1.1 INTRODUCTION

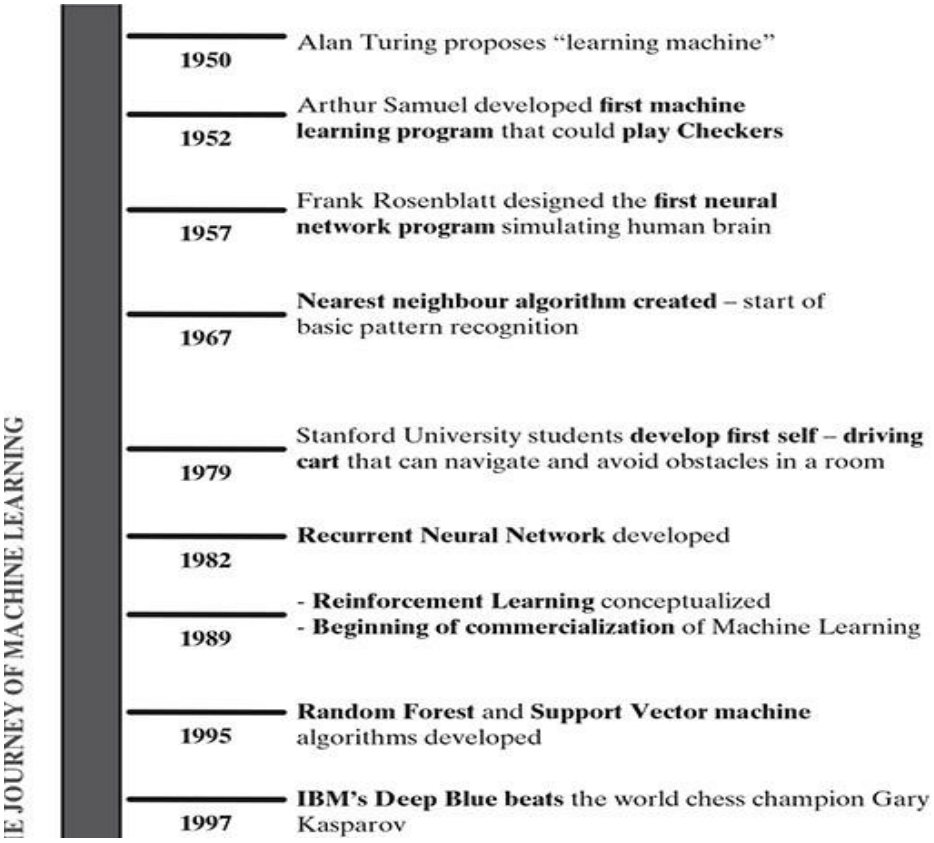
It has been more than 20 years since a computer program defeated the reigning world champion in a game which is considered to need a lot of intelligence to play. The computerprogram was IBM's Deep Blue and it defeated world chess champion, Gary Kasparov. That was the time, probably, whenthe most number of people gave serious attention to a fast-evolving field in computer science or more specificallyartificial intelligence – i.e. machine learning (ML).

As of today, machine learning is a mature technology area finding its application in almost every sphere of life. It can recommend toys to toddlers much in the same way as it can suggest a technology book to a geek or a rich title in literature to a writer.

The foundation of machine learning started in the 18th and 19th centuries. The first related work dates back to 1763. In that year, Thomas Bayes's work 'An Essay towards solving a Problem in the Doctrine of Chances' was published two years after his death. This is the work underlying Bayes Theorem, a fundamental work on which a number of algorithms of machine learning is based upon. In 1812, the Bayes theorem was actually formalized by the French mathematician Pierre- Simon Laplace. The method of least squares, which is the foundational concept to solve regression problems, was formalized in 1805. In 1913, Andrey Markov came up with theconcept of Markov chains.

The evolution of machine learning from 1950 is depicted inFigure 1.1.

The rapid development in the area of machine learning hastriggered a question in everyone's mind – can machines learnbetter than human? To find its answer, the first step would beto understand what learning is from a human perspective.
Then, more light can be shed on what machine learning is. Inthe end, we need to know whether machine learning has already surpassed or has the potential to surpass human learning in every facet of life.



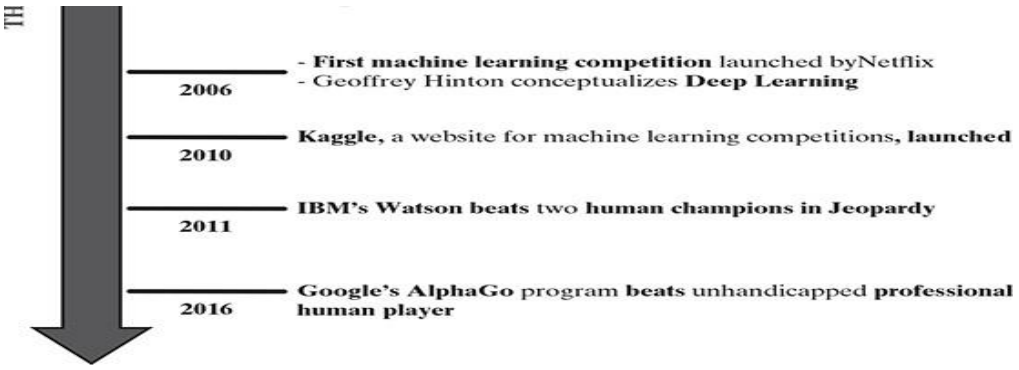


FIG. 1.1 Evolution of machine learning

1.2 WHAT IS HUMAN LEARNING?

In cognitive science, learning is typically referred to as the process of gaining information through observation. And why do we need to learn? In our daily life, we need to carry out multiple activities. It may be a task as simple as walking downthe street or doing the homework. Or it may be some complex task like deciding the angle in which a rocket should be launched so that it can have a particular trajectory. To do a taskin a proper way, we need to have prior information on one or more things related to the task. Also, as we keep learning moreor in other words acquiring more information, the efficiency in doing the tasks keep improving. For example, with more knowledge, the ability to do homework with less number of mistakes increases. In the same way, information from past rocket launches helps in taking the right precautions and makes more successful rocket launch. Thus, with more learning, tasks can be performed more efficiently.

1.3 TYPES OF HUMAN LEARNING

Thinking intuitively, human learning happens in one of the three ways – (1) either somebody who is an expert in the subject directly teaches us, (2) we build our own notion indirectly based on what we have learnt from the expert in thepast, or (3) we do it ourselves, may be after multiple attempts,some being unsuccessful. The first type of learning, we may call, falls under the category of learning directly under expert guidance, the second type falls under learning guided by knowledge gained from experts and the third type is learning by self or self-learning. Let's look at each of these types deeply using real-life examples and try to understand what they mean.

1.3.1 Learning under expert guidance

An infant may inculcate certain traits and characteristics, learning straight from its guardians. He calls his hand, a 'hand', because that is the information he gets from his parents. The sky is 'blue' to him because that is what his parents have taught him. We say that the baby 'learns' thingsfrom his parents.

The next phase of life is when the baby starts going to school. In school, he starts with basic familiarization of alphabets and digits. Then the baby learns how to form wordsfrom the alphabets and numbers from the digits. Slowly morecomplex learning happens in the form of sentences, paragraphs, complex mathematics, science, etc. The baby is able to learn all these things from his teacher who already hasknowledge on these areas.

Then starts higher studies where the person learns aboutmore complex, application-oriented skills. Engineering students get skilled in one of the disciplines like civil, computer science, electrical, mechanical, etc. medical studentslearn about anatomy, physiology, pharmacology,

etc. There aresome experts, in general the teachers, in the respective field who have in-depth subject matter knowledge, who help the students in learning these skills.

Then the person starts working as a professional in some field. Though he might have gone through enough theoreticallearning in the respective field, he still needs to learn more about the hands-on application of the knowledge that he has acquired. The professional mentors, by virtue of the knowledge that they have gained through years of hands-on experience, help all new comers in the field to learn on-job.

In all phases of life of a human being, there is an element ofguided learning. This learning is imparted by someone, purely because of the fact that he/she has already gathered the knowledge by virtue of his/her experience in that field. So guided learning is the process of gaining information from a person having sufficient knowledge due to the past experience.

1.3.2 Learning guided by knowledge gained from experts

An essential part of learning also happens with the knowledge which has been imparted by teacher or mentor at some point oftime in some other form/context. For example, a baby can group together all objects of same colour even if his parents have not specifically taught him to do so. He is able to do so because at some point of time or other his parents have told him which colour is blue, which is red, which is green, etc. A grown-up kid can select one odd word from a set of words because it is a verb and other words being all nouns. He could do this because of his ability to label the words as verbs or nouns, taught by his English teacher long back. In a professional role, a person is able to make out to which customers he should market a campaign from the knowledgeabout preference that was given by his boss long back.

In all these situations, there is no direct learning. It is somepast information shared on some different context, which is used as a learning to make decisions.

1.3.3 Learning by self

In many situations, humans are left to learn on their own. A classic example is a baby learning to walk through obstacles. He bumps on to obstacles and falls down multiple times till helearns that whenever there is an obstacle, he needs to cross over it. He faces the same challenge while learning to ride a cycle as a kid or drive a car as an adult. Not all things are taught by others. A lot of things need to be learnt only from mistakes made in the past. We tend to form a check list on things that we should do, and things that we should not do, based on our experiences.

1.4 WHAT IS MACHINE LEARNING?

Before answering the question ‘What is machine learning?’more fundamental questions that peep into one’s mind are

- Do machines really learn?If
- so, how do they learn?
- Which problem can we consider as a well-posed learning problem? What arethe important features that are required to well-define a learning problem?

At the onset, it is important to formalize the definition of machine learning. This will itself address the first question, i.e.if machines really learn. There are multiple ways to define machine learning. But the one which is perhaps most relevant, concise and accepted universally is the one stated by Tom M.Mitchell, Professor of Machine Learning Department, Schoolof Computer Science, Carnegie Mellon University. Tom M.

Mitchell has defined machine learning as

'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 in T, as measured by P, improves with experience E.'

What this essentially means is that a machine can be considered to learn if it is able to gather experience by doing acertain task and improve its performance in doing the similar tasks in the future. When we talk about past experience, it means past data related to the task. This data is an input to themachine from some source.

In the context of the learning to play checkers, E represents the experience of playing the game, T represents the task of playing checkers and P is the performance measure indicated by the percentage of games won by the player. The same mapping can be applied for any other machine learning problem, for example, image classification problem. In contextof image classification, E represents the past data with images having labels or assigned classes (for example whether the image is of a class cat or a class dog or a class elephant etc.), Tis the task of assigning class to new, unlabelled images and P is the performance measure indicated by the percentage of images correctly classified.

The first step in any project is defining your problem. Evenif the most powerful algorithm is used, the results will be meaningless if the wrong problem is solved.

1.4.1 How do machines learn?

The basic machine learning process can be divided into threeparts.

1. **Data Input:** Past data or information is utilized as a basis for futuredecision-making
2. **Abstraction:** The input data is represented in a broader way through the underlying algorithm
3. **Generalization:** The abstracted representation is generalized to form a framework for making decisions

Figure 1.2 is a schematic representation of the machinelearning process.

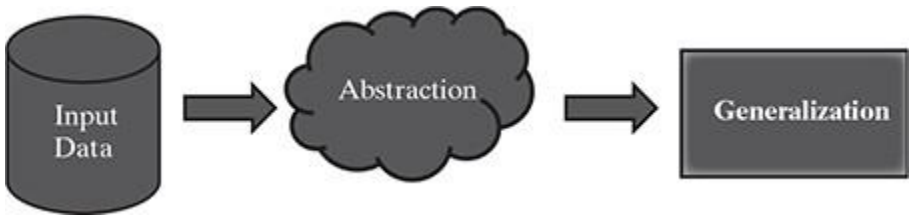


FIG. 1.2 Process of machine learning

Let's put the things in perspective of the human learning process and try to understand the machine learning process more clearly. Reason is, in some sense, machine learning process tries to emulate the process in which humans learn to alarge extent.

Let's consider the situation of typical process of learning from classroom and books and preparing for the examination. It is a tendency of many students to try and memorize (we often call it 'learn by heart') as many things as possible. This may work well when the scope of learning is not so vast. Also,the kinds of questions which are asked in the examination are pretty much simple and straightforward. The questions can be answered by simply writing the same things which have been memorized. However, as the scope gets broader and the questions asked

in the examination gets more complex, the strategy of memorizing doesn't work well. The number of topics may get too vast for a student to memorize. Also, thecapability of memorizing varies from student to student.
Together with that, since the questions get more complex, a direct reproduction of the things memorized may not help. Thesituation continues to get worse as the student graduates to higher classes.

So, what we see in the case of human learning is that just bygreat memorizing and perfect recall, i.e. just based on knowledge input, students can do well in the examinations only till a certain stage. Beyond that, a better learning strategyneeds to be adopted:

1. to be able to deal with the vastness of the subject matter and the relatedissues in memorizing it
2. to be able to answer questions where a direct answer has not been learnt

A good option is to figure out the key points or ideas amongst a vast pool of knowledge. This helps in creating an outline of topics and a conceptual mapping of those outlined topics with the entire knowledge pool. For example, a broad pool of knowledge may consist of all living animals and their characteristics such as whether they live in land or water, whether they lay eggs, whether they have scales or fur or none,etc. It is a difficult task for any student to memorize the characteristics of all living animals – no matter how much photographic memory he/she may possess. It is better to draw a notion about the basic groups that all living animals belong to and the characteristics which define each of the basic groups. The basic groups of animals are invertebrates and vertebrates. Vertebrates are further grouped as mammals, reptiles, amphibians, fishes, and birds. Here, we have mapped animal groups and their salient characteristics.

1. Invertebrate: Do not have backbones and skeletons
2. Vertebrate
    1. Fishes: Always live in water and lay eggs
    2. Amphibians: Semi-aquatic i.e. may live in water or land; smoothskin; lay eggs
    3. Reptiles: Semi-aquatic like amphibians; scaly skin; lay eggs;cold-blooded
    4. Birds: Can fly; lay eggs; warm-blooded
    5. Mammals: Have hair or fur; have milk to feed their young;warm-blooded

This makes it easier to memorize as the scope now reducesto know the animal groups that the animals belong to. Rest ofthe answers about the characteristics of the animals may be derived from the concept of mapping animal groups and theircharacteristics.

Moving to the machine learning paradigm, the vast pool of knowledge is available from the data input. However, rather than using it in entirety, a concept map, much in line with the animal group to characteristic mapping explained above, is drawn from the input data. This is nothing but knowledge abstraction as performed by the machine. In the end, the abstracted mapping from the input data can be applied to makecritical conclusions. For example, if the group of an animal is given, understanding of the characteristics can be automatically made. Reversely, if the characteristic of an unknown animal is given, a definite conclusion can be made about the animal group it belongs to. This is generalization in context of machine learning.

1.4.1.1 Abstraction

During the machine learning process, knowledge is fed in theform of input data. However, the

data cannot be used in the original shape and form. As we saw in the example above, abstraction helps in deriving a conceptual map based on the input data. This map, or a **model** as it is known in the machinelearning paradigm, is summarized knowledge representation ofthe raw data. The model may be in any one of the following forms

- Computational blocks like if/else rules
- Mathematical equations
- Specific data structures like trees or graphsLogical
- groupings of similar observations

The choice of the model used to solve a specific learning problem is a human task. The decision related to the choice ofmodel is taken based on multiple aspects, some of which are listed below:

- The type of problem to be solved: Whether the problem is related to forecastor prediction, analysis of trend, understanding the different segments or groups of objects, etc.
- Nature of the input data: How exhaustive the input data is, whether the datahas no values for many fields, the data types, etc.
- Domain of the problem: If the problem is in a business critical domain with a high rate of data input and need for immediate inference, e.g. fraud detection problem in banking domain.

Once the model is chosen, the next task is to fit the model based on the input data. Let's understand this with an example.In a case where the model is represented by a mathematical equation, say '$y = c_1 + c_2x$' (the model is known as simple linear regression which we will study in a later chapter), basedon the input data, we have to find out the values of c_1 and c_2. Otherwise, the equation (or the model) is of no use. So, fittingthe model, in this case, means finding the values of the unknown coefficients or constants of the equation or the model. This process of fitting the model based on the input data is known as training. Also, the input data based on whichthe model is being finalized is known as training data.

1.4.1.2 *Generalization*

The first part of machine learning process is abstraction i.e. abstract the knowledge which comes as input data in the formof a model. However, this abstraction process, or more popularly training the model, is just one part of machine learning. The other key part is to tune up the abstracted knowledge to a form which can be used to take future decisions. This is achieved as a part of generalization. This part is quite difficult to achieve. This is because the model is trained based on a finite set of data, which may possess a limited set of characteristics. But when we want to apply the model to take decision on a set of unknown data, usually termed as test data, we may encounter two problems:

1. The trained model is aligned with the training data too much, hencemay not portray the actual trend.
2. The test data possess certain characteristics apparently unknown to thetraining data.

Hence, a precise approach of decision-making will not work. An approximate or heuristic approach, much like gut- feeling-based decision-making in human beings, has to be adopted. This approach has the risk of not making a correct decision – quite obviously because certain assumptions that are made may not be true in reality. But just like machines, same mistakes can be made by humans too when a decision ismade based on intuition or gut-feeling – in a situation where exact reason-based decision-making is not possible.

1.4.2 Well-posed learning problem

For defining a new problem, which can be solved using machine learning, a simple framework, highlighted below, canbe used. This framework also helps in deciding whether the problem is a right candidate to be solved using machine learning. The framework involves answering three questions:

1. What is the problem?
2. Why does the problem need to be solved?
3. How to solve the problem?

Step 1: What is the Problem?

A number of information should be collected to know whatis the problem.

Informal description of the problem, e.g. I need a program that will prompt the next word as and when I type aword.

Formalism

Use Tom Mitchell's machine learning formalism stated aboveto define the T, P, and E for the problem.

For example:

- Task (T): Prompt the next word when I type a word.
- Experience (E): A corpus of commonly used English words and phrases.Performance
- (P): The number of correct words prompted considered as apercentage (which in machine learning paradigm is known as learning accuracy).

Assumptions - Create a list of assumptions about theproblem.

Similar problems

What other problems have you seen or can you think of thatare similar to the problem that you are trying to solve?

Step 2: Why does the problem need to be solved?

Motivation

What is the motivation for solving the problem? Whatrequirement will it fulfil?

For example, does this problem solve any long-standingbusiness issue like finding out potentially fraudulent transactions? Or the purpose is more trivial like trying to suggest some movies for upcoming weekend.

Solution benefits

Consider the benefits of solving the problem. Whatcapabilities does it enable?

It is important to clearly understand the benefits of solvingthe problem. These benefits can be articulated to sell the project.

Solution use

How will the solution to the problem be used and the life timeof the solution is expected to have?

Step C: How would I solve the problem?

Try to explore how to solve the problem manually.

Detail out step-by-step data collection, data preparation, andprogram design to solve the problem. Collect all these details and update the previous sections of the problem definition, especially the assumptions.

Summary

- **Step 1: What is the problem?** Describe the problem informally andformally and list assumptions and similar problems.
- **Step 2: Why does the problem need to be solved?** List the motivation forsolving the problem, the benefits that the solution will provide and how the solution will be used.
- **Step C: How would I solve the problem?** Describe how the problem wouldbe solved manually to flush domain knowledge.

1.5 TYPES OF MACHINE LEARNING

As highlighted in Figure 1.3, Machine learning can beclassified into three broad categories:

1. Supervised learning – Also called predictive learning. A machine predicts the class of unknown objects based on prior class-related information of similar objects.
2. Unsupervised learning – Also called descriptive learning. A machine finds patterns in unknown objects by grouping similar objects together.
3. Reinforcement learning – A machine learns to act on its own to achieve the given goals.

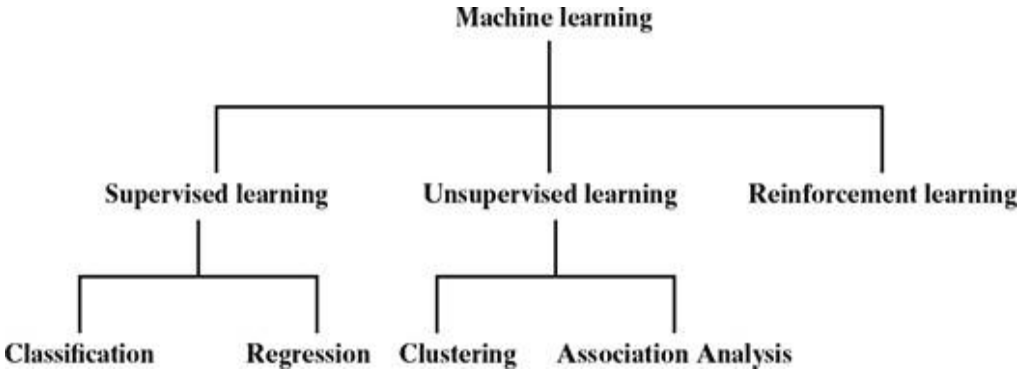


FIG. 1.C Types of machine learning

1.5.1 Supervised learning

The major motivation of supervised learning is to learn from past information. So what kind of past information does the machine need for supervised learning? It is the information about the task which the machine has to execute. In context ofthe definition of machine learning, this past information is theexperience. Let’s try to understand it with an example.

Say a machine is getting images of different objects as inputand the task is to segregate the images by either shape or colour of the object. If it is by shape, the images which are of round-shaped objects need to be separated from images of triangular-shaped objects, etc. If the segregation needs to happen based on colour, images of blue objects need to be separated from images of green objects. But how can the machine know what is round shape, or triangular shape? Sameway, how can the machine distinguish image of an object based on whether it is blue or green in colour? A machine is very much like a little child whose parents or adults need to guide him with the basic information on shape and colour before he can start doing the task. A machine needs the basic information to be provided to it. This basic input, or the experience in the paradigm of machine learning, is given in theform of **training data** . Training data is the past information on a specific task. In context of the image segregation problem, training data will have past data on different aspects or features on a number of images, along with a tag on whether the image is round or triangular, or blue or green in colour. The tag is called ' **label'** and we say that the training data is labelled in case of supervised learning.

Figure 1.4 is a simple depiction of the supervised learningprocess. Labelled training data containing past information comes as an input. Based on the training data, the machine builds a predictive model that can be used on test data to assign a label for each record in the test data.

