GATE in Data Science and AI Study Materials
Machine Learning
By Piyush Wairale

Instructions:

- Kindly go through the lectures/videos on our website www.piyushwairale.com
- Read this study material carefully and make your own handwritten short notes. (Short notes must not be more than 5-6 pages)
- Attempt the question available on portal.
- Revise this material at least 5 times and once you have prepared your short notes, then revise your short notes twice a week
- **If you are not able to understand any topic or required detailed explanation, please mention it in our discussion forum on webiste**
- **Let me know, if there are any typos or mistake in study materials. Mail me at piyushwairale100@gmail.com**

1 Introduction to Machine Learning

Defination

- Machine Learning is the field of study that gives computers the capability to learn without being explicitly programmed. ML is one of the most exciting technologies that one would have ever come across. As it is evident from the name, it gives the computer that makes it more similar to humans: The ability to learn. Machine learning is actively being used today, perhaps in many more places than one would expect.
- Machine learning is programming computers to optimize a performance criterion using example data or past experience. We have a model defined up to some parameters, and learning is the execution of a computer program to optimize the parameters of the model using the training data or past experience. The model may be predictive to make predictions in the future, or descriptive to gain knowledge from data, or both.
- The field of study known as machine learning is concerned with the question of how to construct computer programs that automatically improve with experience

Defination of Learning

A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks T, as measured by P, improves with experience E.

A computer program which learns from experience is called a machine learning program or simply a learning program. Such a program is sometimes also referred to as a learner.

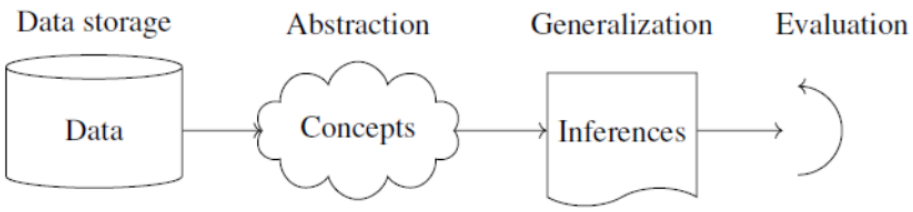
Examples

1. Handwriting recognition learning problem
   - Task T: Recognising and classifying handwritten words within images
   - Performance P: Percent of words correctly classified
   - Training experience E: A dataset of handwritten words with given classifications
2. A robot driving learning problem
   - Task T: Driving on highways using vision sensors
   - Performance measure P: Average distance traveled before an error
   - training experience: A sequence of images and steering commands recorded while observing a human driver
3. A chess learning problem.

- Task T: Playing chess
- Performance measure P: Percent of games won against opponents
- Training experience E: Playing practice games against itself as measured by P, improves with experience E.

How Machine Learn?

The learning process, whether by a human or a machine, can be divided into four components, namely, data storage, abstraction, generalization and evaluation.



1.1 Introduction to Data in Machine Learning

What is data?
It can be any unprocessed fact, value, text, sound, or picture that is not being interpreted and analyzed. Data is the most important part of all Data Analytics, Machine Learning, and Artificial Intelligence.
Without data, we can't train any model and all modern research and automation will go in vain.

- Data is a crucial component in the field of Machine Learning. It refers to the set of observations or measurements that can be used to train a machine-learning model.
- The quality and quantity of data available for training and testing play a significant role in determining the performance of a machine-learning model.
- Data can be in various forms such as numerical, categorical, or time-series data, and can come from various sources such as databases, spreadsheets, or APIs.
- Machine learning algorithms use data to learn patterns and relationships between input variables and target outputs, which can then be used for prediction or classification tasks.

Understanding data
Since an important component of the machine learning process is data storage, we briefly consider in this section the different types and forms of data that are encountered in the machine learning process.
Unit of observation
By a unit of observation we mean the smallest entity with measured properties of interest for a study.
Examples

- A person, an object or a thing
- A time point
- A geographic region
- A measurement

Sometimes, units of observation are combined to form units such as person-years.
Examples and features
Datasets that store the units of observation and their properties can be imagined as collections of data consisting of the following:
Examples
An "example" is an instance of the unit of observation for which properties have been recorded.
An "example" is also referred to as an "instance", or "case" or "record." (It may be noted

that the word "example" has been used here in a technical sense.)

Features

A "feature" is a recorded property or a characteristic of examples. It is also referred to as "attribute", or "variable" or "feature."

Examples for "examples" and "features"

1. Cancer detection

Consider the problem of developing an algorithm for detecting cancer. In this study we note the following.

(a) The units of observation are the patients.

(b) The examples are members of a sample of cancer patients.

(c) The following attributes of the patients may be chosen as the features:

- gender
- age
- blood pressure
- the findings of the pathology report after a biopsy

2. Pet selection

Suppose we want to predict the type of pet a person will choose.

(a) The units are the persons.

(b) The examples are members of a sample of persons who own pets

(c) The features might include age, home region, family income, etc. of persons who own pets.

features

year	model	price	mileage	color	transmission
2011	SEL	21992	7413	Yellow	AUTO
2011	SEL	20995	10926	Gray	AUTO
2011	SEL	19995	7351	Silver	AUTO
2011	SEL	17809	11613	Gray	AUTO
2012	SE	17500	8367	White	MANUAL
2010	SEL	17495	25125	Silver	AUTO
2011	SEL	17000	27393	Blue	AUTO
2010	SEL	16995	21026	Silver	AUTO
2011	SES	16995	32655	Silver	AUTO

examples

Figure 1: Example for "examples" and "features" collected in a matrix format (data relates to automobiles and their features)

Type of Data

Data is typically divided into two types:

1. **Labeled data**
2. **Unlabeled data**

Labeled data includes a label or target variable that the model is trying to predict, whereas **unlabeled data** does not include a label or target variable. The data used in machine learning is typically numerical or categorical. Numerical data includes values that can be ordered and measured, such as age or income. Categorical data includes values that represent categories, such as gender or type of fruit.

- Data can be divided into training and testing sets.
- The training set is used to train the model, and the testing set is used to evaluate the performance of the model.
- It is important to ensure that the data is split in a random and representative way.
- Data preprocessing is an important step in the machine learning pipeline. This step can include cleaning and normalizing the data, handling missing values, and feature selection or engineering.

How do we split data in Machine Learning?

1. **Training Data:** The part of data we use to train our model. This is the data that your model actually sees(both input and output) and learns from.
2. **Validation Data:** The part of data that is used to do a frequent evaluation of the model, fit on the training dataset along with improving involved hyperparameters (initially set parameters before the model begins learning). This data plays its part when the model is actually training.
3. **Testing Data:** Once our model is completely trained, testing data provides an unbiased evaluation. When we feed in the inputs of Testing data, our model will predict some values(without seeing actual output).

   After prediction, we evaluate our model by comparing it with the actual output present in the testing data. This is how we evaluate and see how much our model has learned from the experiences feed in as training data, set at the time of training.

Different forms of data

1. **Numeric data** If a feature represents a characteristic measured in numbers, it is called a numeric feature.
2. **Categorical or nominal** A categorical feature is an attribute that can take on one of a limited, and usually fixed, number of possible values on the basis of some qualitative property. A categorical feature is also called a nominal feature.

3. **Ordinal data** This denotes a nominal variable with categories falling in an ordered list. Examples include clothing sizes such as small, medium, and large, or a measurement of customer satisfaction on a scale from "not at all happy" to "very happy."

Examples In the data given in Fig.1, the features "year", "price" and "mileage" are numeric and the features "model", "color" and "transmission" are categorical.

Properties of Data

- **Volume:** Scale of Data. With the growing world population and technology at exposure, huge data is being generated each and every millisecond.
- **Variety:** Different forms of data – healthcare, images, videos, audio clippings.
- **Velocity:** Rate of data streaming and generation.
- **Value:** Meaningfulness of data in terms of information that researchers can infer from it.
- **Veracity:** Certainty and correctness in data we are working on.
- **Viability:** The ability of data to be used and integrated into different systems and processes.
- Security: The measures taken to protect data from unauthorized access or manipulation.
- **Accessibility:** The ease of obtaining and utilizing data for decision-making purposes. Integrity: The accuracy and completeness of data over its entire lifecycle.
- **Usability:** The ease of use and interpretability of data for end-users.

1.2 Different types of learning

In general, machine learning algorithms can be classified into three types.

1. **Supervised learning**

   - Supervised learning is the machine learning task of learning a function that maps an input to an output based on example input-output pairs.
   - In supervised learning, each example in the training set is a pair consisting of an input object (typically a vector) and an output value.
   - A supervised learning algorithm analyzes the training data and produces a function, which can be used for mapping new examples.
   - In the optimal case, the function will correctly determine the class labels for unseen instances.
   - Both **classification and regression problems** are supervised learning problems.
   - A wide range of supervised learning algorithms are available, each with its strengths and weaknesses. There is no single learning algorithm that works best on all supervised learning problems.
   - **Important Point** :A "supervised learning" is so called because the process of an algorithm learning from the training dataset can be thought of as a teacher supervising the learning process. We know the correct answers (that is, the correct outputs), the algorithm iteratively makes predictions on the training data and is corrected by the teacher. Learning stops when the algorithm achieves an acceptable level of performance.

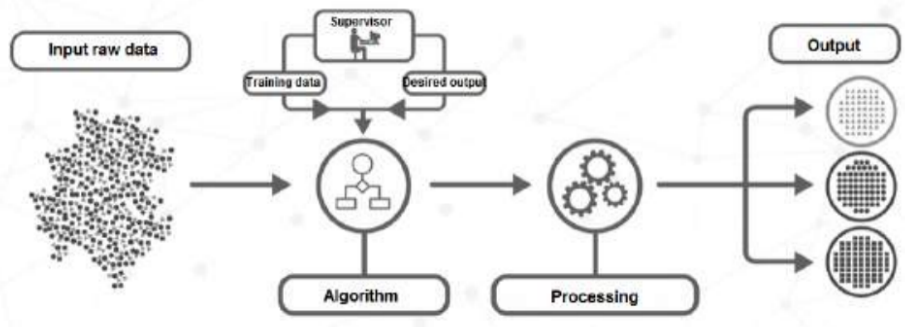


Fig 2:Supervised learning

Example:
Consider the following data regarding patients entering a clinic. The data consists of the gender and age of the patients and each patient is labeled as "healthy" or "sick".

gender	age	label
M	48	sick
M	67	sick
F	53	healthy
M	49	healthy
F	34	sick
M	21	healthy

Based on this data, when a new patient enters the clinic, how can one predict whether he/she is healthy or sick?

2. **Unsupervised learning**

   - Unsupervised learning is a type of machine learning algorithm used to draw inferences from datasets consisting of input data without labeled responses.
   - In unsupervised learning algorithms, a classification or categorization is not included in the observations.
   - There are no output values and so there is no estimation of functions. Since the examples given to the learner are unlabeled, the accuracy of the structure that is output by the algorithm cannot be evaluated.
   - The most common unsupervised learning method is cluster analysis, which is used for exploratory data analysis to find hidden patterns or grouping in data

   Example Consider the following data regarding patients entering a clinic. The data consists of the gender and age of the patients.

gender	age
M	48
M	67
F	53
M	49
F	34
M	21

   Based on this data, can we infer anything regarding the patients entering the clinic?

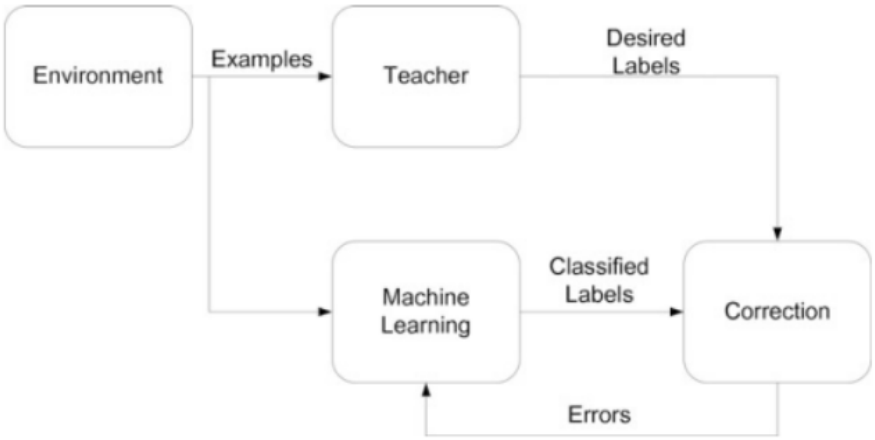
3. **Reinforcement learning**

   - Reinforcement learning is the problem of getting an agent to act in the world so as to maximize its rewards.

