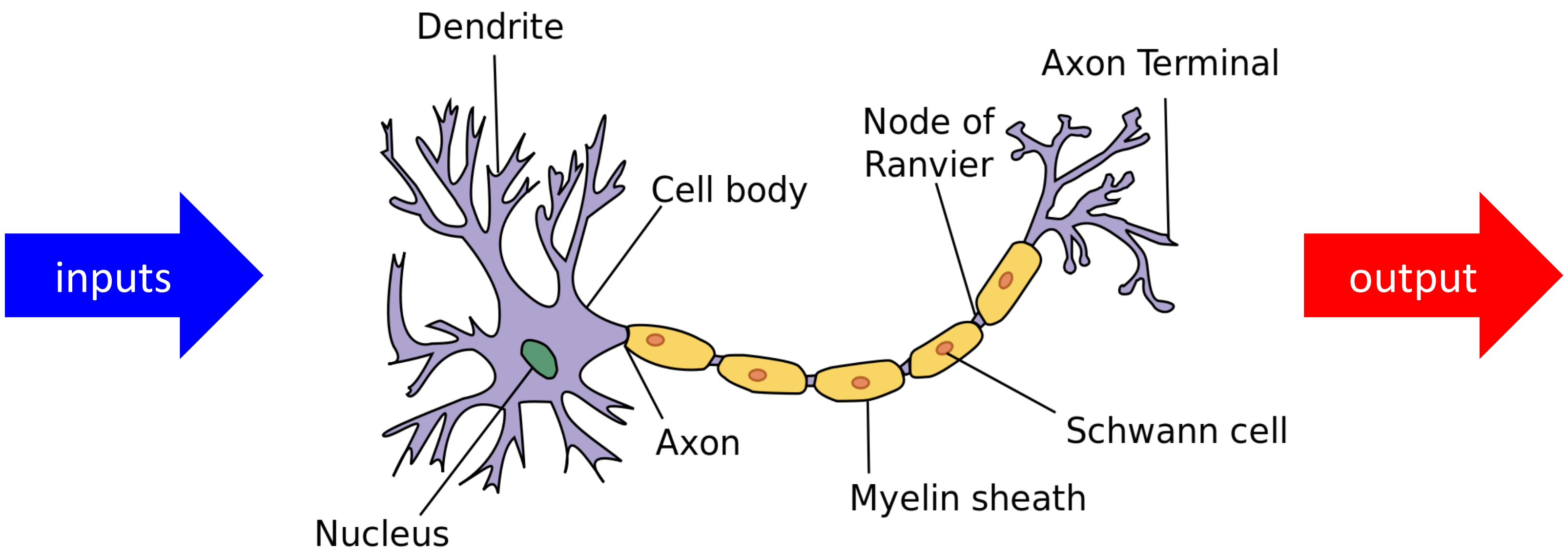
- Strengths & weaknesses of logistic regression

Perceptron (Neural Networks)

- **Biological** and **artificial** neurons
- **Activation** functions
- **Linear regression** with a perceptron
- **Linear classification** with a perceptron
- **Gradient descent**
- Practical implementations

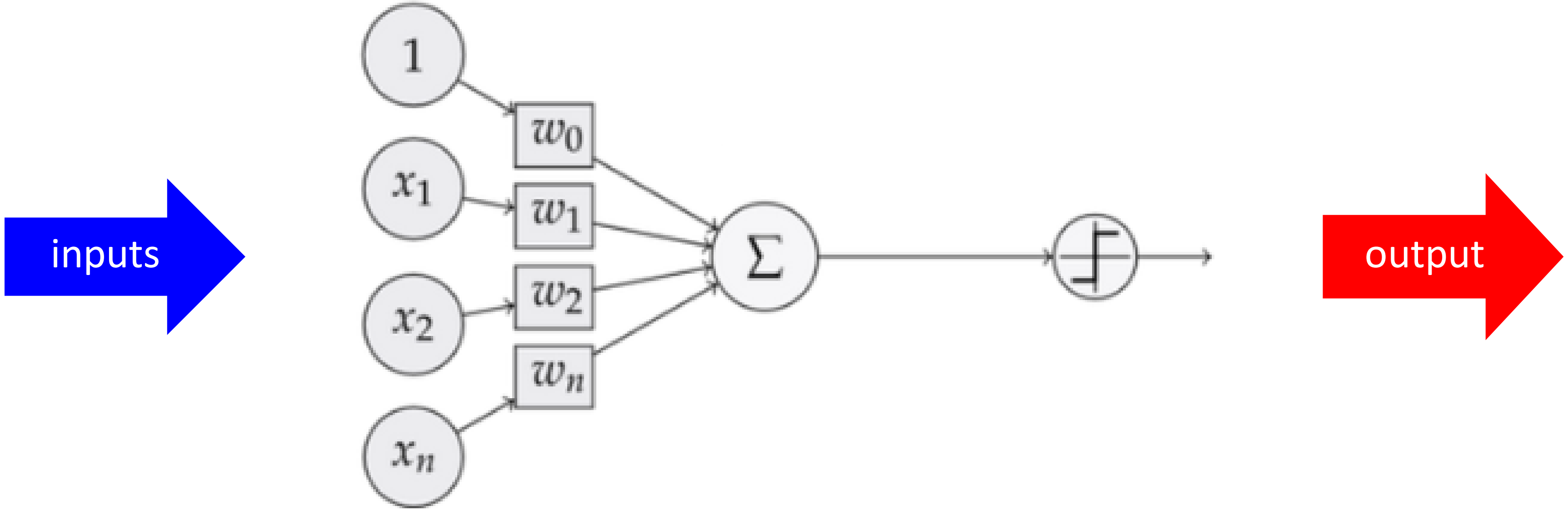
How does a nerve cell make a decision?

- Neuron receives inputs at antennae-like structures (‘**dendrites**’)
- Each incoming connection is **dynamically strengthened or weakened** by:
  - frequency of use (‘weighting’)
  - neurotransmitters
- **Weighted inputs** are summed in the cell body (transformed into a new signal)
- New signal is **propagated** along the cell’s axon to be detected by other neurons



The Perceptron

- A **basic imitation** of the natural neuron
- Inputs are given **weights**
- **Weighted** signals are summed
- summed signal is transformed by an **activation function** to produce an output