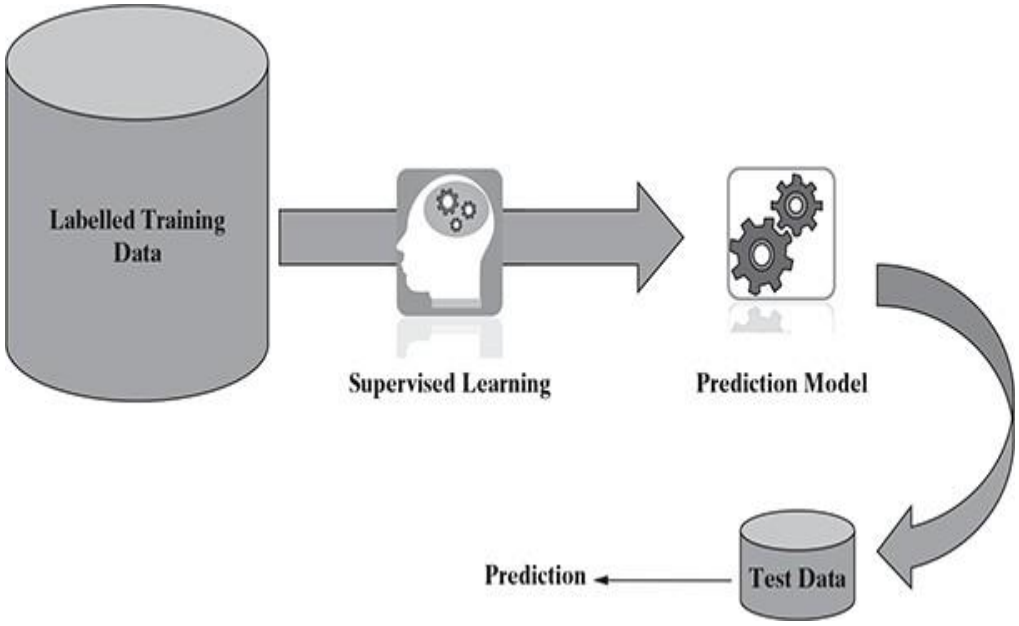


FIG. 1.4 Supervised learning

Some examples of supervised learning are

- Predicting the results of a game
- Predicting whether a tumour is malignant or benign Predicting the
- price of domains like real estate, stocks, etc.
- Classifying texts such as classifying a set of emails as spam or non-spam

Now, let's consider two of the above examples, say 'predicting whether a tumour is malignant or benign' and 'predicting price of domains such as real estate'. Are these two problems same in nature? The answer is 'no'. Though both of them are prediction problems, in one case we are trying to predict which category or class an unknown data belongs to whereas in the other case we are trying to predict an absolute value and not a class. When we are trying

to predict a categorical or nominal variable, the problem is known as a **classification** problem. Whereas when we are trying to predicta real-valued variable, the problem falls under the category of **regression.**

Let's try to understand these two areas of supervised learning, i.e. classification and regression in more details.

1.5.1.1 *Classification*

Let's discuss how to segregate the images of objects based on the shape . If the image is of a round object, it is put under onecategory, while if the image is of a triangular object, it is put under another category. In which category the machine shouldput an image of unknown category, also called a **test data** in machine learning parlance, depends on the information it gets from the past data, which we have called as training data.
Since the training data has a label or category defined for eachand every image, the machine has to map a new image or test data to a set of images to which it is similar to and assign the same label or category to the test data.

So we observe that the whole problem revolves around assigning a label or category or class to a test data based on thelabel or category or class information that is imparted by the training data. Since the target objective is to assign a class label, this type of problem as classification problem. Figure

1.5 depicts the typical process of classification.

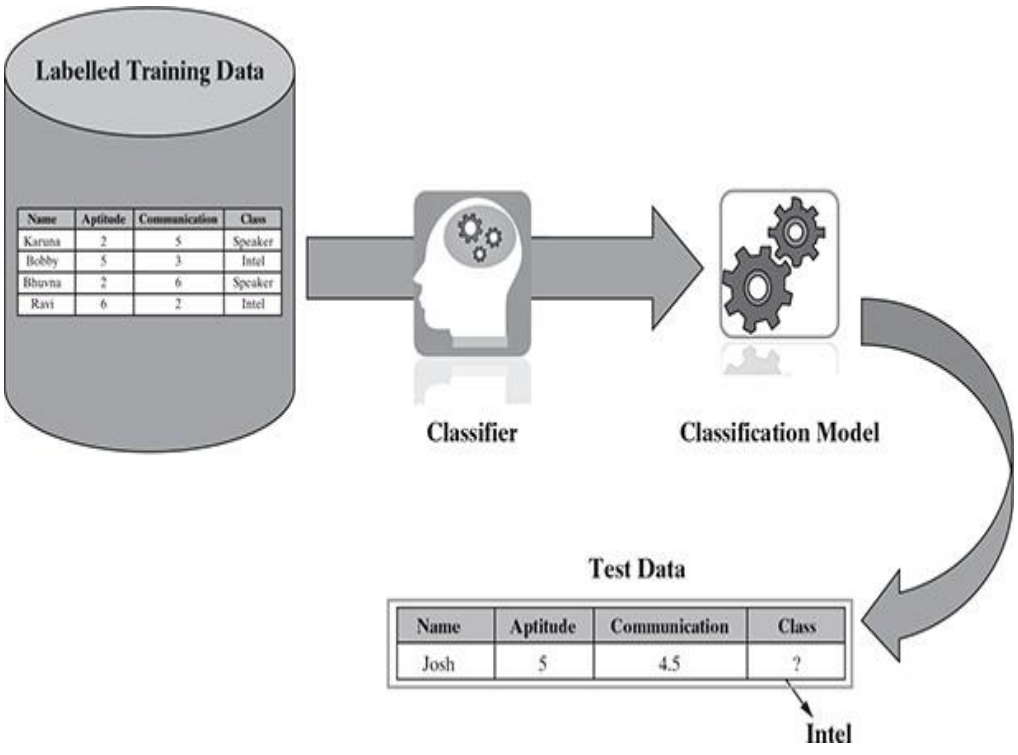


FIG. 1.5 Classification

There are number of popular machine learning algorithms which help in solving classification problems. To name a few,Naïve Bayes, Decision tree, and k-Nearest Neighbour algorithms are adopted by many machine learning practitioners.

A critical classification problem in context of banking domain is identifying potential fraudulent transactions. Since there are millions of transactions which have to be scrutinizedand assured whether it might be a fraud transaction, it is not possible for any human being to carry out this task. Machine learning is effectively leveraged to do this task and this is a classic case

of classification. Based on the past transaction data, specifically the ones labelled as fraudulent, all new incoming transactions are marked or labelled as normal or

suspicious. The suspicious transactions are subsequentlysegregated for a closer review.

In summary, classification is a type of supervised learning where a target feature, which is of type categorical, is predicted for test data based on the information imparted by training data. The target categorical feature is known as **class**.

Some typical classification problems include:

- Image classification Prediction
- of disease Win–loss prediction of
- games
- Prediction of natural calamity like earthquake, flood, etc.
- Recognition of handwriting

1.5.1.2. Regression

In linear regression, the objective is to predict numerical features like real estate or stock price, temperature, marks in an examination, sales revenue, etc. The underlying predictor variable and the target variable are continuous in nature. In case of linear regression, a straight line relationship is 'fitted' between the predictor variables and the target variables, using the statistical concept of least squares method. As in the case of least squares method, the sum of square of error between actual and predicted values of the target variable is tried to be minimized. In case of simple linear regression, there is only one predictor variable whereas in case of multiple linear regression, multiple predictor variables can be included in themodel.

Let's take the example of yearly budgeting exercise of the sales managers. They have to give sales prediction for the nextyear based on sales figure of previous years vis-à-vis investment being put in. Obviously, the data related to past as well as the data to be predicted are continuous in nature. In a basic approach, a simple linear regression model can be applied with investment as predictor variable and sales revenue as the target variable.

Figure 1.6 shows a typical simple regression model, where regression line is fitted based on values of target variable withrespect to different values of predictor variable. A typical linear regression model can be represented in the form –

$$y = \alpha + \beta x$$

where '*x*' is the predictor variable and 'y' is the target variable.

The input data come from a famous multivariate data set named Iris introduced by the British statistician and biologistRonald Fisher. The data set consists of 50 samples from each of three species of Iris – *Iris setosa*, *Iris virginica*, and *Iris versicolor*. Four features were measured for each sample – sepal length, sepal width, petal length, and petal width. These features can uniquely discriminate the different species of theflower.

The Iris data set is typically used as a training data for solving the classification problem of predicting the flower species based on feature values. However, we can also demonstrate regression using this data set, by predicting the value of one feature using another feature as predictor. In Figure 1.6, petal length is a predictor variable which, when fitted in the simple linear regression model, helps in predictingthe value of the target variable sepal length.

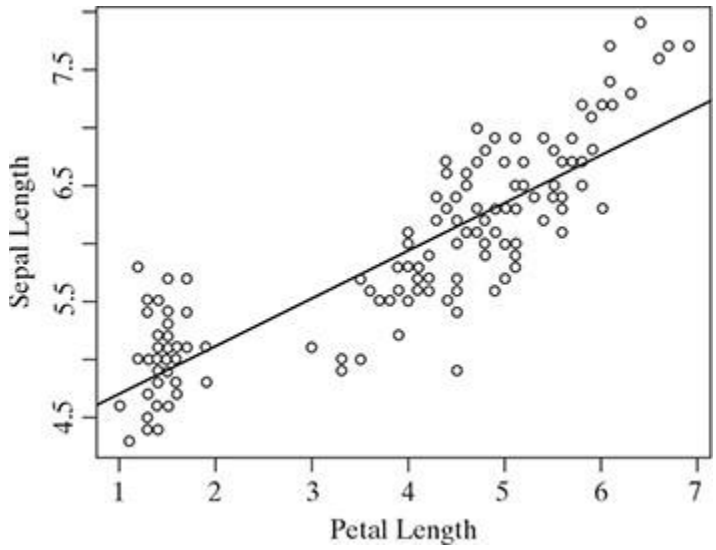


FIG. 1.6 Regression

Typical applications of regression can be seen in

- Demand forecasting in retails
- Sales prediction for managers
- Price prediction in real estate
- Weather forecast
- Skill demand forecast in job market

1.5.2 Unsupervised learning

Unlike supervised learning, in unsupervised learning, there isno labelled training data to learn from and no prediction to be made. In unsupervised learning, the objective is to take a dataset as input and try to find natural groupings or **patterns** within the data elements or records. Therefore, unsupervised learning is often termed as **descriptive model** and the process of unsupervised learning is referred as **pattern discovery** or **knowledge discovery**. One critical application of unsupervised learning is customer segmentation.

Clustering is the main type of unsupervised learning. It intends to group or organize similar objects together. For that reason, objects belonging to the same cluster are quite similarto each other while objects belonging to different clusters are quite dissimilar. Hence, the objective of clustering to discoverthe intrinsic grouping of unlabelled data and form clusters, as depicted in Figure 1.7. Different measures of similarity can beapplied for clustering. One of the most commonly adopted similarity measure is distance. Two data items are considered as a part of the same cluster if the distance between them is less. In the same way, if the distance between the data items ishigh, the items do not generally belong to the same cluster.
This is also known as distance-based clustering. Figure 1.8depicts the process of clustering at a high level.

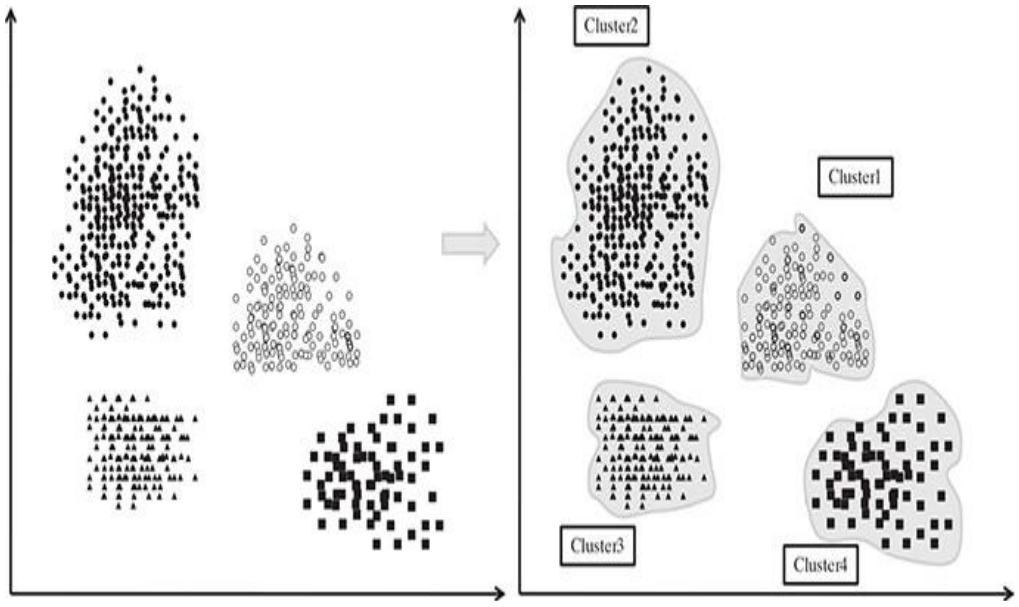


FIG. 1.7 Distance-based clustering

Other than clustering of data and getting a summarized viewfrom it, one more variant of unsupervised learning is **association analysis**. As a part of association analysis, the association between data elements is identified. Let's try to understand the approach of association analysis in context of one of the most common examples, i.e. market basket analysisas shown in Figure 1.9. From past transaction data in a grocerystore, it may be observed that most of the customers who have bought item A, have also bought item B and item C or at least one of them. This means that there is a strong association of the event 'purchase of item A' with the event 'purchase of itemB', or 'purchase of item C'. Identifying these sorts of associations is the goal of association analysis. This helps in boosting up sales pipeline, hence a critical input for the sales group. Critical applications of association analysis include market basket analysis and recommender systems.

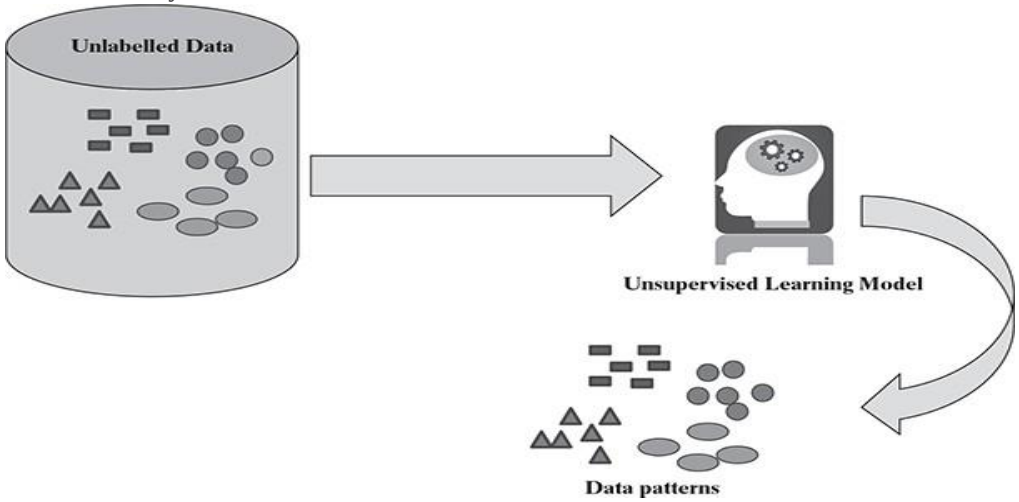


FIG. 1.8 Unsupervised learning

TransID	Items Bought
1	{Butter, Bread}
2	{Diaper, Bread, Milk, Beer}
3	{Milk, Chicken, Beer, Diaper}
4	{Bread, Diaper, Chicken, Beer}
5	{Diaper, Beer, Cookies, Ice cream}
...	...

Market Basket transactions
Frequent itemsets → (Diaper, Beer)
Possible association: Diaper → Beer

FIG. 1.9 Market basket analysis

1.5.3 Reinforcement learning

We have seen babies learn to walk without any prior knowledge of how to do it. Often we wonder how they really do it. They do it in a relatively simple way.

First they notice somebody else walking around, for example parents or anyone living around. They understand that legs have to be used, one at a time, to take a step. While walking, sometimes they fall down hitting an obstacle, whereas other times they are able to walk smoothly avoiding bumpy obstacles. When they are able to walk overcoming theobstacle, their parents are elated and appreciate the baby withloud claps / or may be a chocolates. When they fall down while circumventing an obstacle, obviously their parents do not give claps or chocolates. Slowly a time comes when the babies learn from mistakes and are able to walk with much ease.

In the same way, machines often learn to do tasks autonomously. Let's try to understand in context of the example of the child learning to walk. The action tried to be achieved is walking, the child is the agent and the place with hurdles on which the child is trying to walk resembles the environment. It tries to improve its performance of doing the task. When a sub-task is accomplished successfully, a reward is given. When a sub-task is not executed correctly, obviouslyno reward is given. This continues till the machine is able to complete execution of the whole task. This process of learningis known as reinforcement learning. Figure 1.10 captures the high-level process of reinforcement learning.

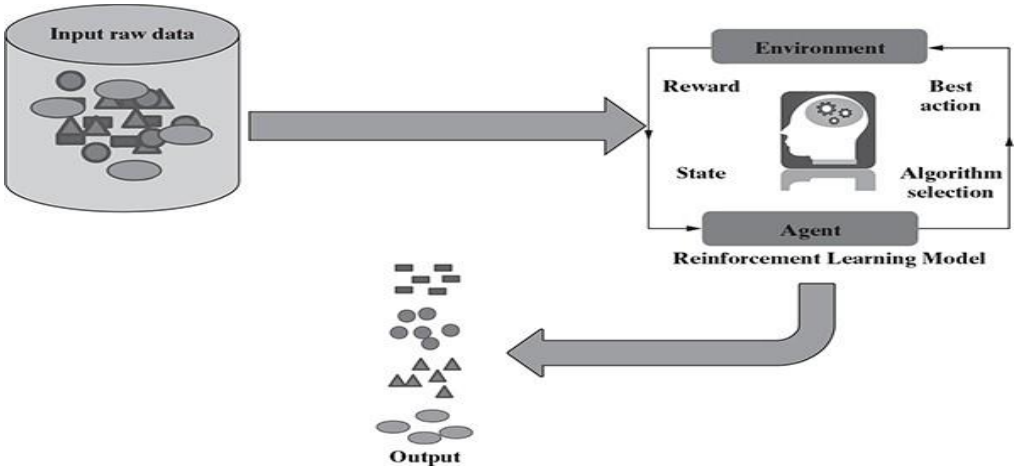


FIG. 1.1O Reinforcement learning

One contemporary example of reinforcement learning isself-driving cars. The critical information which it needs totake care of are speed and speed limit in different road segments, traffic conditions, road conditions, weather conditions, etc. The tasks that have to be taken care of are start/stop, accelerate/decelerate, turn to left / right, etc.

Further details on reinforcement learning have been kept outof the scope of this book.

1.5.4 Comparison – supervised, unsupervised, andreinforcement learning

SUPERVISED	UNSUPERVISED	REINFORCEMENT
This type of learning is used when you know how to classify a given data, or in other words classes or labels are available.	This type of learning is used when there is no idea about the class or label of a particular data. The model has to find pattern in the data.	This type of learning is used when there is no idea about the class or label of a particular data. The model has to do the classification – it will get rewarded if the classification is correct, else get punished.
Labelled training data is needed. Model is built based on training data.	Any unknown and unlabelled data set is given to the model as input and records are grouped.	The model learns and updates itself through reward/ punishment.
The model performance can be evaluated based on how many misclassifications have been done based on a comparison between predicted and actual values.	Difficult to measure whether the model did something useful or interesting. Homogeneity of records grouped together is the only measure.	Model is evaluated by means of the reward function after it had some time to learn.
There are two types of supervised learning problems – classification and regression.	There are two types of unsupervised learning problems – clustering and association.	No such types.
Simplest one to understand.	More difficult to understand and implement than supervised learning.	Most complex to understand and apply.
Standard algorithms include • Naïve Bayes • *k*-nearest neighbour (kNN) • Decision tree • Linear regression • Logistic regression • Support Vector Machine SVM), etc.	Standard algorithms are • *k*-means • Principal Component Analysis (PCA) • Self-organizing map (SOM) • Apriori algorithm • DBSCAN etc.	Standard algorithms are • Q-learning • Sarsa
Practical applications include • Handwriting recognition • Stock market prediction • Disease prediction • Fraud detection, etc.	Practical applications include • Market basket analysis • Recommender systems • Customer segmentation, etc.	Practical applications include • Self-driving cars • Intelligent robots • AlphaGo Zero (the latest version of DeepMind's AI system playing Go)

Machine learning should not be applied to tasks in which humans are very effective or frequent human intervention is needed. For example, air traffic control is a very complex taskneeding intense human involvement. At the same time, for very simple tasks which can be implemented using traditionalprogramming paradigms, there is no sense of using machine learning. For example, simple rule-driven or formula-based applications like price calculator engine, dispute tracking application, etc. do not need machine learning techniques.

Machine learning should be used only when the businessprocess has some lapses. If the task is already optimized, incorporating machine learning will not serve to justify thereturn on investment.

For situations where training data is not sufficient, machine learning cannot be used effectively. This is because, with smalltraining data sets, the impact of bad data is exponentially worse. For the quality of prediction or recommendation to be good, the training data should be sizeable.

1.7 APPLICATIONS OF MACHINE LEARNING

Wherever there is a substantial amount of past data, machine learning can be used to generate actionable insight from the data. Though machine learning is adopted in multiple forms inevery business domain, we have covered below three major domains just to give some idea about what type of actions canbe done using machine learning.

1.7.1 Banking and finance

In the banking industry, fraudulent transactions, especially theones related to credit cards, are extremely prevalent. Since thevolumes as well as velocity of the transactions are extremely high, high performance machine learning solutions are implemented by almost all leading banks across the globe. Themodels work on a real-time basis, i.e. the fraudulent transactions are spotted and prevented right at the time of occurrence. This helps in avoiding a lot of operational hassles in settling the disputes that customers will otherwise raise against those fraudulent transactions.

Customers of a bank are often offered lucrative proposals byother competitor banks. Proposals like higher bank interest, lower processing charge of loans, zero balance savings accounts, no overdraft penalty, etc. are offered to customers, with the intent that the customer switches over to the competitor bank. Also, sometimes customers get demotivated by the poor quality of services of the banks and shift to competitor banks. Machine learning helps in preventing or at least reducing the customer churn. Both descriptive and predictive learning can be applied for reducing customer churn. Using descriptive learning, the specific pockets of problem, i.e. a specific bank or a specific zone or a specific type of offering like car loan, may be spotted where maximumchurn is happening. Quite obviously, these are troubled areas where further investigation needs to be done to find and fix theroot cause. Using predictive learning, the set of vulnerable customers who may leave the bank very soon, can be identified. Proper action can be taken to make sure that the customers stay back.

1.7.2 Insurance

Insurance industry is extremely data intensive. For that reason,machine learning is extensively used in the insurance industry.Two major areas in the insurance industry where machine learning is used are risk prediction during new customer

onboarding and claims management. During customer onboarding, based on the past information the risk profile of anew customer needs to be predicted. Based on the quantum of risk predicted, the quote is generated for the prospective customer. When a customer claim comes for settlement, past information related to historic claims along with the adjustor notes are considered to predict whether there is any possibilityof the claim to be fraudulent. Other than the past information related to the specific customer, information related to similar customers, i.e. customer belonging to the same geographical location, age group, ethnic group, etc., are also considered to formulate the model.

1.7.3 Healthcare

Wearable device data form a rich source for applying machine learning and predict the health conditions of the person real time. In case there is some health issue which is predicted by the learning model, immediately the person is alerted to take preventive action. In case of some extreme problem, doctors orhealthcare providers in the vicinity of the person can be alerted. Suppose an elderly person goes for a morning walk in a park close to his house. Suddenly, while walking, his blood pressure shoots up beyond a certain limit, which is tracked by the wearable. The wearable data is sent to a remote server and a machine learning algorithm is constantly analyzing the streaming data. It also has the history of the elderly person andpersons of similar age group. The model predicts some fatalityunless immediate action is taken. Alert can be sent to the person to immediately stop walking and take rest. Also, doctors and healthcare providers can be alerted to be on standby.

Machine learning along with computer vision also plays acrucial role in disease diagnosis from medical imaging.

1.8 STATE-OF-THE-ART LANGUAGES/TOOLS IN MACHINE LEARNING

The algorithms related to different machine learning tasks are known to all and can be implemented using any language/platform. It can be implemented using a Java platform or C / C++ language or in .NET. However, there are certain languages and tools which have been developed with afocus for implementing machine learning. Few of them, whichare most widely used, are covered below.

1.8.1 Python

Python is one of the most popular, open source programminglanguage widely adopted by machine learning community. Itwas designed by Guido van Rossum and was first released in 1991. The reference implementation of Python, i.e. CPython, is managed by Python Software Foundation, which is a non- profit organization.