- A learner (the program) is not told what actions to take as in most forms of machine learning, but instead must discover which actions yield the most reward by trying them.
- In the most interesting and challenging cases, actions may affect not only the immediate reward but also the next situations and, through that, all subsequent rewards.
- **For example:**, consider teaching a dog a new trick: we cannot tell it what to do, but we can reward/punish it if it does the right/wrong thing. It has to find out what it did that made it get the reward/punishment. We can use a similar method to train computers to do many tasks, such as playing backgammon or chess, scheduling jobs, and controlling robot limbs.
- Reinforcement learning is different from supervised learning. Supervised learning is learning from examples provided by a knowledgeable expert.

2 Supervised Learning

In supervised learning, the training data you feed to the algorithm includes the desired solutions, called labels. These methods use a training set that consists of labeled data points (for which we know the correct label values). We refer to a data point as labeled if its label value is known. Labeled data points might be obtained from human experts that annotate ("label") data points with their label values.



- Supervised learning is a machine learning paradigm where algorithms aim to optimize parameters to minimize the difference between target and computed outputs, commonly used in tasks like classification and regression.
- In supervised learning, training examples are associated with target outputs (initially labeled) and computed outputs (generated by the learning algorithm), and the goal is to minimize misclassification or error.
- The learning process in supervised learning involves initializing parameters randomly, computing output values for labeled examples, and updating parameters iteratively to minimize errors or achieve convergence.

Type of Supervised Learning:
1.Regression
2.Classification

3 Regression:

- In machine learning, a regression problem is the problem of predicting the value of a numeric variable based on observed values of the variable.
- The value of the output variable may be a number, such as an integer or a floating point value. These are often quantities, such as amounts and sizes. The input variables may be discrete or real-valued.
- Regression algorithms are used if there is a relationship between the input variable and the output variable.
- It is used for the prediction of continuous variables, such as Weather forecasting, Market Trends, etc.

General Approach
Let x denote the set of input variables and y the output variable. In machine learning, the general approach to regression is to assume a model, that is, some mathematical relation between x and y, involving some parameters say, θ, in the following form:
$y = f(x, \theta)$
The function $f(x, \theta)$ is called the regression function. The machine learning algorithm optimizes the parameters in the set θ such that the approximation error is minimized; that is, the estimates of the values of the dependent variable y are as close as possible to the correct values given in the training set.

Example
For example, if the input variables are "Age", "Distance" and "Weight" and the output variable is "Price", the model may be

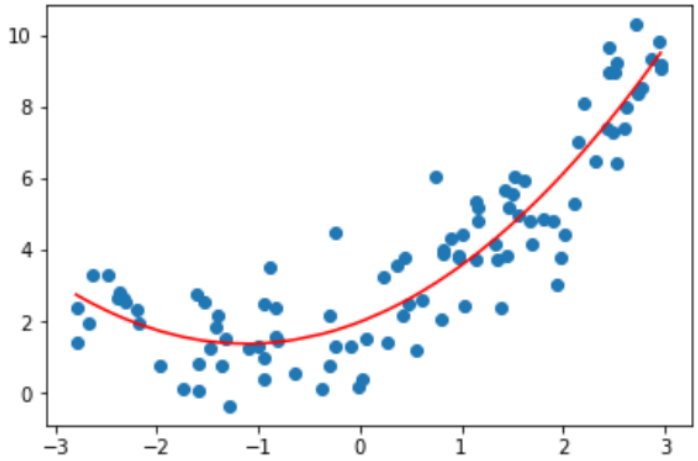
$$y = f(x, \theta)$$
$$\text{Price} = a_0 + a_1 \times (\text{Age}) + a_2 \times (\text{Distance}) + a_3 \times (\text{Weight})$$

where x =(Age, Distance, Weight) denotes the set of input variables and $\theta = (a_0, a_1, a_2, a_3)$ denotes the set of parameters of the model.
Various types of regression techniques These techniques mostly differ in three aspects, namely, the number and type of independent variables, the type of dependent variables and the shape of regression line. Some of these are listed below.

1. Simple linear regression: There is only one continuous independent variable x and the assumed relation between the independent variable and the dependent variable y is $y = a + bx$

2. Multivariate linear regression: There are more than one independent variable, say $x1, ..., xn$, and the assumed relation between the independent variables and the dependent variable is $y = a_0 + a_1x_1 + ... + a_nx_n$

3. Polynomial regression: There is only one continuous independent variable x and the assumed model is $y = a_0 + a_1x + ... + a_nx^n$
   It is a variant of the multiple linear regression model, except that the best fit line is curved rather than straight.



4. Ridge regression: Ridge regression is one of the types of linear regression in which a small amount of bias is introduced so that we can get better long-term predictions. Ridge regression is a regularization technique, which is used to reduce the complexity of the model. It is also called as L2 regularization.

5. Logistic regression: The dependent variable is binary, that is, a variable which takes only the values 0 and 1. The assumed model involves certain probability distributions.

3.0.1 Linear Regression

Simple linear regression is a basic machine learning technique used for modeling the relationship between a single independent variable (often denoted as "x") and a dependent variable (often denoted as "y"). It assumes a linear relationship between the variables and aims to find the best-fitting line (typically represented by the equation $y = mx + b$) that minimizes the sum of squared differences between the observed data points and the values predicted by the model.

Equation: The linear regression model is represented by the equation
$y = ax + b$,
where:
y is the dependent variable (the one you want to predict).
x is the independent variable (the one used for prediction).
a is the slope (also called the regression coefficient), representing how much y changes for each unit change in x.
b is the y-intercept, representing the value of y when x is 0.

In order to determine the optimal estimates of a and b, an estimation method known as Ordinary Least Squares (OLS) is used.
Formulas to find a and b
The means of x and y are given by

$$\bar{x} = \frac{1}{n}\sum x_i$$
$$\bar{y} = \frac{1}{n}\sum y_i$$

and also that the variance of x is given by

$$\text{Var}\,(x) = \frac{1}{n-1}\sum(x_i - \bar{x_i})^2.$$

The covariance of x and y, denoted by Cov(x, y) is defined as

$$\text{Cov}(x, y) = \frac{1}{n-1}\sum(x_i - \bar{x})(y_i - \bar{y})$$

It can be shown that the values of a and b can be computed using the following formulas:

$$b = \frac{\text{Cov}(x, y)}{\text{Var}(x)}$$

$$a = \bar{y} - b\bar{x}$$

Advantages of Simple Linear Regression:

- Simplicity and ease of interpretation.
- Transparent modeling with clear coefficient interpretations.
- Computational efficiency, suitable for large datasets.
- A baseline model for assessing feature significance.
- Effective when the relationship between variables is linear.

Disadvantages of Simple Linear Regression:

- Limited to linear relationships, may perform poorly for nonlinear data.
- Sensitive to outliers, leading to parameter influence.
- Prone to underfitting when facing complex relationships.
- Assumptions of independent and normally distributed errors are critical.
- Suitable only when one independent variable is involved in the analysis.

Example
Obtain a linear regression for the data in below table assuming that y is the independent variable.

x	1.0	2.0	3.0	4.0	5.0
y	1.00	2.00	1.30	3.75	2.25

$$
\begin{aligned}
n &= 5 \\
\bar{x} &= \frac{1}{5}(1.0 + 2.0 + 3.0 + 4.0 + 5.0) \\
&= 3.0 \\
\bar{y} &= \frac{1}{5}(1.00 + 2.00 + 1.30 + 3.75 + 2.25) \\
&= 2.06 \\
\text{Cov}\,(x, y) &= \frac{1}{4}[(1.0 - 3.0)(1.00 - 2.06) + \cdots + (5.0 - 3.0)(2.25 - 2.06)] \\
&= 1.0625 \\
\text{Var}\,(x) &= \frac{1}{4}[(1.0 - 3.0)^2 + \cdots + (5.0 - 3.0)^2] \\
&= 2.5 \\
b &= \frac{1.0625}{2.5} \\
&= 0.425 \\
a &= 2.06 - 0.425 \times 3.0 \\
&= 0.785
\end{aligned}
$$

Therefore, the linear regression model for the data is $y = 0.785 + 0.425x$

3.0.2 Multivariate Linear Regression

Multiple Linear Regression is a machine learning technique used to model the relationship between a dependent variable (target) and multiple independent variables (features) by fitting a linear equation to the data.
The model can be expressed as: $y = \beta_0 + \beta_1 x_1 + ... + \beta_N x_N$
Where:
y is the dependent variable (the one you want to predict).
$x_1, x_2, ..., x_n$ are the independent variables.
β_0 is the y-intercept.
$\beta_1, \beta_2, ...\beta_n$ are the coefficients associated with each independent variable.

Let there also be n observed values of these variables:

Variables (features)	Values (examples)			
	Example 1	Example 2	⋯	Example n
x_1	x_{11}	x_{12}	⋯	x_{1n}
x_2	x_{21}	x_{22}	⋯	x_{2n}
⋯				
x_N	x_{N1}	x_{N2}	⋯	x_{Nn}
y (outcomes)	y_1	y_2	⋯	y_n

As in simple linear regression, here also we use the ordinary least squares method to obtain the optimal estimates of $\beta_0, \beta_1, ...\beta_n$ The method yields the following procedure for the computation of these optimal estimates. Let

$$X = \begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{N1} \\ 1 & x_{12} & x_{22} & \cdots & x_{N2} \\ \vdots & & & & \\ 1 & x_{1n} & x_{2n} & \cdots & x_{Nn} \end{bmatrix}, \quad Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad B = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_N \end{bmatrix}$$

Then it can be shown that the regression coefficients are given by
$B = (X^T X)^{-1} X^T Y$

Advantages:

- The multivariate regression method helps you find a relationship between multiple variables or features.
- It also defines the correlation between independent variables and dependent variables.

Disadvantages:

- Multivariate regression technique requires high-level mathematical calculations.
- It is complex.
- The output of the multivariate regression model is difficult to analyse.
- The loss can use errors in the output.
- Multivariate regression yields better results when used with larger datasets rather than small ones.

Example:
Fit a multiple linear regression model to the following data:

x_1	1	1	2	0
x_2	1	2	2	1
y	3.25	6.5	3.5	5.0

In this problem, there are two independent variables and four sets of values of the variables. Thus, in the notations used above, we have n = 2 and N = 4. The multiple linear regression model for this problem has the form $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$

$$X = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 2 & 2 \\ 1 & 0 & 1 \end{bmatrix}, \quad Y = \begin{bmatrix} 3.25 \\ 6.5 \\ 3.5 \\ 5.0 \end{bmatrix}, \quad B = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

$$X^T X = \begin{bmatrix} 4 & 4 & 6 \\ 4 & 6 & 7 \\ 6 & 7 & 10 \end{bmatrix}$$

$$(X^T X)^{-1} = \begin{bmatrix} \frac{11}{4} & \frac{1}{2} & -2 \\ \frac{1}{2} & 1 & -1 \\ -2 & -1 & 2 \end{bmatrix}$$

$$B = (X^T X)^{-1} X^T Y$$

$$= \begin{bmatrix} 2.0625 \\ -2.3750 \\ 3.2500 \end{bmatrix}$$

The required model is $y = 2.0625 - 2.3750x_1 + 3.2500x_2$

3.0.3 Ridge Regression

(Important for GATE DA)
Ridge Regression, also known as L2 regularization, is a machine learning technique used to mitigate the issues of multicollinearity and overfitting in Multiple Linear Regression. It adds a regularization term to the regression equation, modifying the loss function, and aims to minimize the sum of squared errors along with the sum of the squared coefficients, which can be expressed as:

$$\sum_{i=1}^{M}(y_i - y'_i)^2 = \sum_{i=1}^{M}\left(y_i - \sum_{j=0}^{n}\beta_j * x_{ij}\right)^2 + \lambda\sum_{j=0}^{n}\beta_j{}^2$$

- When data exhibits multicollinearity, that is, the ridge regression technique is applied when the independent variables are highly correlated. While least squares estimates are unbiased in multicollinearity, their variances are significant enough to cause the observed value to diverge from the actual value. Ridge regression reduces standard errors by biassing the regression estimates.
- The lambda (λ) variable in the ridge regression equation resolves the multicollinearity problem.
- Lambda (λ) is the penalty term. So, by changing the values of (λ), we are controlling the penalty term. The higher the values of (λ), the bigger is the penalty and therefore the magnitude of coefficients is reduced.
- In this technique, the cost function is altered by adding the penalty term to it. The amount of bias added to the model is called **Ridge Regression penalty**. We can calculate it by multiplying with the lambda to the squared weight of each individual feature.
- In the above equation, the penalty term regularizes the coefficients of the model, and hence ridge regression reduces the amplitudes of the coefficients that decreases the complexity of the model.
- As we can see from the above equation, if the values of (λ) tend to zero, the equation becomes the cost function of the linear regression model. Hence, for the minimum value of (λ) , the model will resemble the linear regression model.
- A general linear or polynomial regression will fail if there is high collinearity between the independent variables, so to solve such problems, Ridge regression can be used.
- It helps to solve the problems if we have more parameters than samples.

