Conceptual Session
FDS, DAV & ML
MIT ADSP

Topics

- Hypothesis testing
  - Hypothesis Formulation
  - One Tailed Test vs Two Tailed Test
  - Type | and Type || Errors
- Data Exploration and Networks
  - Testing issues and correction networks
  - Dimensionality Reduction
  - Data analysis using Graph Networks
- Unsupervised Learning
  - Different clustering Algorithms
- Regression
  - Simple Linear and Multiple Regression
  - Overfitting, Bias variance tradeoff and Regularisation
  - Cross validation and Bootstrapping
- Classification
  - Logistic Regression and KNN
  - Performance Measures Classification

Hypothesis Testing

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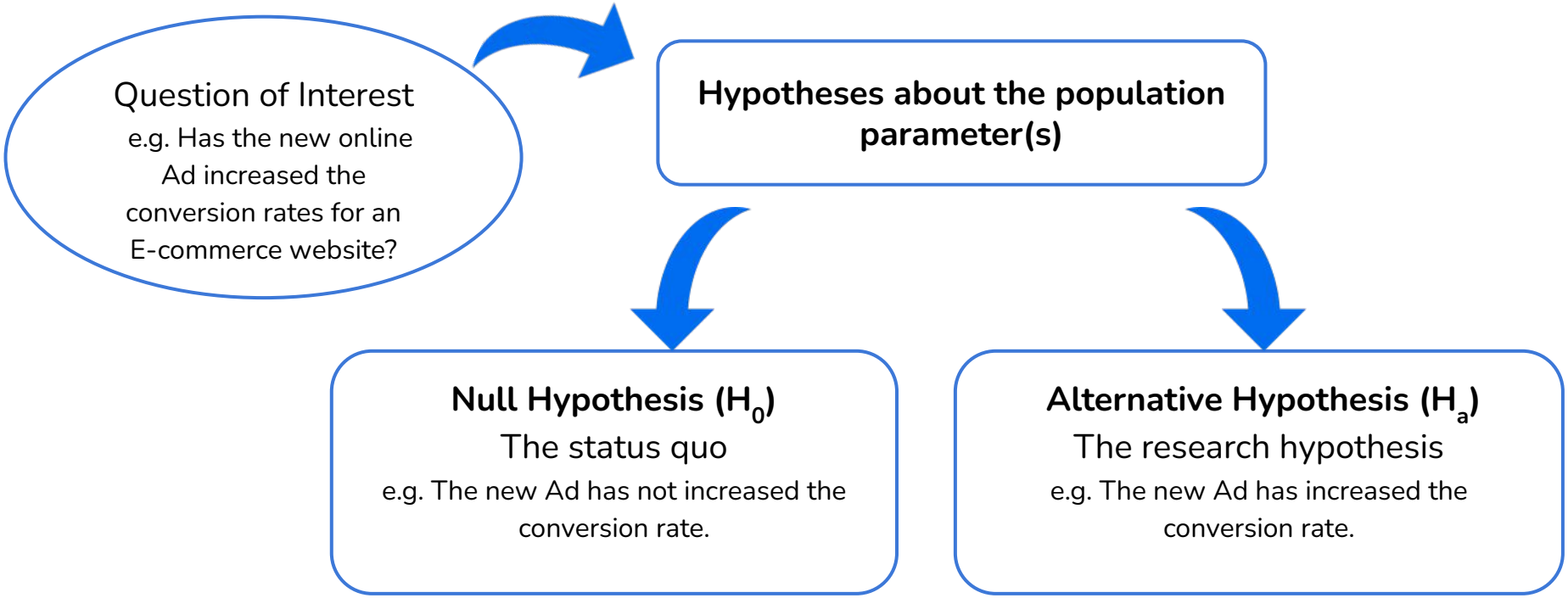
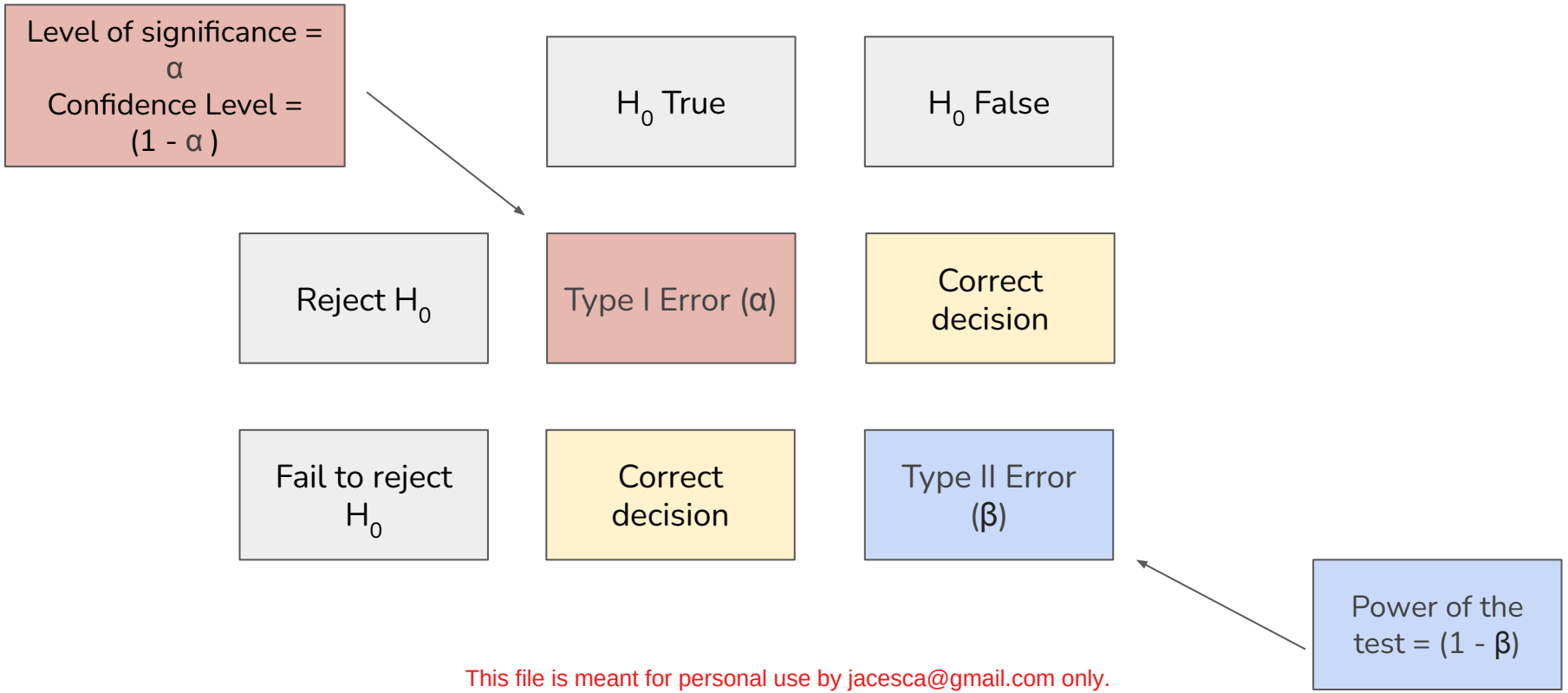
Introduction to Hypothesis Testing



Key terms in Hypothesis Testing

P-Value	• Probability of observing equal or more extreme results than the computed test statistic, under the null hypothesis. • The smaller the p-value, the stronger the evidence against the null hypothesis.
Level of Significance	• The significance level (denoted by α), is the probability of rejecting the null hypothesis when it is true. • It is a measure of the strength of the evidence that must be present in the sample data to reject the null hypothesis.
Acceptance or Rejection Region	• The total area under the distribution curve of the test statistic is partitioned into acceptance and rejection region • Reject the null hypothesis when the test statistic lies in the rejection region, else we fail to reject it
Types of Error	• There are two types of errors - Type I and Type II

Type I and Type II errors



Let's go through an example

Problem Statement: The store manager believes that the average waiting time for the customers at checkouts has become worse than 15 minutes. Formulate the Null and the Alternate hypotheses.