Python has very strong libraries for advanced mathematical functionalities (NumPy), algorithms and mathematical tools (SciPy) and numerical plotting (matplotlib). Built on these libraries, there is a machine learning library named **scikit- learn**, which has various classification, regression, and clustering algorithms embedded in it.

1.8.2 R

R is a language for statistical computing and data analysis. It isan open source language, extremely popular in the academic community – especially among statisticians and data miners. Ris considered as a variant of S, a GNU project which was

developed at Bell Laboratories. Currently, it is supported bythe R Foundation for statistical computing.

R is a very simple programming language with a huge set oflibraries available for different stages of machine learning.
Some of the libraries standing out in terms of popularity are plyr/dplyr (for data transformation), caret ('Classification and Regression Training' for classification), RJava (to facilitate integration with Java), tm (for text mining), ggplot2 (for data visualization). Other than the libraries, certain packages like Shiny and R Markdown have been developed around R to develop interactive web applications, documents and dashboards on R without much effort.

1.8.3 Matlab

MATLAB (matrix laboratory) is a licenced commercial software with a robust support for a wide range of numericalcomputing. MATLAB has a huge user base across industry and academia. MATLAB is developed by MathWorks, a company founded in 1984. Being proprietary software, MATLAB is developed much more professionally, tested rigorously, and has comprehensive documentation.

MATLAB also provides extensive support of statistical functions and has a huge number of machine learning algorithms in-built. It also has the ability to scale up for largedatasets by parallel processing on clusters and cloud.

1.8.4 SAS

SAS (earlier known as 'Statistical Analysis System') is another licenced commercial software which provides strong

support for machine learning functionalities. Developed in Cby SAS Institute, SAS had its first release in the year 1976.

SAS is a software suite comprising different components. The basic data management functionalities are embedded in the Base SAS component whereas the other components like SAS/INSIGHT, Enterprise Miner, SAS/STAT, etc. help in specialized functions related to data mining and statistical analysis.

1.8.5 Other languages/tools

There are a host of other languages and tools that also supportmachine learning functionalities. Owned by IBM, **SPSS** (originally named as Statistical Package for the Social Sciences) is a popular package supporting specialized data mining and statistical analysis. Originally popular for statistical analysis in social science (as the name reflects), SPSS is now popular in other fields as well.

Released in 2012, **Julia** is an open source, liberal licence programming language for numerical analysis and computational science. It has baked in all good things of MATLAB, Python, R, and other programming languages usedfor machine learning for which it is gaining steady attention from machine learning development community. Another bigpoint in favour of Julia is its ability to implement high- performance machine learning algorithms.

1.9 ISSUES IN MACHINE LEARNING

Machine learning is a field which is relatively new and stillevolving. Also, the level of research and kind of use of machine learning tools and technologies varies drastically from country to country. The laws and regulations, cultural

background, emotional maturity of people differ drastically indifferent countries. All these factors make the use of machinelearning and the issues originating out of machine learning usage are quite different.

The biggest fear and issue arising out of machine learning isrelated to privacy and the breach of it. The primary focus of learning is on analyzing data, both past and current, and coming up with insight from the data. This insight may be related to people and the facts revealed might be private enough to be kept confidential. Also, different people have a different preference when it comes to sharing of information. While some people may be open to sharing some level of information publicly, some other people may not want to shareit even to all friends and keep it restricted just to family members. Classic examples are a birth date (not the day, but the date as a whole), photographs of a dinner date with family, educational background, etc. Some people share them with all in the social platforms like Facebook while others do not, or ifthey do, they may restrict it to friends only. When machine learning algorithms are implemented using those information, inadvertently people may get upset. For example, if there is a learning algorithm to do preference-based customer segmentation and the output of the analysis is used for sendingtargeted marketing campaigns, it will hurt the emotion of people and actually do more harm than good. In certain countries, such events may result in legal actions to be taken by the people affected.

Even if there is no breach of privacy, there may be situationswhere actions were taken based on machine learning may create an adverse reaction. Let's take the example of knowledge discovery exercise done before starting an election campaign. If a specific area reveals an ethnic majority or

skewness of a certain demographic factor, and the campaign pitch carries a message keeping that in mind, it might actuallyupset the voters and cause an adverse result.

So a very critical consideration before applying machine learning is that proper human judgement should be exercised before using any outcome from machine learning. Only then the decision taken will be beneficial and also not result in anyadverse impact. reparing to Model

2.1 INTRODUCTION

In the last chapter, we got introduced to machine learning. In the beginning, we got a glimpse of the journey of machine learning as an evolving technology. It all started as a proposition from the renowned computer scientist Alan Turing

— machines can 'learn' and become artificially intelligent. Gradually, through the next few decades path-breaking innovations came in from Arthur Samuel, Frank Rosenblatt, John Hopfield, Christopher Watkins, Geoffrey Hinton and many other computer scientists. They shaped up concepts of Neural Networks, Recurrent Neural Network, Reinforcement Learning, Deep Learning, etc. which took machine learning to new heights. In parallel, interesting applications of machine learning kept on happening, with organizations like IBM and Google taking a lead. What started with IBM's Deep Blue beating the world chess champion Gary Kasparov, continued with IBM's Watson beating two human champions in a Jeopardy competition.Google also started with a series of innovations applying machine learning. The Google Brain, Sibyl, Waymo, AlphaGo programs – are all extremely advanced applications of machine learning which have taken the technology a few notches up. Now we can see an all-pervasive presence of machine learning technology in all walks of life.

We have also seen the types of human learning and howthat, in some ways, can be related to the types of machine learning – supervised, unsupervised, and reinforcement.
Supervised learning, as we saw, implies learning from past data, also called training data, which has got known values or classes. Machines can 'learn' or get 'trained' from the past data and assign classes or values to unknown data, termed as test data. This helps in solving problems related to prediction. This is much like human learning through expert guidance as happens for infants from parents or students through teachers.So, supervised learning in case

of machines can be perceived as guided learning from human inputs. Unsupervised machine learning doesn't have labelled data to learn from. It tries to find patterns in unlabelled data. This is much like human beings trying to group together objects of similar shape. This learning is not guided by labelled inputs but uses the knowledge gained from the labels themselves. Last but not theleast is reinforcement learning in which machine tries to learn

by itself through penalty/ reward mechanism – again prettymuch in the same way as human self-learning happens.

Lastly, we saw some of the applications of machine learningin different domains such as banking and finance, insurance, and healthcare. Fraud detection is a critical business case which is implemented in almost all banks across the world anduses machine learning predominantly. Risk prediction for newcustomers is a similar critical case in the insurance industry which finds the application of machine learning. In the healthcare sector, disease prediction makes wide use of machine learning, especially in the developed countries.

While development in machine learning technology has been extensive and its implementation has become widespread, to start as a practitioner, we need to gain some basic understanding. We need to understand how to apply the array of tools and technologies available in the machine learning to solve a problem. In fact, that is going to be very specific to the kind of problem that we are trying to solve. If itis a prediction problem, the kind of activities that will be involved is going to be completely different vis-à-vis if it is a problem where we are trying to unfold a pattern in a data without any past knowledge about the data. So how a machinelearning project looks like or what are the salient activities thatform the core of a machine learning project will depend on whether it is in the area of supervised or unsupervised or reinforcement learning area. However, irrespective of the variation, some foundational knowledge needs to be built before we start with the core machine learning concepts and key algorithms. In this section, we will have a quick look at a few typical machine learning activities and focus on some of the foundational concepts that all practitioners need to gain as

pre-requisites before starting their journey in the area ofmachine learning.

2.2 MACHINE LEARNING ACTIVITIES

The first step in machine learning activity starts with data. In case of supervised learning, it is the labelled training data set followed by test data which is not labelled. In case of unsupervised learning, there is no question of labelled data butthe task is to find patterns in the input data. A thorough reviewand exploration of the data is needed to understand the type ofthe data, the quality of the data and relationship between the different data elements. Based on that, multiple pre-processingactivities may need to be done on the input data before we cango ahead with core machine learning activities. Following are the typical **preparation** activities done once the input data comes into the machine learning system:

- Understand the type of data in the given input data set.Explore
- the data to understand the nature and quality.
- Explore the relationships amongst the data elements, e.g. inter-featurerelationship.
- Find potential issues in data.
- Do the necessary remediation, e.g. impute missing data values, etc., ifneeded.
- Apply pre-processing steps, as necessary.
- Once the data is prepared for modelling, then the learning tasks start off. Asa part of it, do the following activities:
  - The input data is first divided into parts – the training data and the testdata (called holdout). This step is applicable for supervised learning only.
  - Consider different models or learning algorithms for selection. Train the
  - model based on the training data for supervised learningproblem and apply

to unknown data. Directly apply the chosen unsupervised model on the input data for unsupervised learning problem.

After the model is selected, trained (for supervised learning), and applied on input data, the performance of the model is evaluated. Based on options available, specific actions can be taken to improve the performance of the model,if possible.

Figure 2.1 depicts the four-step process of machine learning.

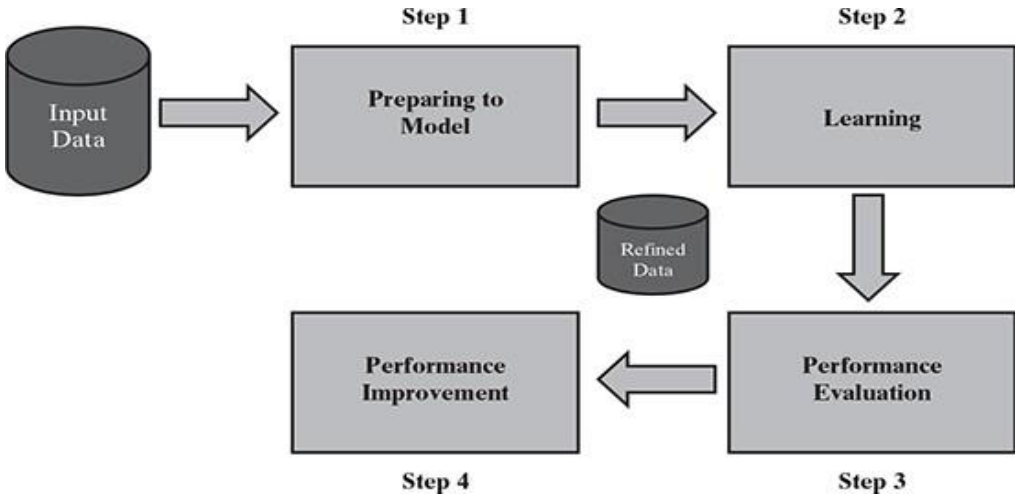


FIG. 2.1 Detailed process of machine learning

Table 2.1 contains a summary of steps and activitiesinvolved:

Table 2.1 *Activities in Machine Learning*

Step #	Step Name	Activities Involved
Step 1	Preparing to Model	• Understand the type of data in the given input data set • Explore the data to understand data quality • Explore the relationships amongst the data elements, e.g. inter-feature relationship • Find potential issues in data • Remediate data, if needed • Apply following pre-processing steps, as necessary: ✓ Dimensionality reduction ✓ Feature subset selection
Step 2	Learning	• Data partitioning/holdout • Model selection • Cross-validation
Step 3	Performance evaluation	• Examine the model performance, e.g. confusion matrix in case of classification • Visualize performance trade-offs using ROC curves
Step 4	Performance improvement	• Tuning the model • Ensembling • Bagging • Boosting

In this chapter, we will cover the first part, i.e. preparing tomodel. The remaining parts, i.e. learning, performance evaluation, and performance improvement will be covered inChapter 3.

2.3 BASIC TYPES OF DATA IN MACHINE LEARNING

Before starting with types of data, let's first understand what adata set is and what are the elements of a data set. A data set is a collection of related information or records. The information may be on some entity or some subject area. For example (Fig.2.2), we may have a data set on students in which each record consists of information about a specific student. Again, we can have a data set on student performance which has records providing performance, i.e. marks on the individual subjects.

Each row of a data set is called a record. Each data set also has multiple attributes, each of which gives information on a specific characteristic. For example, in the data set on students, there are four attributes namely Roll Number, Name, Gender, and Age, each of which understandably is a specific characteristic about the student entity. Attributes can also be termed as feature, variable, dimension or field. Both the data sets, Student and Student Performance, are having four features or dimensions; hence they are told to have four- dimensional data space. A row or record represents a point in the four-dimensional data space as each row has specific values for each of the four attributes or features. Value of an attribute, quite understandably, may vary from record to record. For example, if we refer to the first two records in the Student data set, the value of attributes Name, Gender, and Age are different (Fig. 2.3).

Student data set:

Roll Number	Name	Gender	Age
129/011	Mihir Karmarkar	M	14
129/012	Geeta Iyer	F	15
129/013	Chanda Bose	F	14
129/014	Sreenu Subramanian	M	14
129/015	Pallav Gupta	M	16
129/016	Gajanan Sharma	M	15

Student performance data set:

Roll Number	Maths	Science	Percentage
129/011	89	45	89.33%
129/012	89	47	90.67%
129/013	68	29	64.67%
129/014	83	38	80.67%
129/015	57	23	53.33%
129/016	78	35	75.33%

FIG. 2.2 Examples of data set

Roll Number	Name	Gender	Age
129/011	Mihir Karmarkar	M	14
129/012	Geeta Iyer	F	15

FIG. 2.C Data set records and attributes

Now that a context of data sets is given, let's try to understand the different types of data that we generally comeacross in machine learning problems. Data can broadly be divided into following two types:

1. Qualitative data
2. Quantitative data

Qualitative data provides information about the quality ofan object or information which cannot be measured. For

example, if we consider the quality of performance of studentsin terms of ‘Good’, ‘Average’, and ‘Poor’, it falls under the category of qualitative data. Also, name or roll number of students are information that cannot be measured using some scale of measurement. So they would fall under qualitative data. Qualitative data is also called **categorical data**.
Qualitative data can be further subdivided into two types asfollows:

1. Nominal data
2. Ordinal data

Nominal data is one which has no numeric value, but a named value. It is used for assigning named values to attributes. Nominal values cannot be quantified. Examples ofnominal data are

1. Blood group: A, B, O, AB, etc.
2. Nationality: Indian, American, British, etc.
3. Gender: Male, Female, Other

It is obvious, mathematical operations such as addition, subtraction, multiplication, etc. cannot be performed on nominal data. For that reason, statistical functions such as mean, variance, etc. can also not be applied on nominal data.

However, a basic count is possible. So mode, i.e. most frequently occurring value, can be identified for nominal data.

Ordinal data, in addition to possessing the properties of nominal data, can also be naturally ordered. This means ordinal data also assigns named values to attributes but unlike nominal data, they can be arranged in a sequence of increasingor decreasing value so that we can say whether a value is better than or greater than another value. Examples of ordinal data are

1. Customer satisfaction: ‘Very Happy’, ‘Happy’, ‘Unhappy’, etc.
2. Grades: A, B, C, etc.
3. Hardness of Metal: ‘Very Hard’, ‘Hard’, ‘Soft’, etc.

Like nominal data, basic counting is possible for ordinal data. Hence, the mode can be identified. Since ordering is possible in case of ordinal data, median, and quartiles can be identified in addition. Mean can still not be calculated.

Quantitative data relates to information about the quantity of an object – hence it can be measured. For example, if we consider the attribute ‘marks’, it can be measured using a scaleof measurement. Quantitative data is also termed as numeric data. There are two types of quantitative data:

1. Interval data
2. Ratio data

Interval data is numeric data for which not only the order is known, but the exact difference between values is also known. An ideal example of interval data is Celsius temperature. The difference between each value remains the same in Celsius temperature. For example, the difference between 12°C and 18°C degrees is measurable and is 6°C as in

the case of difference between 15.5°C and 21.5°C. Otherexamples include date, time, etc.

For interval data, mathematical operations such as additionand subtraction are possible. For that reason, for interval data,the central tendency can be measured by mean, median, or mode. Standard deviation can also be calculated.

However, interval data do not have something called a 'truezero' value. For example, there is nothing called '0 temperature' or 'no temperature'. Hence, only addition and subtraction applies for interval data. The ratio cannot be applied. This means, we can say a temperature of 40°C is equal to the temperature of 20°C + temperature of 20°C. However, we cannot say the temperature of 40°C means it is twice as hot as in temperature of 20°C.

Ratio data represents numeric data for which exact valuecan be measured. Absolute zero is available for ratio data.
Also, these variables can be added, subtracted, multiplied, ordivided. The central tendency can be measured by mean, median, or mode and methods of dispersion such as standarddeviation. Examples of ratio data include height, weight, age,salary, etc.

Figure 2.4 gives a summarized view of different types of data that we may find in a typical machine learning problem.

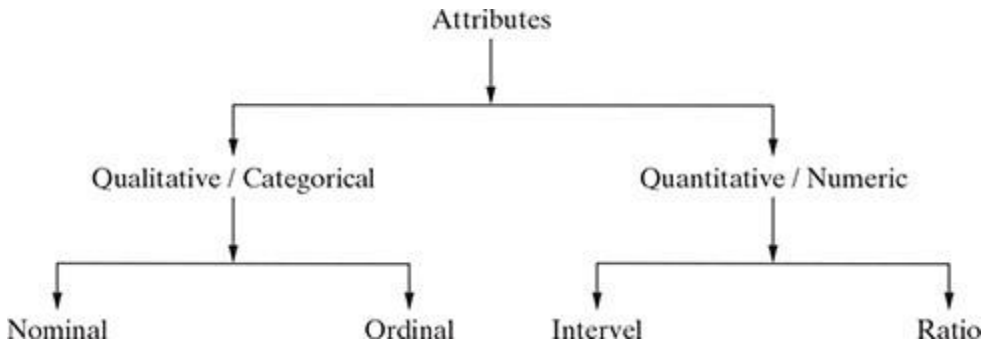


FIG. 2.4 Types of data

Apart from the approach detailed above, attributes can also be categorized into types based on a number of values that canbe assigned. The attributes can be either discrete or continuous based on this factor.

Discrete attributes can assume a finite or countably infinitenumber of values. Nominal attributes such as roll number, street number, pin code, etc. can have a finite number of values whereas numeric attributes such as count, rank of students, etc. can have countably infinite values. A special type of discrete attribute which can assume two values only iscalled binary attribute. Examples of binary attribute include male/ female, positive/negative, yes/no, etc.

Continuous attributes can assume any possible value whichis a real number. Examples of continuous attribute include length, height, weight, price, etc.

2.4 EXPLORING STRUCTURE OF DATA

By now, we understand that in machine learning, we come across two basic data types – numeric and categorical. With this context in mind, we can delve deeper into understanding adata set. We need to understand that in a data set, which of the attributes are numeric and which are categorical in nature. Thisis because, the approach of exploring numeric data is different than the approach of exploring categorical data. In case of a standard data set, we may have the data dictionary available for reference. Data dictionary is a metadata repository, i.e. the repository of all information related to the structure of each data element contained in the data set. The data dictionary gives detailed information on each of the attributes – the description as well as the data type and other relevant details.
In case the data dictionary is not available, we need to use standard library function of the machine learning tool that weare using and get the details. For the time being, let us move ahead with a standard data set from UCI machine learning repository.

The data set that we take as a reference is the Auto MPGdata set available in the UCI repository. Figure 2.5 is a snapshot of the first few rows of the data set.

mpg	cylinder	displace-ment	horse-power	weight	accel-eration	model year	origin	car name
18	8	307	130	3504	12	70	1	Chevrolet chev-elle malibu
15	8	350	165	3693	11.5	70	1	Buick skylark 320
18	8	318	150	3436	11	70	1	Plymouth satellite
16	8	304	150	3433	12	70	1	Amc rebel sst
17	8	302	140	3449	10.5	70	1	Ford torino
15	8	429	198	4341	10	70	1	Ford galaxie 500
14	8	454	220	4354	9	70	1	Chevrolet impala
14	8	440	215	4312	8.5	70	1	Plymouth fury iii
14	8	455	225	4425	10	70	1	Pontiac catalina
15	8	390	190	3850	8.5	70	1	Amc acbassador dpl
15	8	383	170	3563	10	70	1	Dodge challenger se
14	8	340	160	3609	8	70	1	Plymouth ' cuda 340
15	8	400	150	3761	9.5	70	1	Chevrolet monte carlo
14	8	455	225	3086	10	70	1	Buick estate wagon (sw)
24	4	113	95	2372	15	70	3	Toyota corona mark ii
22	6	198	95	2933	15.5	70	1	Plymouth duster
18	6	199	97	2774	15.5	70	1	Amc hornet

FIG. 2.5 Auto MPG data set

As is quite evident from the data, the attributes such as ‘mpg’, ‘cylinders’, ‘displacement’, ‘horsepower’, ‘weight’, ‘acceleration’, ‘model year’, and ‘origin’ are all numeric. Outof these attributes, ‘cylinders’, ‘model year’, and ‘origin’ are

discrete in nature as the only finite number of values can be assumed by these attributes. The remaining of the numeric attributes, i.e. ‘mpg’, ‘displacement’, ‘horsepower’, ‘weight’,and ‘acceleration’ can assume any real value.

Hence, these attributes are continuous in nature. The only remaining attribute ‘car name’ is of type categorical, or more specifically nominal. This data set is regarding prediction of fuel consumption in miles per gallon, i.e. the numeric attribute‘mpg’ is the target attribute.

With this understanding of the data set attributes, we canstart exploring the numeric and categorical attributes separately.

2.4.1 Exploring numerical data

There are two most effective mathematical plots to explore numerical data – box plot and histogram. We will explore allthese plots one by one, starting with the most critical one, which is the box plot.

2.4.1.1 Understanding central tendency

To understand the nature of numeric variables, we can applythe measures of central tendency of data, i.e. mean and median. In statistics, measures of central tendency help us understand the central point of a set of data. Mean, by definition, is a sum of all data values divided by the count ofdata elements. For example, mean of a set of observations – 21, 89, 34, 67, and 96 is calculated as below.

$$\text{Mean} = \frac{21 + 89 + 34 + 67 + 96}{5} = 61.4.$$

If the above set of numbers represents marks of 5 studentsin a class, the mean marks, or the falling in the middle of therange is 61.4.

Median, on contrary, is the value of the element appearing in the middle of an ordered list of data elements. If we consider the above 5 data elements, the ordered list would be –21, 34, 67, 89, and 96. Since there are 5 data elements, the 3rdelement in the ordered list is considered as the median. Hence,the median value of this set of data is 67.

There might be a natural curiosity to understand why two measures of central tendency are reviewed. The reason is meanand median are impacted differently by data values appearing at the beginning or at the end of the range. Mean being calculated from the cumulative sum of data values, is impactedif too many data elements are having values closer to the far end of the range, i.e. close to the maximum or minimum values. It is especially sensitive to outliers, i.e. the values which are unusually high or low, compared to the other values.Mean is likely to get shifted drastically even due to the presence of a small number of outliers. If we observe that forcertain attributes the deviation between values of mean and median are quite high, we should investigate those attributesfurther and try to find out the root cause along with the need for remediation.

