

Classification – Fundamentals & Practical Applications



Course Learning Objectives



Understand what Classification is and its applicability to many real-world scenarios



Perform simple classification tasks using logistic regression in Excel



Understand the implicit assumptions behind Classification techniques and algorithms



Create classification models in Python using statsmodels and sklearn modules



Interpret and evaluate the performance of classification models, outputs and parameters



Explore more advanced evaluation techniques such as PDP plots and SHAP values to expand your horizons.





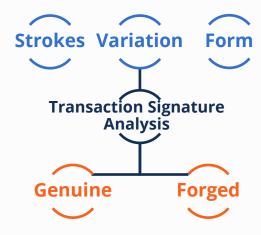
Classification Basics

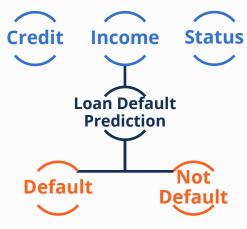


Machine Learning Use Cases

Machine Learning can be used across a wide variety of tasks in Finance.

- The target categories should be discrete variables
- Predictions are made using one or more input variables







Recap: The Machine Learning Ecosystem

There are four main types of **Machine Learning** algorithms:

Supervised Machine Learning

...uses **labelled** datasets to train algorithms in classifying data

Classification

Regression

Unsupervised Machine Learning

...uses **unlabelled datasets** to train algorithms in classifying data

Clustering

Association

Reinforcement Learning

...uses reward maximization such that the algorithm determines the optimal behaviour in an environment

Deep Learning

...learns data patterns and structure from the data itself and is scalable to big data. It can be used for supervised and unsupervised learning



Types of Classification

Binary

- Classification tasks that have two class labels
- Outcomes must be **ONE** of the two classes
- Algorithm that only deals with binary classification include Logistic Regression and Support Vector Machines

Use Case	Input Variables	Output Classes
Tumour diagnosis	Variation, Texture, Contrast, Growth Rate etc	Malignant OR Benign
Customer Prediction	Purchase History, Click history, Customer Profile	Will Buy OR Will Not Buy
Email Spam Detection	Spelling Errors, Grammatical Errors, Email domain	Spam OR Not Spam



Types of Classification

Multi-Class

- Has more than two class labels
- Outcomes must be ONE of a range of classes
- Algorithm suited for multi-class problems include decision trees and random forests.

Use Case	Input Variables	Output Classes
Tumour diagnosis	Variation, Texture, Contrast, Growth Rate etc	Malignant OR Benign OR Premalignant
Customer Prediction	Purchase History, Click history, Customer Profile	Will Buy OR Will Not Buy OR Insufficient Data
Email Spam Detection	Spelling Errors, Grammatical Errors, Email domain	Spam OR Not Spam OR Unsafe



Types of Classification

Multi-label

- Has two or more class labels
- Outcome can be ONE or MORE of the class labels
- Difference between multi-label and multi-class is that each label in the former one represents a different but related classification problem

For example, a multi-label classifier may classify an email as both spam and unsafe, or classify the tumor as both benign and premalignant

Use Case	Input Variables	Output Classes (Labels)
Tumour diagnosis	Variation, Texture, Contrast, Growth Rate etc	Malignant OR /AND Benign OR / AND Premalignant
Customer Prediction	Purchase History, Click history, Customer Profile	Will Buy OR / AND Will Not Buy OR / AND Insufficient Data
Email Spam Detection	Spelling Errors, Grammatical Errors, Email domain	Spam OR / AND Not Spam OR / AND Unsafe



Common Classification Use Cases

Binary

- Machinery Outage Prediction Failure OR Not Failure
- Anomaly Detection Fraud OR Not Fraud
- Credit Card Default Customer Likely to Default OR Not Likely to Default

Multi-Class

- Product Classification Red Wine OR White Wine OR Rose Wine
- News Classification of Articles Sports OR Lifestyle OR Economy OR Current Affairs
- Facial Image Recognition Happy OR Sad OR Angry

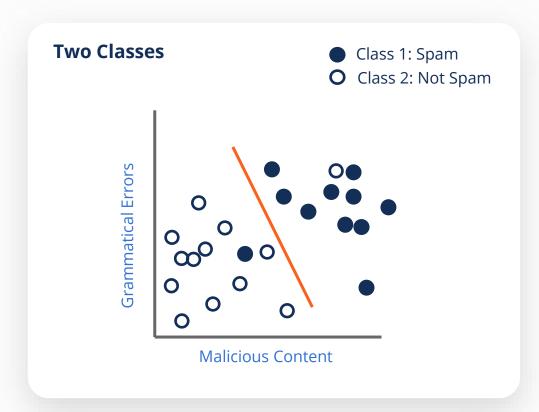
Multi-Label

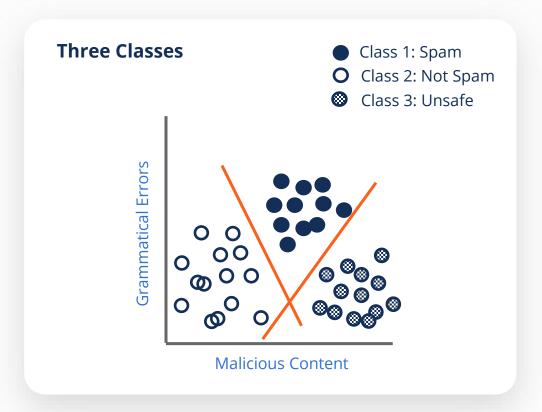
Social Tag Selection - #TogetherAtHome OR / AND #COVID19 OR / AND #WorkFromHome



Visualizing Classification

For simple scenarios, it can help to visualize the **input variables** and **output classes** on a chart.