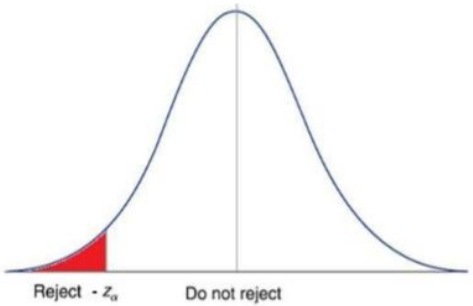
Null Hypothesis (H_0): The average waiting time at checkouts is less than equal to 15 minutes.

Alternate Hypothesis (H_a): The average waiting time at checkouts is more than 15 minutes.

Type I error (False Positive): Reject Null hypothesis when it is indeed true. "The fact is that the average waiting time at checkout is less than equal to 15 minutes but the store manager has identified that it is more than 15 minutes".

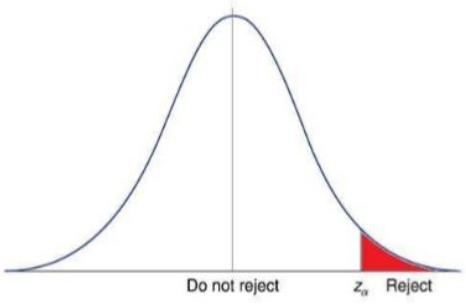
Type II error (False Negative): Fail to reject Null hypothesis when it is indeed false. "The fact is that the average waiting time at checkout is more than 15 minutes but the store manager has identified that it is less than equal to 15 minutes".

One-tailed vs Two-tailed Test



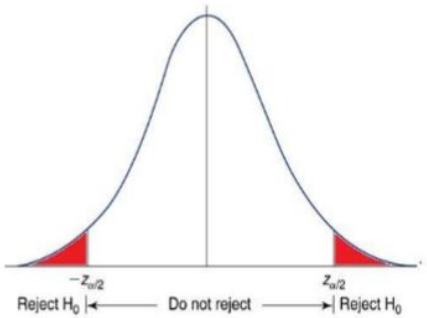
- Lower tail test.
- H_1: $\mu <$ .....

Reject H_0 if the value of test statistic is too small



- Upper tail test.
- H_1: $\mu >$ .....

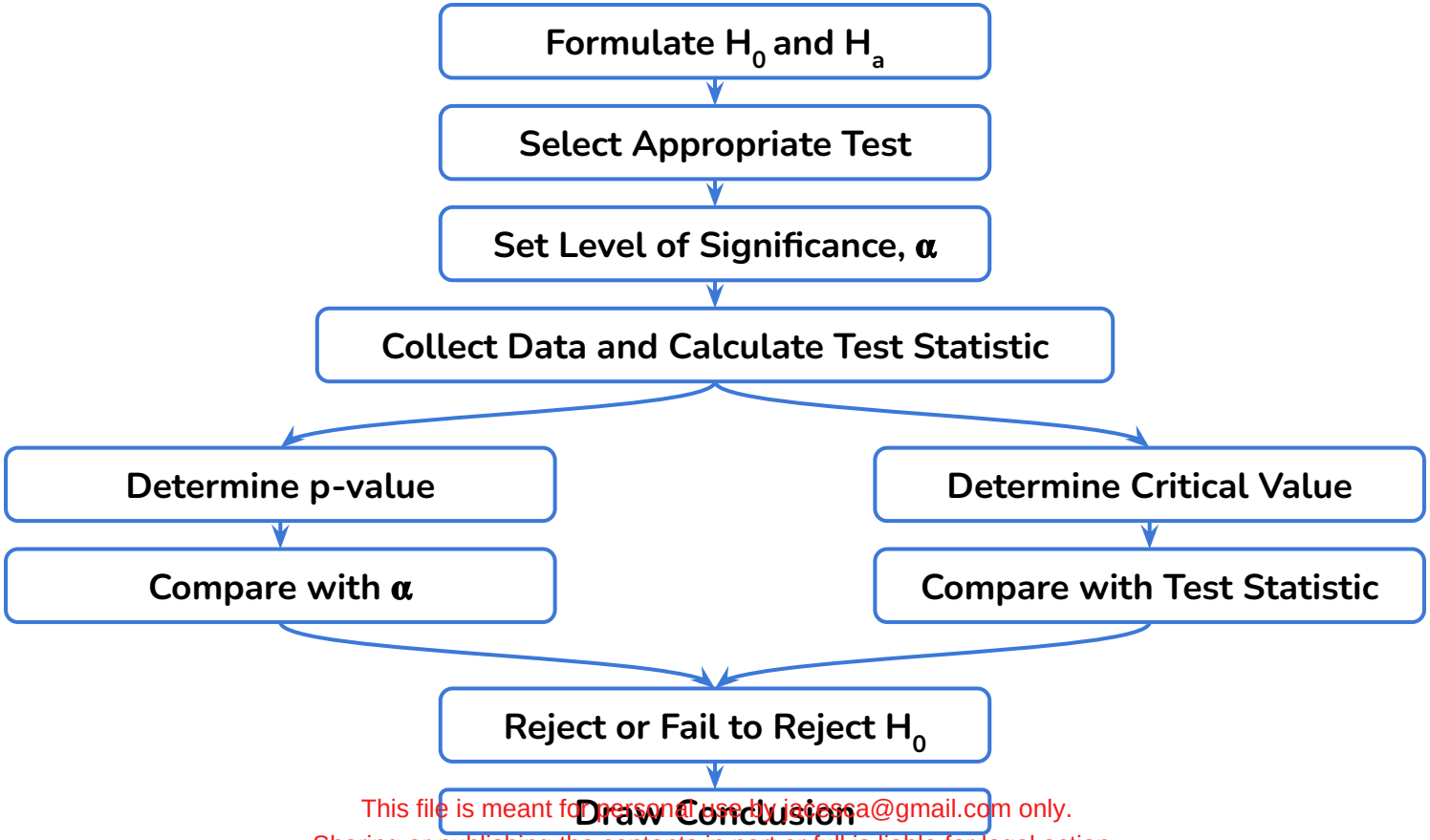
Reject H_0 if the value of test statistic is too large



- Two tail test.
- H_1: $\mu \neq$ .....

Reject H_0 if the value of test statistic is either too small or too large

Hypothesis Testing Steps



Data Exploration and Networks

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Multiple testing issues and their corrections

Multiple testing problem

- This problem arises when multiple hypotheses are tested simultaneously
- The number of false positives increases as you test more hypotheses

The following are the correction methods that can be used to deal with this problem:

- **The Bonferroni correction**
  - It states that the corrected significance level for all the test combined is **α/m.** where **m** is the total number of hypothesis tests performed
  - Reject null hypothesis H_0 when **p-value ≤ α/m or m*p-value ≤ α**
- **The Holm-Bonferroni correction**
  - Sort p-values in increasing order: p(1) ≤ · · · ≤ p(m), The corrected significance level for the ith test is **α/(m-i+ 1)**
  - Reject null hypothesis H_0 **p(i) ≤ α/(m-i + 1) or (m – i + 1)*p(i) ≤ α**
- **The Benjamini-Hochberg correction:**
  - Sort p-values in increasing order: p(1) ≤ · · · ≤ p(m), The corrected significance level for the ith test is **α*i/(m)**
  - Reject null hypothesis H_0 **p(i) ≤ α*i/(m) or m*p(i)/i ≤ α**