So, in the context of the Auto MPG data set, let’s try to findout for each of the numeric attributes the values of mean and median. We can also find out if the deviation between these values is large. In Figure 2.6, the comparison between mean and median for all the attributes has been shown. We can see that for the attributes such as ‘mpg’, ‘weight’, ‘acceleration’, and ‘model.year’ the deviation between mean and median is not significant which means the chance of these attributes having too many outlier values is less. However, the deviation is significant for the attributes ‘cylinders’, ‘displacement’ and ‘origin’. So, we need to further drill down and look at some more statistics for these attributes. Also, there is some problemin the values of the attribute ‘horsepower’ because of which the mean and median calculation is not possible.

	mpg	cylin-ders	dis-place-ment	horse-power	weight	accel-eration	model year	origin
Median	23	4	148.5	?	2804	15.5	76	1
Mean	23.51	5.455	193.4	?	2970	15.57	76.01	1.573
Deviation	2.17	26.67%	23.22%		5.59%	0.45%	0.01%	36.43%
	Low	High	High		Low	Low	Low	High

FIG. 2.6 Mean vs. Median for Auto MPG

With a bit of investigation, we can find out that the problem is occurring because of the 6 data elements, as shown in Figure2.7, do not have value for the attribute 'horsepower'.

mpg	cylinders	displace-ment	horse-power	weight	accel-eration	model year	origin	car name
25	4	98	?	2046	19	71	1	Ford pinto
21	6	200	?	2875	17	74	1	Ford maverick
40.9	4	85	?	1835	17.3	80	2	Renault lecar deluxe
23.6	4	140	?	2905	14.3	80	1	Ford mustang cobra
34.5	4	100	?	2320	15.8	81	2	Renault 18i
23	4	151	?	3035	20.5	82	1	Amc concord di

FIG. 2.7 Missing values of attribute 'horsepower' in Auto MPG

For that reason, the attribute 'horsepower' is not treated as anumeric. That's why the operations applicable on numeric variables, like mean or median, are failing. So we have to firstremediate the missing values of the attribute 'horsepower' before being able to do any kind of exploration. However, we will cover the approach of remediation of missing values a little later.

2.4.1.2 *Understanding data spread*

Now that we have explored the central tendency of the different numeric attributes, we have a clear idea of which attributes have a large deviation between mean and median. Let's look closely at those attributes. To drill down more, we need to look at the entire range of values of the attributes, though not at the level of data elements as that may be too vastto review manually. So we will take a granular view of the data spread in the form of

1. Dispersion of data
2. Position of the different data values

2.4.1.2.1 *Measuring data dispersion*

Consider the data values of two attributes

1. Attribute 1 values : 44, 46, 48, 45, and 47
2. Attribute 2 values : 34, 46, 59, 39, and 52

Both the set of values have a mean and median of 46.
However, the first set of values that is of attribute 1 is more concentrated or clustered around the mean/median value whereas the second set of values of attribute 2 is quite spread out or dispersed. To measure the extent of dispersion of a data,or to find out how much the different values of a data are spread out, the variance of the data is measured. The variance of a data is measured using the formula given below:

Variance $(x) = \frac{\sum_{i=1}^{n} x_i^2}{n} - \left(\frac{\sum_{i=1}^{n} x_i}{n}\right)^2$, where *x* is the variable or attribute whose variance is to be measured and *n* is the numberof observations or values of variable x.

Standard deviation of a data is measured as follows:

$$\text{Standard deviation } (x) = \sqrt{\text{Variance } (x)}$$

Larger value of variance or standard deviation indicates more dispersion in the data and vice versa. In the above example, let's calculate the variance of attribute 1 and that ofattribute 2. For attribute 1,

$$\text{Variance} = \frac{\sum_{i=1}^{n} x_i^2}{n} - \left(\frac{\sum_{i=1}^{n} x_i}{n}\right)^2$$

$$= \frac{44^2 + 46^2 + 48^2 + 45^2 + 47^2}{5} - \left(\frac{44 + 46 + 48 + 45 + 47}{5}\right)^2$$

$$= \frac{1936 + 2116 + 2304 + 2025 + 2209}{5} - \left(\frac{230}{5}\right)^2 = \frac{10590}{5} - (46)^2 = 2$$

For attribute 2,

$$\text{Variance} = \frac{\sum_{i=1}^{n} x_i^2}{n} - \left(\frac{\sum_{i=1}^{n} x_i}{n}\right)^2$$

$$= \frac{34^2 + 46^2 + 59^2 + 39^2 + 52^2}{5} - \left(\frac{34 + 46 + 59 + 39 + 52}{5}\right)^2$$

$$= \frac{1156 + 2116 + 3481 + 1521 + 2704}{5} - \left(\frac{230}{5}\right)^2 = \frac{10978}{5} - (46)^2 = 79.6$$

So it is quite clear from the measure that attribute 1 valuesare quite concentrated around the mean while attribute 2 values are extremely spread out. Since this data was small, avisual inspection and understanding were possible and that matches with the measured value.

2.4.1.2.2 Measuring data value position

When the data values of an attribute are arranged in an increasing order, we have seen earlier that median gives the central data value, which divides the entire data set into two halves. Similarly, if the first half of the data is divided into twohalves so that each half consists of one-quarter of the data set,

then that median of the first half is known as first quartile or Q_1. In the same way, if the second half of the data is divided into two halves, then that median of the second half is known as third quartile or Q_3. The overall median is also known as second quartile or Q_2. So, any data set has five values - minimum, first quartile (Q1), median (Q2), third quartile (Q3),and maximum.

Let's review these values for the attributes 'cylinders', 'displacement', and 'origin'. Figure 2.8 captures a summary ofthe range of statistics for the attributes. If we take the exampleof the attribute 'displacement', we can see that the difference between minimum value and Q1 is 36.2 and the difference between Q1 and median is 44.3. On the contrary, the difference between median and Q3 is 113.5 and Q3 and the maximum value is 193. In other words, the larger values are more spread out than the smaller ones. This helps in understanding why the value of mean is much higher than thatof the median for the attribute 'displacement'. Similarly, in case of attribute 'cylinders', we can observe that the differencebetween minimum value and median is 1 whereas the difference between median and the maximum value is 4. For the attribute 'origin', the difference between minimum value and median is 0 whereas the difference between median and the maximum value is 2.

	cylinders	displacement	origin
Minimum	3	68	1
Q1	4	104.2	1
Median	4	148.5	1
Q3	8	262	2
Maximum	8	455	3

FIG. 2.8 Attribute value drill-down for Auto MPG

However, we still cannot ascertain whether there is any outlier present in the data. For that, we can better adopt somemeans to visualize the data. Box plot is an excellent visualization medium for numeric data.

2.4.2 Plotting and exploring numerical data

2.4.2.1 Box plots

Now that we have a fairly clear understanding of the data set attributes in terms of spread and central tendency, let's try to make an attempt to visualize the whole thing as a box-plot. A box plot is an extremely effective mechanism to get a one-shotview and understand the nature of the data. But before we get to review the box plot for different attributes of Auto MPG data set, let's first try to understand a box plot in general and the interpretation of different aspects in a box plot. As we can see in Figure 2.9, the box plot (also called box and whisker plot) gives a standard visualization of the five-number summary statistics of a data, namely minimum, first quartile (Q1), median (Q2), third quartile (Q3), and maximum. Below is a detailed interpretation of a box plot.

- The central rectangle or the box spans from first to third quartile (i.e. Q1 toQ3), thus giving the inter-quartile range (IQR).
- Median is given by the line or band within the box.
- The lower whisker extends up to 1.5 times of the inter-quartile range (or IQR) from the bottom of the box, i.e. the first quartile or Q1. However, the actual length of the lower whisker depends on the lowest data value that fallswithin (Q1 − 1.5 times of IQR). Let's try to understand this with an example.Say for a specific set of data, Q1 = 73, median = 76 and Q3 = 79. Hence, IQR will be 6 (i.e. Q3 – Q1).So, lower whisker can extend maximum till (Q1
  – 1.5 × IQR) = 73 – 1.5 × 6 = 64. However, say there are lower range data values such as 70, 63, and 60. So, the lower whisker will come at 70 as thisis the lowest data value larger than 64.
- The upper whisker extends up to 1.5 as times of the inter-quartile range (or IQR) from the top of the box, i.e. the third quartile or Q3. Similar to lower whisker, the actual length of the upper whisker will also depend on the highest data value that falls within (Q3 + 1.5 times of IQR). Let's try to understand this with an example. For the same set of data mentioned in the above point, upper whisker can extend maximum till (Q3 + 1.5 × IQR) = 79
  + 1.5 × 6 = 88. If there is higher range of data values like 82, 84, and 89. So, the upper whisker will come at 84 as this is the highest data value lower than 88.
- The data values coming beyond the lower or upper whiskers are the oneswhich are of unusually low or high values respectively. These are the outliers, which may deserve special consideration.

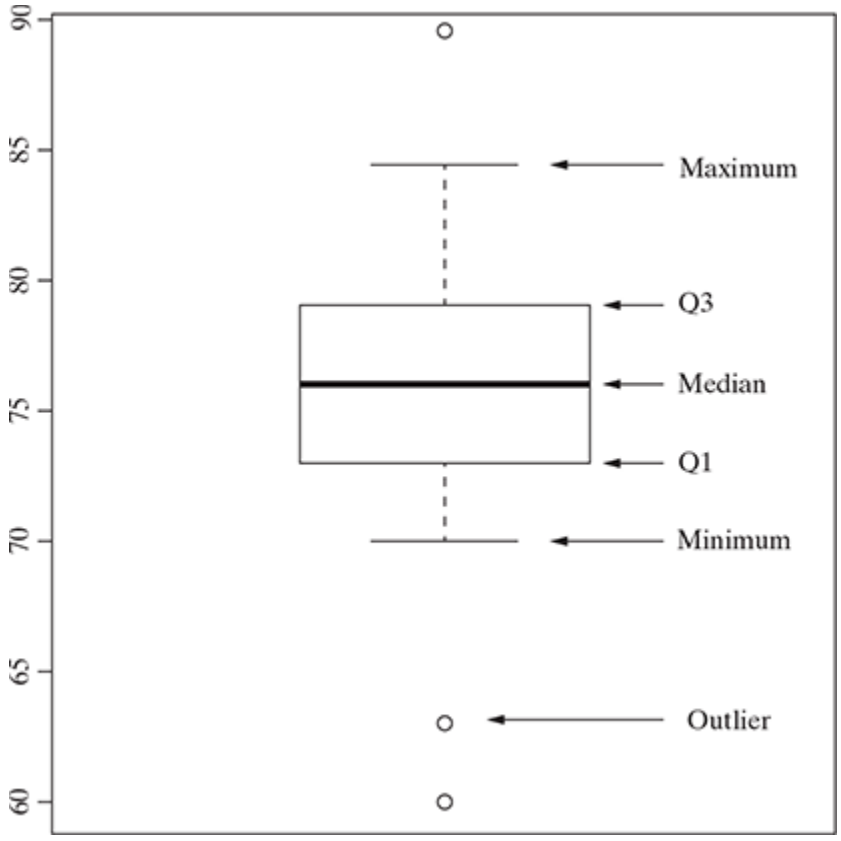


FIG. 2.9 Box plot

Let's visualize the box plot for the three attributes - 'cylinders', 'displacement', and 'origin'. We will also review the box plot of another attribute in which the deviation between mean and median is very little and see what the basic difference in the respective box plots is. Figure 2.10 presentsthe respective box plots.

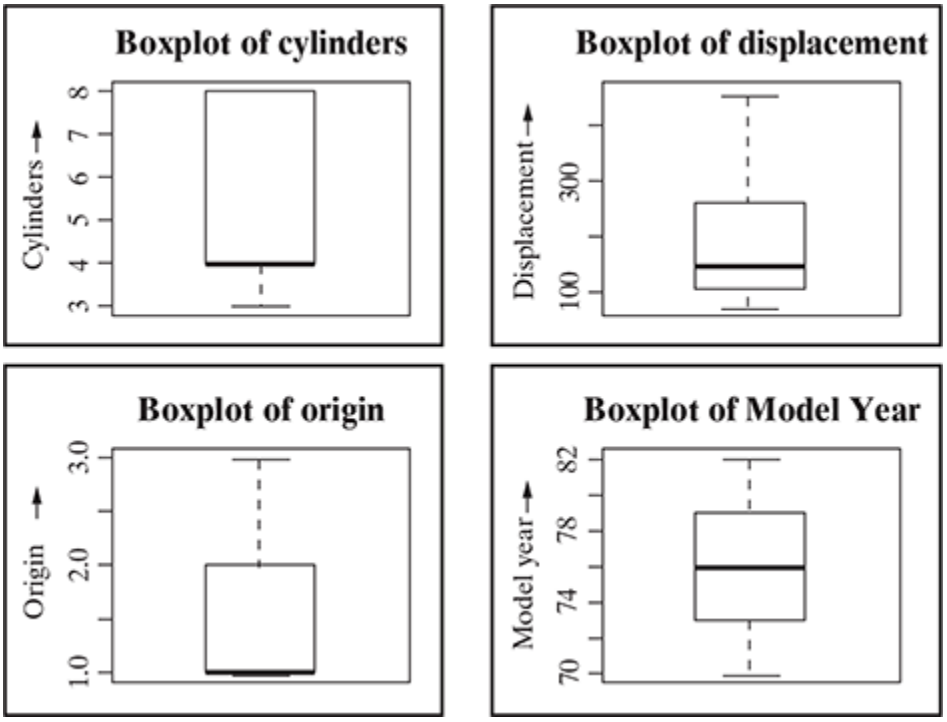


FIG. 2.1O Box plot of Auto MPG attributes

2.4.2.1.1 Analysing box plot for 'cylinders'

The box plot for attribute 'cylinders' looks pretty weird in shape. The upper whisker is missing, the band for median fallsat the bottom of the box, even the lower whisker is pretty small compared to the length of the box! Is everything right?

The answer is a big YES, and you can figure it out if you delve a little deeper into the actual data values of the attribute.The attribute 'cylinders' is discrete in nature having values from 3 to 8. Table 2.2 captures the frequency and cumulative frequency of it.

Table 2.2 *Frequency of "Cylinders" Attribute*

Cylinders	Frequency	Cumulative Frequency
3	4	4
4	204	208 (= 4 + 204)
5	3	211 (= 208 + 3)
6	84	295 (= 211 + 84)
7	0	295 (= 295 + 0)
8	103	398 (= 295 + 103)

As can be observed in the table, the frequency is extremely high for data value 4. Two other data values where the frequency is quite high are 6 and 8. So now if we try to find the quartiles, since the total frequency is 398, the first quartile (Q1), median (Q2), and third quartile (Q3) will be at a cumulative frequency 99.5 (i.e. average of 99th and 100th observation), 199 and 298.5 (i.e. average of 298th and 299th observation), respectively. This way Q1 = 4, median = 4 and Q3 = 8. Since there is no data value beyond 8, there is no upper whisker. Also, since both

Q1 and median are 4, the bandfor median falls on the bottom of the box. Same way, though the lower whisker could have extended till -2 (Q1 – 1.5 × IQR

= 4 – 1.5 × 4 = –2), in reality, there is no data value lower than

3. Hence, the lower whisker is also short. In any case, a valueof cylinders less than 1 is not possible.

2.4.2.1.2 Analysing box plot for 'origin'

Like the box plot for attribute 'cylinders', the box plot for attribute 'cylinders' also looks pretty weird in shape. Here thelower whisker is missing and the band for median falls at the bottom of the box! Let's verify if everything right?

Just like the attribute 'cylinders', attribute 'origin' is discrete in nature having values from 1 to 3. Table 2.3 captures

the frequency and cumulative frequency (i.e. a summation of frequencies of all previous intervals) of it.

Table 2.C *Frequency of "Origin" Attribute*

origin	Frequency	Cumulative Frequency
1	249	249
2	70	319 (= 249 + 70)
3	79	398 (= 319 + 79)

As can be observed in the table, the frequency is extremely high for data value 1. Since the total frequency is 398, the firstquartile (Q1), median (Q2), and third quartile (Q3) will be at a cumulative frequency 99.5 (i.e. average of 99th and 100th observation), 199 and 298.5 (i.e. average of 298th and 299th observation), respectively. This way Q1 = 1, median = 1, and Q3 = 2. Since Q1 and median are same in value, the band for median falls on the bottom of the box. There is no data value lower than Q1. Hence, the lower whisker is missing.

2.4.2.1.3 Analysing box plot for 'displacement'

The box plot for the attribute 'displacement' looks better thanthe previous box plots. However, still, there are few small abnormalities, the cause of which needs to be reviewed.
Firstly, the lower whisker is much smaller than an upper whisker. Also, the band for median is closer to the bottom ofthe box.

Let's take a closer look at the summary data of the attribute 'displacement'. The value of first quartile, Q1 = 104.2, median

= 148.5, and third quartile, Q3 = 262. Since (median – Q1) =

44.3 is greater than (Q3 – median) = 113.5, the band for the median is closer to the bottom of the box (which represents Q1). The value of IQR, in this case, is 157.8. So the lower whisker can be 1.5 times 157.8 less than Q1. But minimum data value for the attribute 'displacement' is 68. So, the lower whisker at 15% [(Q1 – minimum)/1.5 × IQR = (104.2 – 68) / (1.5 × 157.8) = 15%] of the permissible length. On the other hand, the maximum data value is 455. So the upper whisker is 81% [(maximum – Q3)/1.5 × IQR = (455 – 262) / (1.5 × 157.8) = 81%] of the permissible length. This is why the upperwhisker is much longer than the lower whisker.

2.4.2.1.4 Analysing box plot for 'model Year'

The box plot for the attribute 'model. year' looks perfect. Let'svalidate is it really what expected

to be.

For the attribute ‘model.year’:First quartile,

Q1 = 73 Median, Q2 = 76

Third quartile, Q3 = 79

So, the difference between median and Q1 is exactly equalto Q3 and median (both are 3). That is why the band for the median is exactly equidistant from the bottom and top of the box.

I QR = Q3 9 Q1 = 7 9 - 7 3 = 6

Difference between Q1 and minimum data value (i.e. 70) is also same as maximum data value (i.e. 82) and Q3 (both are 3). So both lower and upper whiskers are expected to be of thesame size which is 33% [3 / (1.5 × 6)] of the permissible length.

2.4.2.2 *Histogram*

Histogram is another plot which helps in effective visualization of numeric attributes. It helps in understanding the distribution of a numeric data into series of intervals, alsotermed as 'bins'. The important difference between histogramand box plot is

- The focus of histogram is to plot ranges of data values (acting as 'bins'), thenumber of data elements in each range will depend on the data distribution. Based on that, the size of each bar corresponding to the different ranges will vary.
- The focus of box plot is to divide the data elements in a data set into fourequal portions, such that each portion contains an equal number of data elements.

Histograms might be of different shapes depending on the nature of the data, e.g. skewness. Figure 2.11 provides a depiction of different shapes of the histogram that are generally created. These patterns give us a quick understanding of the data and thus act as a great data exploration tool.

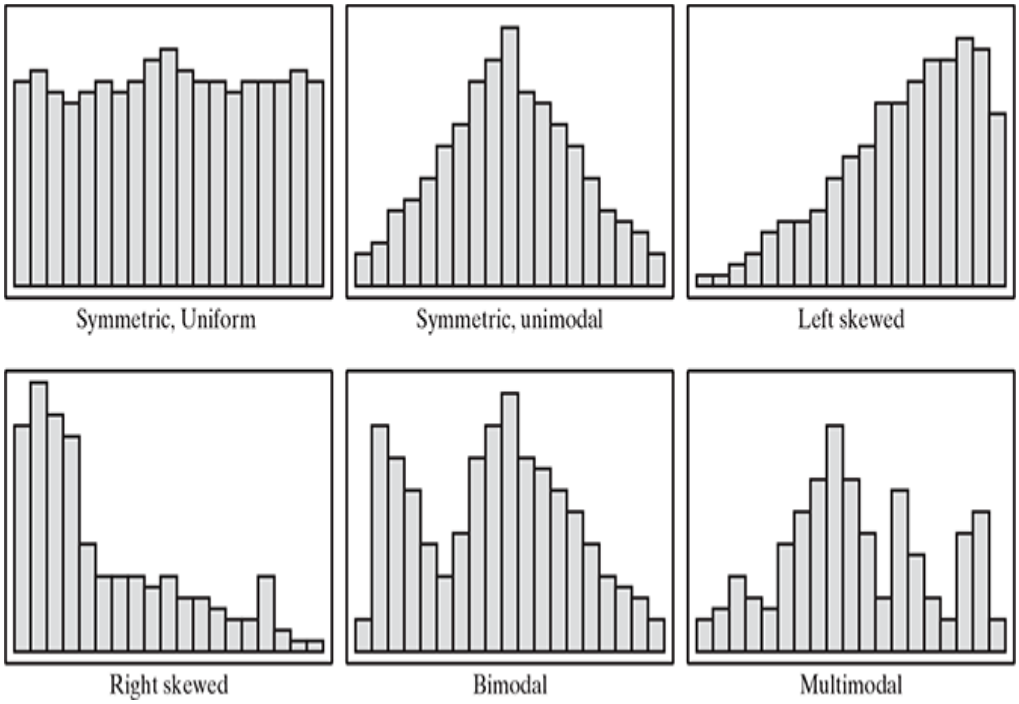


FIG. 2.11 General Histogram shapes

Let's now examine the histograms for the different attributesof Auto MPG data set presented in Figure 2.12. The histograms for 'mpg' and 'weight' are right-skewed. The histogram for 'acceleration' is symmetric and unimodal, whereas the one for 'model.year' is symmetric and uniform.
For the remaining attributes, histograms are multimodal innature.

Now let's dig deep into one of the histograms, say the one for the attribute 'acceleration'. The histogram is composed of anumber of bars, one bar appearing for each of the 'bins'. The height of the bar reflects the total count of data elements whose value falls within the specific bin value, or the frequency. Talking in context of the histogram for acceleration,each 'bin'

represents an acceleration value interval of 2 units.
So the second bin, e.g., reflects acceleration value of 10 to 12units. The corresponding bar chart height reflects the count of

all data elements whose value lies between 10 and 12 units. Also, it is evident from the histogram that it spans over the acceleration value of 8 to 26 units. The frequency of data elements corresponding to the bins first keep on increasing, tillit reaches the bin of range 14 to 16 units. At this range, the baris tallest in size. So we can conclude that a maximum number of data elements fall within this range. After this range, the barsize starts decreasing till the end of the whole range at the acceleration value of 26 units.

Please note that when the histogram is uniform, as in the case of attribute 'model. year', it gives a hint that all values areequally likely to occur.

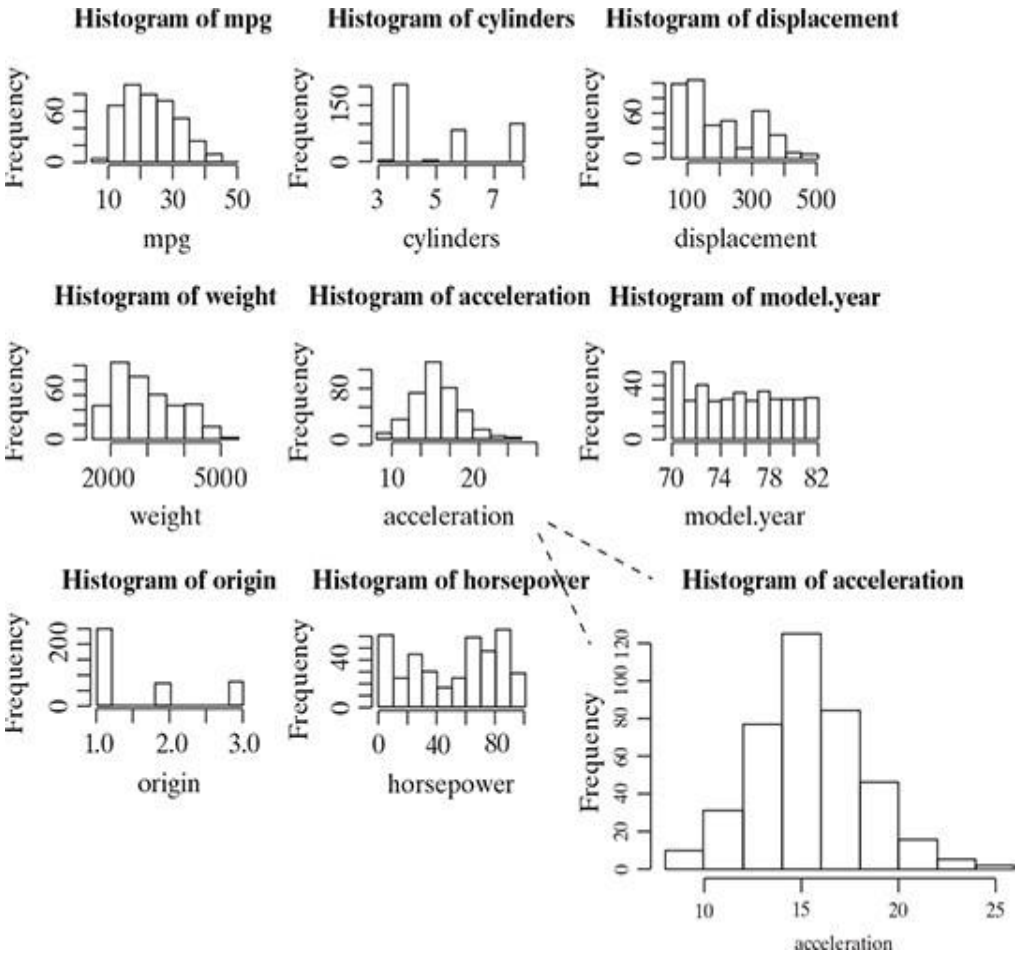


FIG. 2.12 Histogram Auto MPG attributes

2.4.3 Exploring categorical data

We have seen there are multiple ways to explore numeric data.However, there are not many options for exploring categorical data. In the Auto MPG data set, attribute 'car.name' is categorical in nature. Also, as we discussed earlier, we may consider 'cylinders' as a categorical variable instead of a numeric variable.