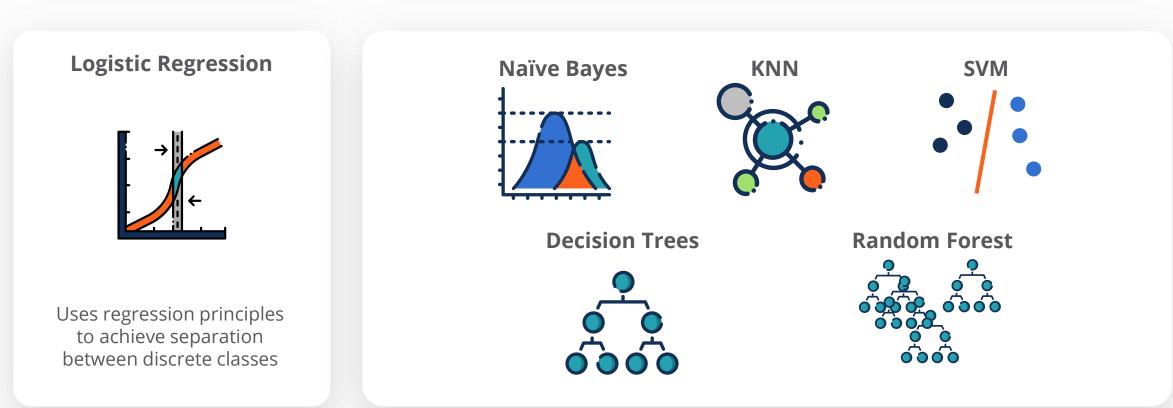


In each case, the goal is to use the input data to **separate the classes** as cleanly as possible.



Classification Algorithms

Throughout the course, we'll explore the most common classification algorithms.



We will look at the benefits of each and how to interpret and evaluate the outputs.









Understand and learn the fundamental concepts of Logistic Regression



Understand and calculate the probabilities, log odds and how these impact model interpretation



Learn how to interpret log odds and the assumptions behind Logistic regression



Be comfortable with the mathematics behind Logistic Regression and how to manipulate it



Be able to comprehend and interpret the outputs of logistic regression algorithm for business scenarios.



Practice a basic logistic regression example in Excel and Python.



Logistic regression makes a classification based on the **probability of an event happening.**

"What is the probability that this customer will purchase medical supplies?"



We determine a **threshold** (typically 0.5 or 50%) as the **cut off between prediction classes**.

In this case: customers lower than the threshold are predicted to NOT buy.

customers higher than the threshold are predicted to WILL buy.



Changing the threshold will **change the prediction class** of some observations.

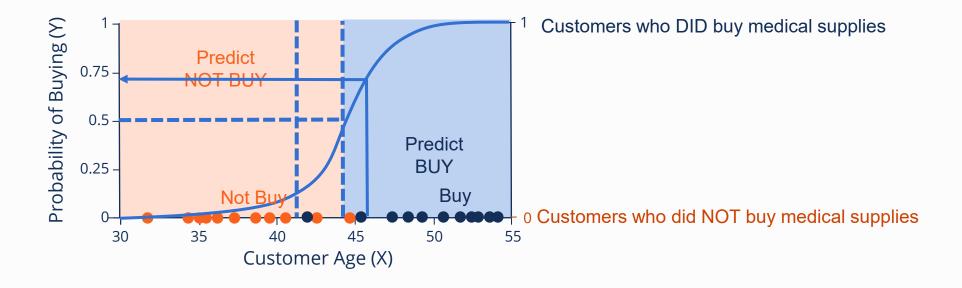


We can use **evaluation metrics** to help us decide on the **most appropriate threshold**.



Visualizing Logistic Regression

Logistic Regression probabilities are estimated using one or more input variables



Logistic Regression uses a curved line to summarize our observed data points

The logistic regression line generates probabilities **between 0 and 1**.



Defining the Logistic Regression Curve

- The logistic regression is based on the logistic function, also called the **sigmoid function**
- Mathematically this is defined as

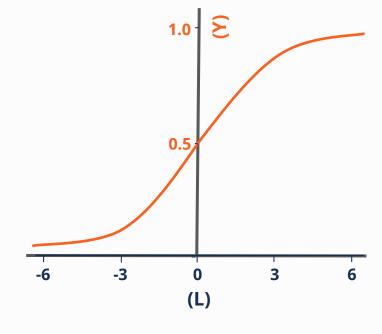
$$f(x) = \frac{1}{1 + e^{-L}}$$

(Where 'e' is the base of the natural logarithm)









At input (L) 0, output (y) = 0.5. As input (L) increases, output (y) increases.



Defining the Logistic Regression Curve

To transform a linear regression into a logistic regression we take the linear regression equation...

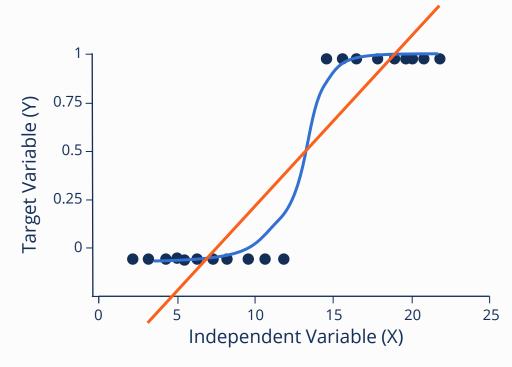
$$\beta_0 + \beta_1 x$$

and substitute it for L in our Logistic function...