Perceptron Activation Function

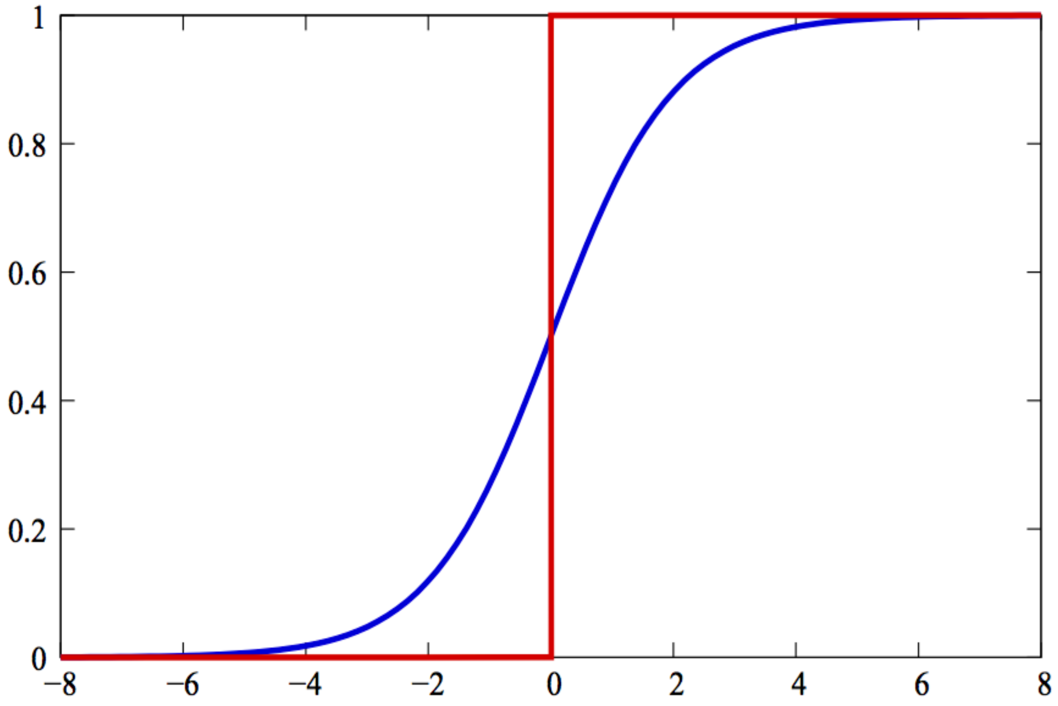
- z is the **weighted sum of inputs** (similar to Logistic Regression):

$$z = \sum_{j=0}^{n} w_j \, x_j$$

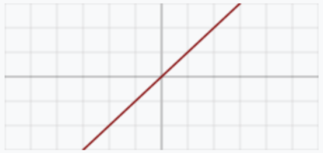
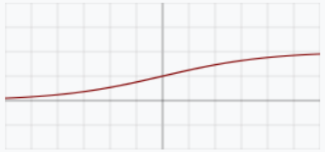
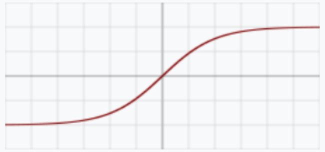
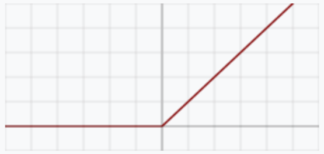
- A transfer function f(z) converts z to the output of the node
- f(z) is called the **activation function**

example:

$$f_{log}(z) = \frac{1}{1 + e^{-z}}$$



Perceptron Activation Functions

	$f(x) = x$
	$f(x) = \dfrac{1}{1 + e^{-x}}$
	$f(x) = \tanh(x) = \dfrac{2}{1 + e^{-2x}} - 1$
	$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$

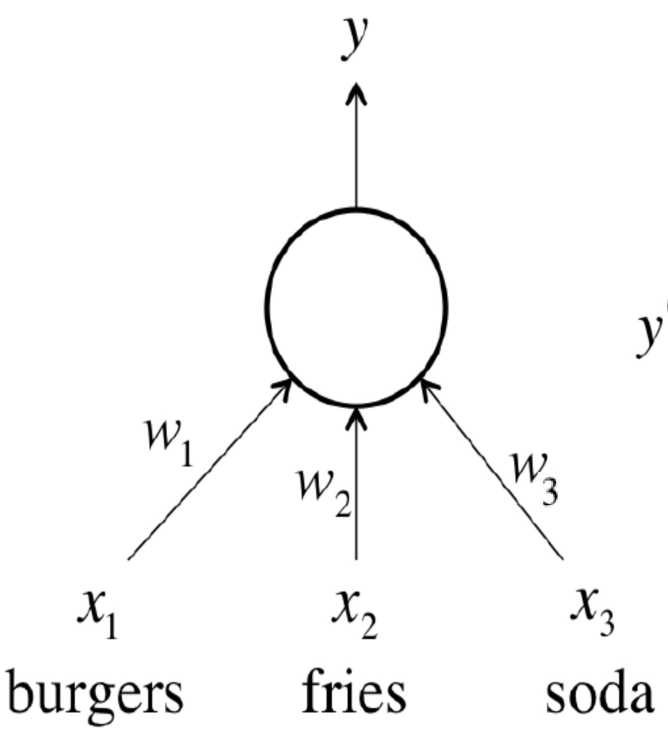
- Linear
- Logistic
- Hyperbolic tangent
- **Rectified linear unit (ReLU)**

Linear Regression Perceptron

- Example: given a set of fast food orders and total prices, can we predict the unit prices?
- let

  x_1 = number of burgers
  x_2 = number of fries
  x_3 = number of sodas
  y = total price
  for any order
- object:

  compute the weights
  w_1, w_2, w_3
  that minimise the residuals of y



$$y^{(i)} = w_1 x_1^{(i)} + w_2 x_2^{(i)} + w_3 x_3^{(i)}$$

Linear Classification Perceptron

- Given
  - a set of n-D **features** X
  - a set of **labels** (response var) y

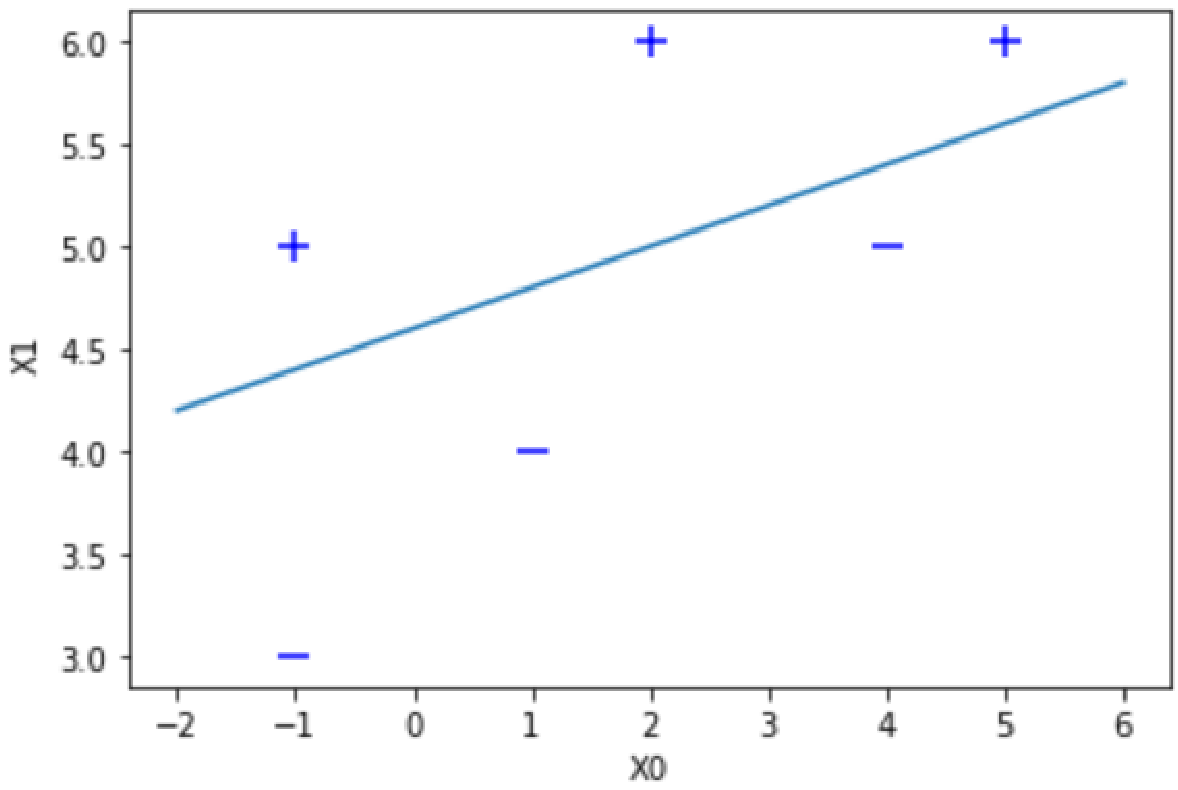
- Objective:

compute the weights
$w_1, w_2, \dots w_n$

that describe the ***hyperplane*** that separates points X by class y

example: labels $y \in \{-1, 1\}$

SEE LAB 5.2



Learning the weights

How to **compute the weights**?