The first summary which we may be interested in noting ishow many unique names are there for the attribute 'car name'

or how many unique values are there for 'cylinders' attribute.We can get this as follows:

For attribute ‘car name’

1. Chevrolet chevelle malibu
2. Buick skylark 320
3. Plymouth satellite
4. Amc rebel sst
5. Ford torino
6. Ford galaxie 500
7. Chevrolet impala
8. Plymouth fury iii
9. Pontiac catalina
10. Amc ambassador dpl

For attribute ‘cylinders’8 4 6 3 5

We may also look for a little more details and want to get atable consisting the categories of the attribute and count of thedata elements falling into that category. Tables 2.4 and 2.5 contain these details.

For attribute ‘car name’

Table 2.4 *Count of Categories for ‘car name’ Attribute*

Attribute Value	amc ambas-sador brougham	amc ambas-sador dpl	amc ambassa-dor sst	amc concord	amc concord d/l	amc con-cord dl 6	amc gremlin	...
Count	1	1	1	1	2	2	4	...

For attribute “cylinders”

Table 2.5 *Count of Categories for ‘Cylinders’ Attribute*

Attribute Value	3	4	5	6	8
Count	4	204	3	84	103

In the same way, we may also be interested to know the proportion (or percentage) of count of data elements belongingto a category. Say, e.g., for the attributes ‘cylinders’, the proportion of data elements belonging to the category 4 is 204
÷ 398 = 0.513, i.e. 51.3%. Tables 2.6 and 2.7 contain the summarization of the categorical attributes by proportion ofdata elements.

For attribute ‘car name’

Table 2.6 *Proportion of Categories for ‘“Cylinders’ Attribute*

Attribute Value	Amc ambas-sador brougham	Amc ambassa-dor dpl	Amc ambassa-dor sst	Amc concord	Amc concord d/l	Amc concord dl 6	Amc gremlin	...
Count	0.003	0.003	0.003	0.003	0.005	0.005	0.01	...

For attribute ‘cylinders’

Table 2.7 *Proportion of Categories for “Cylinders” Attribute*

Attribute Value	3	4	5	6	8
Count	0.01	0.513	0.008	0.211	0.259

Last but not the least, as we have read in the earlier section on types of data, statistical measure “mode” is applicable on categorical attributes. As we know, like mean and median, mode is also a statistical measure for central tendency of a data. Mode of a data is the data value which appears most often. In context of categorical attribute, it is the category which has highest number of data values. Since mean and median cannot be applied for categorical variables, mode is thesole measure of central tendency.

Let’s try to find out the mode for the attributes ‘car name’ and ‘cylinders’. For cylinders, since the number of categories is less and we have the entire table listed above, we can see that the mode is 4, as that is the data value for which frequencyis highest. More than 50% of data elements belong to the category 4. However, it is not so evident for the attribute ‘car name’ from the information given above. When we probe and try to find the mode, it is found to be

category ‘ford pinto’ for which frequency is of highest value 6.

An attribute may have one or more modes. Frequency distribution of an attribute having single mode is called ‘unimodal’, two modes are called ‘bimodal’ and multiplemodes are called ‘multimodal’.

2.4.4 Exploring relationship between variables

Till now we have been exploring single attributes in isolation. One more important angle of data exploration is to explore relationship between attributes. There are multiple plots to enable us explore the relationship between variables. The basicand most commonly used plot is scatter plot.

2.4.4.1 Scatter plot

A scatter plot helps in visualizing bivariate relationships, i.e. relationship between two variables. It is a two-dimensional plot in which points or dots are drawn on coordinates provided by values of the attributes. For example, in a data set there are two attributes – attr_1 and attr_2. We want to understand the relationship between two attributes, i.e. with a change in valueof one attribute, say attr_1, how does the value of the other attribute, say attr_2, changes. We can draw a scatter plot, withattr_1 mapped to *x*-axis and attr_2 mapped in *y*-axis. So, everypoint in the plot will have value of attr_1 in the *x*-coordinate and value of attr_2 in the *y*-coordinate. As in a two- dimensional plot, attr_1 is said to be the independent variable and attr_2 as the dependent variable.

Let’s take a real example in this context. In the data set AutoMPG, there is expected to be some relation between the attributes ‘displacement’ and ‘mpg’. Let’s try to verify our intuition using the scatter plot of ‘displacement’ and ‘mpg’.

Let’s map ‘displacement’ as the *x*-coordinate and ‘mpg’ as the

*y-c*oordinate. The scatter plot comes as in Figure 2.13.

As is evident in the scatter plot, there is a definite relation between the two variables. The value of ‘mpg’ seems to steadily decrease with the increase in the value of ‘displacement’. It may come in our mind that what is the extent of relationship? Well, it can be reviewed by calculating the correlation between the variables. Refer to chapter 5 if youwant to find more about correlation and how to calculate it.

One more interesting fact to notice is that there are certain datavalues which stand-out of the others. For example, there is onedata element which has a mpg of 37 for a displacement of 250. This record is completely different from other data elements having similar displacement value but mpg value in the range of 15 to 25. This gives an indication that of presence of outlierdata values.

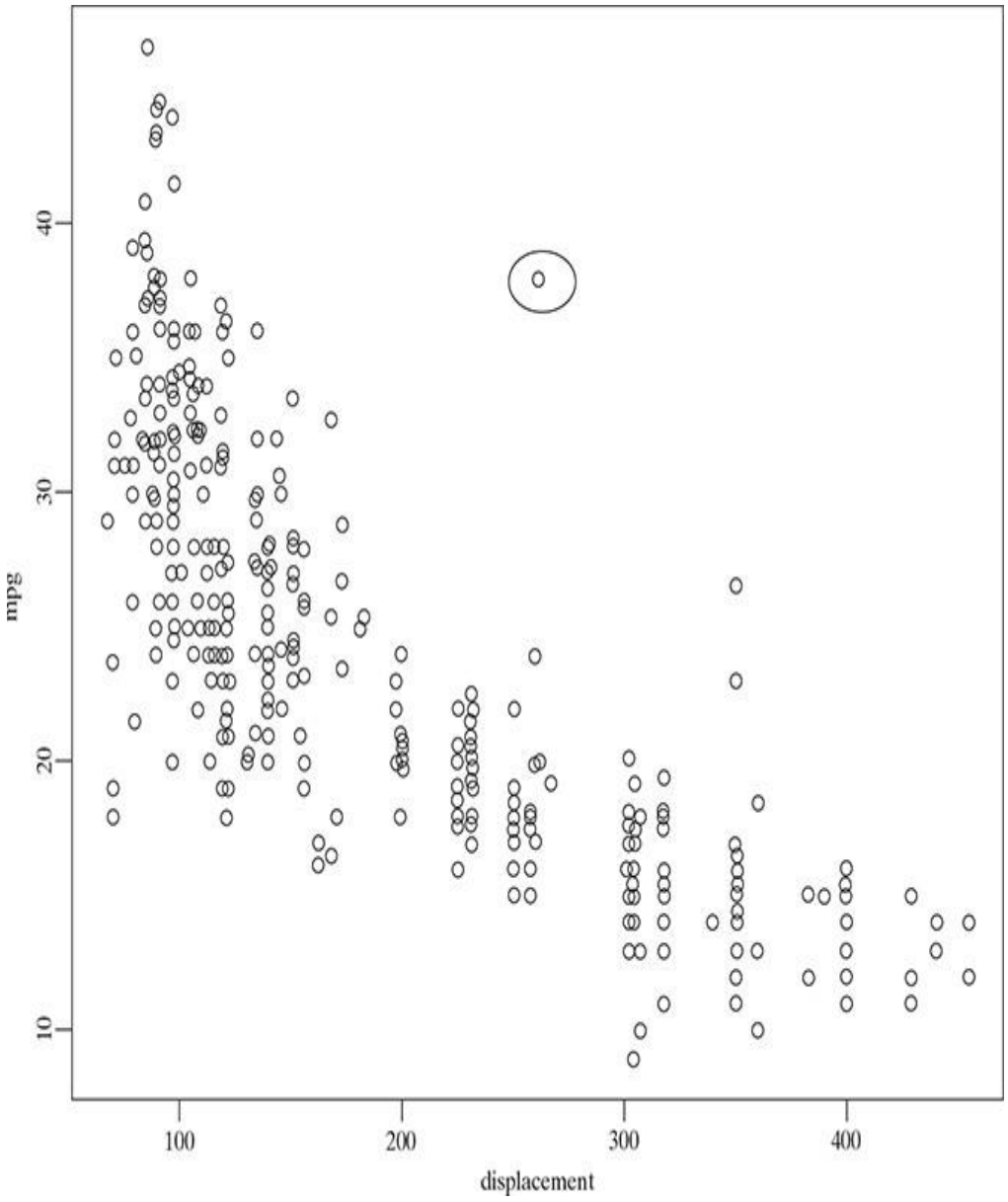


FIG. 2.1C Scatter plot of ‘displacement’ and ‘mpg’

In Figure 2.14, the pair wise relationship among the features

— ‘mpg’, ‘displacement’, ‘horsepower’, ‘weight’, and ‘acceleration’ have been captured. As you can see, in most of the cases, there is a significant relationship between the attribute pairs. However, in some cases, e.g. between attributes‘weight’ and ‘acceleration’, the relationship doesn’t seem to bevery strong.

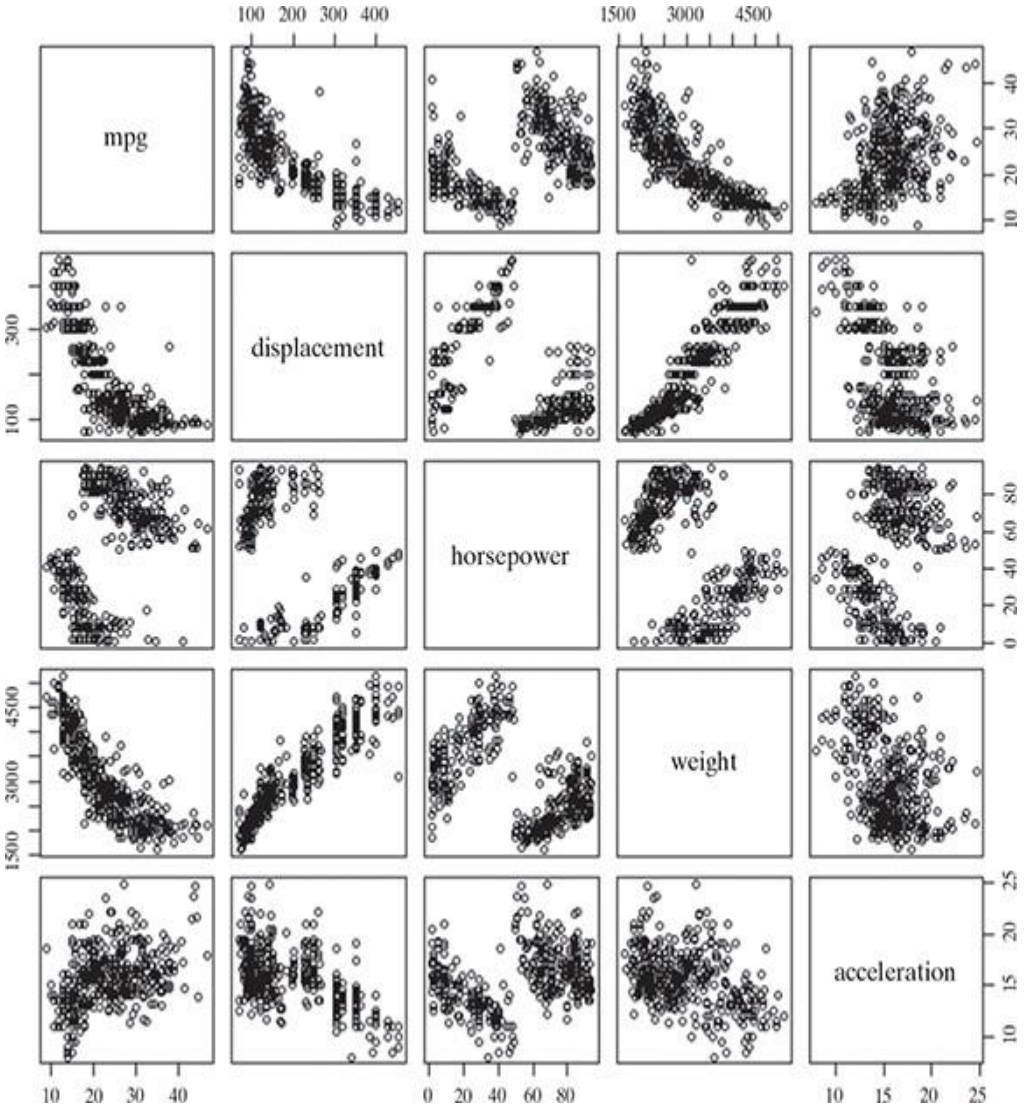


FIG. 2.14 Pair wise scatter plot between different attributes of Auto MPG

2.4.4.2 *Two-way cross-tabulations*

Two-way cross-tabulations (also called cross-tab or contingency table) are used to understand the relationship oftwo categorical attributes in a concise way. It has a matrix format that presents a summarized view of the bivariate frequency distribution. A cross-tab, very much like a scatterplot, helps to understand how much the data values of one attribute changes with the change in data values of another

attribute. Let's try to see with examples, in context of the AutoMPG data set.

Let's assume the attributes 'cylinders', 'model.year', and 'origin' as categorical and try to examine the variation of one with respect to the other. As we understand, attribute 'cylinders' reflects the number of cylinders in a car and assumes values 3, 4, 5, 6, and 8. Attribute 'model.year' captures the model year of each of the car and 'origin' gives the region of the car, the values for origin 1, 2, and 3 corresponding to North America, Europe, and Asia. Below are the cross-tabs. Let's try to understand what information they actually provide.

The first cross-tab, i.e. the one showing relationship between attributes 'model. year' and 'origin' help us understand the number of vehicles per year in each of the regions North America, Europe, and Asia. Looking at it in another way, we can get the count of vehicles per region overthe different years. All these are in the context of the sample data given in the Auto MPG data set.

Moving to the second cross-tab, it gives the number of 3, 4,5, 6, or 8 cylinder cars in every region present in the sample data set. The last cross-tab presents the number of 3, 4, 5, 6, or8 cylinder cars every year.

We may also want to create cross-tabs with a more summarized view like have a cross-tab giving a number of carshaving 4 or less cylinders and more than 4 cylinders in each region or by the years. This can be done by rolling up data values by the attribute 'cylinder'. Tables 2.8–2.10 present cross-tabs for different attribute combinations.

'Model year' vs. 'origin'

Table 2.8 *Cross-tab for* 'Model year' *vs.* 'Origin'

Origin \ Model Year	70	71	72	73	74	75	76	77	78	79	80	81	82
1	22	20	18	29	15	20	22	18	22	23	7	13	20
2	5	4	5	7	6	6	8	4	6	4	9	4	2
3	2	4	5	4	6	4	4	6	8	2	13	12	9

'Cylinders' vs. 'Origin'

Table 2.9 *Cross-tab for 'Cylinders' vs. 'Origin'*

Cylinders \ Origin	1	2	3
3	0	0	4
4	72	63	69
5	0	3	0
6	74	4	6
8	103	0	0

'Cylinders' vs. 'Model year'

Table 2.1O *Cross-tab for 'Cylinders' vs. 'Model year'*

Cylinders \ Model Year	70	71	72	73	74	75	76	77	78	79	80	81	82
3	0	0	1	1	0	0	0	1	0	0	1	0	0
4	7	13	14	11	15	12	15	14	17	12	25	21	28
5	0	0	0	0	0	0	0	0	1	1	1	0	0
6	4	8	0	8	7	12	10	5	12	6	2	7	3
8	18	7	13	20	5	6	9	8	6	10	0	1	0

2.5 DATA QUALITY AND REMEDIATION

2.5.1 Data quality

Success of machine learning depends largely on the quality ofdata. A data which has the right quality helps to achieve betterprediction accuracy, in case of supervised learning. However, it is not realistic to expect that the data will be flawless. We have already come across at least two types of problems:

1. Certain data elements without a value or data with a missing value.
2. Data elements having value surprisingly different from the otherelements, which we term as outliers.

There are multiple factors which lead to these data qualityissues. Following are some of them:

- **Incorrect sample set selection:** The data may not reflect normal or regular quality due to incorrect selection of sample set. For example, if we are selecting a sample set of sales transactions from a festive period and trying touse that data to predict sales in future. In this case, the prediction will be far apart from the actual scenario, just because the sample set has been selected in a wrong time. Similarly, if we are trying to predict poll results using a training data which doesn't comprise of a right mix of voters from different segments such as age, sex, ethnic diversities, etc., the prediction is bound to be a failure. It may also happen due to incorrect sample size. For example, a sample of small size may not be able to capture all aspects or information needed for right learning of the model.
- **Errors in data collection:** resulting in outliers and missing values
  - In many cases, a person or group of persons are responsible for the collection of data to be used in a learning activity. In this manual process, there is the possibility of wrongly recording data either in terms of value (say 20.67 is wrongly recorded as 206.7 or 2.067) or interms of a unit of measurement (say cm. is wrongly recorded as m. or mm.). This may result in data elements which have abnormally high or low value from other elements. Such records are termed as *outliers*.It may also happen that the data is not recorded at all. In case of a survey conducted to collect data, it is all the more possible as survey responders may choose not to respond to a certain question. So the data value for that data element in that responder's record is *missing*.

2.5.2 Data remediation

The issues in data quality, as mentioned above, need to be remediated, if the right amount of efficiency has to be achieved in the learning activity. Out of the two major areas mentioned above, the first one can be remedied by proper sampling technique. This is a completely different area – covered as a specialized subject area in statistics. We will notcover that in this book. However, human errors are bound to happen, no matter whatever checks and balances we put in.
Hence, proper remedial steps need to be taken for the second area mentioned above. We will discuss how to handle outliersand missing values.

2.5.2.1 Handling outliers

Outliers are data elements with an abnormally high value which may impact prediction accuracy, especially in regression models. Once the outliers are identified and the decision has been taken to amend those values, you may consider one of the following approaches. However, if the outliers are natural, i.e. the value of the data element is surprisingly high or low because of a valid reason, then weshould not amend it.

Remove outliers: If the number of records which are outliers is not many, asimple approach may be to remove them.
Imputation: One other way is to impute the value with mean or median ormode. The value of the most similar data element may also be used for imputation.
Capping: For values that lie outside the 1.5|×| IQR limits, we can cap themby replacing those observations below the lower limit with the value of 5th percentile and those that lie above the upper limit, with the value of 95th percentile.

If there is a significant number of outliers, they should betreated separately in the statistical model. In that case, the groups should be treated as two different groups, the modelshould be built for both groups and then the output can be combined.

2.5.2.2 Handling missing values

In a data set, one or more data elements may have missing values in multiple records. As discussed above, it can be caused by omission on part of the surveyor or a person who iscollecting sample data or by the responder, primarily due to his/her unwillingness to respond or lack of understanding needed to provide a response. It may happen that a specific question (based on which the value of a data element originates) is not applicable to a person or object with respectto which data is collected. There are multiple strategies to handle missing value of data elements. Some of those strategies have been discussed below.

2.5.2.2.1 Eliminate records having a missing value of data elements

In case the proportion of data elements having missing values is within a tolerable limit, a simple but effective approach is toremove the records having such data elements. This is possibleif the quantum of data left after removing the data elements having missing values is sizeable.

In the case of Auto MPG data set, only in 6 out of 398 records, the value of attribute ‘horsepower’ is missing. If we get rid of those 6 records, we will still have 392 records, whichis definitely a substantial number. So, we can very well eliminate the records and keep working with the remaining data set.

However, this will not be possible if the proportion of records having data elements with missing value is really highas that will reduce the power of model because of reduction inthe training data size.

2.5.2.2.2 Imputing missing values

Imputation is a method to assign a value to the data elements having missing values. Mean/mode/median is most frequently assigned value. For quantitative attributes, all missing values are imputed with the mean, median, or mode of the remaining values under the same attribute. For qualitative attributes, all missing values are imputed by the mode of all remaining values of the same attribute. However, another strategy may beidentify the similar types of observations whose values are known and use the mean/median/mode of those known values.

For example, in context of the attribute 'horsepower' of theAuto MPG data set, since the attribute is quantitative, we takea mean or median of the remaining data element values and assign that to all data elements having a missing value. So, wemay assign the mean, which is 104.47 and assign it to all the six data elements. The other approach is that we can take a similarity based mean or median. If we refer to the six observations with missing values for attribute 'horsepower' asdepicted in Table 2.11, 'cylinders' is the attribute which is logically most connected to 'horsepower' because with the increase in number of cylinders of a car, the horsepower of the

car is expected to increase. So, for five observations, we can use the mean of data elements of the 'horsepower' attribute having cylinders = 4; i.e. 78.28 and for one observation whichhas cylinders = 6, we can use a similar mean of data elementswith cylinders = 6, i.e. 101.5, to impute value to the missing data elements.

Table 2.11 *Missing Values for 'Horsepower' Attribute*

mpg	cylin-ders	dis-place-ment	horse-power	weight	accel-eration	model year	origin	car name
25	4	98	?	2046	19	71	1	Ford pinto
21	6	200	?	2875	17	74	1	Ford maverick
40.9	4	85	?	1835	17.3	80	2	Renault lecar deluxe
23.6	4	140	?	2905	14.3	80	1	Ford mustang cobra
34.5	4	100	?	2320	15.8	81	2	Renault 18i
23	4	151	?	3035	20.5	82	1	Amc concord dl

2.5.2.2.3 Estimate missing values

If there are data points similar to the ones with missing attribute values, then the attribute values from those similar data points can be planted in place of the missing value. For finding similar data points or observations, distance functioncan be used.

For example, let's assume that the weight of a Russian student having age 12 years and height 5 ft. is missing. Then the weight of any other Russian student having age close to 12years and height close to 5 ft. can be assigned.

2.6 DATA PRE-PROCESSING

2.6.1 Dimensionality reduction

Till the end of the 1990s, very few domains were explored which included data sets with a high number of attributes or features. In general, the data sets used in machine learning used to be in few 10s. However, in the last two decades, therehas been a rapid advent of computational biology like genomeprojects. These projects have produced extremely high- dimensional data sets with 20,000 or more features being verycommon. Also, there has been a wide-spread adoption of social networking leading to a need for text classification for customer behaviour analysis.