Bias and variance trade-off
Bias and variance trade-off is generally complicated when it comes to building ridge regression models on an actual dataset. However, following the general trend which one needs to remember is:

- The bias increases as (λ) increases.
- The variance decreases as (λ) increases.

Assumptions of Ridge Regressions:
The assumptions of ridge regression are the same as that of linear regression: linearity, constant variance, and independence. However, as ridge regression does not provide confidence limits, the distribution of errors to be normal need not be assumed.

- **Linear Relationship:** Ridge Regression assumes that there is a linear relationship between the independent variables and the dependent variable.
- **Homoscedasticity:** Ridge Regression assumes that the variance of the errors is constant across all levels of the independent variables.
- **Independence of errors:** Ridge Regression assumes that the errors are independent of each other, i.e., the errors are not correlated.
- **Normality of errors:** Ridge Regression assumes that the errors follow a normal distribution.

Key points about Ridge Regression in machine learning:

- **Regularization:** Ridge regression adds a penalty term that discourages the magnitude of the coefficients from becoming too large. This helps prevent overfitting.
- **Multicollinearity Mitigation:** It's particularly effective when you have highly correlated independent variables (multicollinearity) by shrinking the coefficients and making the model more stable.
- **Lambda Parameter:** The choice of the lambda parameter (λ) is essential. A small λ is close to standard linear regression, while a large λ results in stronger regularization.
- **Balancing Act:** Ridge regression performs a balancing act between fitting the data well and preventing overfitting. It maintains all predictors but assigns smaller coefficients to less important ones.
- **Model Stability:** It makes the model more stable, especially when you have a high-dimensional dataset with many predictors. This can lead to better generalization to new, unseen data.

- **Interpretability:** Ridge regression may make the model less interpretable because it shrinks coefficients toward zero. It can be challenging to discern the individual importance of predictors.
- **Tuning Lambda:** Cross-validation is often used to tune the lambda parameter and find the optimal trade-off between fitting the data and regularization.

Disadvantages of Ridge Regression:

- **Sensitivity to Lambda:** Proper selection of the regularization parameter (λ) is crucial; an incorrect choice can result in underfitting or ineffective regularization.
- **Loss of Interpretability:** Ridge regression can make the model less interpretable since it shrinks coefficients towards zero, potentially making it harder to discern the individual predictor's importance.
- **Ineffective for Feature Selection:** Ridge regression does not perform feature selection. It retains all predictors in the model but assigns smaller coefficients to less important ones.
- **Less Effective for Sparse Data:** In cases where many predictors are irrelevant or unimportant, Ridge may not eliminate them from the model effectively.

Extra info to understand more about Ridge Regression

What is Regularization?

- Regularization is one of the most important concepts of machine learning. It is a technique to prevent the model from overfitting by adding extra information to it.
- Sometimes the machine learning model performs well with the training data but does not perform well with the test data. It means the model is not able to predict the output when deals with unseen data by introducing noise in the output, and hence the model is called overfitted. This problem can be deal with the help of a regularization technique.
- This technique can be used in such a way that it will allow to maintain all variables or features in the model by reducing the magnitude of the variables. Hence, it maintains accuracy as well as a generalization of the model.
- It mainly regularizes or reduces the coefficient of features toward zero. In simple words, "In regularization technique, we reduce the magnitude of the features by keeping the same number of features."

What is Shrinkage?

- Shrinkage refers to the process of shrinking the estimated regression coefficients towards zero. This is done by adding a penalty term to the sum of squared residuals in the regression equation, which is called the regularization term.
- The regularization term is proportional to the square of the magnitude of the regression coefficients, and it is controlled by a tuning parameter, usually denoted as λ. The higher the value of λ, the more the coefficients are shrunk towards zero.
- Shrinkage helps to reduce the variance of the estimates and can improve the prediction accuracy of the model.

What is Multicollinearity?

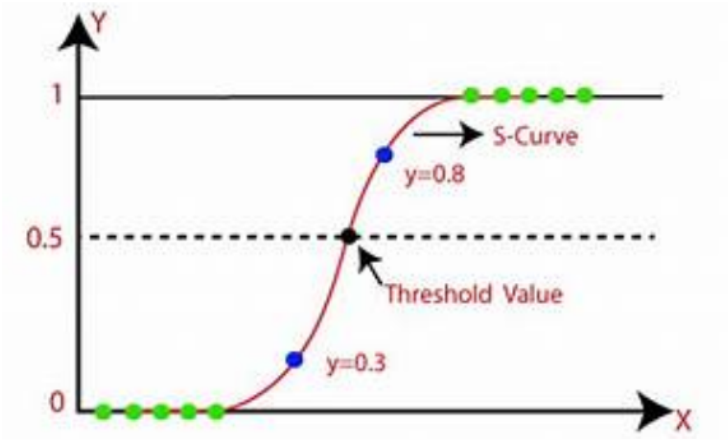
- Multicollinearity is a phenomenon where one predicted value in several regression models is linearly predicted with others.
- Multicollinearity basically happens when more than two anticipated variables have substantial correlations with one another.
- In modeled data, multicollinearity could be defined as the presence of a correlation between independent variables. Estimates of the regression coefficient may become inaccurate as a result. It can potentially raise the standard errors of the regression coefficients and reduce the efficacy of any t-tests.
- In addition to increasing model redundancy and decreasing predictability's effectiveness and dependability, multicollinearity can provide false results and p-values.
- Multicollinearity can be introduced by using multiple data sources. This could happen as a result of limitations placed on linear or demographic models, an overly precise model, outliers, or model design or choice made during the data collection process.
- Multicollinearity may be introduced during the data collection process if the data were gathered using an inappropriate sampling method. Even if the sample size is smaller than expected, it could still happen.
- Because there are more variables than data, multicollinearity will be visible if the model is overspecified.

4 Logistic Regression

- Logistic Regression is a machine learning algorithm used for binary classification tasks, modeling the probability of an event occurring or not, by fitting a logistic curve to the data. It's expressed as the logistic function, which maps the linear combination of input features to values between 0 and 1.
- Logistic regression predicts the output of a categorical dependent variable. Therefore the outcome must be a categorical or discrete value. It can be either Yes or No, 0 or 1, true or False, etc. but instead of giving the exact value as 0 and 1, it gives the probabilistic values which lie between 0 and 1.
- Logistic Regression is much similar to the Linear Regression except that how they are used. Linear Regression is used for solving Regression problems, whereas Logistic regression is used for solving the classification problems.
- In Logistic regression, instead of fitting a regression line, we fit an "S" shaped logistic function, which predicts two maximum values (0 or 1). The curve from the logistic function indicates the likelihood of something such as whether the cells are cancerous or not, a mouse is obese or not based on its weight, etc.
- Logistic Regression is a significant machine learning algorithm because it has the ability to provide probabilities and classify new data using continuous and discrete datasets.
- Logistic Regression can be used to classify the observations using different types of data and can easily determine the most effective variables used for the classification.
- It is used for predicting the categorical dependent variable using a given set of independent variables.

4.1 Logistic Function (Sigmoid Function)

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



- The sigmoid function is a mathematical function used to map the predicted values to probabilities. It maps any real value into another value within a range of 0 and 1. o The value of the logistic regression must be between 0 and 1, which cannot go beyond this limit, so it forms a curve like the "S" form.
- The S-form curve is called the Sigmoid function or the logistic function.
- In logistic regression, we use the concept of the threshold value, which defines the probability of either 0 or 1. Such as values above the threshold value tends to 1, and a value below the threshold values tends to 0.

4.2 Type of Logistic Regression:

On the basis of the categories, Logistic Regression can be classified into three types:

- **Binomial:** In binomial Logistic regression, there can be only two possible types of the dependent variables, such as 0 or 1, Pass or Fail, etc.
- **Multinomial:** In multinomial Logistic regression, there can be 3 or more possible unordered types of the dependent variable, such as "cat", "dogs", or "sheep"
- **Ordinal:** In ordinal Logistic regression, there can be 3 or more possible ordered types of dependent variables, such as "low", "Medium", or "High".

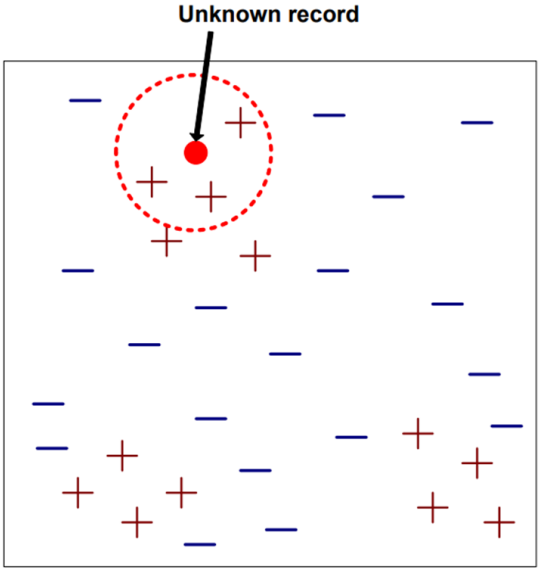
Key points about Logistic Regression include:

- **Binary Classification:** It's primarily used for two-class classification problems, where the output is either 0 or 1, indicating the absence or presence of an event.
- **Logistic Function:** Utilizes the logistic (sigmoid) function to convert a linear combination of input features into a probability value between 0 and 1.
- **Coefficient Interpretation:** Coefficients represent the impact of each feature on the probability of the event, making the model interpretable.
- **Maximum Likelihood Estimation:** The model is trained using maximum likelihood estimation to find the optimal parameters that best fit the data.
- **Decision Boundary:** Logistic Regression calculates a decision boundary to separate the classes, making it a linear classifier by default.
- **Regularization:** Regularization techniques, such as L1 (Lasso) and L2 (Ridge), can be applied to prevent overfitting and improve model generalization.
- **Evaluating Performance:** Common performance metrics include accuracy, precision, recall, F1 score, and the ROC-AUC curve.
- **Extensions:** Multinomial (softmax) logistic regression is used for multi-class classification tasks.
- **Applications:** Logistic Regression is applied in various fields, including medical diagnosis, finance, spam detection, and sentiment analysis.

5 K-Nearest Neighbors

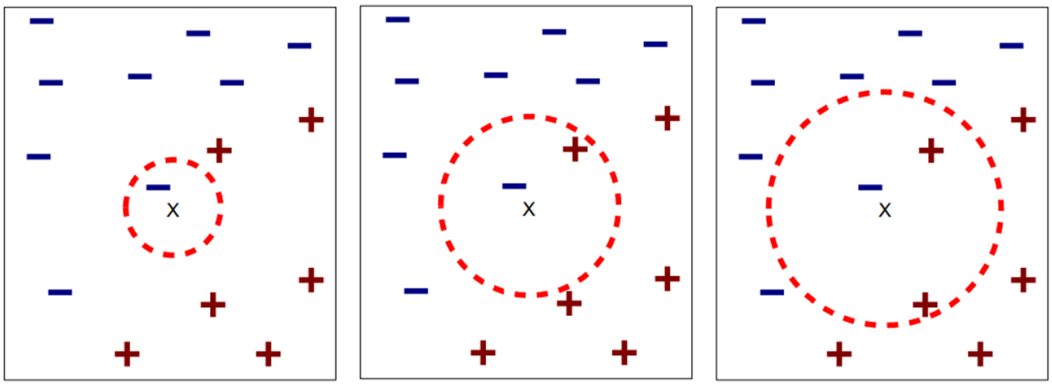
- K-Nearest Neighbors (KNN) is a simple and intuitive machine-learning algorithm used for both classification and regression tasks.
- It is a non-parametric and instance-based learning method, which means it doesn't make any assumptions about the underlying data distribution and makes predictions based on the similarity of data points.
- K-NN algorithm assumes the similarity between the new case/data and available cases and put the new case into the category that is most similar to the available categories.
- K-NN algorithm stores all the available data and classifies a new data point based on the similarity. This means when new data appears then it can be easily classified into a well suite category by using K- NN algorithm.
- K-NN is a non-parametric algorithm, which means it does not make any assumption on underlying data.
- It is also called a lazy learner algorithm because it does not learn from the training set immediately instead it stores the dataset and at the time of classification, it performs an action on the dataset.
- KNN tries to predict the correct class for the test data by calculating the distance between the test data and all the training points. Then select the K number of points which is closest to the test data. The KNN algorithm calculates the probability of the test data belonging to the classes of 'K' training data and class that holds the highest probability will be selected. In the case of regression, the value is the mean of the 'K' selected training points.