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

$$P(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$

(where P(Y=1|X) is the probability of Y=1 given X input features)

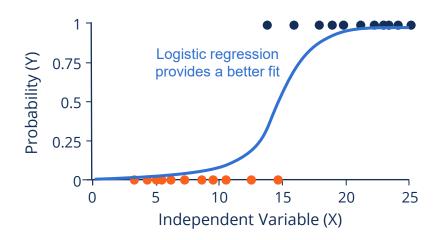


The logistic curve has been **transformed to fit** the input data.



Summary of Logistic Vs Linear Regression

Logistic Regression



- Probabilities always sit between 0 and 1.
- More suitable for predicting a binary outcome.
- More suitable for **Classification**.

Linear Regression



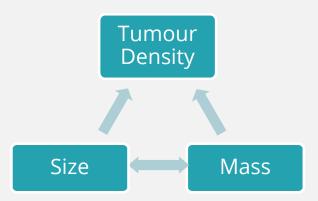
- Probabilities are not limited to a sensible range.
- Suited to predicting number of something.



Logistic regression assumptions

- The dependent variable is binary i.e. fits into one of two clear-cut categories
- There should be no, or very little, multicollinearity between the predictor variables— meaning the independent variables should be independent of each other
- 3. Logistic regression requires **large sample sizes**—the larger the sample size, the more reliable the results
- 4. The independent variables should be **linearly related** to the log odds

With **multicollinear** variables, the algorithm would be **unable to separate their effects** likely causing errors



Multicollinearity would happen because **size** and mass hold similar information.



Probability, Odds and Log Odds

 Probabilities are the chance of something happening, relative to all outcomes.

 Odds are the chance of something happening, relative to other outcomes.

- Log Odds are simply the log of the odds.
- Log odds are easier for statistical models to work with.



Odds Of Winning =
$$\frac{p(W)}{p(L)} = \frac{0.6}{0.4} = 1.5 = \frac{p(W)}{1 - p(W)}$$

Log Odds Of Winning =
$$\ln \left(\frac{60}{40} \right) = \ln \left(1.5 \right)$$



Logistic Probabilities, Odds and Log Odds

Interpreting the impact of a change in an input variable appears to be difficult at first.

$$P(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$
 Here x is our input variable.

Rearranging our logistic regression equation we can reach the following:

$$P(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$



$$P(Y = 1|X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$
REARRANGE
$$\ln\left(\frac{P(Y = 1)}{1 - P(Y = 1)}\right) = \ln\left(\frac{P(Y = 1)}{P(Y = 0)}\right) = \beta_0 + \beta_1 x$$

$$\ln\left(\frac{P(Y=1)}{1-P(Y=1)}\right) = \beta_0 + \beta_1 x$$

Log Odds of being 1

Linear Inputs



Interpreting Coefficients

We can interpret the coefficients in two ways:

$$Log(\frac{Odds \, of}{being \, 1}) = \beta_0 + \beta_1 x$$

For every **unit change in** $\boldsymbol{\mathcal{X}}$

the **log odds** will change by β_1 .

Odds of being 1 =
$$\exp(\beta_0 + \beta_1 x)$$

For every **unit change in** $\boldsymbol{\mathcal{X}}$

the **odds** will change by $exp(\beta_1)$

Odds are generally easier to interpret than log odds.



Interpretation Scenario

You are tasked by your company with **predicting the likelihood of purchase** of medical supplies (Y).

Input features:

Equation

- X₁ = Customer tenure
- X₂ = Purchased in the last year

Odds of Purchase = $\exp (\beta_0 + \beta_{Tenure} x_1 + \beta_{Purchased} x_2)$

Coefficients:

- Customer loyalty coefficient $\beta_{Tenure} = 0.6$
- Purchased last year coefficient $\beta_{Purchased} = 0.2$

Odds Interpretations:

- $\exp(\beta_{Tenure}) = 1.82$ "Every extra year as a customer **increases the odds** of purchase by a factor of **1.82**.
- $\exp(\beta_{Purchased})$ = **1.22** "Customers that purchased in the last year have **22% higher odds** to buy again this year.

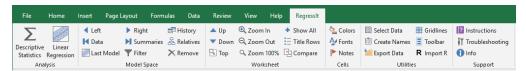


Logistic Regression in Practice

Excel

Regressit is a powerful Excel add-in tool that performs multivariate descriptive data analysis and linear as well as logistic regression





Python packages



Scikit-learn provides a range of supervised and unsupervised learning algorithms

statsmodels statsmodels provides classes and functions for many different statistical models and tests





Classification Algorithms



Classification Algorithms



Learn about the basic Classification algorithms and when and how to use them



Understand the underlying considerations and assumptions of these algorithms



Learn the inner workings of the algorithms and understand how they categorize observations



Understand how to interpret the parameters, outputs and evaluation metrics for the algorithms



Be able to apply these to real-world scenarios and learn about their applications

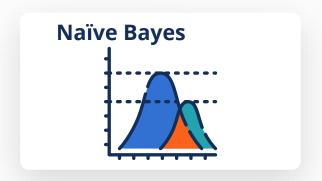


Apply each classification algorithm in Python identify the quality of results from each.