High-dimensional data sets need a high amount of computational space and time. At the same time, not all features are useful – they degrade the performance of machinelearning algorithms. Most of the machine learning algorithms perform better if the dimensionality of data set, i.e. the numberof features in the data set, is reduced. Dimensionality reduction helps in reducing irrelevance and redundancy in features. Also, it is easier to understand a model if the number of features involved in the learning activity is less.

Dimensionality reduction refers to the techniques of reducing the dimensionality of a data set by creating new attributes by combining the original attributes. The most common approach for dimensionality reduction is known as Principal Component Analysis (PCA). PCA is a statistical technique to convert a set of correlated variables into a set of transformed, uncorrelated variables called principal components. The principal components are a linear combination of the original variables. They are orthogonal toeach other. Since principal components are uncorrelated, they

capture the maximum amount of variability in the data. However, the only challenge is that the original attributes arelost due to the transformation.

Another commonly used technique which is used for dimensionality reduction is Singular Value Decomposition(SVD).

More about these concepts have been discussed in Chapter 4.

2.6.2 Feature subset selection

Feature subset selection or simply called feature selection, both for supervised as well as unsupervised learning, try to find out the optimal subset of the entire feature set which significantly reduces computational cost without any major impact on the learning accuracy. It may seem that a feature subset may lead to loss of useful information as certain features are going to be excluded from the final set of featuresused for learning. However, for elimination only features which are not relevant or redundant are selected.

A feature is considered as irrelevant if it plays an insignificant role (or contributes almost no information) in classifying or grouping together a set of data instances. All irrelevant features are eliminated while selecting the final feature subset. A feature is potentially redundant when the information contributed by the feature is more or less same asone or more other features. Among a

group of potentially redundant features, a small number of features can be selectedas a part of the final feature subset without causing any negative impact to learn model accuracy.

There are different ways to select a feature subset. In Chapter 4, we will be discussing feature selection in details.

Chapter 3 Modelling and Evaluation

1.1 INTRODUCTION

The learning process of machines may seem quite magical to somebody who is new to machine learning. The thought that a machine is able to think and take intelligent action may be mesmerizing – much like a science fiction or a fantasy story.

However, delving a bit deeper helps them realize that it is notas magical as it may seem to be. In fact, it tries to emulate human learning by applying mathematical and statistical formulations. In that sense, both human and machine learningstrives to build formulations or mapping based on a limited number of observations. As introduced in Chapter 1, the basiclearning process, irrespective of the fact that the learner is a human or a machine, can be divided into three parts:

1. Data Input
2. Abstraction
3. Generalization

Though in Chapter 1 we have understood these aspects in details, let's quickly refresh our memory with an example. It'sa fictitious situation. The detective department of New City Police has got a tip that in a campaign gathering for the upcoming election, a criminal is going to launch an attack on the main candidate. However, it is not known who the person is and quite obviously the person might use some disguise.
The only thing that is for sure is the person is a history-sheeteror a criminal having a long record of serious crime. From the criminal database, a list of such criminals along with their photographs has been collected. Also, the photos taken by security cameras positioned at different places near the gathering are available with the detective department. They have to match the photos from the criminal database with the faces in the gathering to spot the potential attacker. So the main problem here is to spot the face of the criminal based on the match with the photos in the criminal database.

This can be done using human learning where a person fromthe detective department can scan through each shortlisted photo and try to match that photo with the faces in the gathering. A person having a strong memory can take a glance at the photos of all criminals in one shot and then try to find a face in the gathering which closely resembles one of the criminal photos that she has viewed. Easy, isn't it? But that is not possible in reality. The number of criminals in the databaseand hence the count of photos runs in hundreds, if not thousands. So taking a look at all the photos and memorizing them is not possible. Also, an exact match is out of the question as the criminal, in most probability, will come in disguise. The strategy to be taken here is to match the photos in smaller counts and also based on certain salient physical features like the shape of the jaw, the slope of the forehead, thesize of the eyes, the structure of the ear, etc. So, the photos from the criminal database form the input data. Based on it, key features can be abstracted. Since human matching for eachand every photo may soon lead to a visual as well as mental fatigue, a generalization of abstracted feature-based data is a good way to detect potential criminal faces in the gathering.

For example, from the abstracted feature-based data, say it is
observed that most of the criminals have a shorter distance between the inner corners of the eyes, a smaller angle betweenthe nose and the corners of the mouth, a higher curvature to the upper lip, etc. Hence, a face in the gathering may be classified as 'potentially criminal' based on whether they match with these generalized observations. Thus, using the input data, feature-based abstraction could be built and by applying generalization of the abstracted data, human learningcould classify the faces as potentially criminal ultimately leading to spotting of the

criminal.

The same thing can be done using machine learning too.
Unlike human detection, a machine has no subjective baggage,no emotion, no bias due to past experience, and above all no mental fatigue. The machine can also use the same input data, i.e. criminal database photos, apply computational techniques to abstract feature-based concept map from the input data and generalize the same in the form of a classification algorithm todecide whether a face in the gathering is potentially criminal or not.

When we talk about the learning process, abstraction is a significant step as it represents raw input data in a summarizedand structured format, such that a meaningful insight is obtained from the data. This structured representation of raw input data to the meaningful pattern is called a **model**. The model might have different forms. It might be a mathematical equation, it might be a graph or tree structure, it might be a computational block, etc. The decision regarding which modelis to be selected for a specific data set is taken by the learning task, based on the problem to be solved and the type of data.
For example, when the problem is related to prediction and thetarget field is numeric and continuous, the regression model isassigned. The process of assigning a model, and fitting a specific model to a data set is called model **training**. Once themodel is trained, the raw input data is summarized into an abstracted form.

However, with abstraction, the learner is able to only summarize the knowledge. This knowledge might be still verybroad-based – consisting of a huge number of feature-based data and inter-relations. To generate actionable insight from such broad-based knowledge is very difficult. This is where generalization comes into play. Generalization searches through the huge set of abstracted knowledge to come up witha small and manageable set of key findings. It is not possible to do an exhaustive search by reviewing each of the abstractedfindings one-by-one. A heuristic search is employed, an approach which is also used for human learning (often termedas ‘gut-feel’). It is quite obvious that the heuristics sometimes result in erroneous result. If the outcome is systematicallyincorrect, the learning is said to have a **bias**.

1.2 SELECTING A MODEL

Now that you are familiar with the basic learning process and have understood model abstraction and generalization in that context, let’s try to formalize it in context of a motivating example. Continuing the thread of the potential attack during the election campaign, New City Police department has succeeded in foiling the bid to attack the electoral candidate. However, this was a wake-up call for them and they want to take a proactive action to eliminate all criminal activities in theregion. They want to find the pattern of criminal activities in the recent past, i.e. they want to see whether the number of criminal incidents per month has any relation with an average income of the local population, weapon sales, the inflow of immigrants, and other such factors. Therefore, an association between potential causes of disturbance and criminal incidentshas to be determined. In other words, the goal or target is to develop a model to infer how the criminal incidents change based on the potential influencing factors mentioned above.

In machine learning paradigm, the potential causes of disturbance, e.g. average income of the local population, weapon sales, the inflow of immigrants, etc. are input variables. They are also called predictors, attributes, features, independent variables, or simply variables. The number of criminal incidents is an output variable (also called response ordependent variable). Input variables can be denoted by X, while individual input variables are represented as X_1, X_2, X_3,
…, X_n and output variable by symbol Y. The relationship between X and Y is represented in the general form: $Y = f(X) + e$, where 'f' is the **target function** and 'e' is a random error term.

Just like a target function with respect to a machine learning model, some other functions which are frequentlytracked are

A **cost function** (also called **error function**) helps to measure the extent to which the model is going wrong in estimating the relationship between X and Y. In that sense, cost function can tell how bad the modelis performing. For example, R-squared (to be discussed later in this chapter) is a cost function of regression model.

Loss function is almost synonymous to cost function – only differencebeing loss function is usually a function defined on a data point, while cost function is for the entire training data set.

Machine learning is an optimization problem. We try to define a model and tune the parameters to find the most suitable solution to a problem. However, we need to have a way to evaluate the quality or optimality ofa solution. This is done using **objective function**. Objective means goal.

Objective function takes in data and model (along with parameters) as input and returns a value. Target is to find values of model parameter to maximize or minimize the return value. When the objective is to minimize the value, it becomes synonymous to cost function. Examples:

maximize the reward function in reinforcement learning, maximize the posterior probability in Naive Bayes, minimize squared error in regression.

But the problem that we just talked about is one specific type of problem in machine learning. We have seen in Chapter1 that there are three broad categories of machine learning approaches used for resolving different types of problems.

Quickly recapitulating, they are

1. Supervised
    1. Classification
    2. Regression
2. Unsupervised
    1. Clustering
    2. Association analysis
3. Reinforcement

For each of the cases, the model that has to be created/trained is different. Multiple factors play a role when we try to select the model for solving a machine learning problem. The most important factors are (i) the kind of problem we want to solve using machine learning and (ii) the nature of the underlying data. The problem may be related to the prediction of a class value like whether a tumour is malignant or benign, whether the next day will be snowy or rainy, etc.

It may be related to prediction – but of some numerical value like what the price of a house should be in thenext quarter, what is the expected growth of a certain IT stockin the next 7 days, etc. Certain problems are related to grouping of data like finding customer segments that are usinga certain product, movie genres which have got more box office success in the last one year, etc. So, it is very difficult togive a generic guidance related to which machine learning has to be selected. In other words, there is no one model that works best for every machine learning problem. This is what'**No Free Lunch'** theorem also states.

Any learning model tries to simulate some real-world aspect. However, it is simplified to a large extent removing all intricate details. These simplifications are based on certain assumptions – which are quite dependent on situations. Based on the exact situation, i.e. the problem in hand and the data characteristics, assumptions may or may not hold. So the same model may yield remarkable results in a certain situation whileit may completely fail in a different situation. That's why, while doing the data exploration, which we covered in the previous chapter, we need to understand the data characteristics, combine this understanding with the problem we are trying to solve and then decide which model to be selected for solving the problem.

Let's try to understand the philosophy of model selection ina structured way. Machine learning algorithms are broadly of two types: models for supervised learning, which primarily focus on solving predictive problems and models for unsupervised learning, which solve descriptive problems.

3.2.1 Predictive models

Models for supervised learning or predictive models, as is understandable from the name itself, try to predict certain value using the values in an input data set. The learning modelattempts to establish a relation between the target feature, i.e. the feature being predicted, and the predictor features. The predictive models have a clear focus on what they want to learn and how they want to learn.

Predictive models, in turn, may need to predict the value ofa category or class to which a data instance belongs to. Beloware some examples:

1. Predicting win/loss in a cricket match
2. Predicting whether a transaction is fraud
3. Predicting whether a customer may move to another product

The models which are used for prediction of target featuresof categorical value are known as classification models. The target feature is known as a class and the categories to which classes are divided into are called levels. Some of the popularclassification models include *k*-Nearest Neighbor (kNN), Naïve Bayes, and Decision Tree.

Predictive models may also be used to predict numericalvalues of the target feature based on the predictor features.Below are some examples:

1. Prediction of revenue growth in the succeeding year
2. Prediction of rainfall amount in the coming monsoon
3. Prediction of potential flu patients and demand for flu shots next winter

The models which are used for prediction of the numerical value of the target feature of a data instance are known as regression models. Linear Regression and Logistic Regression models are popular regression models.

3.2.2 Descriptive models

Models for unsupervised learning or descriptive models areused to describe a data set or gain insight from a data set.
There is no target feature or single feature of interest in case ofunsupervised learning. Based on the value of all features, interesting patterns or insights are derived about the data set.

Descriptive models which group together similar data instances, i.e. data instances having a similar value of the different features are called clustering models. Examples ofclustering include

1. Customer grouping or segmentation based on social, demographic, ethnic,etc. factors
2. Grouping of music based on different aspects like genre, language, time-period, etc.
3. Grouping of commodities in an inventory

The most popular model for clustering is *k*-Means.

Descriptive models related to pattern discovery is used for market basket analysis of transactional data. In market basket analysis, based on the purchase pattern available in the transactional data, the possibility of purchasing one product based on the purchase of another product is determined. For example, transactional data may reveal a pattern that generallya customer who purchases milk also purchases biscuit at the same time. This can be useful for targeted promotions or in- store set up. Promotions related to biscuits can be sent to customers of milk products or vice versa. Also, in the store products related to milk can be placed close to biscuits.

1.3 TRAINING A MODEL (FOR SUPERVISED LEARNING)

1.3.1 Holdout method

In case of supervised learning, a model is trained using the labelled input data. However, how can we understand the performance of the model? The test data may not be available immediately. Also, the label value of the test data is not known. That is the reason why a part of the input data is held back (that is how the name holdout originates) for evaluation of the model. This subset of the input data is used as the test data for evaluating the performance of a trained model. In general 70%–80% of the input data (which is obviously labelled) is used for model training. The remaining 20%–30% is used as test data for validation of the performance of the model. However, a different proportion of dividing the input data into training and test data is also acceptable. To make surethat the data in both the buckets are similar in nature, the division is done randomly. Random numbers are used to assigndata items to the partitions. This method of partitioning the input data into two parts – training and test data (depicted in

Figure 3.1), which is by holding back a part of the input datafor validating the trained model is known as holdout method.

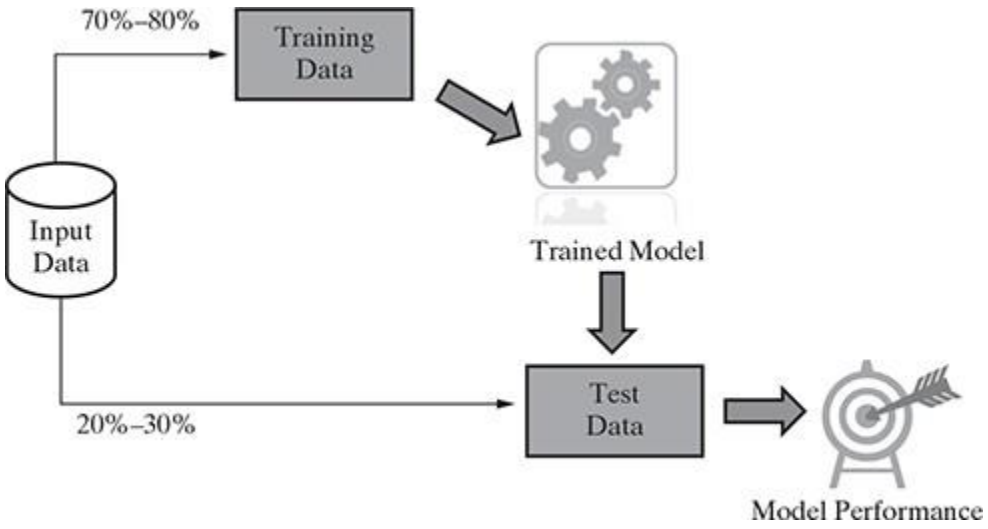


FIG. C.1 Holdout method

Once the model is trained using the training data, the labels of the test data are predicted using the model's target function.Then the predicted value is compared with the actual value of the label. This is possible because the test data is a part of the input data with known labels. The performance of the model isin general measured by the accuracy of prediction of the label value.

In certain cases, the input data is partitioned into three portions – a training and a test data, and a third validation data.The validation data is used in place of test data, for measuring the model performance. It is used in iterations and to refine themodel in each iteration. The test data is used only for once, after the model is refined and finalized, to measure and report the final performance of the model as a reference for future learning efforts.

An obvious problem in this method is that the division of data of different classes into the training and test data may not be proportionate. This situation is worse if the overall percentage of data related to certain classes is much less compared to other classes. This may happen despite the fact that random sampling is employed for test data selection. This problem can be addressed to some extent by applying stratifiedrandom sampling in place of sampling. In case of stratified random sampling, the whole data is broken into several homogenous groups or strata and a random sample is selected from each such stratum. This ensures that the generated random partitions have equal proportions of each class.

1.3.2 *K*-fold Cross-validation method

Holdout method employing stratified random sampling approach still heads into issues in certain specific situations. Especially, the smaller data sets may have the challenge to divide the data of some of the classes proportionally amongst training and test data sets. A special variant of holdout method, called repeated holdout, is sometimes employed to ensure the randomness of the composed data sets. In repeated holdout, several random holdouts are used to measure the model performance. In the end, the average of all performances is taken. As multiple holdouts have been drawn,the training and test data (and also validation data, in case it isdrawn) are more likely to contain representative data from all classes and resemble the original input data closely. This process of repeated holdout is the basis of *k*-fold cross-validation technique. In *k*-fold cross-validation, the data set is divided into *k*-completely distinct or non-overlapping random partitions called folds. Figure 3.2 depicts an overall approach for *k*-fold cross-validation.

The value of '*k*' in *k*-fold cross-validation can be set to anynumber. However, there are two approaches which are extremely popular:

1. 10-fold cross-validation (10-fold CV)
2. Leave-one-out cross-validation (LOOCV)

10-fold cross-validation is by far the most popular approach.
In this approach, for each of the 10-folds, each comprising of approximately 10% of the data, one of the folds is used as the test data for validating model performance trained based on the remaining 9 folds (or 90% of the data). This is repeated 10 times, once for each of the 10 folds being used as the test data and the remaining folds as the training data.The average performance across all folds is being reported. Figure 3.3 depicts the detailed approach of selecting the '*k*' folds in *k*-foldcross-validation. As can be observed in the figure, each of the circles resembles a record in the input data set whereas the different colors indicate the different classes that the records belong to.The entire data set is broken into '*k*' folds – out of which one fold is selected in each iteration as the test data set. The fold selected as test data set in each of the '*k*' iterations is different. Also, note that though in figure 3.3 the circles resemble the records in the input data set, the contiguous circles represented as folds do not mean that they are subsequent records in the data set. This is more a virtual representation and not a physical representation. As already mentioned, the records in a fold are drawn by using random sampling technique.

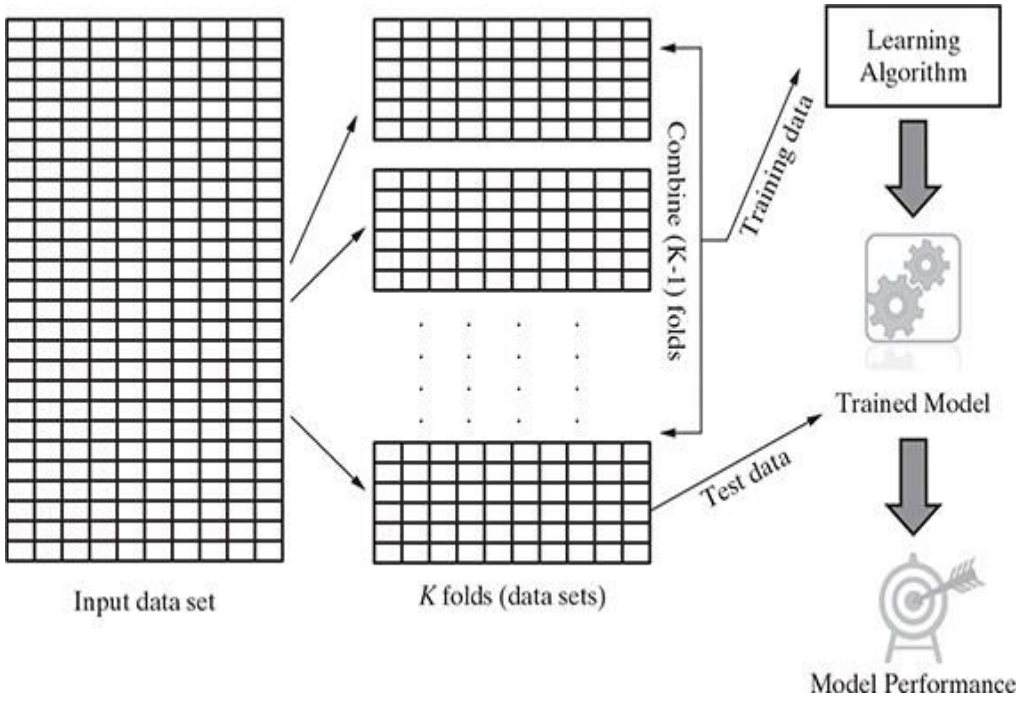


FIG. C.2 Overall approach for *K*-fold cross-validation

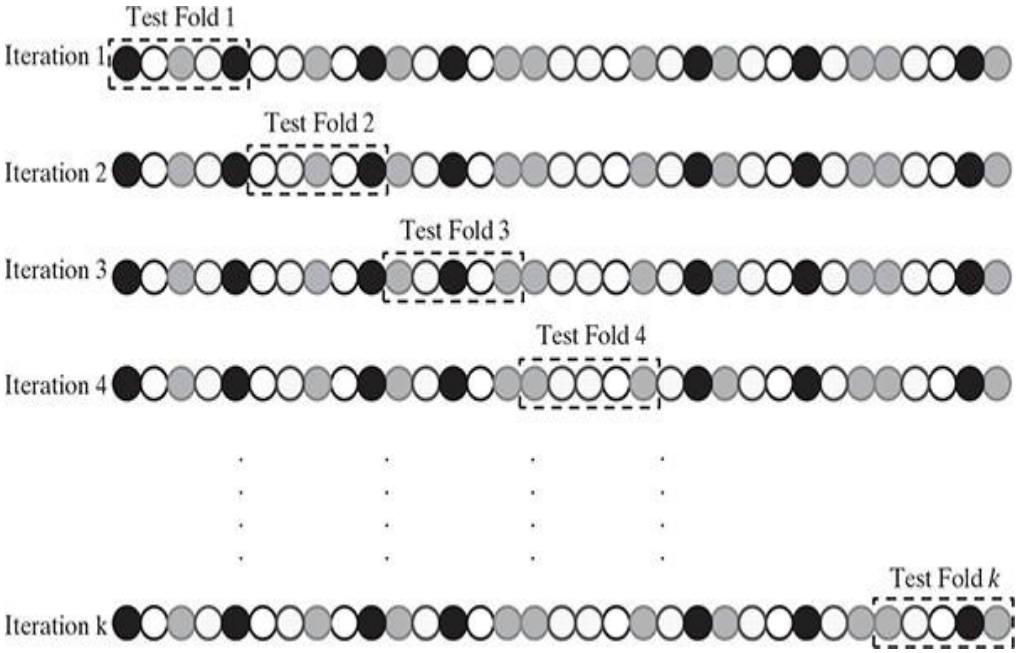


FIG. C.C Detailed approach for fold selection

Leave-one-out cross-validation (LOOCV) is an extreme case of *k*-fold cross-validation using one record or data instance at a time as a test data. This is done to maximize the count of data used to train the model. It is obvious that the number of iterations for which it has to be run is equal to the total number of data in the input data set. Hence, obviously, it is computationally very expensive and not used much in practice.

1.3.3 Bootstrap sampling

Bootstrap sampling or simply bootstrapping is a popular way to identify training and test data sets from the input data set. It uses the technique of Simple Random Sampling with Replacement (SRSWR), which is a well-known technique in sampling theory for drawing random samples. We have seen earlier that *k*-fold cross-validation divides the data into separate partitions – say 10 partitions in case of 10-fold cross-validation. Then it uses data instances from partition as test data and the remaining partitions as training data. Unlike this approach adopted in case of *k*-fold cross- validation, bootstrapping randomly picks data instances from the input data set, with the possibility of the same data instance to be picked multiple times. This essentially means that from the input data set having '*n*' data instances, bootstrapping can create one or more training data sets having '*n*' data instances,some of the data instances being repeated multiple times.

Figure 3.4 briefly presents the approach followed in bootstrap sampling.

This technique is particularly useful in case of input datasets of small size, i.e. having very less number of data instances.