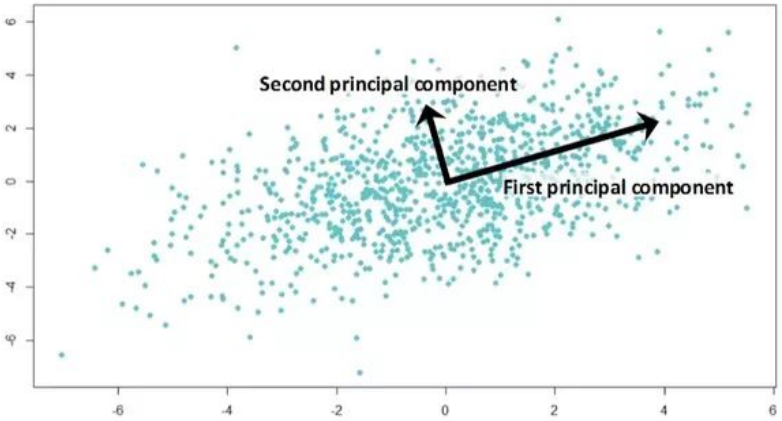
Need for dimensionality reduction

- Dimensionality reduction is the idea of reducing the number of dimensions in the feature space.
- In machine learning, we tend to add many features to get more accurate results. However, after a certain point, the performance and robustness of the model starts decreasing and computational complexity starts increasing as we increase the number of features. This is called the curse of dimensionality, where the sample density decreases exponentially with the increase of dimensionality.
    - We use dimensionality reduction to transform the data into low dimensions while keeping most of the information intact.
    - It also helps us to visualize high dimensional data in 2D & 3D.
- The following are two techniques we can use for dimensionality reduction:
    - PCA
    - t-SNE

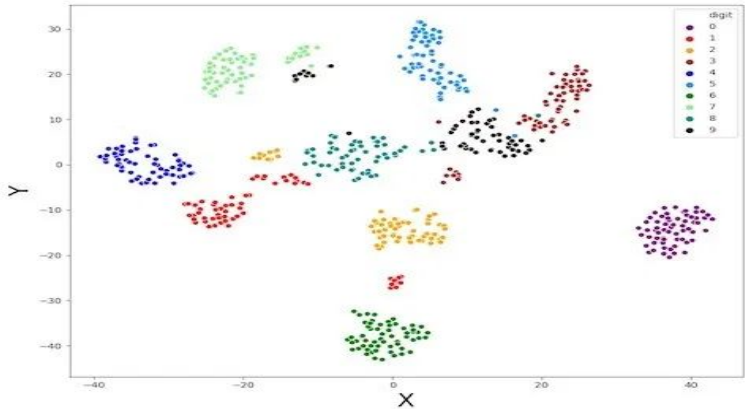
PCA and t-SNE

Principal component analysis (PCA) is a dimensionality reduction technique used for the identification of a smaller number of uncorrelated variables known as principal components from a larger dataset. The technique is widely used to emphasize variation and capture strong patterns in a dataset.

t-Distributed Stochastic Neighbor Embedding (t-SNE) is a technique for dimensionality reduction that is particularly well suited for the visualization of high-dimensional datasets.



PCA



t-SNE

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Differences between PCA and t-SNE

PCA	t-SNE
It tries to capture the linear structure in the data	It tries to capture the non-linear structure in the data
It focuses on preserving the global structure of the data	It focuses on preserving the local structure (i.e. clusters) of the data
There are no hyperparameters involved in PCA	There are some hyperparameters like perplexity, no. of dimensions, etc. in t-SNE
PCA works by separating points as far as possible based on the highest variance	t-SNE works by grouping points as close as possible based on the characteristics of the point
It might easily get affected by outliers	It can handle outliers as well

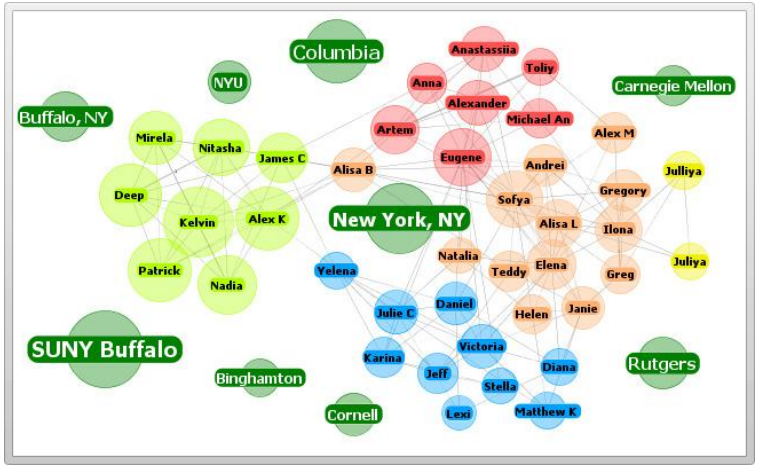
Why do we study Graphs and Networks?

A Graph is basically the study of relationships. It has certain nodes (vertices) and links (edges) that create these relationships.

It can be used to model and create many types of relations and processes in physical, social, biological, and information systems, and has a wide range of applications:

- Community networks (through social media)
- Google maps
- DNA/RNA sequencing
- Search engine rankings

Example: This friendship network shows us a bunch of friends, the networks they belong to, and the social cliques they are part of.



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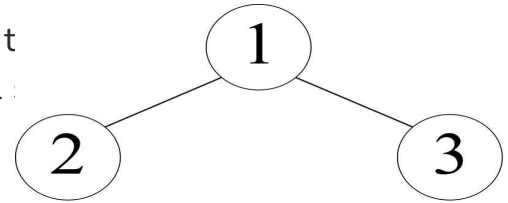
The Adjacency Matrix

We can represent the graph as an adjacency matrix, where the row and column indices represent the nodes, and the entries in the matrix represent the absence or presence of an edge between the nodes.

Example: For a graph 2-1-3, the adjacency matrix will be -

$$\begin{pmatrix} 0,1,1 \\ 1,0,0 \\ 1,0,0 \end{pmatrix}$$

An adjacency matrix is t h into a mathematical form that tells us whether there are any edges between all his matrix will always be zero if there are no self-loops in the network.



Unsupervised Learning

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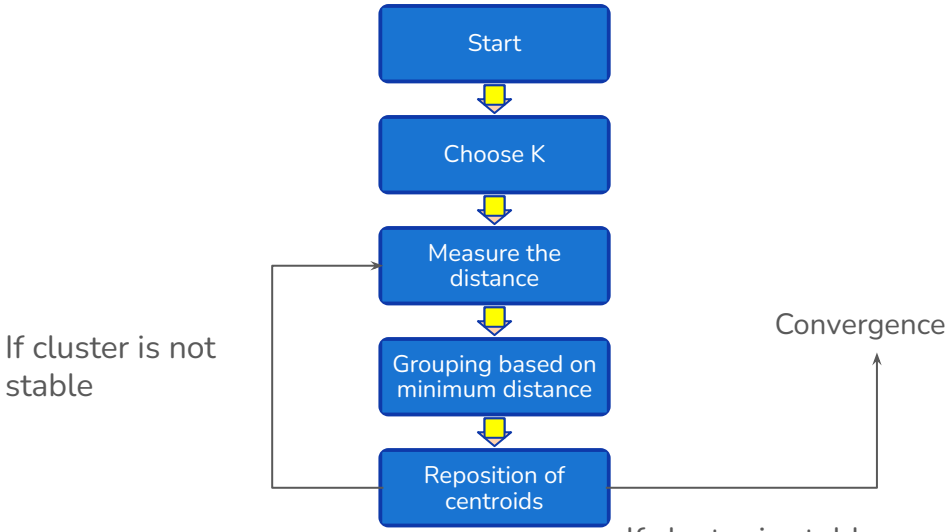
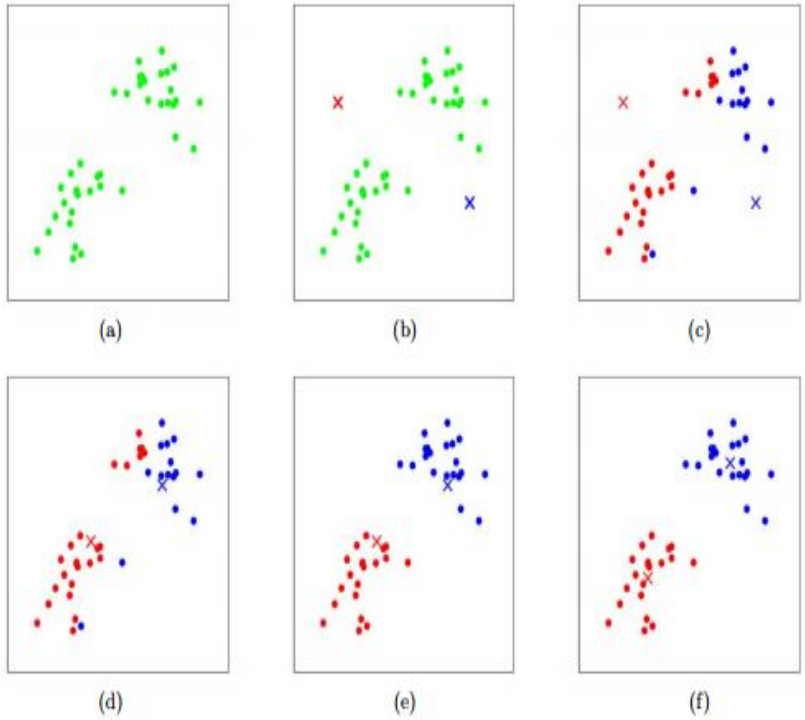
K-Means clustering