Algorithms Overview

We will review five common algorithms used to build classification models:













Naïve Bayes

- Naïve Bayes is a probabilistic model based on Bayes theorem; it gives us classifications based on probabilities
- Bayes theorem generates the probability of one event, given the probabilities of other events

Strengths

- Easy to use and good for large datasets
- Can be used to solve multi-class prediction problems

Weaknesses

- Assumes independence in features, which makes it less applicable on most real-world datasets
- Bayes Theorem states the **probability (P)** of an event A happening given that an event B occurred can be given by:

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

Where A is the *hypothesis* or *outcome variable*, and B is the *evidence* or *features*



Naïve Bayes – Example

We want to predict the likelihood of an email being spam, given it contains a grammatical error.

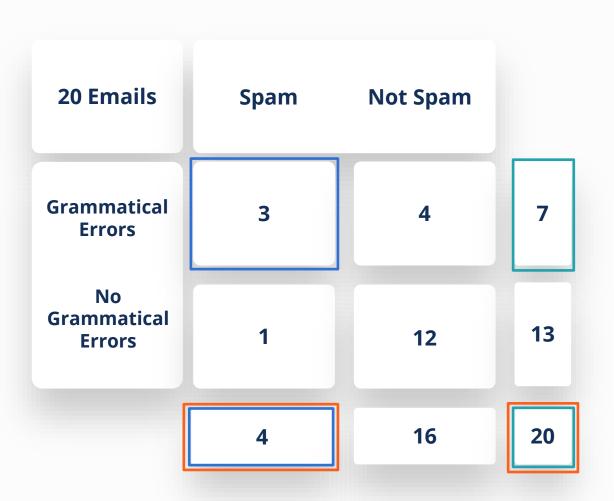
Observation	Spam Email?	Grammatical Errors?	
1	Yes	Yes	
2	No	No	
3	No	Yes	
4	No	No	
5	No	No	
6	Yes	No	
7	No	No	
8	No	No	
9	No	Yes	
10	No	No	
•••	•••	•••	

20 Emails	Spam	Not Spam	
Grammatical Errors	3	4	7
No Grammatical Errors	1	12	13
	4	16	20



Naïve Bayes - Example

We want to predict the likelihood of an email being spam, given it contains a grammatical error.



•
$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

P(Spam | Error) =

•
$$P(Error|Spam) = 3/4 \text{ or } 0.75$$

•
$$P(Spam) = 4/20 \text{ or } 0.20$$

•
$$P(Error) = 7/20 \text{ or } 0.35$$

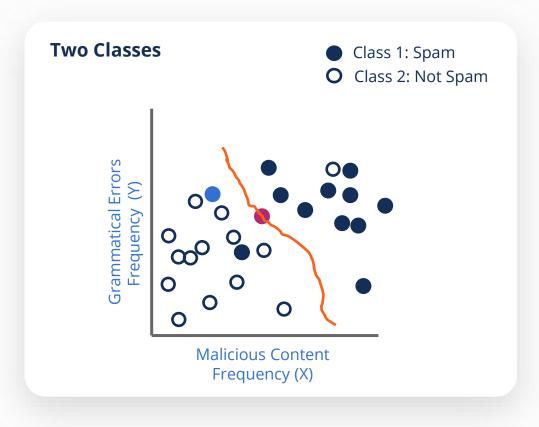
• P(Spam | Error) =
$$\frac{0.75*0.20}{0.35}$$
 = **0.43** or **43% likely**



K-Nearest Neighbours (KNN)

KNN assigns output classes based on the most similar observations in our sample space.

By similar, we mean those who have the closest input values.



New observation - Which class would you likely assign it to? Not Spam!

The new observation is closer to the Not Spam observations, meaning its characteristics are more similar.

• New observation - The nearest observation is Spam.

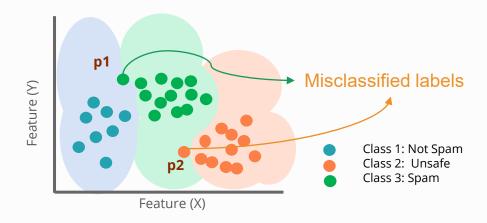
However, the next 3 closest are Not Spam.

How many of the nearest observations should we choose?

Once we have optimized this number of nearest neighbours, we can visualize our decision boundary, which represents the boundary between Spam and Not Spam.



K-Nearest Neighbours - Example



As the misclassified point **p1** (Not Spam) has a green point (Spam) closest, a value of K=1 misclassifies the Not Spam email as Spam.

The exact thing happens in the case of p2

Strengths

- Simple and easy implementation (no assumptions)
- Can be used for classification and regression

Choosing the right value for K is critical

K=1 will simply classify the data point on the basis of one closest neighbour

K=1000 will not identify categories in the data at all

Increasing K improves prediction due to averaging of the distance, the algorithm selects the most suitable point

An optimal value of K must be selected depending on the size of the dataset

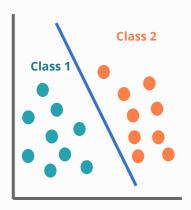
Weaknesses

 Performance decreases as the number of examples and/or independent variables increases

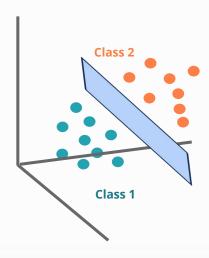


Support Vector Machines (SVM)