- Iteratively **adjust the weights** over the entire dataset until the algorithm converges to a solution:

  error (at output) < *tolerance*

How to implement this?

Gradient descent

- Error at a node is a function of the weights on the inputs flowing into the node
- Use gradient of error function to step in direction of decreasing error until minimum is found
- Update weight with a Learning Rate times the error and direction of the error (which is the derivative of the cost function)
- w = w + Learning Rate * (expected - predicted) * x

The Perceptron in Practice

- in the *burgers/fries/sodas* example there should be an exact solution
  - (unless the unit process vary over the course of the dataset, in which case we would end up predicting the average price of each item)

- in general ...
  - the data will not permit an exact solution
  - presence of local minima may cause convergence to fail

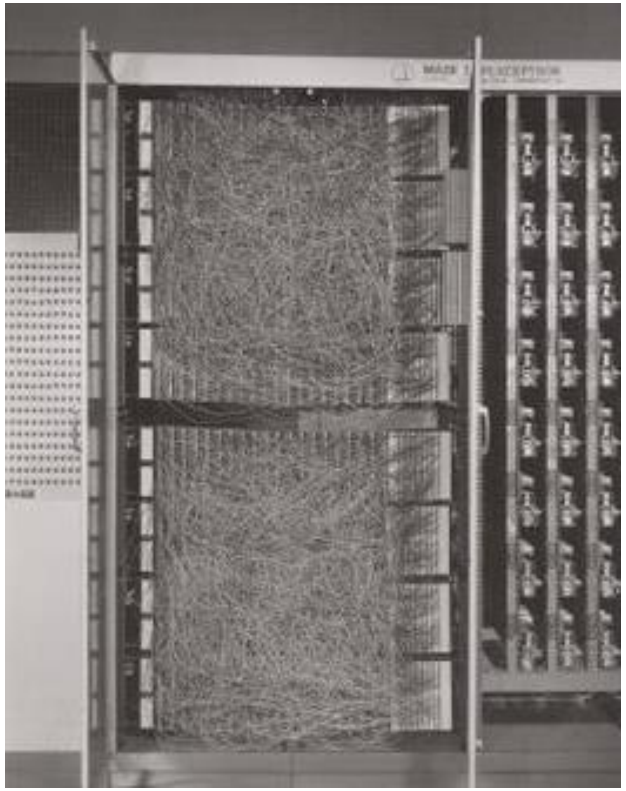
- in practice ...
  - use many perceptrons (***nodes***), organised into ***layers*** to learn more complex problems

  > neural network and Deep Learning

Lab 5.2: Classification with a Perceptron

- Purpose:
  - To evaluate a simple perceptron for predicting classes from numeric features.

- Materials:
  - ‘Lab 5.2.ipynb’



Mark 1 Perceptron

By Source (WP:NFCC#4), Fair use, https://en.wikipedia.org/w/index.php?curid=47541432

Discussion

- Strengths & weaknesses of perceptron-based prediction

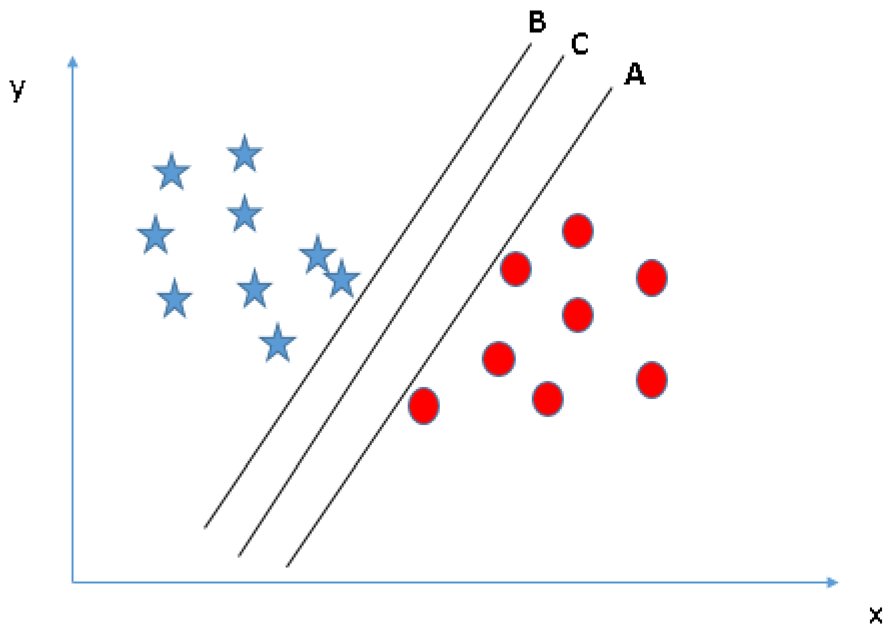
Support Vector Machines

- Concepts
- Linear SVMs
- Nonlinear SVMs
- Limitations
- Applications

Support Vector Machines

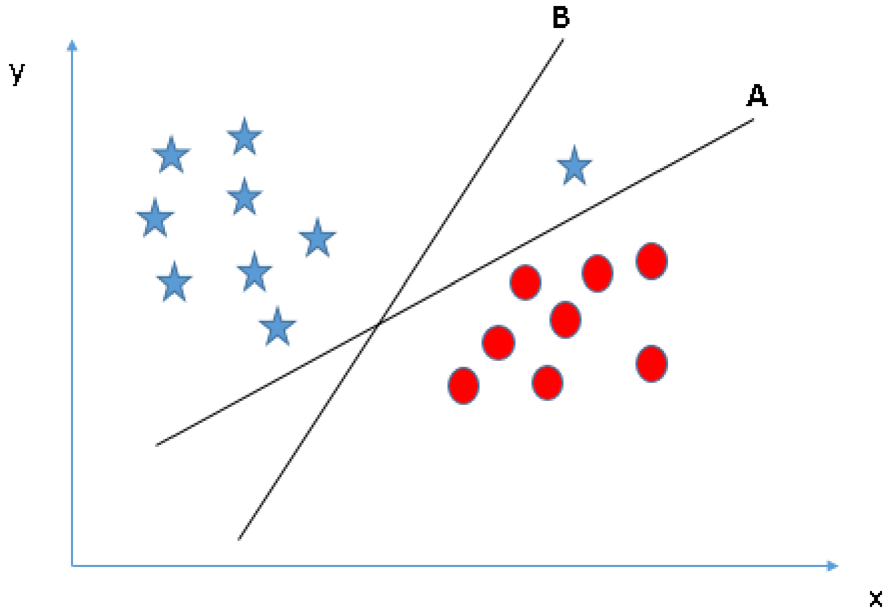
- A **linear** algebraic method for separating ***n*-dimensional** data into classes
  - Data points are separated by a ***hyperplane*** (i.e. a boundary that has dimensionality *n*−1)

example: 2D



- lines A, B, C are **hyperplanes** in a 2D space
- each line correctly separates the two classes
- line C is preferred, because it **maximises** the average squared distance (***margin***) between the boundary and the points