Nearest-Neighbor Classifiers



- Requires three things
  - The set of stored records
  - Distance Metric to compute distance between records
  - The value of *k*, the number of nearest neighbors to retrieve
- To classify an unknown record:
  - Compute distance to other training records
  - Identify *k* nearest neighbors
  - Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

Definition of Nearest Neighbor

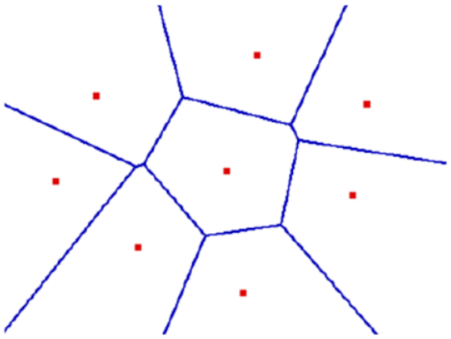


(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

K-nearest neighbors of a record x are data points that have the k smallest distance to x

Voronoi diagram, deals with when value of K =1

Describes the areas that are nearest to any given point, given a set of data. Each line segment is equidistant between two points of opposite class



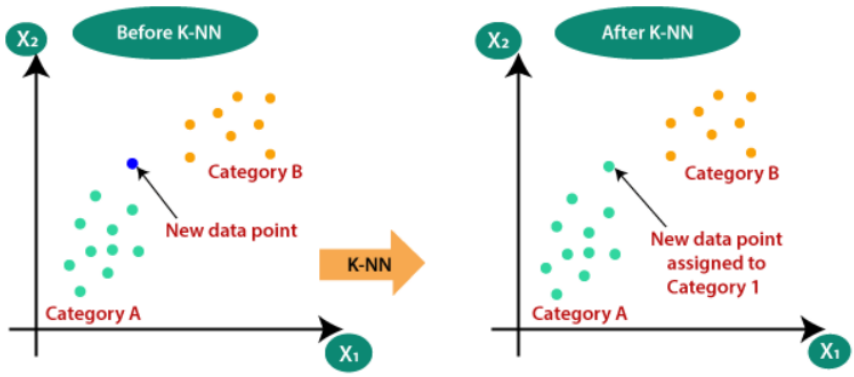
Choosing Value of K

- Larger k may lead to better performance But if we set k too large we may end up looking at samples that are not neighbors (are far away from the query)
- We can use cross-validation to find k
- Rule of thumb is k ¡ sqrt(n), where n is the number of training example
- Larger k produces smoother boundary effect
- When K==N, always predict the majority class

5.1 Working

The K-NN working can be explained on the basis of the below algorithm:

1. Select the number K of the neighbors
2. Calculate the Euclidean distance of K number of neighbors
3. Take the K nearest neighbors as per the calculated Euclidean distance.
4. Among these k neighbors, count the number of the data points in each category.
5. Assign the new data points to that category for which the number of the neighbor is maximum.
6. Our model is ready.



5.2 K-Nearest Neighbors (KNN) Classification Example

Suppose we have a dataset with the following points:

Data Point	Feature 1 (X1)	Feature 2 (X2)	Class
A	1	2	Blue
B	2	3	Blue
C	2	1	Red
D	3	3	Red
E	4	2	Blue

Now, let's say we want to classify a new data point with features $X1 = 2.5$ and $X2 = 2.5$ using a KNN algorithm with $k = 3$ (i.e., considering the three nearest neighbors).

1. Calculate Euclidean Distances:

$$\text{Distance to A: } \sqrt{(2.5-1)^2 + (2.5-2)^2} = \sqrt{1.5}$$
$$\text{Distance to B: } \sqrt{(2.5-2)^2 + (2.5-3)^2} = \sqrt{1.5}$$
$$\text{Distance to C: } \sqrt{(2.5-2)^2 + (2.5-1)^2} = \sqrt{1.5}$$
$$\text{Distance to D: } \sqrt{(2.5-3)^2 + (2.5-3)^2} = \sqrt{2.5}$$
$$\text{Distance to E: } \sqrt{(2.5-4)^2 + (2.5-2)^2} = \sqrt{4.5}$$

2. Find K Nearest Neighbors: Identify the three nearest neighbors based on the calculated distances. In this case, the three closest points are A, B, and C.

3. Majority Voting: Determine the majority class among the three nearest neighbors. Since A and B are Blue, and C is Red, the majority class is Blue.

4. Prediction: Predict that the new point $X1 = 2.5, X2 = 2.5$ belongs to the majority class, which is Blue.

5.3 Advantages of K-Nearest Neighbors (KNN):

- **Simplicity:** KNN is easy to understand and implement, making it a good choice for simple classification and regression tasks.
- **No Training Period:** KNN is a lazy learner, meaning it doesn't require a lengthy training period. It stores the entire training dataset and makes predictions when needed.
- **Non-parametric:** KNN doesn't make any assumptions about the underlying data distribution, making it versatile for a wide range of applications.
- **Adaptability:** KNN can be used for both classification and regression tasks, and it can handle multi-class problems without modification.
- **Interpretability:** The algorithm provides human-interpretable results, as predictions are based on the majority class or the average of the nearest neighbors.

5.4 Disadvantages of K-Nearest Neighbors (KNN):

- **Computational Intensity:** KNN can be computationally expensive, especially for large datasets, as it requires calculating distances to all data points during prediction.
- **Sensitivity to Feature Scaling:** KNN is sensitive to the scale of features, so it's essential to normalize or standardize your data before applying the algorithm.
- **Curse of Dimensionality:** KNN's performance degrades as the number of features or dimensions increases, as distances between data points become less meaningful in high-dimensional spaces.
- **Determining the Optimal K:** Selecting the right value for K is crucial, and choosing an inappropriate K can lead to underfitting or overfitting. There's no universally optimal value, and it often requires experimentation.
- **Imbalanced Data:** KNN can be biased towards the majority class in imbalanced datasets. It's essential to balance the dataset or adjust the class weights when necessary.

6 Naive Bayes Classifier

Naïve Bayes algorithm is a supervised learning algorithm, which is based on Bayes theorem and used for solving classification problems. It is mainly used in text classification that includes a high-dimensional training dataset. Naïve Bayes Classifier is one of the simple and most effective Classification algorithms which helps in building the fast machine learning models that can make quick predictions. It is a probabilistic classifier, which means it predicts on the basis of the probability of an object. Some popular examples of Naïve Bayes Algorithm are spam filtration, Sentimental analysis, and classifying articles.

6.1 Bayes' Theorem

Bayes' theorem is also known as Bayes' Rule or Bayes' law, which is used to determine the probability of a hypothesis with prior knowledge. It depends on the conditional probability. The formula for Bayes' theorem is given as: Where,

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

P(A—B) is Posterior probability: Probability of hypothesis A on the observed event B.

P(B—A) is Likelihood probability: Probability of the evidence given that the probability of a hypothesis is true. P(A) is Prior Probability: Probability of hypothesis before observing the evidence.

P(B) is Marginal Probability: Probability of Evidence.

Assumption

The fundamental Naive Bayes assumption is that each feature makes an **independent** and **equal** contribution to the outcome.

With relation to our dataset, this concept can be understood as:

We assume that no pair of features are dependent. For example, the temperature being 'Hot' has nothing to do with the humidity or the outlook being 'Rainy' has no effect on the winds. Hence, the features are assumed to be independent.

Secondly, each feature is given the same weight(or importance). For example, knowing only temperature and humidity alone can't predict the outcome accurately. None of the attributes is irrelevant and assumed to be contributing equally to the outcome.

Here are the key concepts and characteristics of the Naive Bayes classifier:

- **Bayes' Theorem:** The classifier is based on Bayes' theorem, which calculates the probability of a hypothesis (in this case, a class label) given the evidence (features or attributes). Mathematically, it is expressed as P(class—evidence) = [P(evidence—class) * P(class)] / P(evidence).

- **Independence Assumption:** The "Naive" in Naive Bayes refers to the assumption that all features are independent of each other, given the class label. In reality, this assumption is often not true, but the simplification makes the algorithm computationally efficient and easy to implement.
- **Types of Naive Bayes Classifiers:**
  1. Multinomial Naive Bayes: Typically used for text classification where features represent word counts.
  2. Gaussian Naive Bayes: Suitable for continuous data and assumes a Gaussian distribution of features.
  3. Bernoulli Naive Bayes: Applicable when features are binary, such as presence or absence.
- **Prior Probability (P(class)):** This is the probability of a class occurring before observing any evidence. It can be calculated from the training data.
- **Likelihood (P(evidence—class)):** This represents the probability of observing a specific set of features given a class label. For text classification, this might involve counting the occurrence of words in documents.
- **Posterior Probability (P(class—evidence)):** It is the probability of a class label given the evidence, which is what the Naive Bayes classifier calculates for each class.
- **Classification:** To classify a new data point, the classifier calculates the posterior probabilities for each class and selects the class with the highest probability.

Bayes Classifiers

- Bayesian classifiers use **Bayes theorem**, which says

$$p(c_j \mid d) = \frac{p(d \mid c_j)\, p(c_j)}{p(d)}$$

- $p(c_j \mid d)$ = probability of instance d being in class c_j,
  This is what we are trying to compute
- $p(d \mid c_j)$ = probability of generating instance d given class c_j,
  We can imagine that being in class c_j, causes you to have feature d with some probability
- $p(c_j)$ = probability of occurrence of class c_j,
  This is just how frequent the class c_j, is in our database
- $p(d)$ = probability of instance d occurring

  This can actually be ignored, since it is the same for all classes

- To simplify the task, **naïve Bayesian classifiers** assume attributes have independent distributions, and thereby estimate

$$p(d|c_j) = p(d_1|c_j) * p(d_2|c_j) * \ldots * p(d_n|c_j)$$

The probability of class c_j generating instance d, equals….

The probability of class c_j generating the observed value for feature 1, multiplied by..

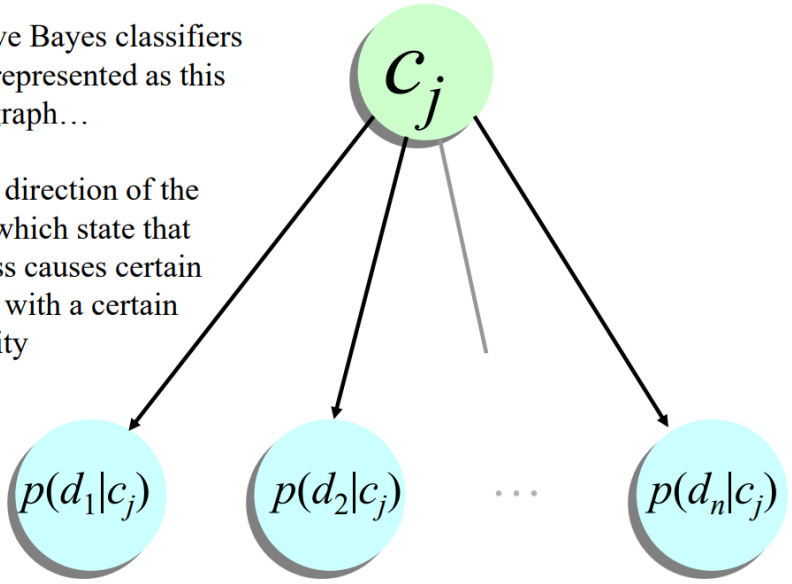
The probability of class c_j generating the observed value for feature 2, multiplied by..