In 2D sample space, separation is created using a line



In 3D sample space, separation is created using a plane



SVMs separate data points with a line or plane through the sample space

SVM aims to find a plane that maximises the separation distance between data points of both classes

The algorithm defines the criterion for a boundary that is maximally far away from any data point

This distance to the closest data point from the decision surface determines the margin of the classifier

Strengths

 Uses a subset of training points in the decision function so it is memory efficient

Weaknesses

 The algorithm does not directly provide probability estimates, these are calculated using expensive techniques



Decision Trees

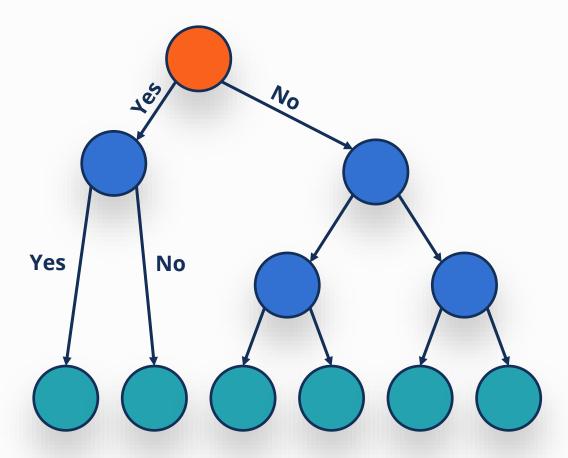
A decision tree is a cascading set of questions, used to incrementally separate classes and improve predictive power.

Strengths

- Simple to understand and interpret (visualise)
- Used for classification or regression
- Requires little data preparation as it can handle both numerical and categorical

Weaknesses

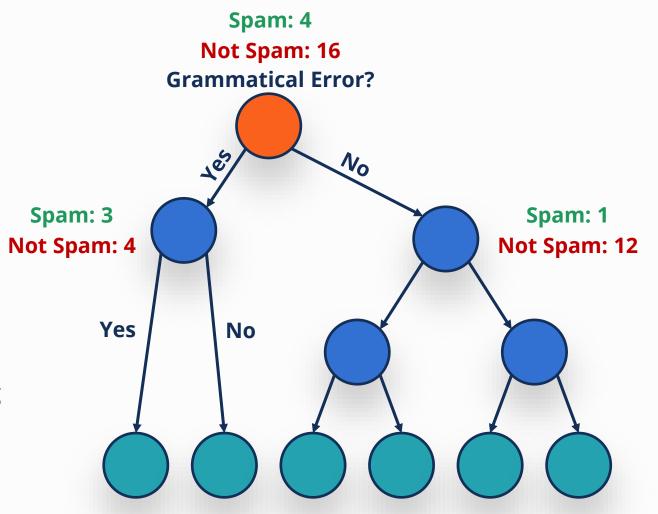
- Tends to overfit (the trained tree doesn't generalise well to unseen data)
- Small changes in data tends to cause big difference in tree (instability)
- Can become expensive to compute with high dimensionality





Decision Trees - Example

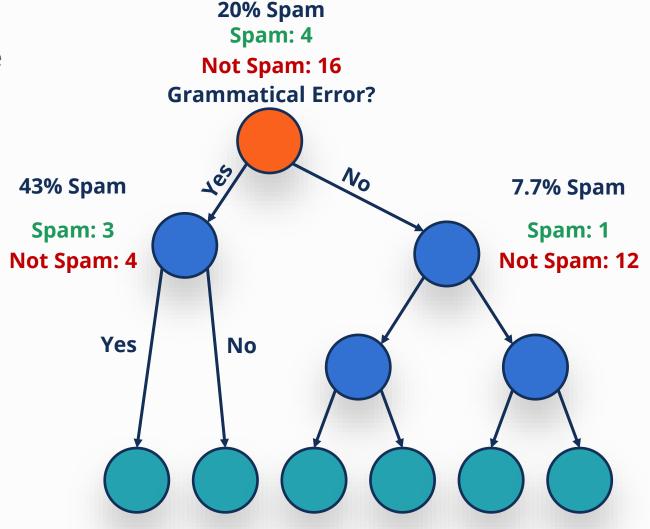
- Each node represents a feature/attribute of the data set and branches represent a decision
- The decision tree starts at the root node
- We go down the tree asking true/false questions at decision nodes...
- ...until the leaf node (or outcome) is reached
- Once the tree is completed, it can be used to evaluate each email by answering the questions until a leaf node is reached and a prediction is made.





Decision Trees - Example

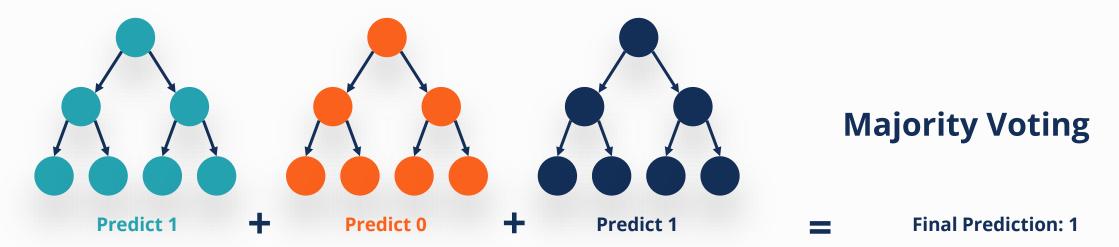
- Splitting is the process of dividing a node into child nodes
- The goal is to make each of the child nodes more "pure" or homogenous – containing more similar classes of observations
- Separating emails according to grammatical errors adds predictive value to the model





Random Forest

A random forest is known as an ensemble model since it combines the results from multiple other models; in this case decision trees.