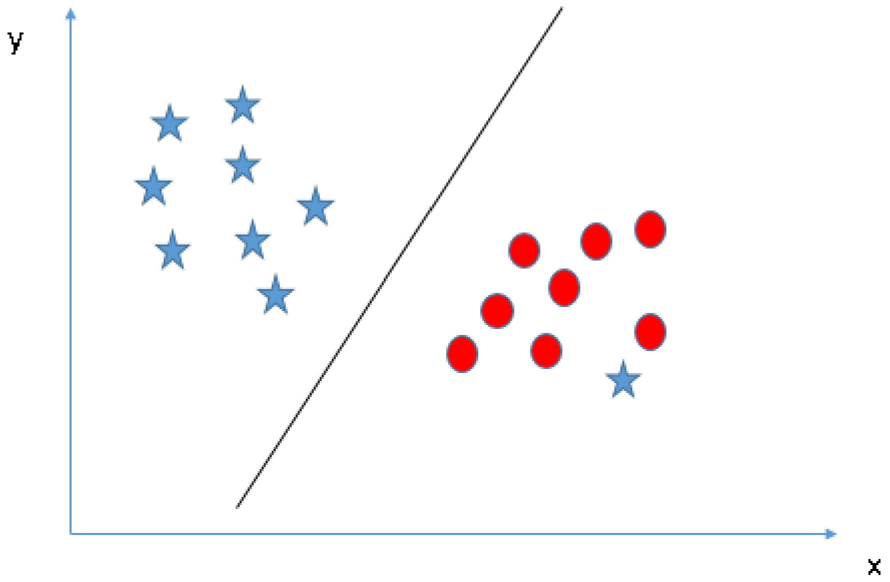
Support Vector Machines – cont’d



- line B gives a larger margin
- line A correctly separates the classes

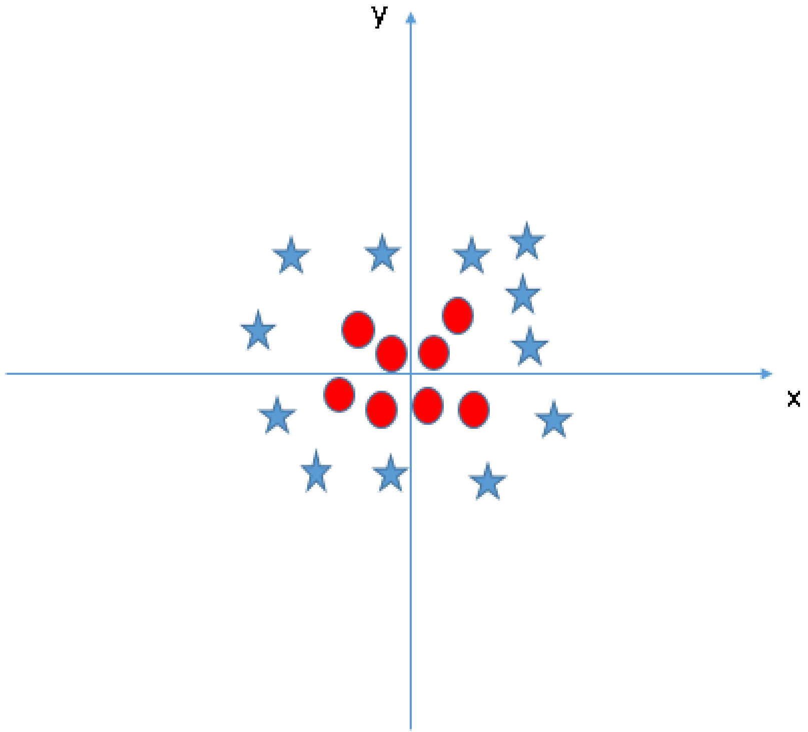
- line B will be chosen
  - **maximum separation** of classes is the first priority

Support Vector Machines – cont’d



- the line separates the classes except for one outlier
- the presence of the outlier does not shift the line to the right
  - **SVMs are robust against outliers**

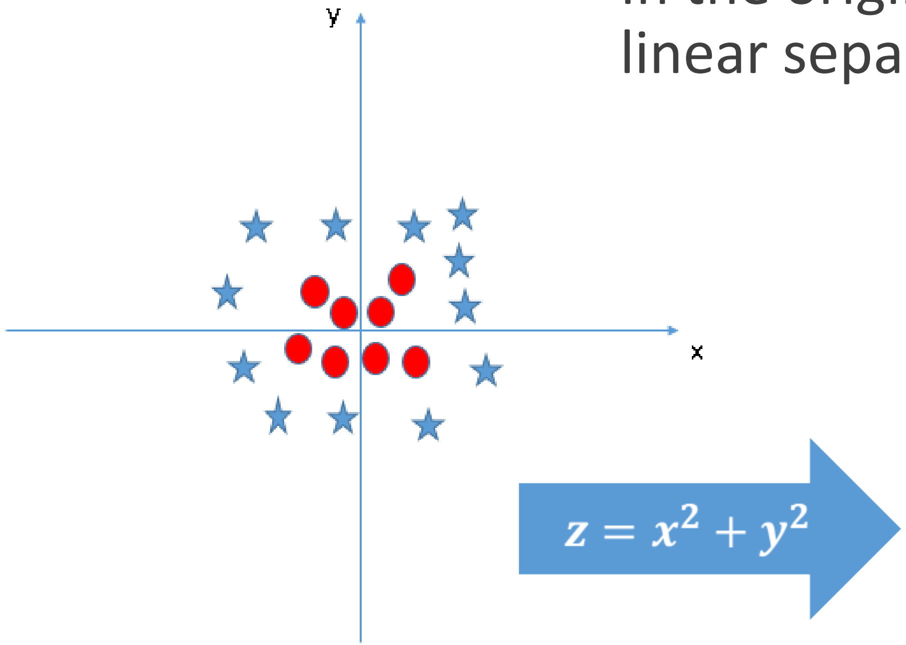
Support Vector Machines – cont'd

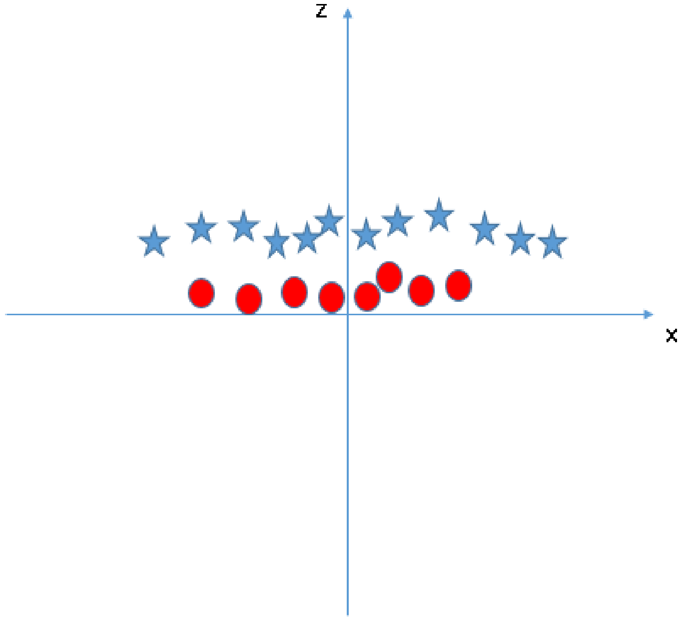


- there is no line that can separate these classes
  - will an SVM fail, here?
  - *Hint: we could* ***transform*** *the coordinates or create a new feature*