- To simplify the task, **naïve Bayesian classifiers** assume attributes have independent distributions, and thereby estimate

$$p(d|c_j) = p(d_1|c_j) * p(d_2|c_j) * \ldots * p(d_n|c_j)$$

The Naive Bayes classifiers is often represented as this type of graph…

Note the direction of the arrows, which state that each class causes certain features, with a certain probability

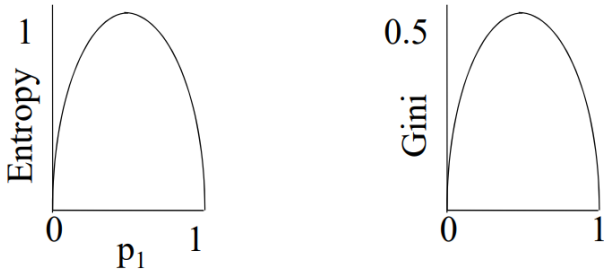


- Approach:
  - compute the posterior probability P(C | A_1, A_2, …, A_n) for all values of C using the Bayes theorem

$$P(C \mid A_1 A_2 \ldots A_n) = \frac{P(A_1 A_2 \ldots A_n \mid C) P(C)}{P(A_1 A_2 \ldots A_n)}$$

  - Choose value of C that maximizes
    P(C | A_1, A_2, …, A_n)
  - Equivalent to choosing value of C that maximizes
    P(A_1, A_2, …, A_n|C) P(C)

- How to estimate P(A_1, A_2, …, A_n | C)?



- Information gain on partitioning S into r subsets
- Impurity (S) - sum of weighted impurity of each subset

$$Gain(S, S_1..S_r) = Entropy(S) - \sum_{j=1}^{r} \frac{S_j}{S} Entropy(S_j)$$

6.2 Advantages of Naive Bayes:

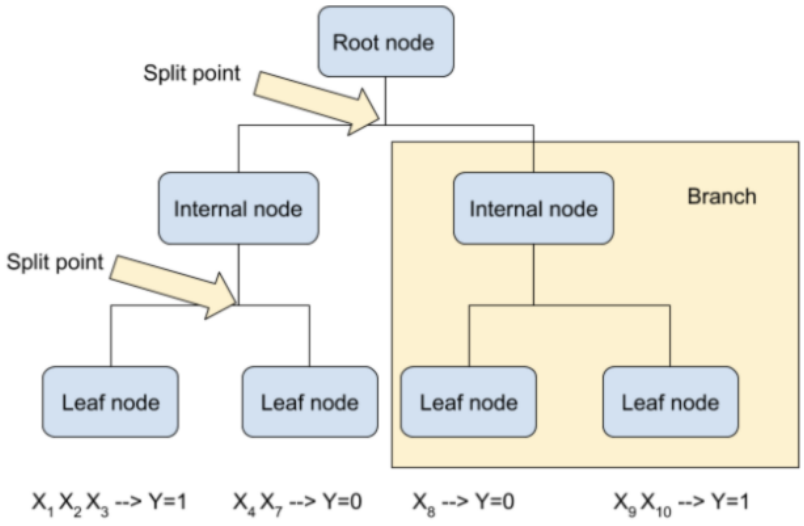
- Simplicity: Naive Bayes is easy to implement and understand, making it a good choice for quick classification tasks.
- Efficiency: It can handle a large number of features efficiently, particularly in text classification.
- Works Well with Small Datasets: It can perform reasonably well even with limited training data.
- Multiclass Classification: It can be used for multiclass classification problems.
- Interpretable: The results are easy to interpret, as it provide the probability of belonging to each class.

6.3 Disadvantages of Naive Bayes:

- **Independence Assumption:** The assumption of feature independence doesn't always hold, which can affect accuracy.
- Sensitivity to Feature Distribution: It may not perform well when features have complex, non-Gaussian distributions.
- Requires Sufficient Data: For some cases, Naive Bayes might not perform well when there is a scarcity of data.
- Zero Probability Problem: If a feature-class combination does not exist in the training data, the probability will be zero, causing issues. Smoothing techniques are often used to address this.

7 Decision Trees

- A decision tree is a simple model for supervised classification. It is used for classifying a single discrete target feature.
- Each internal node performs a Boolean test on an input feature (in general, a test may have more than two options, but these can be converted to a series of Boolean tests). The edges are labeled with the values of that input feature.
- Each leaf node specifies a value for the target feature
- Classifying an example using a decision tree is very intuitive. We traverse down the tree, evaluating each test and following the corresponding edge. When a leaf is reached, we return the classification on that leaf.
- Decision Tree is a Supervised learning technique that can be used for both classification and Regression problems, but mostly it is preferred for solving Classification problems.
- It is a tree-structured classifier, where internal nodes represent the features of a dataset, branches represent the decision rules and each leaf node represents the outcome.
- In a Decision tree, there are two nodes, which are the Decision Node and Leaf Node. Decision nodes are used to make any decision and have multiple branches, whereas Leaf nodes are the output of those decisions and do not contain any further branches.
- The decisions or the test are performed on the basis of features of the given dataset. It is a graphical representation for getting all the possible solutions to a problem/decision based on given conditions.
- It is called a decision tree because, similar to a tree, it starts with the root node, which expands on further branches and constructs a tree-like structure.
- In order to build a tree, we use the CART algorithm, which stands for Classification and Regression Tree algorithm.
- A decision tree simply asks a question, and based on the answer (Yes/No), it further split the tree into subtrees.



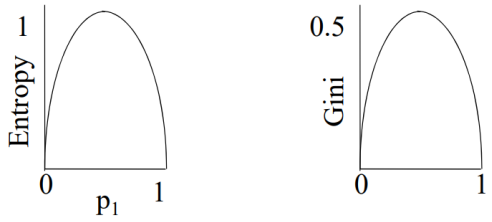
7.1 Terminologies

- **Root Node:** A decision tree's root node, which represents the original choice or feature from which the tree branches, is the highest node.
- **Internal Nodes (Decision Nodes):** Nodes in the tree whose choices are determined by the values of particular attributes. There are branches on these nodes that go to other nodes.
- **Leaf Nodes (Terminal Nodes):** The branches' termini, when choices or forecasts are decided upon. There are no more branches on leaf nodes.
- **Branches (Edges):** Links between nodes that show how decisions are made in response to particular circumstances.
- **Splitting:** The process of dividing a node into two or more sub-nodes based on a decision criterion. It involves selecting a feature and a threshold to create subsets of data.
- **Parent Node:** A node that is split into child nodes. The original node from which a split originates.
- **Child Node:** Nodes created as a result of a split from a parent node.
- **Decision Criterion:** The rule or condition used to determine how the data should be split at a decision node. It involves comparing feature values against a threshold.
- **Pruning:** The process of removing branches or nodes from a decision tree to improve its generalization and prevent overfitting.

7.2 Measures of impurity

While implementing a Decision tree, the main issue arises that how to select the best attribute for the root node and for sub-nodes. So, to solve such problems there is a technique which is called as Attribute selection measure or ASM. By this measurement, we can easily select the best attribute for the nodes of the tree. There are two popular techniques for ASM, which are:

1. Information Gain



- Information gain on partitioning S into r subsets
- Impurity (S) - sum of weighted impurity of each subset

$$Gain(S, S_1..S_r) = Entropy(S) - \sum_{j=1}^{r} \frac{S_j}{S} Entropy(S_j)$$

- Information gain is the measurement of changes in entropy after the segmentation of a dataset based on an attribute.
- It calculates how much information a feature provides us about a class.
- According to the value of information gain, we split the node and build the decision tree.
- A decision tree algorithm always tries to maximize the value of information gain, and a node/attribute having the highest information gain is split first.

It can be calculated using the below formula:
Information Gain= Entropy(S)- [(Weighted Avg) *Entropy(each feature)
Entropy: Entropy is a metric to measure the impurity in a given attribute.

$$Entropy \quad (S) = -\sum_{i=1}^{k} p_i \log \; p_i$$

It specifies randomness in data. Entropy can be calculated as:

Entropy(s)= -P(yes)log2 P(yes)- P(no) log2 P(no)

2. Gini Index

- Gini index is a measure of impurity or purity used while creating a decision tree in the CART(Classification and Regression Tree) algorithm.
- An attribute with a low Gini index should be preferred as compared to the high Gini index.
- It only creates binary splits, and the CART algorithm uses the Gini index to create binary splits.

Gini index can be calculated using the below formula:

$$Gini\ (S) = 1 - \sum_{i=1}^{k} p_i^{\,2}$$

7.3 Advantages of Decision Trees:

- Interpretability: Decision Trees are easy to interpret, making them a good choice when you need to explain or visualize the model's decisions.
- Handling Non-linearity: Decision Trees can capture non-linear relationships between features and the target variable.
- Feature Selection: They can automatically select the most important features, reducing the need for feature engineering.
- Versatility: Decision Trees can handle both categorical and numerical data.
- Efficiency: They are relatively efficient during prediction, with time complexity logarithmic in the number of data points.

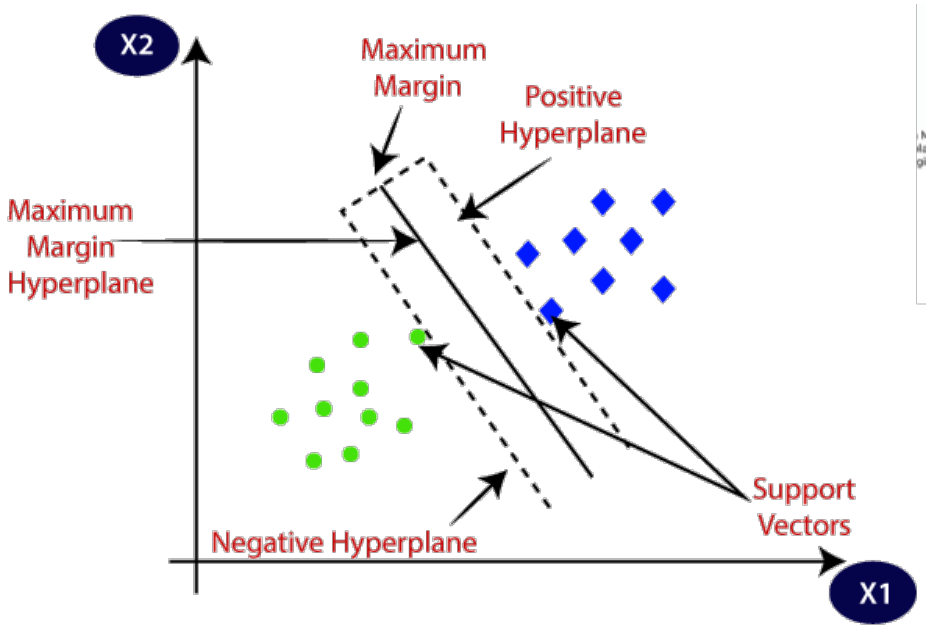
7.4 Disadvantages of Decision Trees:

- Overfitting: Decision Trees can be prone to overfitting, creating complex models that don't generalize well to new data. Pruning and setting appropriate parameters can help mitigate this.
- Bias Toward Dominant Classes: In classification tasks, Decision Trees can be biased toward dominant classes, leading to imbalanced predictions.
- Instability: Small variations in the data can lead to different tree structures, making them unstable models.
- Greedy Algorithm: Decision Trees use a greedy algorithm, making locally optimal decisions at each node, which may not lead to the global optimal tree structure

8 Support Vector Machine

- Support Vector Machine is a system for efficiently training linear learning machines in kernel-induced feature spaces, while respecting the insights of generalisation theory and exploiting optimisation theory.'
- The goal of the SVM algorithm is to create the best line or decision boundary that can segregate n-dimensional space into classes so that we can easily put the new data point in the correct category in the future. This best decision boundary is called a hyperplane.
- SVMs pick best separating hyperplane according to some criterion e.g. maximum margin
- Training process is an optimisation
- Training set is effectively reduced to a relatively small number of support vectors
- SVM chooses the extreme points/vectors that help in creating the hyperplane. These extreme cases are called as support vectors, and hence algorithm is termed as Support Vector Machine.

  Consider the below diagram in which there are two different categories that are classified using a decision boundary or hyperplane:



Here are the key concepts and characteristics of Support Vector Machines:

- **Hyperplane:** There can be multiple lines/decision boundaries to segregate the classes in n-dimensional space, but we need to find out the best decision boundary that helps to classify the data points. This best boundary is known as the hyperplane of SVM.
- In a binary classification problem, an SVM finds a hyperplane that best separates the data points of different classes. This hyperplane is the decision boundary.
- The dimensions of the hyperplane depend on the features present in the dataset, which means if there are 2 features (as shown in image), then hyperplane will be a straight line. And if there are 3 features, then hyperplane will be a 2-dimension plane.