Strengths

- Improved accuracy (reduces overfitting) and more powerful than decision trees
- Used in regression and classification

Weaknesses

- The complexity of the algorithm can cause it to become slow and inefficient
- Real-time predictions can be slow due to large inputs





Evaluation & Interpretability



Evaluation & Interpretability



Understand the basic outcomes of classification and how they are represented visually in a confusion matrix.



Learn how to evaluate and compare models with evaluation metrics such as accuracy, precision and recall.



Understand when certain metrics may be more appropriate than others.



Learn more advanced evaluation metrics that build on basis
Precision and Recall, such as F-scores.



Understand how to interpret AUC-ROC curves and use them to compare model results.



Implement the above model evaluation techniques in Python using SkLearn.



Model Evaluation Basics

- Evaluation metrics are important because they ensure that the model is performing correctly
- To set up our model evaluation, the dataset is often split into training and testing data

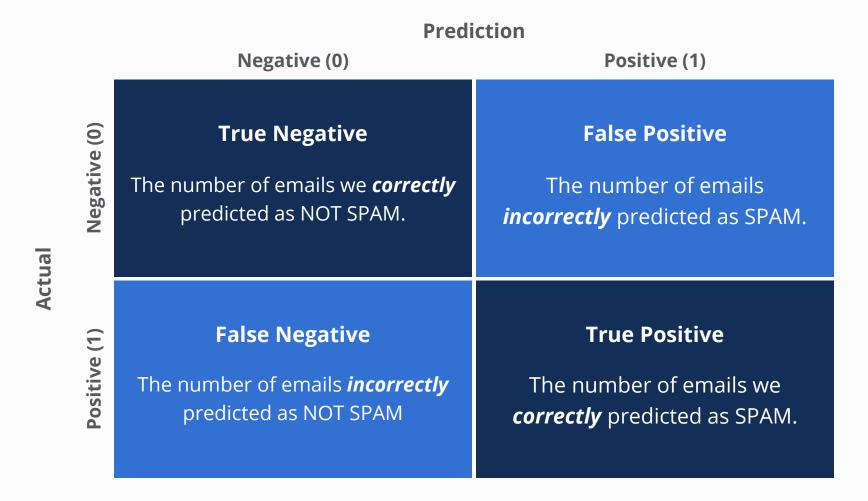


- The model learns from the training data
- The testing data is used to test how well the model performs on new unseen data
- Better evaluation results ensure that the model can be used in real-world on new data reliably



Confusion Matrix

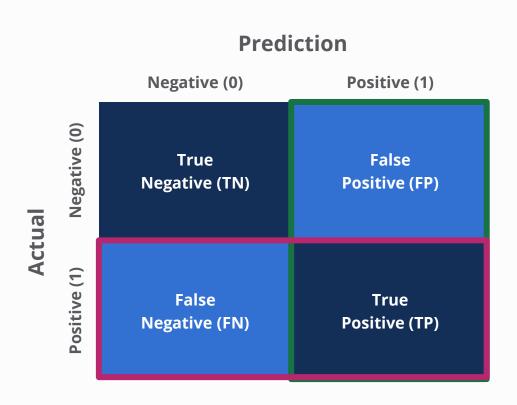
The confusion matrix helps us understand the quality of our predictions.





Evaluation Metrics

There are **four key metrics** that can help summarize the observations in the confusion matrix:





Accuracy = (TN + TP) / Total Predictions

Describes what proportion of predictions were correct (may not always be the best indicator of performance).



Precision = TP / (TP + FP)

How good are the positive predictions? Out of those predicted positive, how many were actually positive?



Recall = TP / (TP + FN)

Describes what proportion of the actual positive cases were correctly identified.



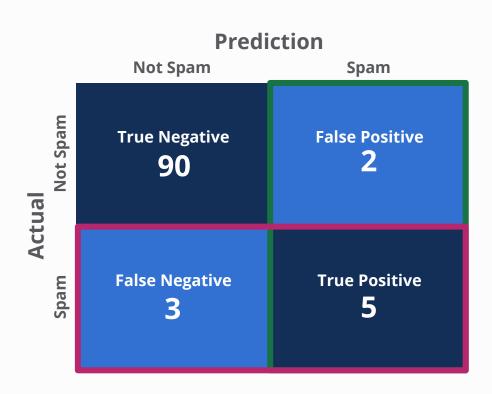
F1 Score = 2 * [(Precision*Recall) / (Precision+Recall)]

Provides a balance between precision and recall.



Evaluation Metrics Example

Consider an example where we have 100 emails and we use a model to predict whether an email is spam or not. Here **SPAM** emails is our positive class and **NOT SPAM** is our negative class.



$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN} = \frac{95}{90 + 3 + 2 + 5} = 0.95$$

$$Precision = \frac{TP}{TP + FP} = \frac{5}{5 + 2} = 0.71$$

$$Recall = \frac{TP}{TP + FN} = \frac{5}{5 + 3} = 0.62$$

In this situation, **Precision** and **Recall** are equally important:

 we don't want to pass any SPAM emails as NOT SPAM (as they could be dangerous)

and at the same time:

• we would not want any NOT SPAM emails going into our SPAM box (as that email could be important to us).