Support Vector Machines – cont’d

- In the original coordinates, linear separation is not possible





- in these **coordinate**, there *is* a line that can separate the classes

  > the **kernel trick**:

  - an inseparable problem can be transformed into a separable problem in a higher dimension
  - the transform function is called the ***kernel***

Linear SVMs

Hard margin

- classes are separable by the margin around the solution hyperplane

Soft margin

- classes are not separable
- the best-fit hyperplane is computed by minimising the *hinge loss* function
  - incorporates a parameter that defines the trade-off between maximising the margin and minimising the number of misclassified points

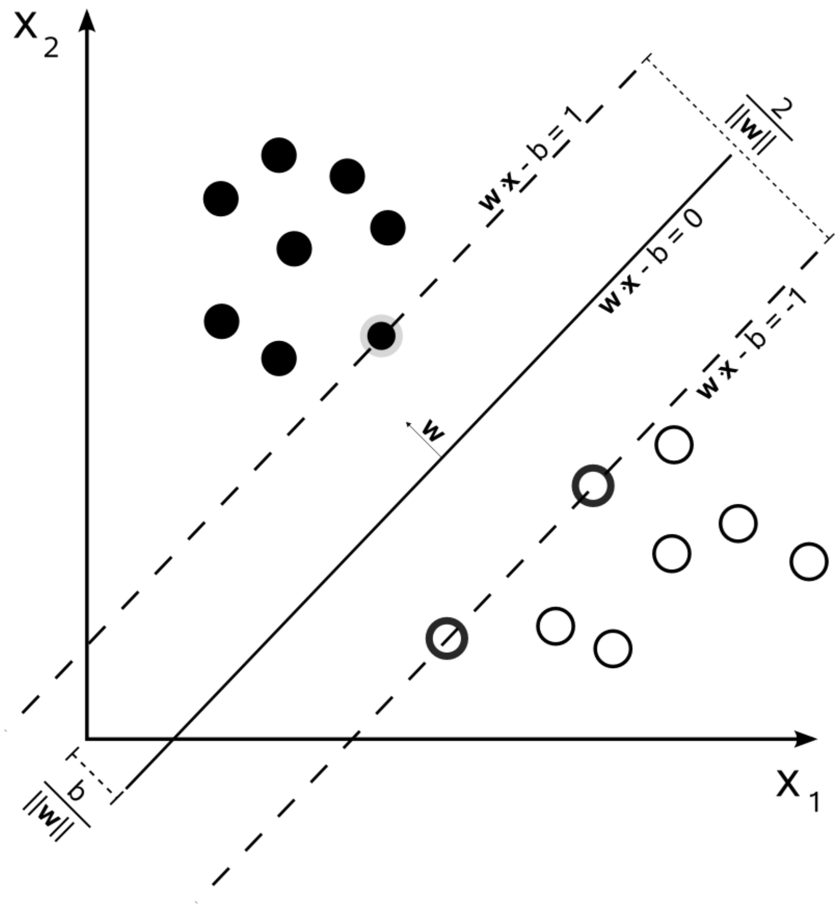
Linear SVM with Hard Margin

- equation of hyperplane is

$$\vec{w} \cdot \vec{x} - b = 0$$

- compute $\vec{w}, b$ so as to maximise width of margin

$$2/||\vec{w}||$$



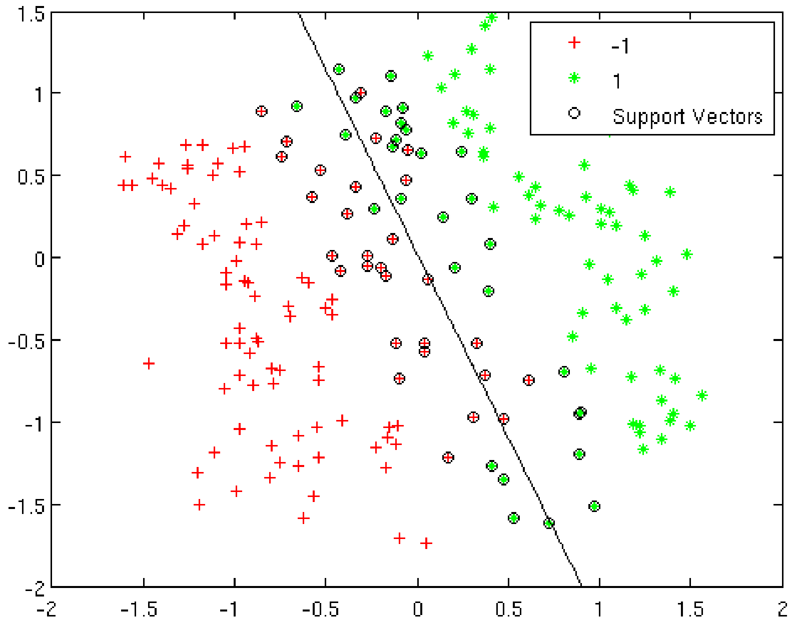
Linear SVM with Soft Margin

- equation of hyperplane is

$$\vec{w} \cdot \vec{x} - b = 0$$

- compute $\vec{w}$, b so as to minimise

$$\left[\frac{1}{n}\sum_{i=1}^{n}\max\left(0, 1 - y_i(\vec{w}\cdot\vec{x}_i - b)\right)\right] + \lambda\|\vec{w}\|^2$$



Nb. This plot also shows that only the nearest points are used to compute the boundary. These points are called the ***support vectors***.

Nonlinear SVMs

- Polynomial kernel
  - with or without constant term
- Gaussian radial basis function (RBF)
- Hyperbolic tangent

Limitations of SVMs

- Generalisation error
  - margin is too small (data too close together) to accurately separate all classes
- Requires full labelling of input data
- Class membership probabilities are uncalibrated
- Does not natively handle more than 2 classes
  - multiclass problems must be reduced to a series of binary problems before applying SVMs
- Solution parameters are difficult to interpret

Applications of SVMs

- Text categorisation
- Image classification
- Handwriting interpretation
- Protein classification
- Customer segmentation

SVMs in Python

- Predictors **X**
- Response **y**
- Test data **Xtest**

- c = **regularisation** parameter: controls sensitivity to outliers
- gamma = kernel coefficient (‘rbf’, ‘poly’ and ‘sigmoid’ kernels): controls influence of nearby points

```
from sklearn import svm

# Create SVM classification object:
model = svm.svc(kernel = 'linear’, c = 1, gamma = 1)

# Train model:
model.fit(X, y)

# Evaluate quality of fit:
model.score(X, y)

#Predict output for test data:
predicted = model.predict(Xtest)
```

Lab 5.3: Support Vector Machines

- Purpose:
  - To apply the SVM method to linear and nonlinear classification problems.
- Materials:
  - ‘Lab 5.3.ipynb’

Discussion

- Strengths & weaknesses of SVMs

Bayesian Inference

- **Frequentist** vs **Bayesian** probability
- **Bayes' theorem**
- Example: Disease detection
- **Bayesian modelling**
- **Naïve Bayes Classification**

Frequentist Probability

- Probability:
  - a proportion of outcomes
- In the frequentist approach, we have some **sample results** from which we calculate the **frequency** of the *positive* result
  - we estimate the future probability of a positive result based entirely on this sample