K-Means Clustering is an iterative **algorithm** that divides the unlabeled dataset into **K** different **clusters** in such a way that each point in the dataset belongs to only one group that has similar properties.





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Advantages and Disadvantages of using K-Means clustering

Advantages:

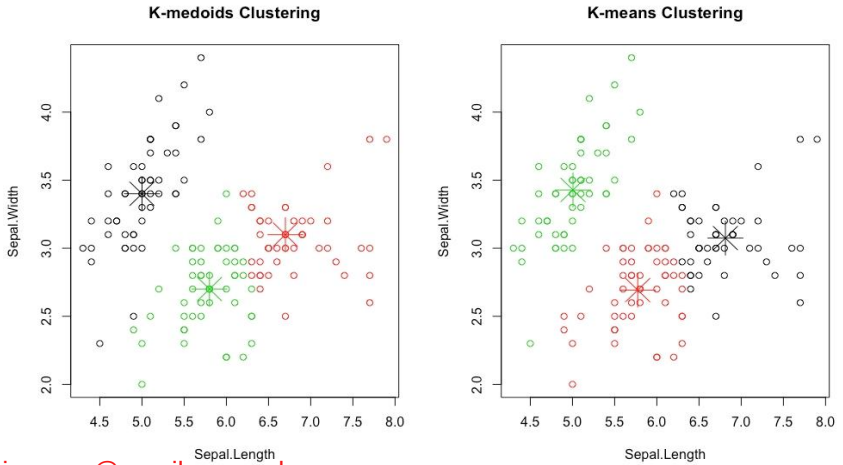
- K-Means is relatively simple to implement.
- It scales to large datasets.
- It also guarantees convergence.
- It can easily be adapted to new examples.

Disadvantages:

- It is difficult to identify the value of K.
- K-Means has trouble clustering data where clusters are of varying sizes and densities.
- It can easily be affected by outliers.
- It assumes the data shape to be spherical and does not perform well on arbitrary data.
- It depends on the initial values assigned to the centroids and gives different results for different initializations.

Alternative to K-Means - PAM (K-Medoids) clustering

- The problem with K-Means is that the final centroids are not interpretable, i.e., centroids are not actual points but the means of the points present in the cluster.
- The idea behind K-Medoids clustering is to make the final centroids as actual data points so that they are interpretable.
- In K-Medoids, we only change one step from K-Means which is to update the centroids. In this process, if there are m points in a cluster, swap the previous centroids with all other (m-1) points from the cluster and finalize the point as new centroid which has minimum loss.
- Because of this, unlike K-Means, it is robust to outliers and converges fast.
- You can see in this image that the centroids in K-Medoids are the actual data points represented as the cross, unlike K-Means.



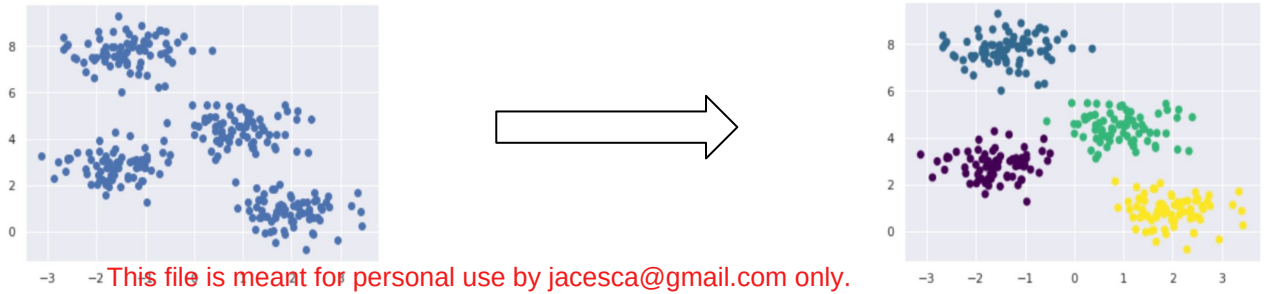
Expectation Maximization in GMM clustering

In GMM, we need the parameters of each Gaussian (mean, variance, etc.) in order to cluster our data, but we need to know which sample belongs to what Gaussian in order to estimate those very same parameters.
That is where we need the EM algorithm. There are two steps involved in this algorithm:

1. **The E-step:** It estimates the probability that a given observation is in a cluster/distribution. This value will be high when the point is assigned to the right cluster and lower otherwise.
2. **The M-step:** In this step, we want to maximize the likelihood that each observation came from the distribution.

After that, we reiterate these two steps and update the probabilities of observation being in a cluster.

Example of GMM clustering



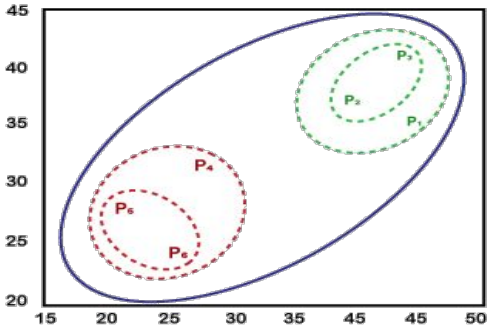
Hierarchical clustering

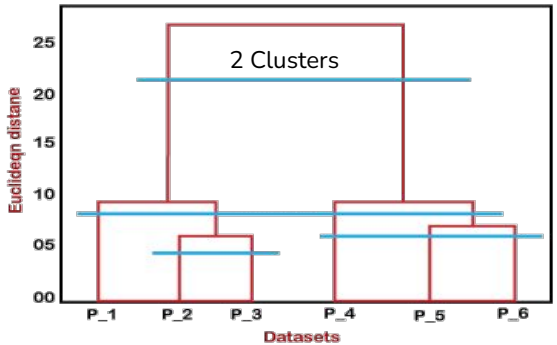
Hierarchical clustering is an unsupervised clustering algorithm that involves creating clusters that have predominant ordering from top to bottom. For example, all files and folders on our hard disk are organized in a hierarchy.

The algorithm groups similar objects into groups called "clusters." The endpoint is a set of clusters or groups, where each cluster is distinct from the other cluster, and the objects within each cluster are broadly similar to each other.