Precision Vs Recall

- Accuracy works well for balanced classes (having roughly equal number of samples of every class)
- Precision is a good choice of metric when we have imbalanced classes and we want to minimized false positives.
- Recall is a good choice of metric when we have imbalanced classes and we want to minimize false negatives.
 - In tumour risk detection, we would want to reduce the number of False Negatives.
 - We cannot afford to miss any malignant samples in the data.
 - **Recall** would be the preferred metric here because it measures the proportion of actual malignant tumours that we detected.
 - Misclassifying a low risk tumour as risky is obviously not ideal, but is a secondary priority.
- Ideally, a model with both a high recall and precision score would be preferred.

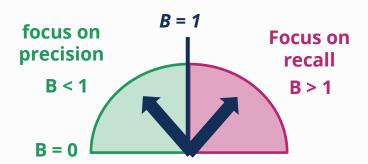


F_{β} –Score

 F_{β} is a combined evaluation metric that balances **precision** and **recall**.

By choosing any value of β , we can modify our equation to control the weight of Precision and Recall in our calculations.

$$F_{\beta} = \frac{1 + \beta^2}{\frac{\beta^2}{Recall} + \frac{1}{Precision}}$$



 F_1 and F_2 are the most common iterations of F_β score



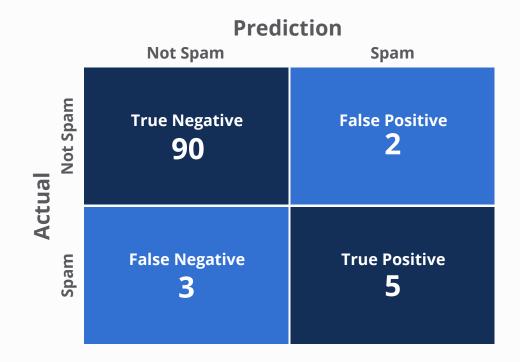
Practical Example F_β

We can calculate F₁ score as:

$$F_1 = \frac{1 + I^2}{\frac{I^2}{0.62} + \frac{1}{0.71}} = 0.66$$

And we can calculate F₂ as:

$$F_2 = \frac{1 + 2^2}{\frac{2^2}{0.62} + \frac{1}{0.71}} = 0.63$$



- F₁ gives equal importance to both **Precision** and **Recall**
- In this example, F₁ would be a relatively better choice as we prefer both Precision and Recall somewhat equally here.



Is Accuracy the Best Choice?

Now consider we have 1000 sample observations:

- Not Spam (-ve) 980 samples
- **Spam** (+ve) 20 samples

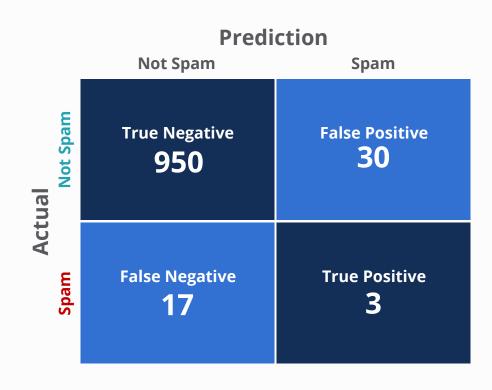
This is an **imbalanced class** problem.

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} = \frac{953}{10+950+30+17} = 0.95 = 95\%$$

However, we are failing to correctly predict the class we care about - the **SPAM** emails, and we can see it in the poor performance of the other metrics:

- Precision: 3/33 = 10%
- Recall: 3/20 = 15%

So **Accuracy may not be the best choice** for all problems





The ROC Curve

The Receiver Operating Characteristic (ROC) curve visualizes the model performance and is a useful way to evaluate the results of a binary classification model.

True Positive Rate

Describes the proportion of **actual positives** that we correctly identified.

Same as recall.

$$TPR = \frac{True\ Positive}{True\ Positive + \ False\ Negative}$$

Random Classifiet

False Positive Rate

Describes the proportion of **actual negatives** that we flagged as positive.

$$FPR = rac{False\ Positive}{True\ Negative +\ False\ Positive}$$

Each classification model we create can be **plotted as a curve** on this chart.

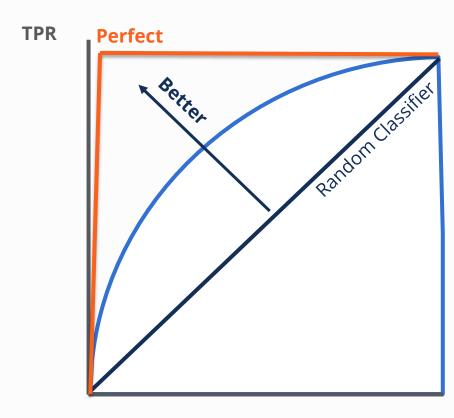
The further the ROC curve from the **random classifier** (towards TPR), **the better the model is at predicting overall results.**

FPR



The ROC Curve - AUC

- AUC stands for Area Under the Curve. It is calculated as the surface or area that sits underneath the curve.
- Helps summarise the ROC curve into a single number between 0 and 1, to help compare different algorithms
- Higher AUC (close to 1) means the model is better at separating classes.
- A perfect model would display a square in order to maximize the area.