Bayesian Probability

- Probability:
  - a degree of belief

- In the Bayesian approach, we also have pre-existing information (a sample or distribution) about something that has a causal connection to the thing we are sampling
  - we use this **prior** distribution in addition to the current sample to estimate the future probability of a positive result

Bayes' Theorem – cont'd

- Suppose event A leads to event B, or that B is seen to be associated with A
- Let

$$p(B|A)$$

be the probability of B given A

- Then

$$p(A|B) = \frac{p(A)p(B|A)}{p(B)}$$

is the probability of A given B

  - the probability that A happened given that the event B happened

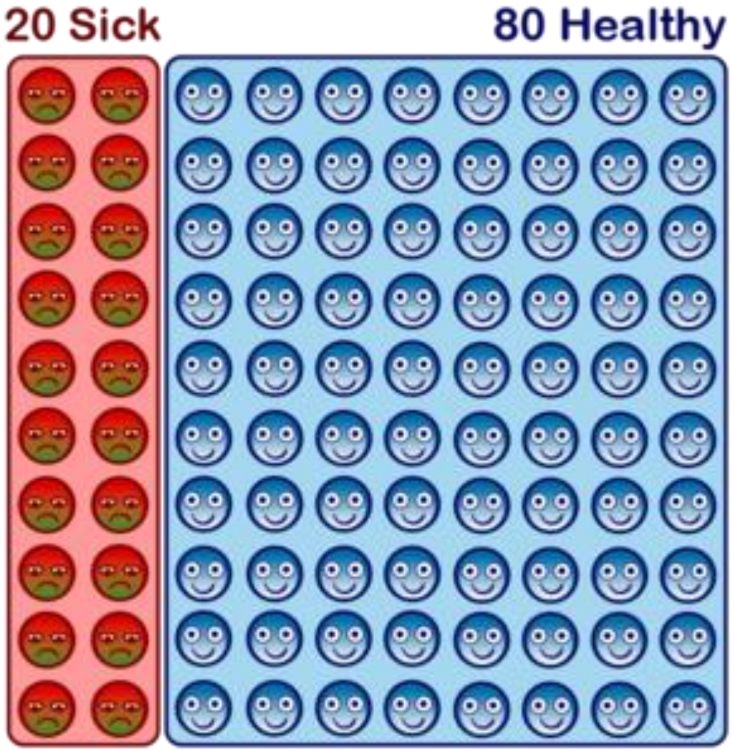
Bayes' Theorem – cont'd

- $$p(A|B) = \frac{p(A)p(B|A)}{p(B)}$$

- $p(A), p(B)$ are **marginal** probabilities
- $p(A|B), p(B|A)$ are **conditional** probabilities
- $p(A)$ is the **prior** probability
- $p(B)$ is the **evidence**

Example: Disease Detection

- prior knowledge:
  - 20% of population has the disease
    P / (P + N) = 0.20
  - in a random sample of 100 people,
    20 will have the disease (on average)



https://arbital.com/p/bayes_frequency_diagram/

Example: Disease Detection

- sensitivity of test:
  - 90% of subjects with disease are correctly detected

  TPR = 0.90 = TP / (TP + FN)

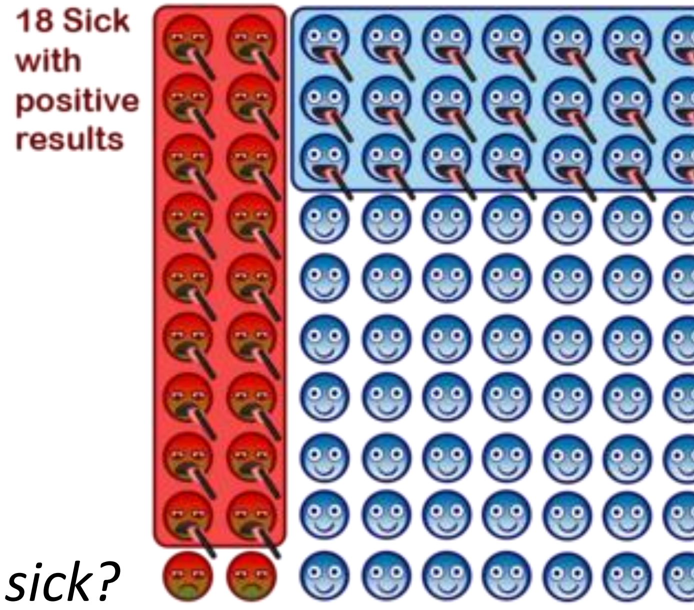
  TP = 0.90 * 20 = 18

- FPR (1 – specificity) of test:
  - 30% of disease-free subjects are erroneously detected

  FPR = 0.30 = FP / (FP + TN)

  FP = 0.30 * 80 = 24

> *if a person tests positive, what is the probability that they are sick?*



Example: Disease Detection

- Probability that a subject with a positive test result is actually sick:

$p(sick|test^+) = TP / (TP + FP)$

$= 18 / (18 + 24)$

$= 18 / 42$

≈ 0.43

Alternatively, using Bayes' Theorem,

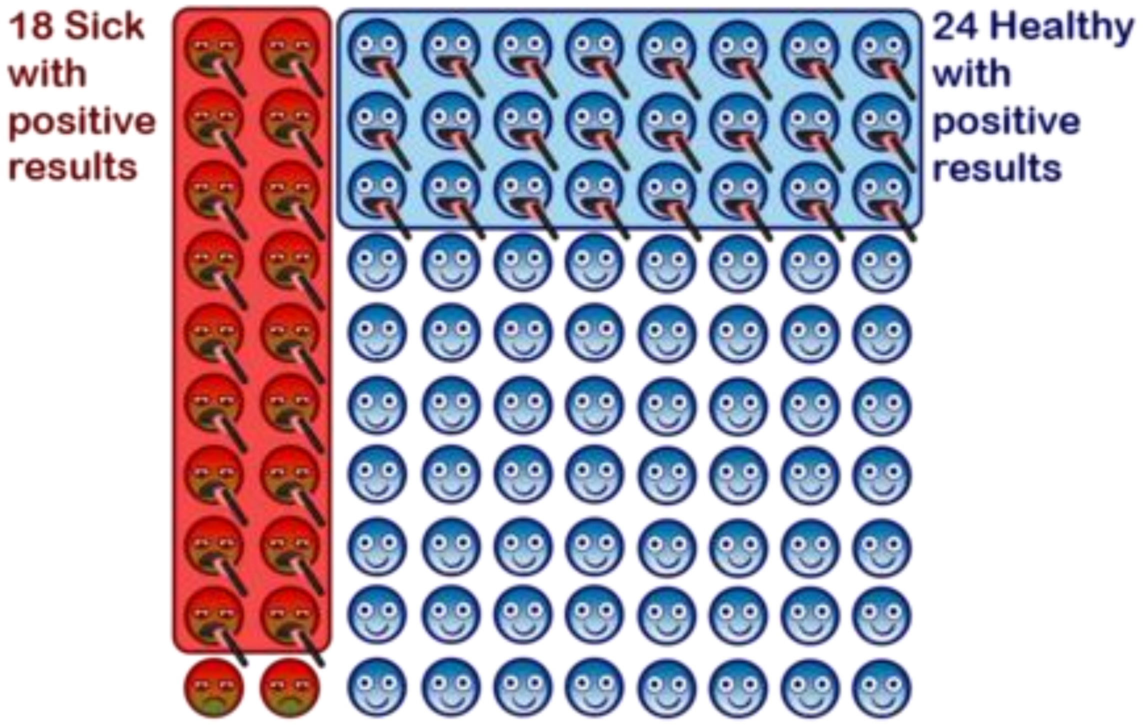
$p(sick|test^+)$

$= p(sick)*p(test^+|sick) / p(test^+)$

$= 0.2*0.9 / (0.2*0.9 + 0.3*0.8)$

$= 0.18 / 0.42$

≈ 0.43



https://arbital.com/p/bayes_frequency_diagram/

Bayesian Modelling

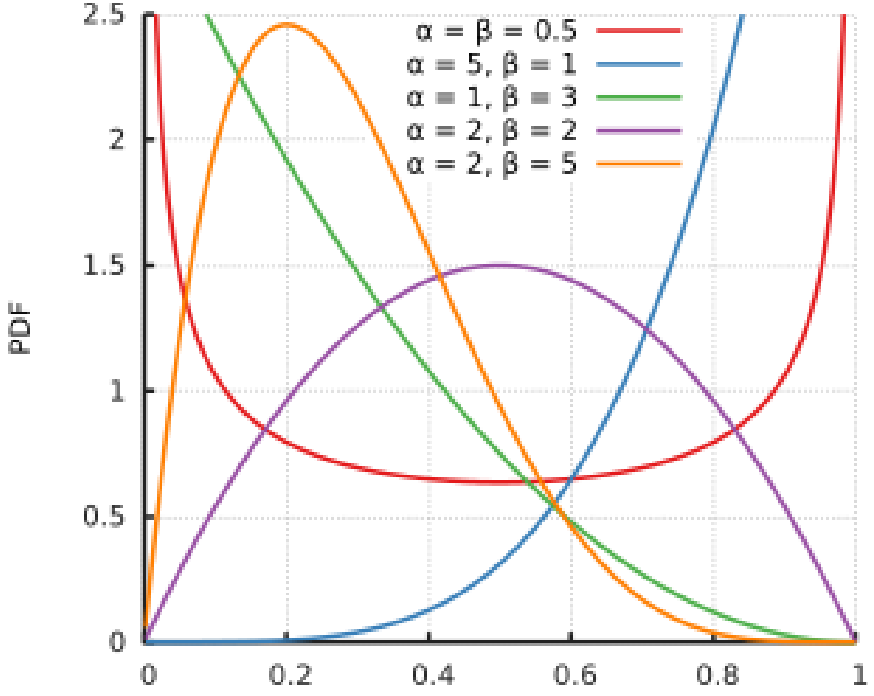
- **Model-based** approach
  - results not dependent on arbitrary ***p*-value, confidence interval**
- **Naïve Bayes** assumption
  - **Predictors are independent**
    - variables come from distributions that do not interact
- prior distribution is not usually known explicitly
  - type of distribution must be assumed:
    - from domain knowledge
    - by choosing a mathematically sound distribution
  - parameters of distribution are fitted to the prior data

How to Choose the Prior Distribution?

- Informative, **empirical**:
  - Data from **related experiments** informs our prior beliefs
  - Prior beliefs will influence final predictions
- Informative, **non-empirical**:
  - Prefer certain values over others (e.g. need to **regularise coefficients**)
  - Prior beliefs will influence final predictions
- Informative, **domain-knowledge**:
  - No supporting data, but certain facts are known to be more true than others
  - Prior beliefs will influence final predictions
- **Non-informative**:
  - Prior beliefs will have little to no effect on our final assessment
  - Current data alone will determine final predictions

Beta Distribution

- a probability density function suitable for modelling the random behaviour of percentages and proportions



$$\text{PDF} = \frac{x^{\alpha-1}\,(1-x)^{\beta-1}}{B(\alpha,\beta)}$$

$\alpha, \beta > 0$

B is the beta function

https://en.wikipedia.org/wiki/Beta_distribution

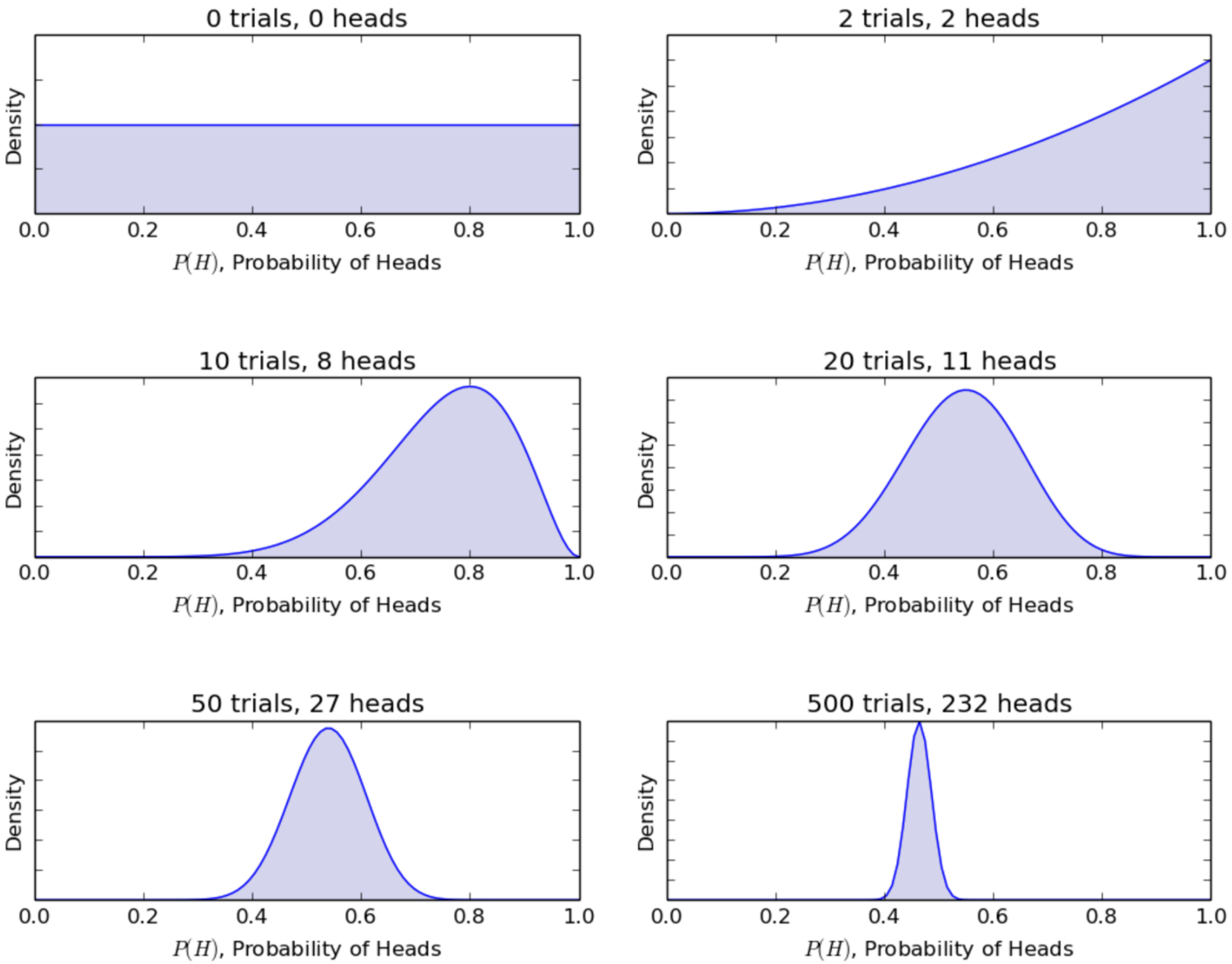
Bayesian Modelling – cont'd

What can we use for the prior probability if we have no information?