Steps:

- Make each data point a single-point cluster → that forms N clusters
- Take the two closest data points and make them one cluster → that forms N-1 clusters
- Take the two closest clusters and make them one cluster → that forms N-2 clusters.
- Repeat step-3 until you are left with only one cluster.





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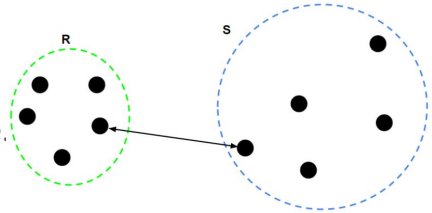
Dissimilarity among clusters in hierarchical clustering

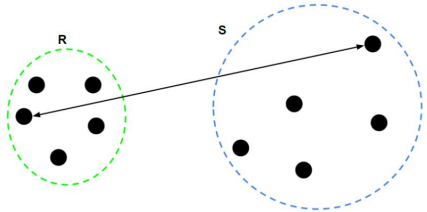
The below are some of the following ways by which we can measure dissimilarity among clusters in hierarchical clustering:

- **Single linkage:** It measures the closest pair of points, i.e., the minimum distance.



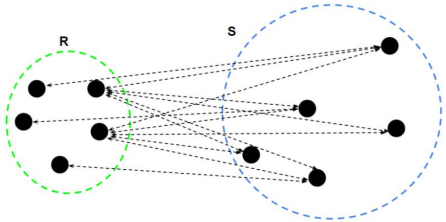
L(R,S) = min(d(i,j)) where i belongs to R and j belongs to S

- **Complete linkage:** It measures the farthest pair of points i.e the maximum distance



L(R,S) = max(d(i,j)) where i belongs to R and j belongs to S

- **Average linkage:** It measures the average dissimilarity over all pairs i.e. the average distance



$$L(R,S) = \frac{1}{n_R+n_S}\sum_{i=1}^{n_R}\sum_{j=1}^{n_S} D(i,j), i\epsilon R, j\epsilon S$$

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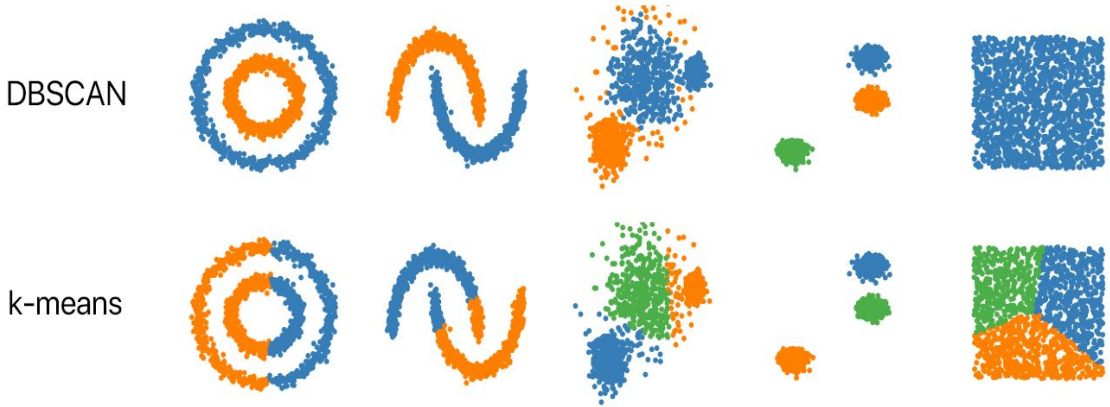
DBSCAN

DBSCAN stands for **D**ensity-**B**ased **S**patial **C**lustering of **A**pplications with **N**oise.

It recognizes groups in the data by looking at the local density of a data point. Unlike K-means, **DBSCAN clustering is not sensitive to outliers** and also does not require the number of clusters to be told beforehand.



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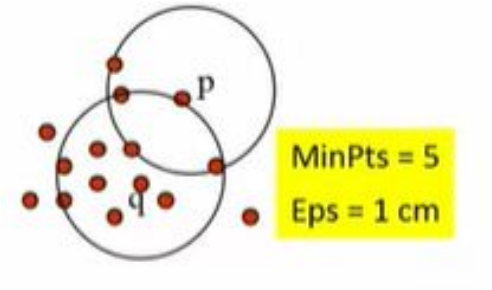
Parameters in DBSCAN

- **eps (‘ε’):** It defines the neighborhood around a data point, i.e., if the distance between two points is lower or equal to 'eps', then they are considered neighbors. If the eps value is chosen too small, then a large part of the data will be considered outliers. If it is chosen very large, then the clusters will merge and the majority of the data points will be in the same clusters. One way to find the eps value is based on the k-distance graph.



- **MinPts:** Minimum number of neighbors (data points) within eps radius. The larger the dataset, the larger value of MinPts must be chosen. As a general rule, the minimum MinPts can be derived from the number of dimensions D in the dataset as MinPts >= D+1. The minimum value of MinPts must be chosen at least.

Regression

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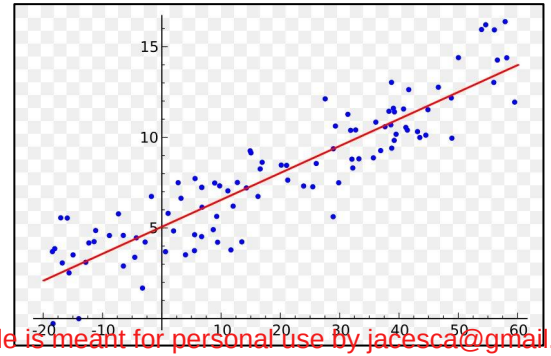
Linear Regression

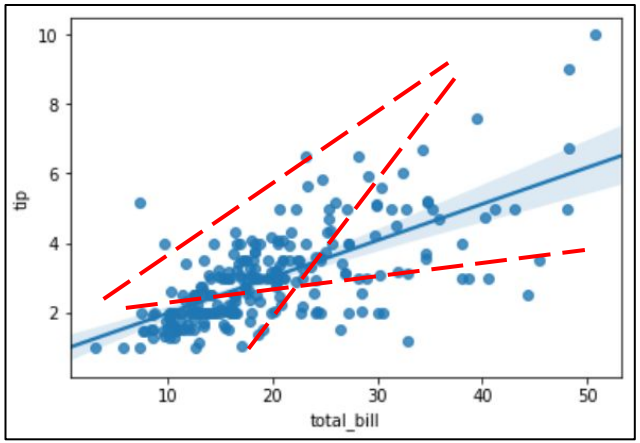
- Linear regression is a way to identify relationship between the independent variable(s) and the dependent variable.
- We can use these relationships to predict values for one variable for given value(s) of other variable(s).
- It assumes the relationship between variables can be modeled through linear equation or an equation of the line.
- The variable, which is used in prediction is termed as independent/explanatory/regressor, whereas the predicted variable is termed as dependent/target/response variable.
- In case of linear regression with a single explanatory variable, the linear combination can be expressed as:

response = intercept + constant * explanatory variable



Best fit line in the linear regression model

- Learning from the data, the model generates a line that fits the data.
- Our aim is to find a regression line that best fits the data.
- By best fit, it means that the line will be such that the cumulative distance of all the points from the line is minimized.
- Mathematically, the line that minimizes the sum of squared error of residuals is called the Regression Line or the Line of Best Fit.



- In the example here, you can see a scatter plot between the total_*tip* amount and the *total_bill* amount.
- We can see that there is a positive correlation between these variables. As the bill amount increases, the tip increases.
- The blue line is the 'best fit' line and those in red are some examples of other lines that are not the 'best fit'.

What is Multiple Linear Regression?

- This is just an extension of the concept of simple linear regression with one variable, to multiple variables.
- In the real world, any phenomenon or outcome could be driven by many different independent variables.
- Therefore there is a need to have a mathematical model that can capture this relationship.