  We always create a hyperplane that has a maximum margin, which means the maximum distance between the data points.
- **Support Vectors:**The data points or vectors that are the closest to the hyperplane and which affect the position of the hyperplane are termed as Support Vector. Since these vectors support the hyperplane, hence called a Support vector. They are critical for defining the margin and determining the location of the hyperplane.
- **Margin:** The margin is the distance between the support vectors and the decision boundary. SVM aims to maximize this margin because a larger margin often leads to better generalization.
- **C Parameter:** The regularization parameter "C" controls the trade-off between maximizing the margin and minimizing the classification error. A smaller "C" value results in a larger margin but may allow some misclassifications, while a larger "C" value allows for fewer misclassifications but a smaller margin.
- **Multi-Class Classification:** SVMs are inherently binary classifiers, but they can be extended to handle multi-class classification using techniques like one-vs-one (OvO) or one-vs-all (OvA) classification.
- **The Scalar Product:**The scalar or dot product is, in some sense, a measure of Similarity $a.b = |a|.|b|cos(\theta)$
- **Decision Function for binary classification**

$$f(x) \in \mathbf{R}$$

$$f(x_i) \geq 0 \Rightarrow y_i = 1$$
$$f(x_i) < 0 \Rightarrow y_i = -1$$

- **Feature Spaces** We may separate data by mapping to a higherdimensional feature space
  – The feature space may even have an infinite number of dimensions!
  • We need not explicitly construct the new feature space

8.1 Kernels

We may use Kernel functions to implicitly map to a new feature space
• Kernel fn: $K(x_1, x_2) \in R$
• Kernel must be equivalent to an inner product in some feature space

- **Kernel Trick:** SVM can handle non-linearly separable data by using a kernel function to map the data into a higher-dimensional space where it becomes linearly separable. Common kernel functions include linear, polynomial, radial basis function (RBF), and sigmoid kernels.

- The linear classifier relies on inner product between vectors $K(\mathbf{x_i},\mathbf{x_j})=\mathbf{x_i}^T\mathbf{x_j}$
- If every datapoint is mapped into high-dimensional space via some transformation Φ: $\mathbf{x} \rightarrow \varphi(\mathbf{x})$, the inner product becomes:

$$K(\mathbf{x_i},\mathbf{x_j})= \varphi(\mathbf{x_i})^T\varphi(\mathbf{x_j})$$

- A *kernel function* is some function that corresponds to an inner product into some feature space.
- Example:

  2-dimensional vectors $\mathbf{x}=[x_1\ x_2]$; let $K(\mathbf{x_i},\mathbf{x_j})=(1 + \mathbf{x_i}^T\mathbf{x_j})^2$,

  Need to show that $K(\mathbf{x_i},\mathbf{x_j})= \varphi(\mathbf{x_i})^T\varphi(\mathbf{x_j})$:

$$K(\mathbf{x_i},\mathbf{x_j})=(1 + \mathbf{x_i}^T\mathbf{x_j})^2 = 1+ x_{i1}^2x_{j1}^2 + 2\,x_{i1}x_{j1}\,x_{i2}x_{j2}+ x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2}=$$
$$= [1\ \ x_{i1}^2\ \sqrt{2}\,x_{i1}x_{i2}\ \ x_{i2}^2\ \sqrt{2}x_{i1}\ \sqrt{2}x_{i2}]^T\,[1\ \ x_{j1}^2\ \sqrt{2}\,x_{j1}x_{j2}\ \ x_{j2}^2\ \sqrt{2}x_{j1}\ \sqrt{2}x_{j2}] =$$
$$= \varphi(\mathbf{x_i})^T\varphi(\mathbf{x_j}), \quad \text{where } \varphi(\mathbf{x}) = [1\ \ x_1^2\ \sqrt{2}\,x_1x_2\ \ x_2^2\ \ \sqrt{2}x_1\ \sqrt{2}x_2]$$

- For some functions $K(\mathbf{x_i},\mathbf{x_j})$ checking that $K(\mathbf{x_i},\mathbf{x_j})= \varphi(\mathbf{x_i})^T\varphi(\mathbf{x_j})$ can be cumbersome.
- Mercer's theorem:

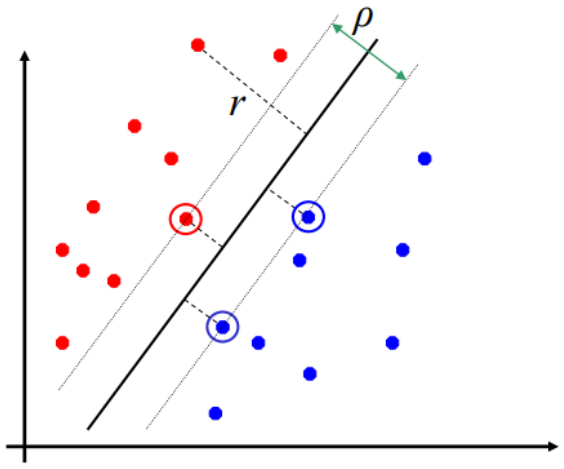
  Every semi-positive definite symmetric function is a kernel

Examples of kernel functions

- Linear: $K(\mathbf{x_i},\mathbf{x_j})= \mathbf{x_i}^T\mathbf{x_j}$
- Polynomial of power p: $K(\mathbf{x_i},\mathbf{x_j})= (1+ \mathbf{x_i}^T\mathbf{x_j})^p$
- Gaussian (radial-basis function network): $K(\mathbf{x_i},\mathbf{x_j})= e^{-\frac{\|\mathbf{x_i}-\mathbf{x_j}\|^2}{2\sigma^2}}$
- Two-layer perceptron: $K(\mathbf{x_i},\mathbf{x_j})= \tanh(\beta_0\mathbf{x_i}^T\mathbf{x_j} + \beta_1)$

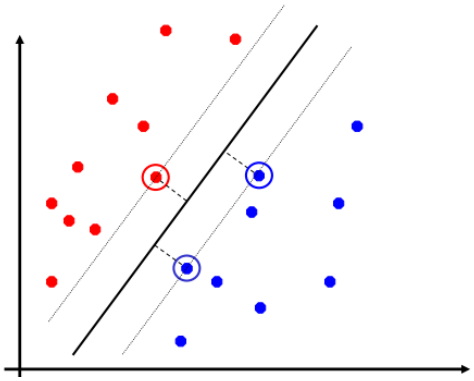
8.2 Classification Margin

- Distance from example data to the separator is $r = \frac{\mathbf{w}^T\mathbf{x}+b}{\|\mathbf{w}\|}$
- Data closest to the hyperplane are ***support vectors***.
- ***Margin*** ρ of the separator is the width of separation between classes.



Maximum Margin Classification

- Maximizing the margin is good according to intuition and theory.
- Implies that only support vectors are important; other training examples are ignorable.



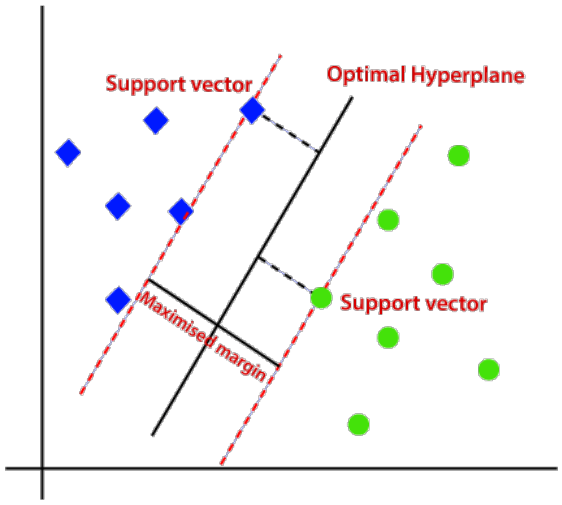
- Misclassification error and the function complexity bound generalization error.
- Maximizing margins minimizes complexity.
- "Eliminates" overfitting.
- Solution depends only on *Support Vectors* not number of attributes.

8.3 Types of SVM

1. Linear SVM: Linear SVM is used for linearly separable data, which means if a dataset can be classified into two classes by using a single straight line, then such data is termed as linearly separable data, and classifier is used called as Linear SVM classifier.

   The working of the SVM algorithm can be understood by using an example. Suppose we have a dataset that has two tags (green and blue), and the dataset has two features x1 and x2. We want a classifier that can classify the pair(x1, x2) of coordinates in either green or blue. So as it is 2-d space so by just using a straight line, we can easily separate these two classes. But there can be multiple lines that can separate these classes.
   Hence, the SVM algorithm helps to find the best line or decision boundary; this best boundary or region is called as a hyperplane. SVM algorithm finds the closest point of the lines from both the classes. These points are called support vectors. The distance between the vectors and the hyperplane is called as margin. And the goal of SVM

is to maximize this margin. The hyperplane with the maximum margin is called the optimal hyperplane.



Linear SVM Mathematically

- Assuming all data is at distance larger than 1 from the hyperplane, the following two constraints follow for a training set $\{(\mathbf{x_i}, y_i)\}$

$$\mathbf{w}^T\mathbf{x_i} + b \geq 1 \quad \text{if } y_i = 1$$
$$\mathbf{w}^T\mathbf{x_i} + b \leq -1 \quad \text{if } y_i = -1$$

- For support vectors, the inequality becomes an equality; then, since each example's distance from the
- hyperplane is $r = \frac{\mathbf{w}^T\mathbf{x} + b}{\|\mathbf{w}\|}$ the margin is: $\rho = \frac{2}{\|\mathbf{w}\|}$

Linear SVMs Mathematically (cont.)

- Then we can formulate the *quadratic optimization problem:*

Find $\mathbf{w}$ and b such that

$\rho = \frac{2}{\|\mathbf{w}\|}$ is maximized and for all $\{(\mathbf{x_i}, y_i)\}$

$\mathbf{w}^T\mathbf{x_i} + b \geq 1$ if y_i=1; $\mathbf{w}^T\mathbf{x_i} + b \leq -1$ if $y_i = -1$

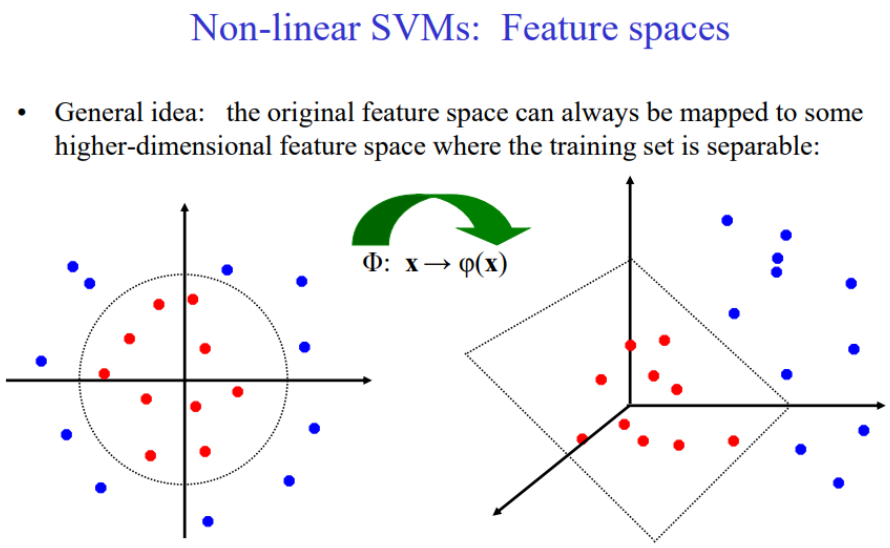
A better formulation:

Find $\mathbf{w}$ and b such that

$\Phi(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{w}$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$

$y_i(\mathbf{w}^T\mathbf{x_i} + b) \geq 1$

2. Non-linear SVM: Non-linear SVM is used for non-linearly separated data, which means if a dataset cannot be classified by using a straight line, then such data is termed as non-linear data and classifier used is called as Non-linear SVM classifier.