> **a beta distribution**

$$\mu = \frac{\alpha}{\alpha + \beta}$$

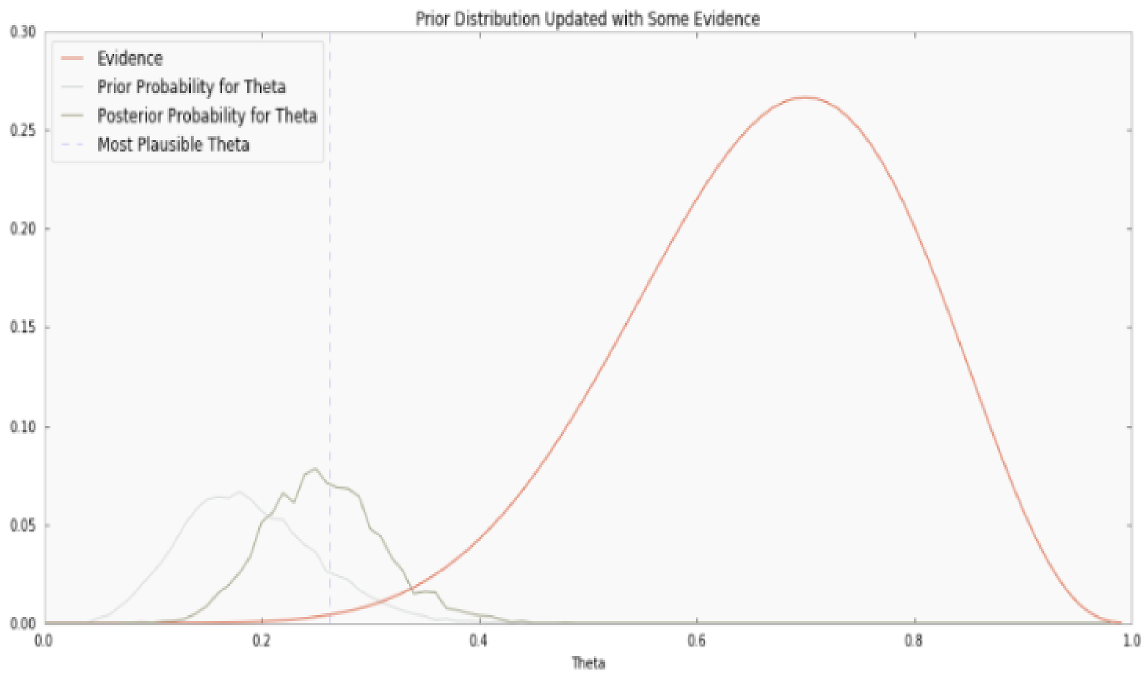
$$\sigma = \sqrt{\frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}}$$



Bayesian Analysis of a Sample

Example:

Campaign to boost click rates on ‘ads’



- new ad yielded 7 clicks from 10 users tested (red line)
    - beta distribution of θ peaks at 0.7 (most likely value)
- previous 100 campaigns yielded much lower click rates (light grey line)
    - prior θ peaks $\lesssim 0.17$
- we don’t believe the new result, so we modify it based on our prior information (result = dark grey line)
    - posterior θ peaks $\lesssim 0.25$

Naïve Bayes Classification

- Probabilistic classification methods

- Assumptions
  - predictors are independent (hence ‘naïve’)
  - predictors are normally distributed

- Applications
  - text classification (spam, topic)
  - medical diagnosis
  - fraud detection
  - insurance risk category

Naïve Bayes Classification – cont'd

- Advantages
  - Algorithms **scale linearly** with number of variables
  - Uses marginal distributions of variables

- Disadvantages
  - **Correlated features** bias the model
  - Absolute probabilities cannot be relied upon
    - only the **probability rankings** should be used
  - Assigns zero probability if a new category appears in test data
    - training data must span all possible levels of categorical features

      or
    - apply a smoothing technique (Sklearn uses Laplace estimation)

Naïve Bayes Classification in Python

sklearn.naive_bayes

GaussianNB
- assumes normally distributed features

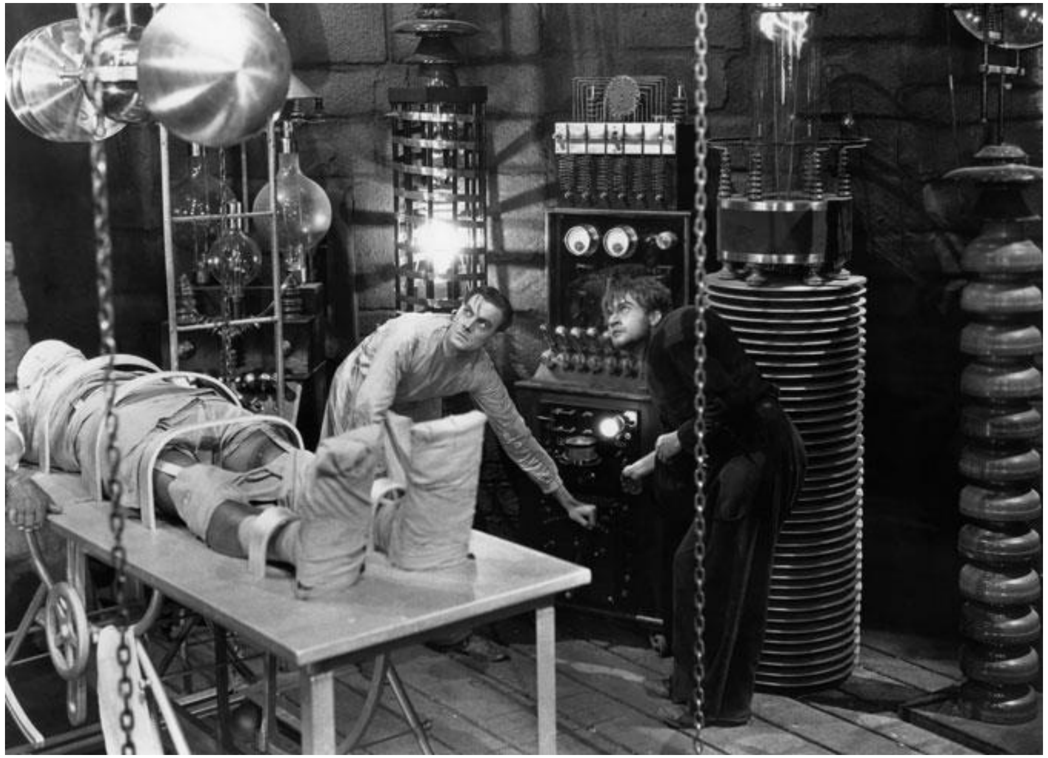
BernoulliNB
- binary/boolean features

MultinomialNB
- discrete features (multinomial distribution)
  - e.g. word counts for text classification
- uses smoothing to account for features not present in the training set

Lab 5.3.1: Comparison of Classification Methods

- Purpose:
  - To compare classification methods in Python, including Naïve Bayes
  - To apply grid search to find optimal parameters

- Materials:
  - 'Lab 5_3_1.ipynb'



Discussion

- more on Bayesian inference:
  - https://www.analyticsvidhya.com/blog/2016/06/bayesian-statistics-beginners-simple-english/
  - https://ankitrathi.com/markdown/bayesian-statistics-for-data-science/
- to be covered in a future module:
  - decision trees (nonlinear classification methods)

Questions?

Appendices

End of Presentation!