  - **Ex:** Predicting the price of a house, we need to consider various attributes such as area, number of rooms, number of kitchens, etc. Such a regression problem is an example of multiple linear regression.
  - The equation for multiple linear regression can be represented by:

target = intercept + constant 1*feature 1 + constant 2*feature 2 + constant 3*feature 3 + ...

- The model aims to find the constants and intercept such that this line is the best fit.

Regression Model Evaluation Metrics

R-squared	Adjusted R-squared	Mean Absolute Error	Root Mean Square Error
• A measure of the % of the variance in the target variable explained by the model • Generally, the first metric to look at for linear regression model performance • Higher the better	• Conceptually, very similar to R-squared but penalizes for the addition of too many variables • Generally, used when you have too many variables as adding more variables always increases R-squared but not Adjusted R-squared • Higher the better	• Simplest metric to check prediction quality • Same unit as the dependent variable • Not sensitive to outliers, i.e. the metric is not affected too much if there are outliers • Difficult to optimize from a mathematical point of view (pure maths logic) • Lower the better	• Another metric to measure the quality of predictions • Same unit as the dependent variable • Sensitive to outliers - errors will be magnified due to the square function • But has other mathematical advantages • Lower the better

$$R^2 = 1 - \frac{\frac{1}{n}\sum_{i=1}^{n}(y_i - yhat_i)^2}{\frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

$$Adjusted\ R^2 = 1 - \frac{(1 - R^2)(N - 1)}{N - p - 1}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - yhat_i|$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - yhat_i)^2}$$

Assumptions of Linear Regression

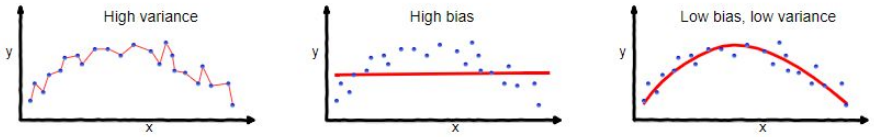
Assumption	How to test	How to fix
There should be a linear relationship between dependent and independent variables	Pair plot / Correlation of each independent variable with dependent variables	Transform variables that appear non-linear (log, square root, etc.)
No multicollinearity in independent variables	Heatmaps of correlations or VIF (Variance Inflation Factor)	Remove correlated variables or merge them
No Heteroskedasticity - residuals should have constant variance	Plot residuals vs. fitted values and check the plot	Non-linear transformation of the dependent variable or adding other important variables
Residuals must be normally distributed	Plot residuals or use a Q-Q plot	Non-linear transformation of independent or dependent variables

Bias-Variance Tradeoff: Underfitting and Overfitting

Bias: Bias is the difference between the prediction of our model and the correct value that we are trying to predict. Models with high bias give less attention to the training data and overgeneralize the model which leads to a high error in the training and the test datasets.

Variance: Models with high variance pay a lot of attention to the training data, including the noise, and do not generalize on the test data. Therefore, such models perform very well on training data but have a high error on the test data.

In supervised learning, **underfitting** happens when a model is not able to capture the underlying pattern of the data. These models usually have high bias and low variance, whereas, **overfitting** happens when our model captures the noise along with the underlying pattern in training data. These models usually have low bias and high variance.



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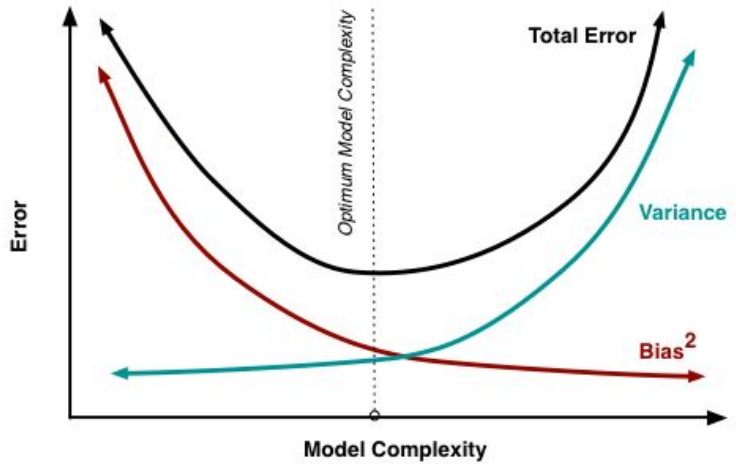
Bias-Variance Tradeoff

If our model is too simple and has very few parameters, then it may have high bias and low variance. On the other hand, if our model has a large number of parameters, then it's going to have high variance and low bias. So, we need to find the right/good balance between overfitting and underfitting the data.
An optimal balance of bias and variance would neither overfit nor underfit the model.



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Regularization and its types

- Regularization is the process that regularizes or shrinks the coefficients towards zero. In other words, this technique discourages learning a more complex or flexible model, to avoid the risk of overfitting.
- Regularization significantly reduces the variance of the model, without a substantial increase in its bias.
- The two most common types of regularization in regression are:
    - **Lasso Regression:** In this technique, we add $\alpha * \sum|\beta|$ as the shrinkage quantity. It only penalizes high coefficients. It has the effect of forcing some of the coefficient estimates to be exactly equal to zero when the tuning parameter α is sufficiently large. This technique is also called L1 regularization.
    - **Ridge Regression:** In this technique, we modify the residual sum of squares by adding the shrinkage quantity $\alpha * \sum\beta^2$ and use α as the tuning hyperparameter that decides how much we want to penalize the flexibility of our model. This technique is also called L2 regularization.

Cross-validation and its types

Cross-validation is a technique in which we train our model using the subset of the dataset and then evaluate using the complementary subset of the dataset.

- It provides some kind of assurance that the model has got most of the pattern from the dataset correct and it is not picking up noise.
- Two most common types of cross-validation techniques are:
    1. K-Fold Cross-Validation
    2. Leave-One-Out Cross-Validation (LOOCV)

Classification

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Contents

Image Source

Why do we use logistic regression?

- Logistic Regression is a supervised learning algorithm that is used for classification problems, i.e., where the dependent variable is categorical.
- In logistic regression, we use the Sigmoid function to calculate the probability of the dependent variable.
- The real-life applications of logistic regression are churn prediction, spam detection, etc.
- The below image shows how logistic regression is different from linear regression in fitting the model.

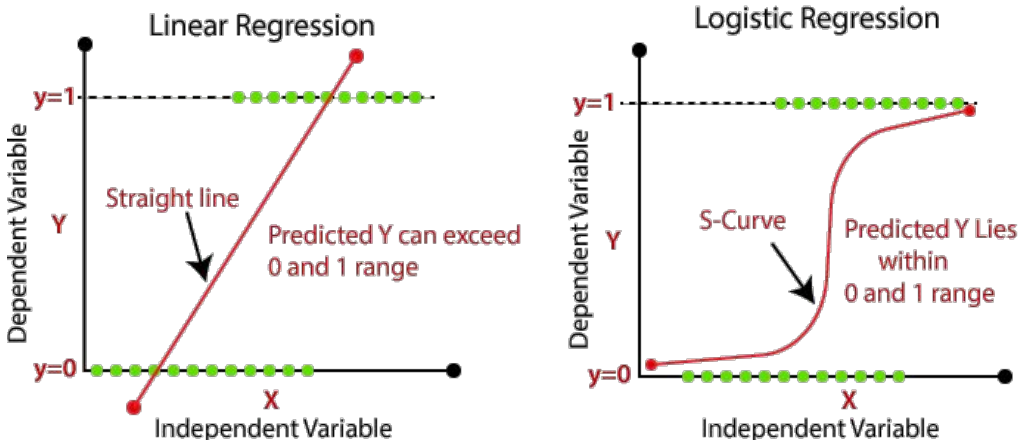
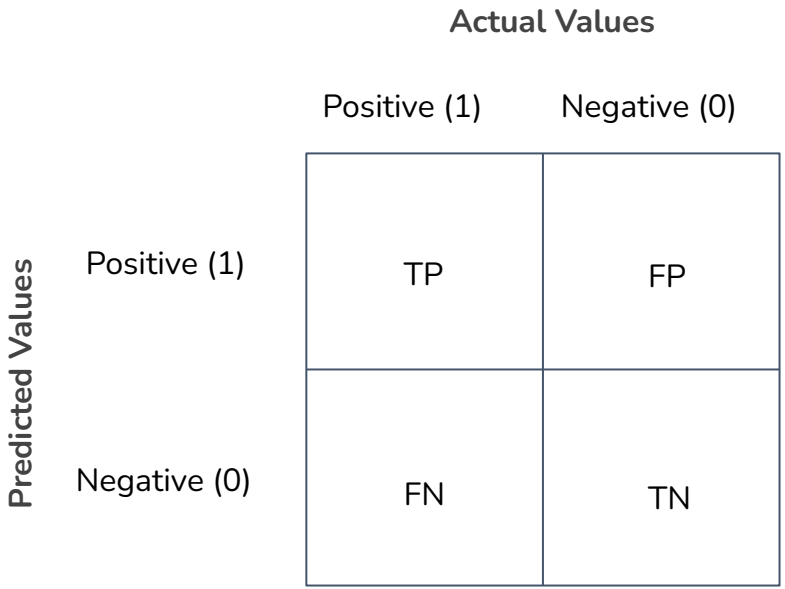