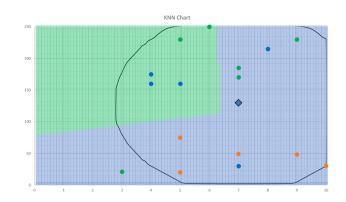


FPR



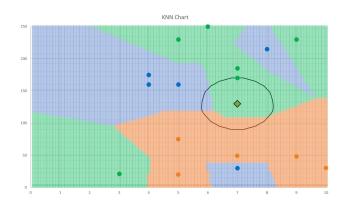
Overfitting Vs Underfitting

Underfitting and Overfitting are terms that helps us summarize the performance of a model.



Underfitting

- Is **too simple** for the scenario
- Does not perform well on the training data
- Oversimplifies patterns in the data
- Will not perform well on testing data



Overfitting

- Learns the training data too well (effectively learns the answers)
- Will perform very well on training data.
- But is unable to look at the bigger picture and generalize trends
- Will likely perform badly on testing (new) data



We've built a good working model, now what?

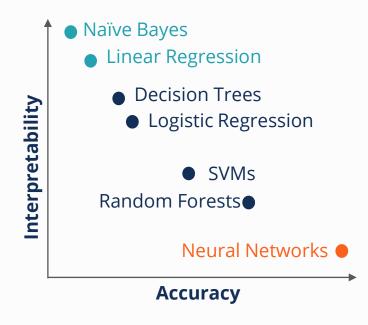
Often a model is the spark for follow up questions, such as:

- To what extent can we explain the reasons why our model makes the predictions that it does?
- What are the main drivers for making this class prediction?
- What are the main drivers for predicting this **customer will purchase my product**?
- What influences positively/negatively on that purchase prediction?
- How large is the influence of each input variable?
- How can we explain the difference between one prediction and the next?



Interpretability of Machine Learning Models

- A model is **interpretable** if it can be understood by anyone without additional explanation.
 - Interpretability ensures that the model is reliable, fair, robust and reasonable
 - Basic models, like Linear models or Naïve Bayes models, are highly interpretable and user-friendly
- A model is **accurate** is it can make higher quality predictions on average.
 - For better accuracy in models that use real-world data we tend to require more complex models (often less interpretable) like Neural Networks.



We must consider the extent to which we are required to dissect and provide interpretable outputs.



Interpretability and Explainability

Interpretability A model is interpretable if you can work out the simple cause and effect relationship between inputs and outputs with relatively simple logic.



Explainability

A model is **explainable** if we can fully dissect each part of the model and explain it's role in the decision making process.

White Box Models are easy to interpret and explain.

Reinforces accountability and audit.

Black Box Models make it difficult to pinpoint causality for a particular outcome.

Less helpful for accountability or audit.



Introduction to Feature Importance

- **Feature importance** helps determine how well each of the individual features helps predict the **overall outcome**.
- The **higher** the total importance, the **more influence** that feature has on what we want to predict.
- This technique tends to be used in tree-based algorithms such as **Decision Trees** or **Random Forests** but can also be used more generally.
- There are different types of feature importance depending on **how we define importance** e.g. *number of times a feature is used to split a branch in a decision tree.*



We can see **genetics**, **age** and **being sedentary** have high importance when **predicting whether a tumor is malignant**.

Strengths

- Model learns better by prioritising important features
- Training time and memory requirements reduces

Weaknesses

- Mostly rely on approximations other than for linear models
- Most methods cannot deal with high-dimensional data



Introduction to Partial Dependence Plots (PDP)

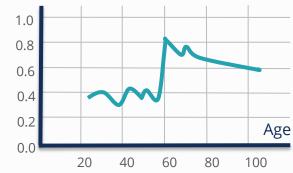
- Partial Dependence Plots (PDP) show the marginal effect of independent feature(s) on model predictions
- They shows whether the relationship between the outcome and predictor variable is **linear**, **monotonic** or **more complex**
- Straight flat PDP indicates that the feature is not important.
- When predicting malignant tumours increase in age (>55)
 and genetic likelihood score (>0.5) means higher likelihood of
 tumour being malignant

Strengths

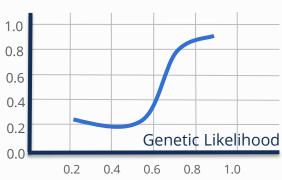
The interpretation of the plots is intuitive and easy to understand

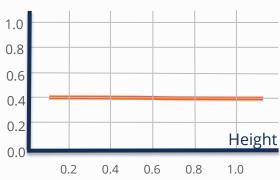
Weaknesses

- Assumes independence in the features
- Limited interpretability with more than 2 features



Malignant Tumour Probability







Introduction to SHapley Additive exPlanations (SHAP)

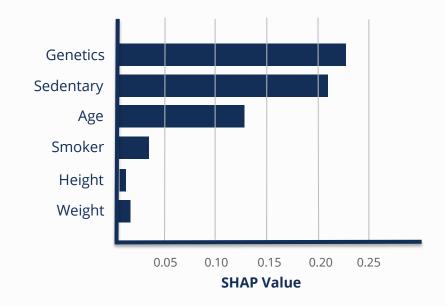
- SHAP values help explain the contribution each feature is making on an individual prediction.
- When we are talking about individual observations, we are talking about local explainability.

Instead of asking:

 How much is the prediction of a tumour being malignant driven by a persons age?

We would ask:

• How much is the prediction of this patients tumour being malignant driven by the fact that she is over 65 years old?



Genetics was the highest driver behind this positive prediction.

Strengths

- Makes black-box models easy to explain to all audiences
- Allows for decomposing of each prediction by all the features

Weaknesses

- SHAP can be slow to plot
- It is possible to create intentionally misleading interpretations that can hide biases