8.4 Advantages of Support Vector Machines:

- Effective in High-Dimensional Spaces: SVMs perform well even in high-dimensional feature spaces.
- Robust to Overfitting: SVMs are less prone to overfitting, especially when the margin is maximized. Accurate for Non-Linear Data: The kernel trick allows SVMs to work effectively on non-linear data by transforming it into higher dimensions.
- Wide Applicability: SVMs can be applied to various tasks, including classification, regression, and outlier detection.
- Strong Theoretical Foundation: SVMs are based on solid mathematical principles.

8.5 Disadvantages of Support Vector Machines:

- Computationally Intensive: Training an SVM can be computationally expensive, especially for large datasets.
- Sensitivity to Kernel Choice: The choice of the kernel function and kernel parameters can significantly impact the SVM's performance.
- Challenging for Large Datasets: SVMs may not be suitable for very large datasets because of their computational complexity.
- Interpretability: The decision boundary learned by SVMs can be challenging to interpret, especially in high-dimensional spaces.

9 Bias-Variance Trade-Off

- The goal of supervised machine learning is to learn or derive a target function that can best determine the target variable from the set of input variables.
- A key consideration in learning the target function from the training data is the extent of generalization. This is because the input data is just a limited, specific view and the new, unknown data in the test data set may be differing quite a bit from the training data.
- The fitness of a target function approximated by a learning algorithm determines how correctly it is able to classify a set of data it has never seen.

9.1 Underfitting

- If the target function is kept too simple, it may not be able to capture the essential nuances and represent the underlying data well.
- A typical case of underfitting may occur when trying to represent a non-linear data with a linear model as demonstrated by both cases of underfitting shown in figure 1.1
- Many times underfitting happens due to the unavailability of sufficient training data.
- Underfitting results in both poor performance with training data as well as poor generalization to test data. Underfitting can be avoided by
  1. using more training data
  2. reducing features by effective feature selection

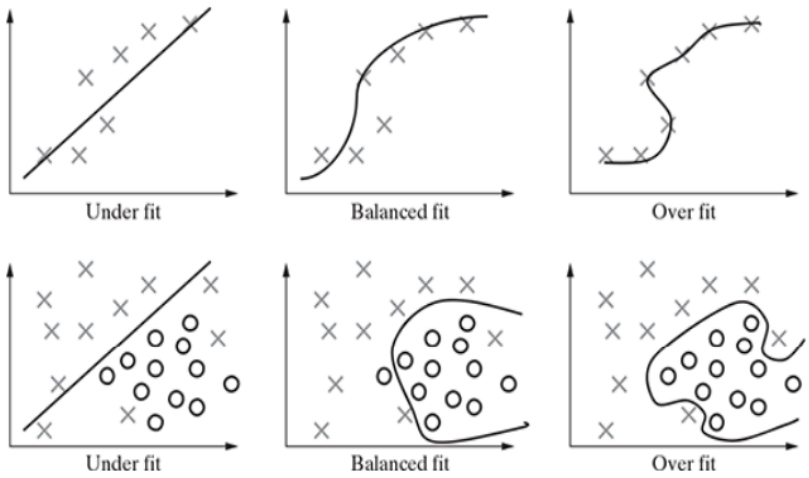


Figure:1.1 Underfitting and Overfitting of models

9.2 Overfitting

- Overfitting refers to a situation where the model has been designed in such a way that it emulates the training data too closely. In such a case, any specific deviation in the training data, like noise or outliers, gets embedded in the model. It adversely impacts the performance of the model on the test data.
- Overfitting, in many cases, occur as a result of trying to fit an excessively complex model to closely match the training data. This is represented with a sample data set in figure 1.1. The target function, in these cases, tries to make sure all training data points are correctly partitioned by the decision boundary. However, more often than not, this exact nature is not replicated in the unknown test data set. Hence, the target function results in wrong classification in the test data set.
- Overfitting results in good performance with training data set, but poor generalization and hence poor performance with test data set. Overfitting can be avoided by
  1. using re-sampling techniques like k-fold cross validation
  2. hold back of a validation data set
  3. remove the nodes which have little or no predictive power for the given machine learning problem.
- Both underfitting and overfitting result in poor classification quality which is reflected by low classification accuracy

9.3 Bias – variance trade-off

Bias-variance trade-off is a fundamental concept in machine learning that refers to the balance between two sources of error that affect the predictive performance of a model: bias and variance.
Bias: Bias is the error due to overly simplistic assumptions in the learning algorithm. High bias can lead to underfitting, where the model is too simple to capture the underlying patterns in the data.
Variance: Variance is the error due to too much complexity in the learning algorithm. High variance can lead to overfitting, where the model is overly sensitive to noise in the training data and fails to generalize well to new, unseen data.
In supervised learning, the class value assigned by the learning model built based on the training data may differ from the actual class value. This error in learning can be of two types – errors due to 'bias' and error due to 'variance'. Let's try to understand each of them in details.

Error due to 'Bias':

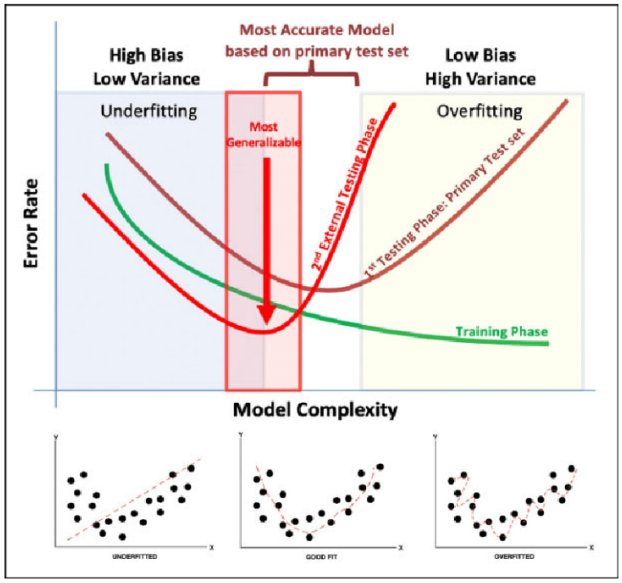
- Errors due to bias arise from simplifying assumptions made by the model to make the target function less complex or easier to learn. In short, it is due to underfitting of the model.

- Parametric models generally have high bias making them easier to understand/interpret and faster to learn.
- These algorithms have a poor performance on data sets, which are complex in nature and do not align with the simplifying assumptions made by the algorithm.
- Underfitting results in high bias.

Errors due to 'Variance':

- Errors due to variance occur from difference in training data sets used to train the model.
- Different training data sets (randomly sampled from the input data set) are used to train the model. Ideally the difference in the data sets should not be significant and the model trained using different training data sets should not be too different.
- However, in case of overfitting, since the model closely matches the training data, even a small difference in training data gets magnified in the model.

So, the problems in training a model can either happen because either
(a) the model is too simple and hence fails to interpret the data grossly or
(b) the model is extremely complex and magnifies even small differences in the training data.



Key points about the bias-variance trade-off:

- **Complex Models vs. Simple Models:** Complex models (e.g., deep neural networks) tend to have low bias but high variance, whereas simple models (e.g., linear regression) tend to have high bias but low variance.

- **Balancing Act:** Machine learning practitioners aim to strike a balance between bias and variance to achieve a model with good generalization, one that performs well on both the training data and new, unseen data.
- **Underfitting and Overfitting:** The trade-off helps address the problems of underfitting (high bias) and overfitting (high variance). Underfit models don't capture enough of the data's complexity, while overfit models fit noise in the data.
- **Model Complexity:** Adjusting model complexity, such as the number of features, the choice of hyperparameters, and regularization techniques, is a way to manage the bias-variance trade-off.
- **Cross-Validation:** Cross-validation techniques, like k-fold cross-validation, help estimate a model's performance on unseen data and guide the selection of the optimal model complexity.
- **Generalization:** Achieving good generalization, where a model performs well on new, unseen data, is the ultimate goal of managing the bias-variance trade-off.

Important Note

Increasing the bias will decrease the variance, and Increasing the variance will decrease the bias On one hand, parametric algorithms are generally seen to demonstrate high bias but low variance. On the other hand, non-parametric algorithms demonstrate low bias and high variance.

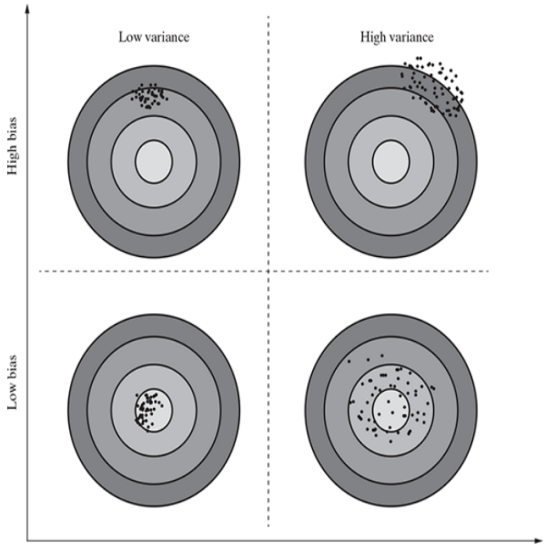


Figure 1.3.1

As can be observed in Figure 1.3.1, the best solution is to have a model with low bias as well as low variance. However, that may not be possible in reality. Hence, the goal of

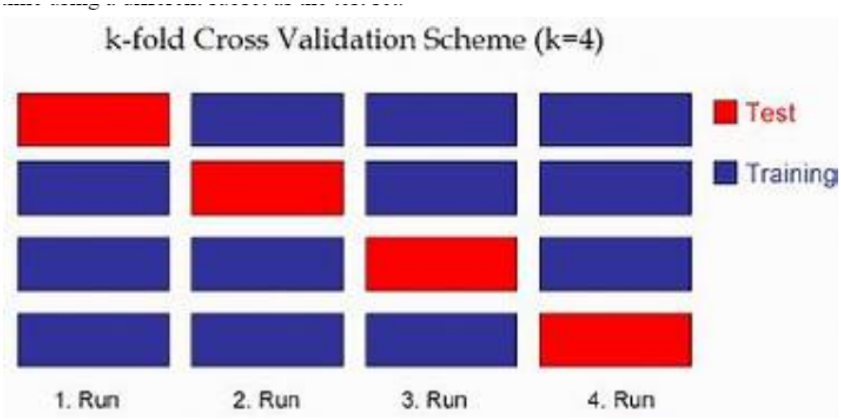
supervised machine learning is to achieve a balance between bias and variance. The learning algorithm chosen and the user parameters which can be configured helps in striking a tradeoff between bias and variance.
For example, in a popular supervised algorithm k-Nearest Neighbors or kNN, the user configurable parameter 'k' can be used to do a trade-off between bias and variance. In one hand, when the value of 'k' is decreased, the model becomes simpler to fit and bias increases. On the other hand, when the value of 'k' is increased, the variance increases.

10 Cross-validation methods

- When the dataset is small, the method is prone to high variance. Due to the random partition, the results can be entirely different for different test sets. To deal with this issue, we use cross-validation to evaluate the performance of a machine-learning model.
- In cross-validation, we don't divide the dataset into training and test sets only once. Instead, we repeatedly partition the dataset into smaller groups and then average the performance in each group. That way, we reduce the impact of partition randomness on the results.
- Many cross-validation techniques define different ways to divide the dataset at hand. We'll focus on the two most frequently used: the k-fold and the leave-one-out methods.

10.1 K-Fold Cross-Validation

K-Fold Cross-Validation is a widely used technique in machine learning for assessing the performance and generalization ability of a model. It involves dividing the dataset into 'k' subsets of approximately equal size, where one of these subsets is used as the test set, and the remaining 'k-1' subsets are used as the training set. This process is repeated 'k' times, each time using a different subset as the test set.