Image Source

Confusion matrix

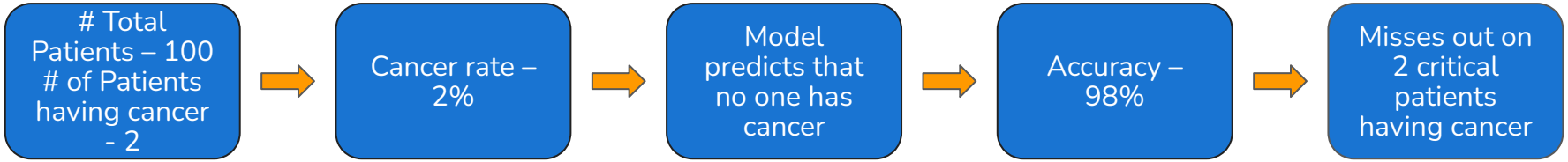
It is used to measure the performance of a classification algorithm. It can be used to calculate the following metrics:

1. **Accuracy:** Proportion of correctly predicted results among the total number of observations
   Accuracy = (TP+TN)/(TP+FP+FN+TN)
2. **Precision:** Proportion of true positives to all the predicted positives, i.e., how valid the predictions are
   Precision = (TP)/(TP+FP)
3. **Recall:** Proportion of true positives to all the actual positives, i.e., how complete the predictions are
   Recall = (TP)/(TP+FN)



Why accuracy is not always a good performance measure

Accuracy is simply the overall % of correct predictions and can be high even for very useless models.

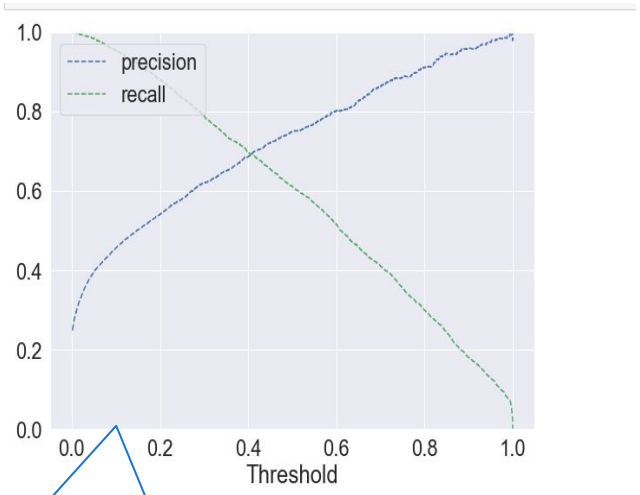


- Here, accuracy will be 98%, even if we simply predict that every patient does not have cancer.
- In this case, Recall should be used as a measure of model performance; high recall imply fewer false negatives.
- Fewer false negatives implies a lower chance of 'missing' a cancer patient, i.e., predicting a cancer patient as one not having cancer.
- This is where we need other metrics to evaluate model performance.

- The other important metrics are Recall and Precision:
  - Recall - What % of actuals 1s did the model capture in prediction?
  - Precision - What % of predicted 1s are actual 1s?
- There is a tradeoff - as you try to increase the Recall, the Precision will reduce and vice versa.
- This tradeoff can be used to figure out the right threshold to use for the model.

How to chose thresholds using the Precision-Recall curve?

- The Precision-Recall curve is a useful measure of the success of prediction when the classes are imbalanced.
- The curve shows the tradeoff between the precision and the recall for different thresholds.
- It can be used to select an optimal threshold as required to improve the model performance.
- Here, as we can see, the precision and the recall are almost equal when the threshold is around 0.4.
- If we want a higher precision, we can increase the threshold.
- If we want a higher recall, we can decrease the threshold.



Choosing different thresholds can completely change the model's performance.
It is important to think about what constitutes the 'sweet spot'.

Is there a performance measure that can cover both Precision and Recall?

- F1 Score is a measure that takes into account both Precision and Recall.
- The F1 Score is the harmonic mean of Precision and Recall. Therefore, this score takes both false positives and false negatives into account.

$$F1\ Score = \frac{2 \times Precision \times Recall}{Precision + Recall}$$

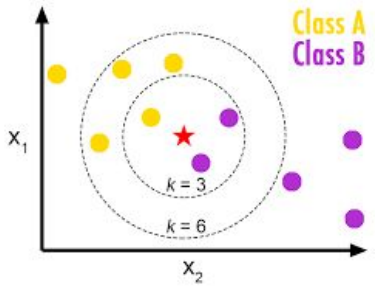
- The highest possible value of the F1 score is 1, indicating perfect precision and recall, and the lowest possible value is 0.

K-Nearest Neighbours (K-NN) algorithm

This algorithm uses features from the training data to predict the values of new data points, which means the new data point will be assigned a value based on how similar it is to the data points in the training set. We can define its working in the following steps:

- Step 1: We need to choose the value of K, i.e., the number of nearest data points to consider. K can be any positive integer.
- Step 2: For each point in the test data do the following:
  - Calculate the distance between the test point and each training point with the help of any of the distance methods, namely: Euclidean, Manhattan, etc. The most commonly used method to calculate the distance is the Euclidean method.
  - Now, based on the distance value, sort them in ascending order.
  - Next, choose the top K rows from the sorted array.
  - Now, assign a class to the test point based on the most frequent class.
- Step 3: Repeat this process until all the test points are classified in a particular class.

We try different values of K and plot them against the test error. The lower the value of the test error, the better the value of K.



Appendix

Data Exploration and Networks

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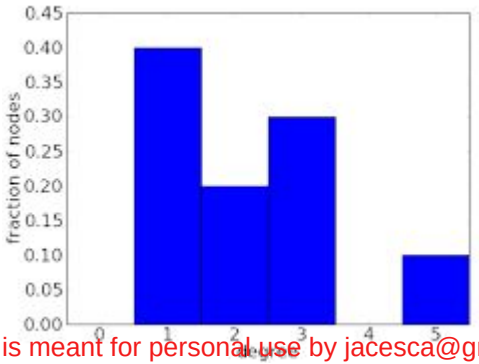
Degree and its calculation

The degree of a node refers to the number of edges that are connected to it. In a directed graph, you can calculate the in-degree and out-degree which means incoming and outgoing connections of a node.
In simple words, it is a popularity measure. The higher the degree, more central the node is.
We can calculate the average degree of a network by using the formula **2*(m/n)**, where **m** is the number of edges and **n** is the number of nodes.
Degree distribution: It is a probability that the random chosen node has k number of connections.