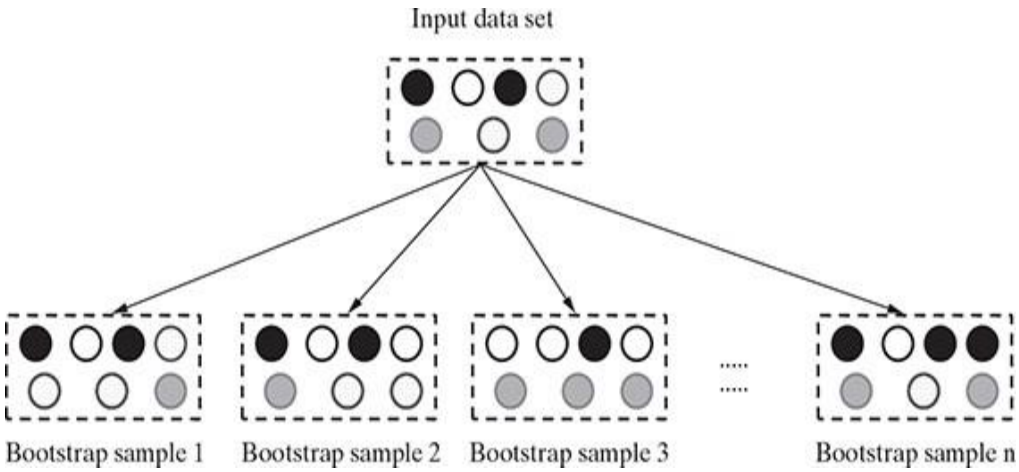


FIG. C.4 Bootstrap sampling

CROSS-VALIDATION	BOOTSTRAPPING
It is a special variant of holdout method, called repeated holdout. Hence uses stratified random sampling approach (without replacement). Data set is divided into 'k' random partitions, with each partition containing approximately $\frac{n}{k}$ number of unique data elements, where 'n' is the total number of data elements and 'k' is the total number of folds.	It uses the technique of Simple Random Sampling with Replacement (SRSWR). So the same data instance may be picked up multiple times in a sample.
The number of possible training/test data samples that can be drawn using this technique is finite.	In this technique, since elements can be repeated in the sample, possible number of training/test data samples is unlimited.

1.3.4 Lazy vs. Eager learner

Eager learning follows the general principles of machine learning – it tries to construct a generalized, input-independenttarget function during the model training phase. It follows the typical steps of machine learning, i.e. abstraction and generalization and comes up with a trained model at the end ofthe learning phase. Hence, when the test data comes in for classification, the eager learner is ready with the model and

doesn't need to refer back to the training data. Eager learnerstake more time in the learning phase than the lazy learners.
Some of the algorithms which adopt eager learning approachinclude Decision Tree, Support Vector Machine, Neural Network, etc.

Lazy learning, on the other hand, completely skips the abstraction and generalization processes, as explained in context of a typical machine learning process. In that respect, strictly speaking, lazy learner doesn't 'learn' anything. It uses the training data in exact, and uses the knowledge to classify the unlabelled test data. Since lazy learning uses training data as-is, it is also known as rote learning (i.e. memorization technique based on repetition). Due to its heavy dependency on the given training data instance, it is also known as instancelearning. They are also called non-parametric learning. Lazy learners take very little time in training because not much of training actually happens. However, it takes quite some time inclassification as for each tuple of test data, a comparison-basedassignment of label happens. One of the most popular algorithm for lazy learning is *k*-nearest neighbor.

1.4 MODEL REPRESENTATION AND INTERPRETABILITY

We have already seen that the goal of supervised machine learning is to learn or derive a target function which can best determine the target variable from the set of input variables. Akey consideration in learning the target function from the training data is the extent of generalization. This is because theinput 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.

Fitness of a target function approximated by a learning algorithm determines how correctly it is able to classify a setof data it has never seen.

1.4.1 Underfitting

If the target function is kept too simple, it may not be able to capture the essential nuances and represent the underlying datawell. 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
3.5. Many times underfitting happens due to unavailability of sufficient training data. Underfitting results in both poor performance with training data as well as poor generalizationto test data. Underfitting can be avoided by

1. using more training data
2. reducing features by effective feature selection

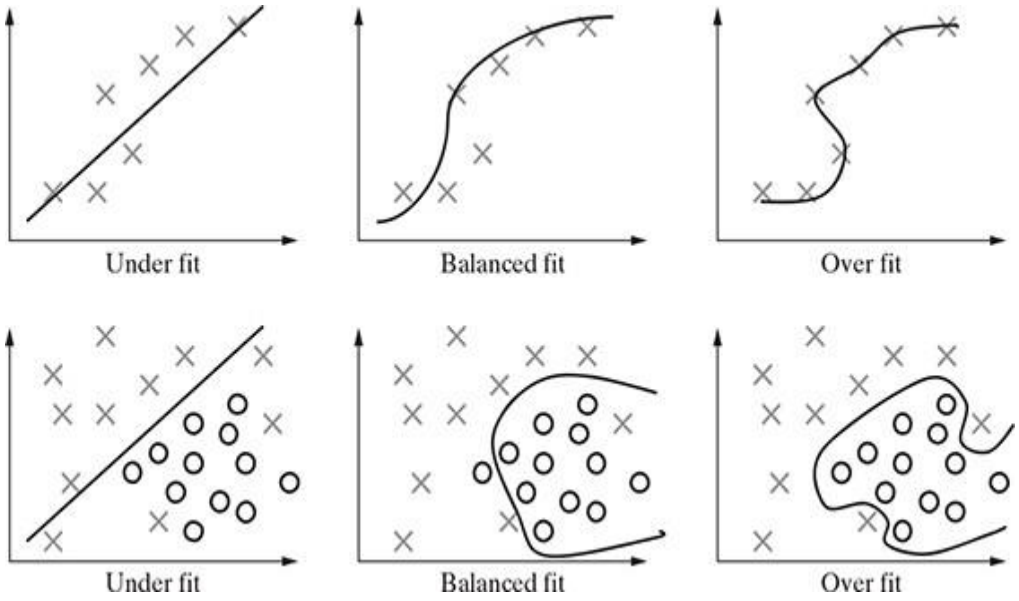


FIG. C.5 Underfitting and Overfitting of models

1.4.2 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 trainingdata. This is represented with a sample data set in figure 3.5 . 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 testdata 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 givenmachine learning problem.

Both underfitting and overfitting result in poor classificationquality which is reflected by low classification accuracy.

1.4.3 Bias – variance trade-off

In supervised learning, the class value assigned by the learningmodel 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.

1.4.3.1 *Errors due to ‘Bias’*

Errors due to bias arise from simplifying assumptions made bythe model to make the target function less complex or easier tolearn. 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 arecomplex in nature and do not align with the simplifying assumptions made by the algorithm. Underfitting results in high bias.

1.4.3.2 *Errors due to ‘Variance’*

Errors due to variance occur from difference in training datasets 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 besignificant 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.

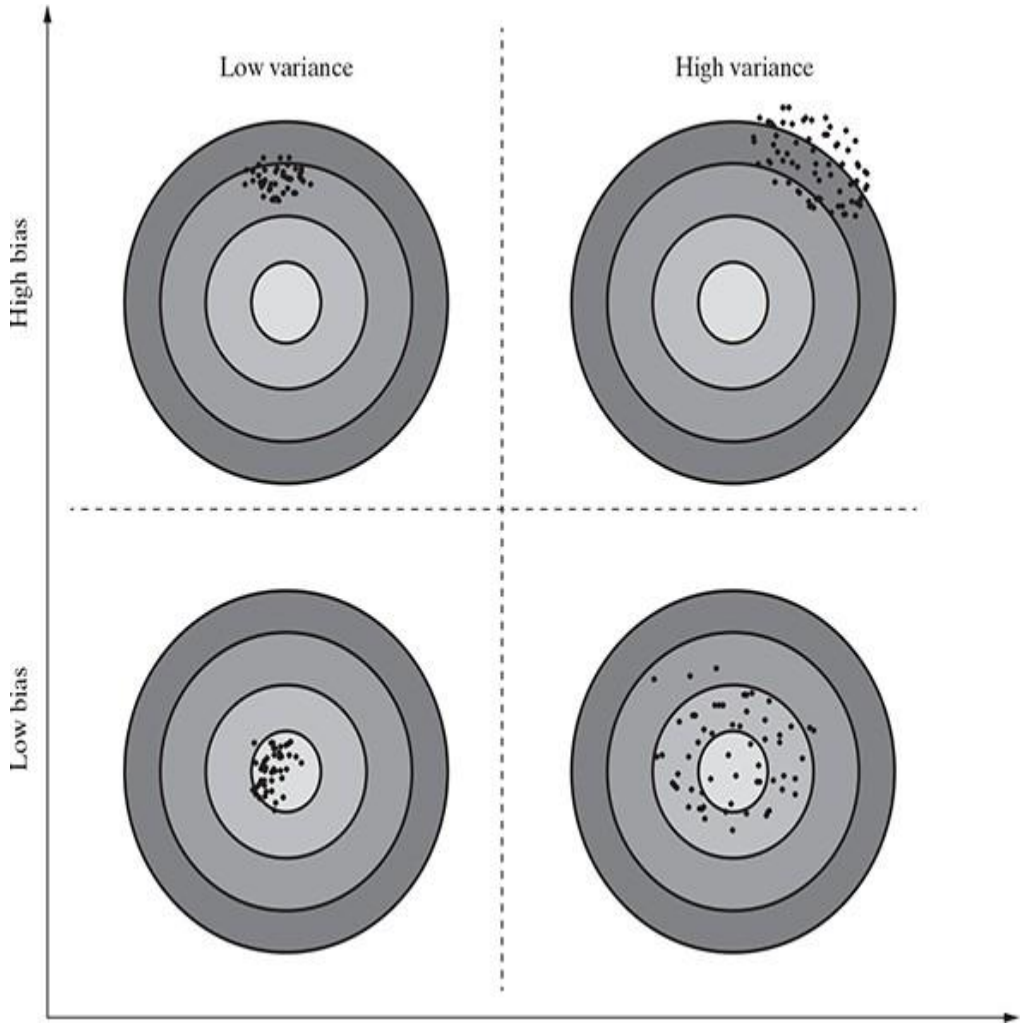


FIG. C.6 Bias-variance trade-off

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

As is quite understandable:

- Increasing the bias will decrease the variance, andIncreasing
- the variance will decrease the bias

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

As can be observed in Figure 3.6 , 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 userparameters which can be configured helps in striking a trade- off between bias and variance. For example, in a popular supervised algorithm *k*-Nearest Neighbors or *k*NN, 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.

1.5 EVALUATING PERFORMANCE OF A MODEL

3.5.1 Supervised learning - classification

In supervised learning, one major task is classification. The responsibility of the classification model is to assign class label to the target feature based on the value of the predictorfeatures. For example, in the problem of predicting the

win/loss in a cricket match, the classifier will assign a class value win/loss to target feature based on the values of other features like whether the team won the toss, number of spinners in the team, number of wins the team had in the tournament, etc. To evaluate the performance of the model, thenumber of correct classifications or predictions made by the model has to be recorded. A classification is said to be correct if, say for example in the given problem, it has been predicted by the model that the team will win and it has actually won.

Based on the number of correct and incorrect classificationsor predictions made by a model, the accuracy of the model is calculated. If 99 out of 100 times the model has classified correctly, e.g. if in 99 out of 100 games what the model has predicted is same as what the outcome has been, then the model accuracy is said to be 99%. However, it is quite relativeto say whether a model has performed well just by looking at the accuracy value. For example, 99% accuracy in case of a sports win predictor model may be reasonably good but the same number may not be acceptable as a good threshold when the learning problem deals with predicting a critical illness. In this case, even the 1% incorrect prediction may lead to loss of many lives. So the model performance needs to be evaluated in light of the learning problem in question. Also, in certain cases, erring on the side of caution may be preferred at the costof overall accuracy. For that reason, we need to look more closely at the model accuracy and also at the same time look at other measures of performance of a model like sensitivity, specificity, precision, etc. So, let's start with looking at model accuracy more closely. And let's try to understand it with an example.

There are four possibilities with regards to the cricket matchwin/loss prediction:

1. the model predicted win and the team won
2. the model predicted win and the team lost
3. the model predicted loss and the team won
4. the model predicted loss and the team lost

In this problem, the obvious class of interest is ‘win’.

The first case, i.e. the model predicted win and the team won is a case where the model has correctly classified data instances as the class of interest. These cases are referred asTrue Positive (TP) cases.

The second case, i.e. the model predicted win and the teamlost is a case where the model incorrectly classified data instances as the class of interest. These cases are referred as False Positive (FP) cases.

The third case, i.e. the model predicted loss and the team won is a case where the model has incorrectly classified as notthe class of interest. These cases are referred as False Negative (FN) cases.

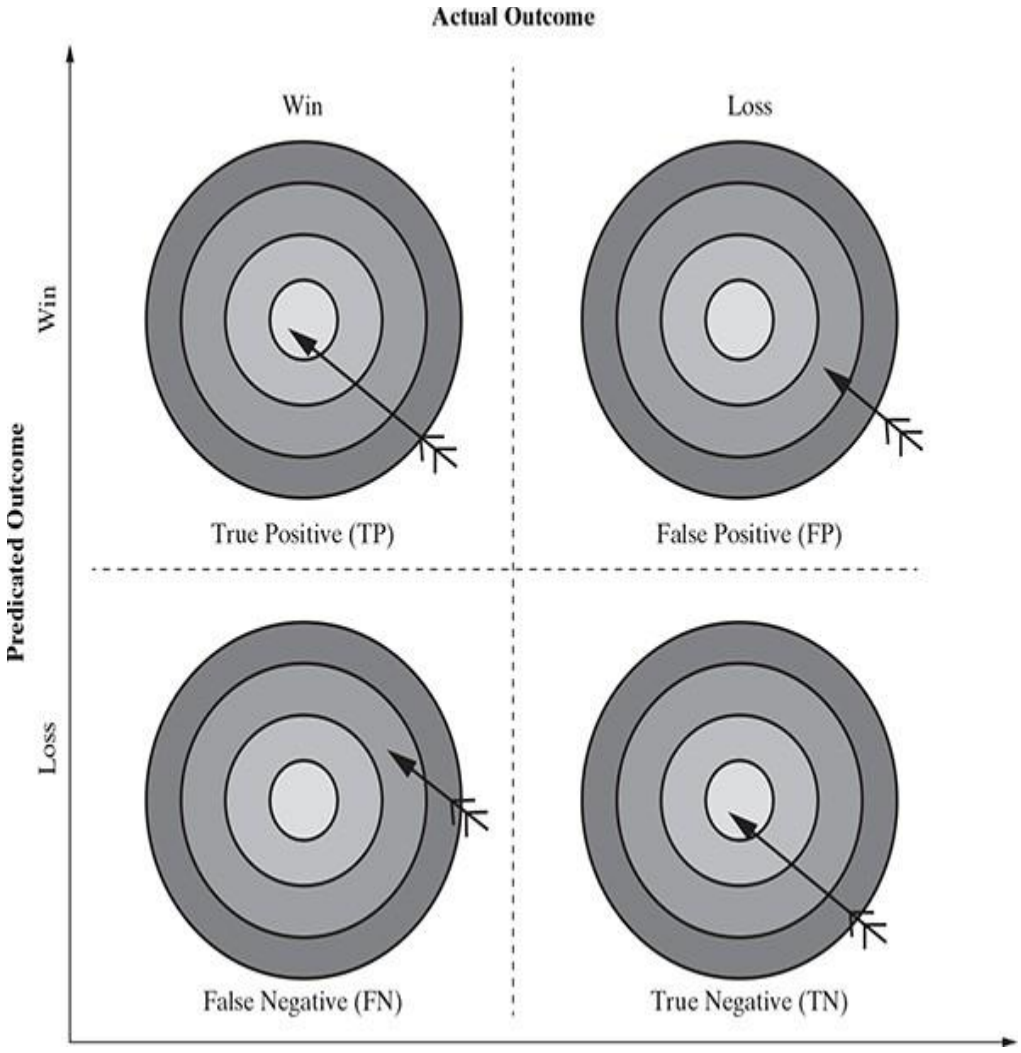


FIG. C.7 Details of model classification

The fourth case, i.e. the model predicted loss and the team lost is a case where the model

has correctly classified as not the class of interest. These cases are referred as True Negative (TN) cases. All these four cases are depicted in Figure 3.7 .

For any classification model, **model accuracy** is given by total number of correct classifications (either as the class of interest, i.e. True Positive or as not the class of interest, i.e. True Negative) divided by total number of classifications done.

$$\text{Model accuracy} = \frac{TP + TN}{TP + FP + FN + TN}$$

A matrix containing correct and incorrect predictions in the form of TPs, FPs, FNs and TNs is known as **confusion matrix**. The win/loss prediction of cricket match has two classes of interest – win and loss. For that reason it will generate a 2 × 2 confusion matrix. For a classification probleminvolving three classes, the confusion matrix would be 3 × 3, etc.

Let's assume the confusion matrix of the win/loss predictionof cricket match problem to be as below:

	ACTUAL WIN	ACTUAL LOSS
Predicted Win	85	4
Predicted Loss	2	9

In context of the above confusion matrix, total count of TPs = 85, count of FPs = 4, count of FNs = 2 and count of TNs = 9.

$$\therefore \text{Model accuracy} = \frac{TP + TN}{TP + FP + FN + TN} = \frac{85 + 9}{85 + 4 + 2 + 9} = \frac{94}{100} = 94\%$$

The percentage of misclassifications is indicated using **error rate** which is measured as

$$\text{Error rate} = \frac{FP + FN}{TP + FP + FN + TN}$$

In context of the above confusion matrix,

$$\text{Error rate} = \frac{FP + FN}{TP + FP + FN + TN} = \frac{4 + 2}{85 + 4 + 2 + 9} = \frac{6}{100} = 6\%$$
$$= 1 - \text{Model accuracy}$$

Sometimes, correct prediction, both TPs as well as TNs, may happen by mere coincidence. Since these occurrences boost model accuracy, ideally it should not happen. **Kappa** value of a model indicates the adjusted the model accuracy. Itis calculated using the formula below:

$$\text{Kappa value (k)} = \frac{P(a) - P(p_r)}{1 - P(p_r)}$$

P(a) = Proportion of observed agreement between actual and predicted in overall data set

$$= \frac{TP + TN}{TP + FP + FN + TN}$$

$P(p_r)$ = Proportion of expected agreement between actual and predicted data both in case of class of interest as well as the other classes

$$= \frac{TP + FP}{TP + FP + FN + TN} \times \frac{TP + FN}{TP + FP + FN + TN} + \frac{FN + TN}{TP + FP + FN + TN} \times \frac{FP + TN}{TP + FP + FN + TN}$$

In context of the above confusion matrix, total count of TPs = 85, count of FPs = 4, count of FNs = 2 and count of TNs = 9.

$$\therefore P(a) = \frac{TP + TN}{TP + FP + FN + TN} = \frac{85 + 9}{85 + 4 + 2 + 9} = \frac{94}{100} = 0.94$$

$$P(p_r) = \frac{85 + 4}{85 + 4 + 2 + 9} \times \frac{85 + 2}{85 + 4 + 2 + 9} + \frac{2 + 9}{85 + 4 + 2 + 9} \times \frac{4 + 9}{85 + 4 + 2 + 9}$$

$$= \frac{89}{100} \times \frac{87}{100} + \frac{11}{100} \times \frac{13}{100} = 0.89 \times 0.87 + 0.11 \times 0.13 = 0.7886$$

$$\therefore k = \frac{0.94 - 0.7886}{1 - 0.7886} = 0.7162$$

As discussed earlier, in certain learning problems it is critical to have extremely low number of FN cases, if needed, at the cost of a conservative classification model. Though it is a clear case of misclassification and will impact model accuracy adversely, it is still required as missing each class ofinterest may have serious consequence. This happens more in problems from medical domains like disease prediction problem. For example, if a tumor is malignant but wrongly classified as benign by the classifier, then the repercussion of such misclassification is fatal. It does not matter if higher number of tumours which are benign are wrongly classified as malignant. In these problems there are some measures of model performance which are more important than accuracy. Two such critical measurements are sensitivity and specificityof the model.

The **sensitivity** of a model measures the proportion of TP examples or positive cases which were correctly classified. Itis measured as

$$\text{Sensitivity} = \frac{TP}{TP + FN}$$

In the context of the above confusion matrix for the cricketmatch win prediction problem,

$$\text{Sensitivity} = \frac{TP}{TP + FN} = \frac{85}{85 + 2} = \frac{85}{87} = 97.7\%$$

So, again taking the example of the malignancy prediction of tumours, class of interest is ‘malignant’. Sensitivity measure gives the proportion of tumours which are actually malignant and have been predicted as malignant. It is quite obvious that for such problems the most critical measure of theperformance of a good model is sensitivity. A high value of sensitivity is more desirable than a high value of accuracy.

Specificity is also another good measure to indicate a good balance of a model being excessively conservative or excessively aggressive. Specificity of a model measures the proportion of negative examples which have been correctly classified. In the context, of malignancy prediction of tumours,specificity gives the proportion of benign tumours which have been correctly classified. In the context of the above confusionmatrix for the cricket match win prediction problem,

$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}} = \frac{9}{9 + 4} = \frac{9}{13} = 69.2\%$$

A higher value of specificity will indicate a better model performance. However, it is quite understandable that a conservative approach to reduce False Negatives might actually push up the number of FPs. Reason for this is that themodel, in order to reduce FNs, is going to classify more tumours as malignant. So the chance that benign tumours willbe classified as malignant or FPs will increase.

There are two other performance measures of a supervised learning model which are similar to sensitivity and specificity. These are **precision** and **recall**. While precision gives the proportion of positive predictions which are truly positive, recall gives the proportion of TP cases over all actually positive cases.

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

Precision indicates the reliability of a model in predicting aclass of interest. When the model is related to win / loss prediction of cricket, precision indicates how often it predicts the win correctly. In context of the above confusion matrix forthe cricket match win prediction problem,

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}} = \frac{85}{85 + 4} = \frac{85}{89} = 95.5\%$$

It is quite understandable that a model with higher precisionis perceived to be more reliable.

Recall indicates the proportion of correct prediction of positives to the total number of positives. In case of win/loss

prediction of cricket, recall resembles what proportion of thetotal wins were predicted correctly.

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

In the context of the above confusion matrix for the cricketmatch win prediction problem,

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}} = \frac{85}{85 + 2} = \frac{85}{87} = 97.7\%$$

3.5.1.1 F-measure

F-measure is another measure of model performance which combines the precision and recall. It takes the harmonic meanof precision and recall as calculated as

$$F\text{-measure} = \frac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

In context of the above confusion matrix for the cricketmatch win prediction problem,

$$F\text{-measure} = \frac{2 \times 0.955 \times 0.977}{0.955 + 0.977} = \frac{1.866}{1.932} = 96.6\%$$

As a combination of multiple measures into one, *F*-score gives the right measure using which performance of different models can be compared. However, one assumption the calculation is based on is that precision and recall have equal weight, which may not always be true in reality. In certain problems, the disease prediction problems, e.g., precision may be given far more weightage. In that case, different weightagesmay be assigned to precision and recall. However, there may be a serious dilemma regarding what value to be adopted for each and what is the basis for the specific value adopted.

3.5.1.1.1 Receiver operating characteristic (ROC) curves

As we have seen till now, though accuracy is the most popularmeasure, there are quite a number of other measures to evaluate the performance of a supervised learning model.
However, visualization is an easier and more effective way to understand the model performance. It also helps in comparingthe efficiency of two models.