K-Fold Cross-Validation

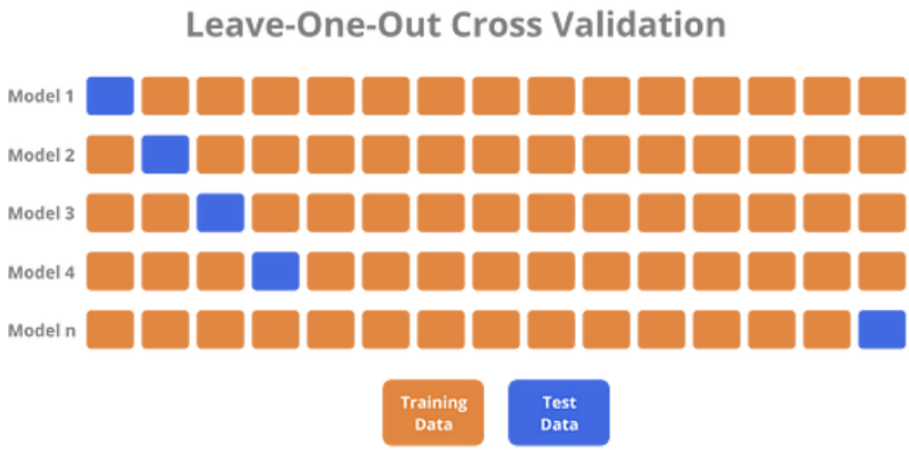
Here are the key points about K-Fold Cross-Validation:

- **Data Splitting:** The dataset is divided into 'k' subsets or folds, where each fold is used as the test set exactly once, and the rest are used for training.
- **Multiple Evaluations:** K-Fold Cross-Validation enables multiple evaluations of the model's performance, providing a more reliable estimate of its generalization ability compared to a single train-test split.

- **Bias-Variance Trade-Off:** It helps in managing the bias-variance trade-off. The model's performance is assessed under different training and test subsets, helping you detect issues like overfitting or underfitting.
- **Hyperparameter Tuning:** K-Fold Cross-Validation is often used for hyperparameter tuning. By trying different hyperparameters on different folds, you can choose the set of hyperparameters that yield the best average performance.
- **K-Fold Variations:** Variations include stratified K-Fold, which ensures that each fold has a similar class distribution, and repeated K-Fold, where the process is repeated multiple times with different random splits.
- **Performance:** The final model performance is typically determined by averaging the results of all 'k' iterations, such as mean accuracy or root mean squared error.
- **Trade-Off:** There's a trade-off between computational cost and model assessment quality. Larger 'k' values lead to a more accurate assessment but require more computation.
- **Usage:** K-Fold Cross-Validation is widely used in various machine learning tasks, including model selection, hyperparameter tuning, and performance estimation.
- **Validation Set:** In practice, a separate validation set might be used to validate the final model after hyperparameter tuning, while K-Fold Cross-Validation helps in assessing the overall performance of the model.

10.2 Leave-One-Out Cross-Validation

Cross-validation methods, including leave-one-out (LOO) cross-validation, are techniques used in machine learning to assess the performance and generalization ability of a model.
In the leave-one-out (LOO) cross-validation, we train our machine-learning model n times where n is to our dataset's size. Each time, only one sample is used as a test set while the rest are used to train our model.



Leave-One-Out Cross-Validation

Here's an explanation of LOO cross-validation and its role:

- **Principle:** LOO cross-validation is a special case of k-fold cross-validation, where k is equal to the number of data points (n) in the dataset. It involves splitting the dataset into n subsets, each containing a single data point. For each iteration, one data point is held out as the test set, and the remaining n-1 data points are used as the training set. This process is repeated n times (once for each data point), and the model's performance is evaluated by averaging the results across all iterations.
- **Comprehensive Evaluation:** LOO cross-validation provides an exhaustive assessment of a model's performance, as each data point is used as a test set exactly once. This makes it suitable for small to moderately sized datasets.
- **Bias and Variance:** It tends to produce a more reliable estimate of a model's performance as it reduces bias compared to other cross-validation methods like k-fold cross-validation. However, LOO can have high variance due to its many iterations, making it computationally expensive.
- **Model Evaluation:** LOO cross-validation allows you to assess how well the model generalizes to unseen data and identify potential issues like overfitting or data leakage.
- **Advantages:** LOO is particularly useful when dealing with imbalanced datasets or when each data point is scarce and valuable, as none are left out during training.
- **Computational Cost:** LOO cross-validation can be computationally expensive, especially for large datasets, as it requires training the model n times. Variance Estimation: It's valuable for estimating the variance of performance metrics, helping you understand the stability and robustness of your model's predictions.

Comparison

An important factor when choosing between the k-fold and the LOO cross-validation methods is the size of the dataset.

When the size is small, LOO is more appropriate since it will use more training samples in each iteration. That will enable our model to learn better representations.

Conversely, we use k-fold cross-validation to train a model on a large dataset since LOO trains n models, one per sample in the data. When our dataset contains a lot of samples, training so many models will take too long. So, the k-fold cross-validation is more appropriate.

Also, in a large dataset, it is sufficient to use less than n folds since the test folds are large enough for the estimates to be sufficiently precise.

11 Feedforward Neural Network (FNN)

Neural networks are a class of machine learning models inspired by the structure and function of the human brain. Feedforward Neural Networks (FNN) represent the simplest form of neural networks, where information travels in one direction, from the input layer to the output layer.

11.1 Architecture of a Feedforward Neural Network

The architecture of a feedforward neural network consists of three types of layers: the input layer, hidden layers, and the output layer. Each layer is made up of units known as neurons, and the layers are interconnected by weights.

- **Input Layer:** This layer consists of neurons that receive inputs and pass them on to the next layer. The number of neurons in the input layer is determined by the dimensions of the input data.
- **Hidden Layers:** These layers are not exposed to the input or output and can be considered as the computational engine of the neural network. Each hidden layer's neurons take the weighted sum of the outputs from the previous layer, apply an activation function, and pass the result to the next layer. The network can have zero or more hidden layers.
- **Output Layer:** The final layer that produces the output for the given inputs. The number of neurons in the output layer depends on the number of possible outputs the network is designed to produce.
- Each neuron in one layer is connected to every neuron in the next layer, making this a fully connected network. The strength of the connection between neurons is represented by weights, and learning in a neural network involves updating these weights based on the error of the output.

The input and hidden layers use sigmoid and linear activation functions whereas the output layer uses a Heaviside step activation function at nodes because it is a two-step activation function that helps in predicting results as per requirements. All units also known as neurons have weights and calculation at the hidden layer is the summation of the dot product of all weights and their signals and finally the sigmoid function of the calculated sum. Multiple hidden and output layer increases the accuracy of the output.

11.2 Neurons,Activation Functions, Weights and Biases

- **Neurons**

  Nodes in the network that receive inputs, perform a weighted sum, and pass the result through an activation function.

- **Activation Functions**

  Non-linear functions applied to the weighted sum to introduce non-linearity and enable the network to learn complex patterns.

- **Weights**

  Parameters that the network learns during training, determining the strength of connections between neurons.

- **Biases**

  Additional parameters that are added to the weighted sum before applying the activation function, allowing the network to better fit the data.

11.3 Feedforward Process

1. The input data is fed into the input layer.
2. Each neuron in the hidden layers processes the input using weights, biases, and activation functions.
3. The output from each hidden layer is passed to the next layer.
4. This process continues until the output layer produces the final prediction.

11.4 How Feedforward Neural Networks Work

The working of a feedforward neural network involves two phases: **the feedforward phase** and the **backpropagation phase.**

- **Feedforward Phase:** In this phase, the input data is fed into the network, and it propagates forward through the network. At each hidden layer, the weighted sum of the inputs is calculated and passed through an activation function, which introduces non-linearity into the model. This process continues until the output layer is reached, and a prediction is made.
- **Backpropagation Phase:** Once a prediction is made, the error (difference between the predicted output and the actual output) is calculated. This error is then propagated back through the network, and the weights are adjusted to minimize this error. The process of adjusting weights is typically done using a gradient descent optimization algorithm.

11.5 Optimization Techniques

- **Gradient Descent**

  An iterative optimization algorithm that adjusts weights and biases to minimize the loss function.

- **Learning Rate**

  A hyperparameter that determines the step size in the weight and bias updates.

- **Mini-Batch Gradient Descent**

  An optimization technique that processes the training data in small batches to speed up convergence.

11.6 Common Activation Functions

- **Sigmoid**

  Outputs values between 0 and 1, commonly used in the output layer for binary classification.

- **Hyperbolic Tangent (tanh)**

  Similar to the sigmoid but outputs values between -1 and 1, often used in hidden layers.

- **Rectified Linear Unit (ReLU)**

  Outputs the input for positive values and zero for negative values, widely used in hidden layers.

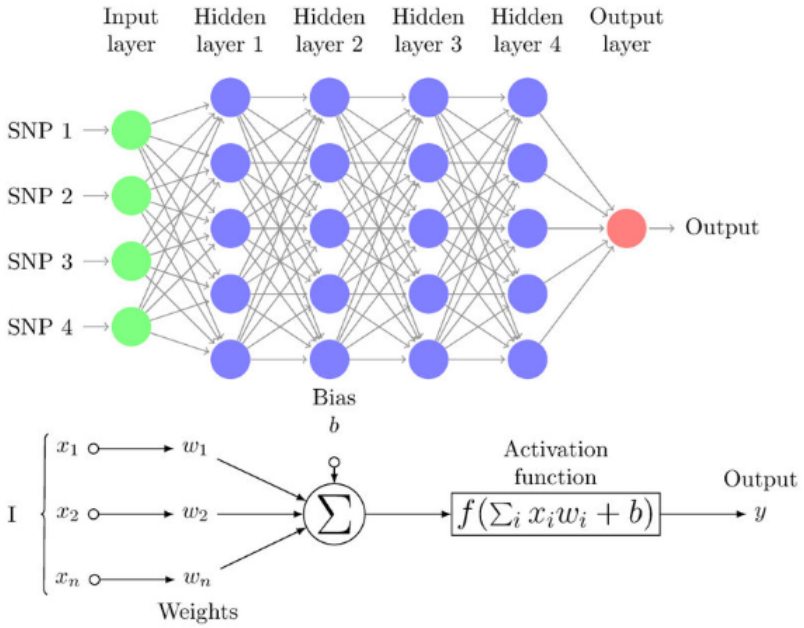
Overfitting
When a model performs well on the training data but poorly on new, unseen data.

Regularization Techniques
Methods like dropout and L2 regularization are employed to prevent overfitting by penalizing overly complex models.

Applications of Feedforward Neural Networks
Image and speech recognition, natural language processing, financial forecasting, and many other tasks where complex patterns need to be learned from data.

12 Multi-Layer Perceptron

- A Multi-Layer Perceptron (MLP) is a class of feedforward artificial neural networks, often used in machine learning and deep learning for various tasks, such as classification, regression, and pattern recognition. An MLP consists of multiple layers of interconnected nodes, where information flows in one direction, from the input layer to the output layer, without feedback loops.
- A multi-layered perceptron consists of interconnected neurons transferring information to each other, much like the human brain. Each neuron is assigned a value. The network can be divided into three main layers.
- The MLP is a feedforward neural network, which means that the data is transmitted from the input layer to the output layer in the forward direction.
- The connections between the layers are assigned weights. The weight of a connection specifies its importance. This concept is the backbone of an MLP's learning process.
- While the inputs take their values from the surroundings, the values of all the other neurons are calculated through a mathematical function involving the weights and values of the layer before it.



Multi-Layer Perceptron

12.1 Architecture:

- **Input Layer:** The input layer is responsible for receiving data from the outside world. Each neuron in the input layer corresponds to one feature, and the values from the dataset are directly fed into these neurons.
- **Hidden Layers:** Between the input and output layers, there can be one or more hidden layers. These layers contain neurons, also known as units or nodes, which are responsible for learning complex patterns and relationships in the data. Hidden layers add the capacity to model non-linear functions. An MLP can have a varying number of hidden layers and units, depending on the problem's complexity.
- **Output Layer:** The output layer is responsible for producing the final results or predictions. The number of output neurons depends on the nature of the task. For instance, in binary classification, there might be a single output neuron that outputs the probability of belonging to one class, while in multi-class classification, there could be multiple output neurons, each corresponding to a class.

12.2 Backpropagation

- Backpropagation is a technique used to optimize the weights of an MLP using the outputs as inputs.
- In a conventional MLP, random weights are assigned to all the connections. These random weights propagate values through the network to produce the actual output. Naturally, this output would differ from the expected output. The difference between the two values is called the error.
- Backpropagation refers to the process of sending this error back through the network, readjusting the weights automatically so that eventually, the error between the actual and expected output is minimized.
- In this way, the output of the current iteration becomes the input and affects the next output. This is repeated until the correct output is produced. The weights at the end of the process would be the ones on which the neural network works correctly.

12.3 Hyperparameter Tuning:

- **Architecture:** Determining the number of hidden layers, the number of neurons in each layer, and the choice of activation functions are important architectural decisions.
- **Learning Rate:**Choosing an appropriate learning rate is crucial for effective training, as it controls the size of weight updates during backpropagation.
- **Regularization:** Regularization techniques like dropout, L1, and L2 regularization are used to prevent overfitting.

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