In this graph, you can observe how the degree is varying with the fraction of nodes.



Centrality measures

Centrality measures capture the importance of a node's position in a network. There are the following types of centrality measures:

1. **Degree centrality:** It is a measure of the popularity of a node in a network. It does not capture the quality vs quantity.
2. **Propagated degree (eigenvector) centrality:** It measures the importance of a node in a graph with respect to the importance of its neighbors. If a node is connected to highly important nodes, it will have a higher score as compared to a node that is connected to less important nodes.
3. **Closeness centrality:** It tracks how close a node is to another by measuring the distance between them. In other words, it measures the node efficiency in terms of connection to other nodes.
4. **Betweenness centrality:** It measures the importance of a node in a network based on how many times it occurs in the shortest path between all pairs of nodes in a graph. It measures the extent to which a node lies on paths between other nodes.

Real life example of a network and its centrality measures

In a **social network:**

- High degree centrality - most popular person who can quickly connect with the wider network
- High eigenvector centrality - most popular person who has a good social network with another popular person
- High closeness centrality - a person who can influence the whole network most quickly
- High betweenness centrality - a person who influences the flow around the network, i.e., removal of that person can break the network

Regression

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Statistics vs Machine Learning

The difference between machine learning and statistical learning is their purpose. Machine learning models are designed to make the most accurate predictions possible, whereas statistical models are designed for inference about the relationships between variables.
The following table highlights the major differences between statistics and the machine learning point of view:

Statistics	Machine Learning
Emphasis on deep theorems on complex models	Emphasis on the underlying algorithm
Focus on hypothesis testing and interpretability	Focus on predicting the accuracy of the model
Inference on parameter estimation, errors, and predictions	Inference on prediction
Deep understanding of simple models	The theory does not always explain the success

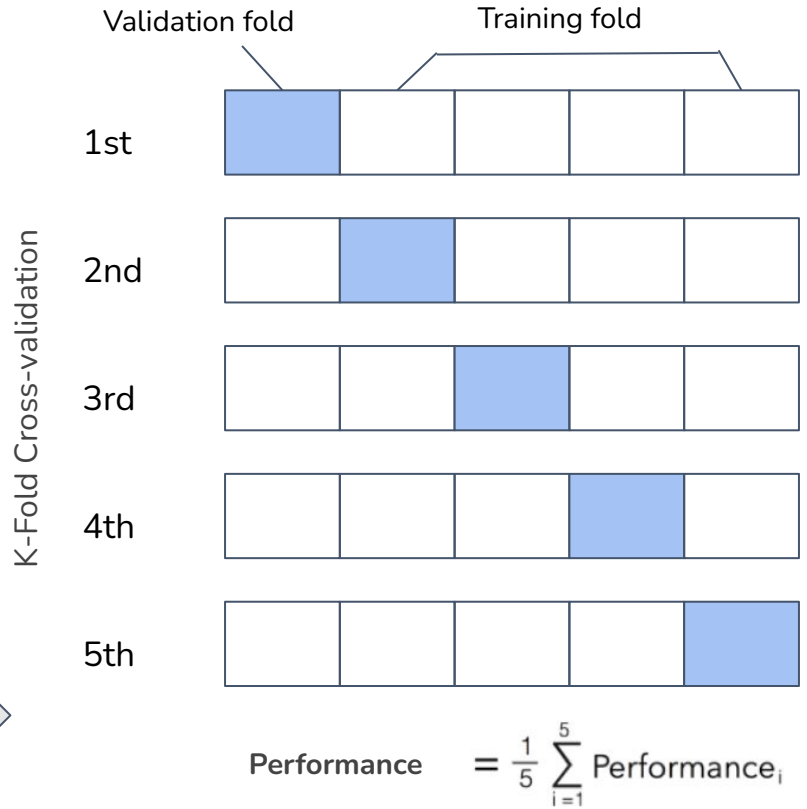
K-Fold Cross-Validation

This algorithm has a single parameter called K which refers to the number of groups that a given dataset is to be split into.

This algorithm has the following procedure:

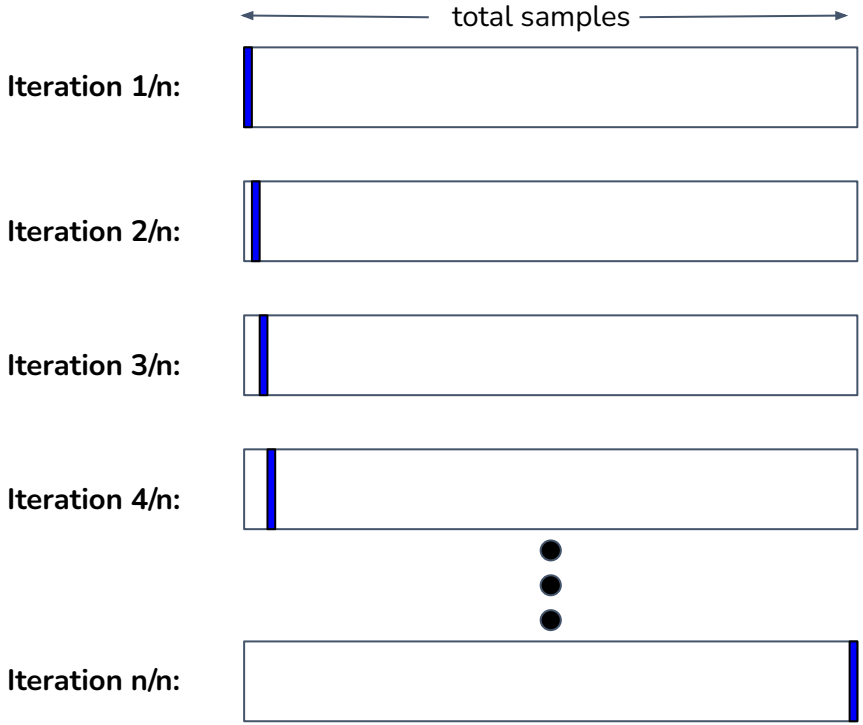
1. Shuffle the dataset randomly.
2. Split the whole dataset into K distinct groups.
3. In each iteration, take one group as a hold-out set and the remaining as the training set.
4. Repeat step 3, K times with a different group, as a validation set, in each iteration.
5. Summarize the skill of the model using the average model evaluation scores of all groups.

Here, K = 5



Leave-One-Out Cross-Validation (LOOCV)

- LOOCV is a special case of K-Fold Cross-Validation where K equals n, n being the number of data points in the dataset.
- This approach leaves 1 data point out of the training data, i.e., if there are n data points in the original dataset, then n-1 data points are used to train the model and 1 data point is used as the validation set.
- This is repeated for all combinations in which the original dataset can be separated this way, and then the error is averaged for all trials, to give an overall model performance.
- The number of possible combinations is equal to the number of data points in the original dataset, i.e., n.



Bootstrapping

Bootstrapping (also called Bootstrap sampling) is a resampling method that involves the drawing of samples from the data repeatedly with replacement to estimate a population parameter.
It involves the following steps:

1. Choose a number of bootstrap samples to perform
2. Choose a sample size n
3. For each bootstrap sample
    1. Draw a sample with replacement with the chosen size
    2. Calculate the statistic on the sample
4. Calculate the mean of the calculated sample statistics

Bootstrap sampling can be used to estimate the parameter of a population, for example, mean, standard error, etc.

Classification

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LDA vs QDA

Linear Discriminant Analysis	Quadratic Discriminant Analysis
It is a linear classifier but much less flexible than QDA	It is a non-linear classifier but more flexible than LDA
It assumes a common covariance matrix for all the classes	It assumes that each class has its covariance matrix
It is preferred when the training set only has a few observations	It is preferred when the training set is very large
It can be used as a dimensionality reduction technique	It cannot be used as a dimensionality reduction technique

Great Learning

Happy Learning !