Receiver Operating Characteristic (ROC) curve helps in visualizing the performance of a classification model. It showsthe efficiency of a model in the detection of true positives while avoiding the occurrence of false positives. To refresh ourmemory, true positives are those cases where the model has correctly classified data instances as the class of interest. For example, the model has correctly classified the tumours as malignant, in case of a tumour malignancy prediction problem. On the other hand, FPs are those cases where the model incorrectly classified data instances as the class of interest.
Using the same example, in this case, the model has incorrectly classified the tumours as malignant, i.e. tumourswhich are actually benign have been classified as malignant.

$$\text{True Positive Rate TPR} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{False Positive Rate FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$

In the ROC curve, the FP rate is plotted (in the horizontal axis) against true positive rate (in the vertical axis) at different classification thresholds. If we assume a lower value of classification threshold, the model classifies more items as positive. Hence, the values of both False Positives and True Positives increase. The area under curve (AUC) value, as shown in figure 3.8a , is the area of the two-dimensional spaceunder the curve extending from (0, 0) to (1, 1), where each point on the curve gives a set of true and false positive values at a specific classification threshold. This curve gives an indication of the predictive quality of a model. AUC value ranges from 0 to 1, with an AUC of less than 0.5 indicating that the classifier has no predictive ability. Figure 3.8b shows the curves of two classifiers – classifier 1 and classifier 2.

Quite obviously, the AUC of classifier 1 is more than the AUC
of classifier 2. So, we can draw the inference that classifier 1 isbetter than classifier 2.

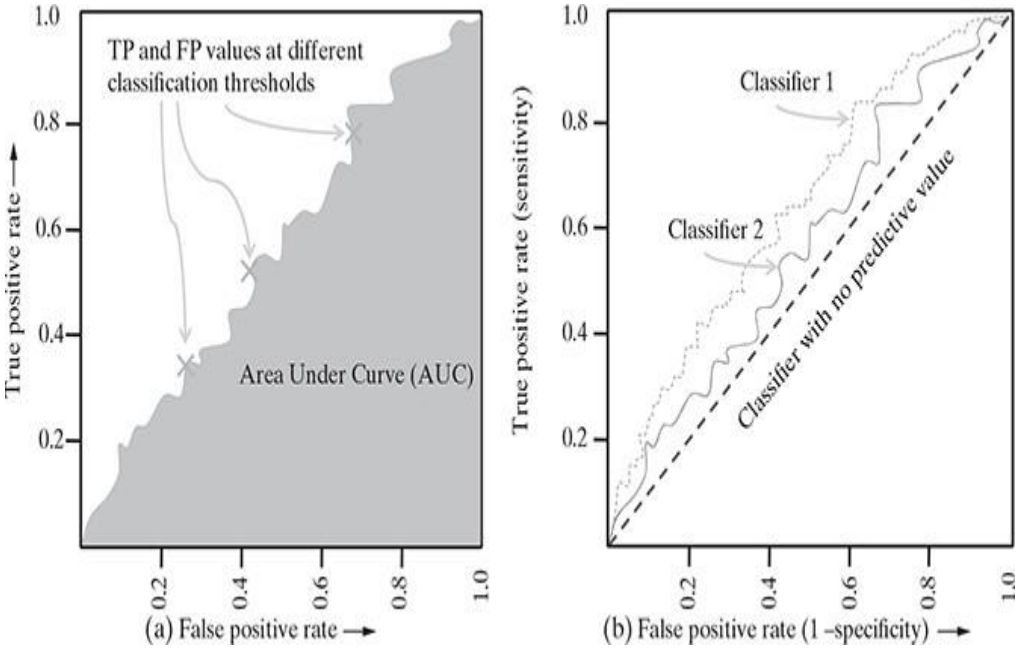


FIG. C.8 ROC curve

A quick indicative interpretation of the predictive valuesfrom 0.5 to 1.0 is given below:

- 0.5 – 0.6 ➔ Almost no predictive ability
- 0.6 – 0.7 ➔ Weak predictive ability
- 0.7 – 0.8 ➔ Fair predictive ability
- 0.8 – 0.9 ➔ Good predictive ability
- 0.9 – 1.0 ➔ Excellent predictive ability

3.5.2 Supervised learning – regression

A well-fitted regression model churns out predicted values close to actual values. Hence, a regression model which ensures that the difference between predicted and actual valuesis low can be considered as a good model. Figure 3.9 represents a very simple problem of real estate value prediction solved using linear regression model. If 'area' is thepredictor variable (say *x*) and 'value' is the target variable (say*y*), the linear regression model can be represented in the form:

$$y = \alpha + \beta x$$

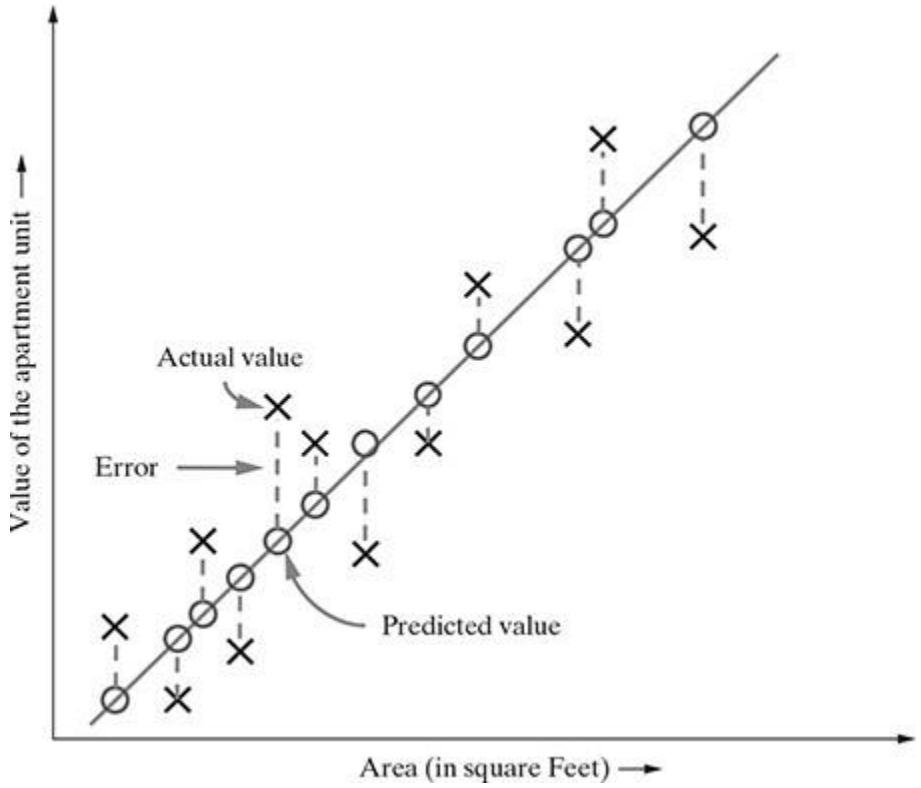


FIG. C.9 Error – Predicted vs. actual value

For a certain value of *x*, say *x*, the value of y is predicted as $\hat{y}$ whereas the actual value of *y* is *Y* (say). The distance between the actual value and the fitted or predicted value, i.e. $\hat{y}$is known as **residual**. The regression model can be considered to be fitted well if the difference between actual and predicted value, i.e. the residual value is less.

R-squared is a good measure to evaluate the model fitness.
It is also known as the coefficient of determination, or for multiple regression, the coefficient of multiple determination.The R-squared value lies between 0 to 1 (0%–100%) with a larger value representing a better fit. It is calculated as:

$$R^2 = \frac{SST - SSE}{SST}$$

Sum of Squares Total (SST) = squared differences of each observation from the overall mean = $\sum_{i=1}^{n} (y_i - \bar{y})^2$ where $\bar{y}$ is the mean.

Sum of Squared Errors (SSE) (of prediction) = sum of the squared residuals = $\sum_{i=1}^{n} (Y_i - \hat{y})^2$ where $\hat{y}_i$ is the predicted value of y_i and Y_i is the actual value of y_i.

3.5.3 Unsupervised learning - clustering

Clustering algorithms try to reveal natural groupings amongst the data sets. However, it is quite tricky to evaluate the performance of a clustering algorithm. Clustering, by nature, is very subjective and whether the cluster is good or bad is open for interpretations. It was noted, 'clustering is in the eye of the beholder'. This stems from the two inherent challenges which lie in the process of clustering:

1. It is generally not known how many clusters can be formulated from a particular data set. It is completely open-ended in most cases and provided as a user input to a clustering algorithm.
2. Even if the number of clusters is given, the same number of clusters can be formed with different groups of data instances.

In a more objective way, it can be said that a clustering algorithm is successful if the clusters identified using the algorithm is able to achieve the right results in the overall problem domain. For example, if clustering is applied for identifying customer segments for a marketing campaign of a new product launch, the clustering can be considered successful only if the marketing campaign ends with a success, i.e. it is able to create the right brand recognition resulting in steady revenue from new product sales. However, there are couple of popular approaches which are adopted for cluster quality evaluation.

1. *Internal evaluation*

   In this approach, the cluster is assessed based on the underlying data that was clustered. The internal evaluation methods generally measure cluster quality based on homogeneity of data belonging to the same cluster and heterogeneity of data belonging to different clusters. The homogeneity/heterogeneity is decided by some similarity measure. For example, **silhouette coefficient**, which is one of the most popular internal evaluation methods, uses distance (Euclidean or Manhattan distances most commonly used) between data elements as a similarity measure. The value of silhouette width ranges between –1 and +1, with a high value indicating high intra-cluster homogeneity and inter-cluster heterogeneity.

   For a data set clustered into '*k*' clusters, silhouette width is calculated as:

$$\text{Silhouette width} = \frac{b(i) - a(i)}{\max\{a(i),\ b(i)\}}$$

$a(i)$ is the average distance between the i th data instance and all other data instances belonging to the same cluster and $b(i)$ is the lowest average distance between the i-the data instance and data instances of all other clusters.

Let's try to understand this in context of the example depicted in figure 3.10. There are four clusters namely cluster 1, 2, 3, and 4. Let's consider an arbitrary data element 'i' in cluster 1, resembled by the asterisk. $a(i)$ is the average of the distances a_{i1}, a_{i2}, …, a_{in1} of the different data elements from the i th data element in cluster 1, assuming there are n_1 data elements in cluster 1. Mathematically,

$$a(i) = \frac{a_{i1} + a_{i2} + \ldots + a_{in_1}}{n_1}$$

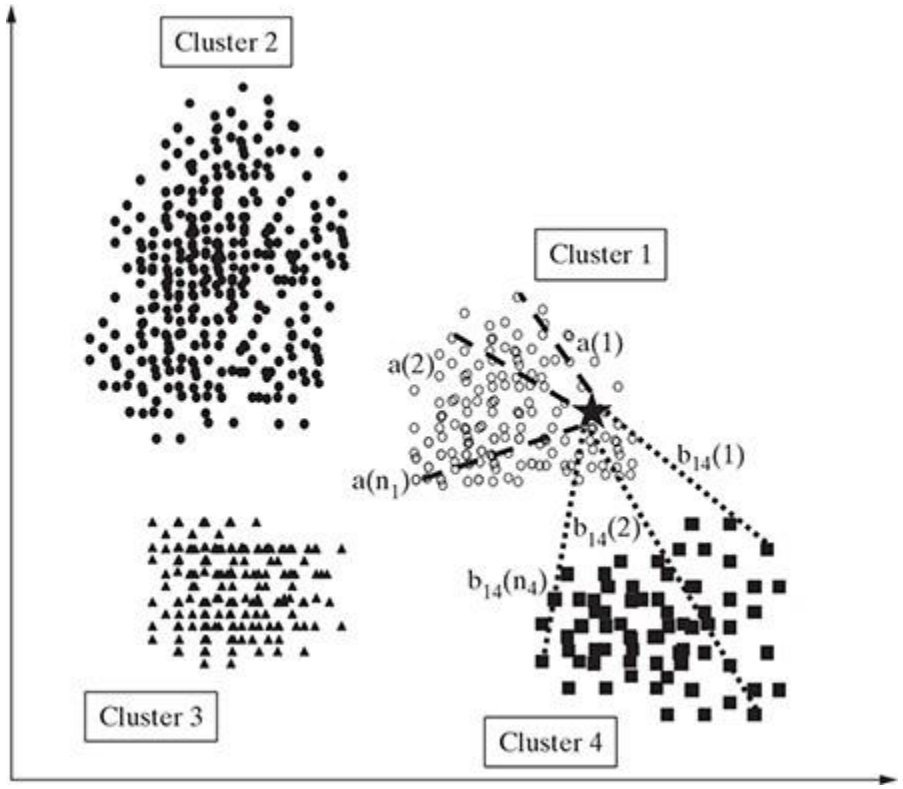


FIG. C.1O Silhouette width calculation

In the same way, let's calculate the distance of an arbitrary data element 'i' in cluster 1 with the different data elements from another cluster, say cluster 4and take an average of all those distances. Hence,

$$b_{14}(\text{average}) = \frac{b_{14}(1) + b_{14}(2) + \ldots + b_{14}(n_4)}{(n_4)}$$

where n_4 is the total number of elements in cluster 4. In the same way, we

can calculate the values of b_{12} (average) and b_{13} (average). b (i) is the

minimum of all these values. Hence, we can say that,

$$b(\text{i}) = \text{minimum } [b_{12}(\text{average}),\ b_{13}(\text{average}),\ b_{14}(\text{average})]$$

2. *External evaluation*

In this approach, class label is known for the data set subjected to clustering. However, quite obviously, the known class labels are not a part of the dataused in clustering. The cluster algorithm is assessed based on how close the

results are compared to those known class labels. For example, **purity** is one of the most popular measures of cluster algorithms – evaluates the extent to which clusters contain a single class.

For a data set having '*n*' data instances and '*c*' known class labels which generates '*k*' clusters, purity is measured as:

$$\text{Purity} = \frac{1}{n}\sum_{k}\max(k \cap c)$$

3.6 IMPROVING PERFORMANCE OF A MODEL

Now we have almost reached the end of the journey of building learning models. We have got some idea about whatmodelling is, how to approach about it to solve a learning problem and how to measure the success of our model. Nowcomes a million dollar question. Can we improve the performance of our model? If so, then what are the levers forimproving the performance? In fact, even before that comes the question of model selection – which model should be selected for which machine learning task? We have already discussed earlier that the model selection is done one severalaspects:

1. Type of learning the task in hand, i.e. supervised or unsupervised
2. Type of the data, i.e. categorical or numeric
3. Sometimes on the problem domain
4. Above all, experience in working with different models to solve problems of diverse domains

So, assuming that the model selection is done, what are thedifferent avenues to improve the performance of models?

One effective way to improve model performance is by tuning model parameter. **Model parameter tuning** is the process of adjusting the model fitting options. For example, inthe popular classification model *k*-Nearest Neighbour (*k*NN), using different values of '*k*' or the number of nearest neigh bours to be considered, the model can be tuned. In the same way, a number of hidden layers can be adjusted to tunethe performance in neural networks model. Most machine learning models have at least one parameter which can be tuned.

As an alternate approach of increasing the performance of one model, several models may be combined together. The models in such combination are complimentary to each other, i.e. one model may learn one type data sets well while strugglewith another type of data set. Another model may perform well with the data set which the first one struggled with. This approach of combining different models with diverse strengthsis known as **ensemble** (depicted in Figure 3.11). Ensemble helps in averaging out biases of the different underlying models and also reducing the variance. Ensemble methods combine weaker learners to create stronger ones. A performance boost can be expected even if models are built asusual and then ensembled.

Following are the typical steps in ensemble process:

- Build a number of models based on the training data
- For diversifying the models generated, the training data subset can be varied using the allocation function. Sampling techniques like bootstrapping may beused to generate unique training data sets.
- Alternatively, the same training data may be used but the models combinedare quite varying, e.g, SVM, neural network, *k*NN, etc.
- The outputs from the different models are combined using a combination function. A very simple strategy of combining, say in case of a prediction task using ensemble, can be majority voting of the different models combined. For example, 3 out of 5 classes predict 'win' and 2 predict 'loss' –then the final outcome of the ensemble using majority vote would be a 'win'.

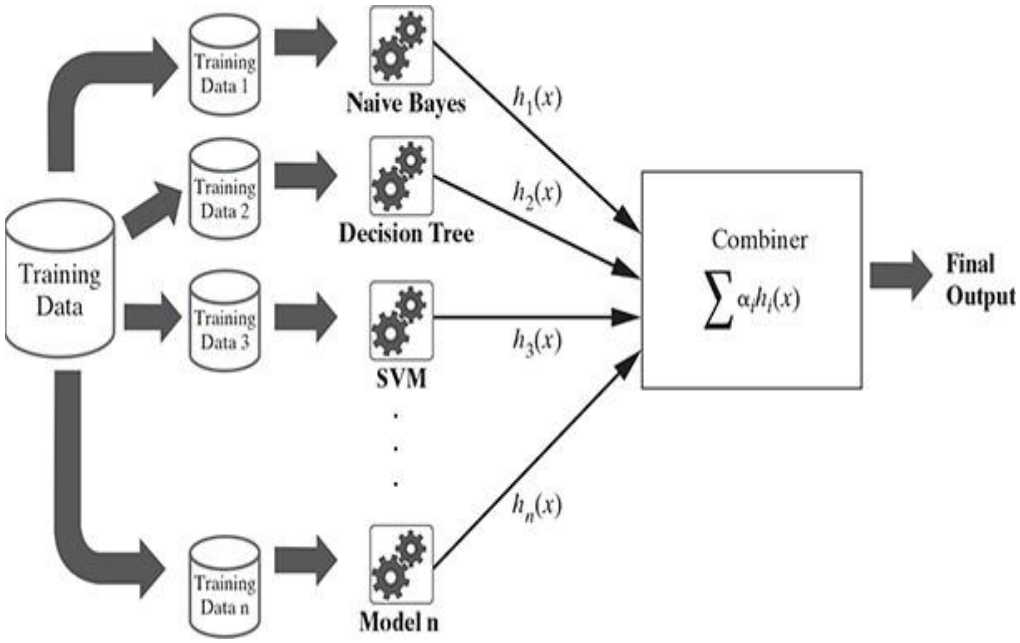


FIG. C.11 Ensemble

One of the earliest and most popular ensemble models is **bootstrap aggregating** or **bagging**. Bagging uses bootstrap sampling method (refer section 3.3.3) to generate multiple training data sets. These training data sets are used to generate(or train) a set of models using the same learning algorithm.
Then the outcomes of the models are combined by majority voting (classification) or by average (regression). Bagging is avery simple ensemble technique which can perform really wellfor unstable learners like a decision tree, in which a slight change in data can impact the outcome of a model significantly.

Just like bagging, **boosting** is another key ensemble-based technique. In this type of ensemble, weaker learning models are trained on resampled data and the outcomes are combined using a weighted voting approach based on the performance ofdifferent models. **Adaptive boosting** or **AdaBoost** is a special

variant of boosting algorithm. It is based on the idea ofgenerating weak learners and slowly learning

Random forest is another ensemble-based technique. It is an ensemble of decision trees – hence the name random forestto indicate a forest of decision trees. It has been discussed in more details in chapter 7.

In this chapter, you have been introduced to the crux of machine learning, i.e. modelling. Thorough understanding ofthe technical aspects elaborated in this chapter is extremely crucial for the success of any machine learning project.
For example, the first dilemma comes about which model to select. Again, in case of supervised learning, how can we deal with the unavailability of sufficient training data. In the same way, once the model is trained in case of supervised learning or the grouping is done in case of clustering, how we can understand whether the model training (for supervised) or grouping done (for unsupervised) is good or bad. All these andmore have been addressed as a part of this chapter.

Chapter 4

Basics of Feature Engineering

OBJECTIVE OF THE CHAPTER

In the last three chapters, you have been introduced to the basic concepts of machine learning. Also, the process to start modelling a problem has also been discussed in details. With this context in mind, in this chapter, we will introduce you to another very important aspect of machine learning, that is feature engineering. Though not a core part of the machine learning processes, feature engineering is a critical allied task that we need to perform to make learning more effective. It has three key components – feature construction, feature selection, and feature transformation, each of which will be covered in details in this chapter.

4.1 INTRODUCTION

In the last three chapters, we had a jumpstart to the machine learning process. We first started with what human learning isand how the different types of machine learning emulate the aspects of human learning. We had a detailed view of the

different types of problem that can be solved using machine learning techniques. Before applying machine learning to solve the problems, there are certain preparatory steps. These preparatory steps have been covered in details. After that, we have done a step-by-step navigation of the different activities of modelling a problem using machine learning. Modelling alone doesn't help us to realize the effectiveness of
machine learning as a problem- solving tool. So we also learnthow to measure the effectiveness of machine learning models in solving problems. In case a specific model is not effective, we can use different levers to boost the effectiveness. Those levers of boosting the model performance were also covered.

Now that we are ready (well almost ready!) to start solving problems using machine learning, we need to touch upon another key aspect which plays a critical role in solving any machine learning problem – feature engineering. Though feature engineering is a part of the preparatory activities whichhave already been covered in Chapter 2, the criticality and vastness of the area call for treating it separately. This area deals with features of the data set, which form an important input of any machine learning problem – be supervised or unsupervised learning. Feature engineering is a critical preparatory process in machine learning. It is responsible for taking raw input data and converting that to well-aligned features which are ready to be used by the machine learning models.

But before we start discussing feature engineering, let's tryto understand more clearly what feature is.

Unstructured data is raw, unorganized data which doesn't follow a specific format or hierarchy. Typical examples of unstructured data include text data from social networks, e.g. Twitter, Facebook, etc. or data from server logs, etc.

4.1.1 What is a feature?

A feature is an attribute of a data set that is used in a machinelearning process. There is a view amongst certain machine learning practitioners that only those attributes which are meaningful to a machine learning problem are to be called asfeatures, but this view has to be taken with a pinch of salt. In fact, selection of the subset of features which are meaningful for machine learning is a sub-area of feature engineering which draws a lot of research interest. The features in a data set are also called its dimensions. So a data set having '*n*' features is called an *n*-dimensional data set.

Let's take the example of a famous machine learning data set, Iris, introduced by the British statistician and biologist Ronald Fisher, partly shown in Figure 4.1. It has five attributesor features namely Sepal.Length, Sepal.Width, Petal.Length, Petal. Width and Species. Out of these, the feature 'Species' represent the class variable and the remaining features are the predictor variables. It is a five-dimensional data set.

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
6.7	3.3	5.7	2.5	Virginica
4.9	3	1.4	0.2	Setosa
5.5	2.6	4.4	1.2	Versicolor
6.8	3.2	5.9	2.3	Virginica
5.5	2.5	4	1.3	Versicolor
5.1	3.5	1.4	0.2	Setosa
6.1	3	4.6	1.4	versicolor

FIG. 4.1 Data set features

4.1.2 What is feature engineering?

Feature engineering refers to the process of translating a dataset into features such that these features are able to represent the data set more effectively and result in a better learning performance.

As we know already, feature engineering is an important pre-processing step for machine learning. It has two major elements:

1. feature transformation
2. feature subset selection

Feature transformation transforms the data – structured or unstructured, into a new set of features which can represent the underlying problem which machine learning is trying to solve. There are two variants of feature transformation:

1. feature construction
2. feature extraction

Both are sometimes known as feature discovery.

Feature construction process discovers missing information about the relationships between features and augments the feature space by creating additional features. Hence, if there are 'n' features or dimensions in a data set, after feature construction 'm' more features or dimensions may get added. So at the end, the data set will become '$n + m$' dimensional.

Feature extraction is the process of extracting or creating a new set of features from the original set of features using some functional mapping.

Unlike feature transformation, in case of **feature subset selection** (or simply **feature selection**) no new feature is generated. The objective of feature selection is to derive a subset of features from the full feature set which is most meaningful in the context of a specific machine learning problem. So, essentially the job of feature selection is to derive a subset F_j (F_1, F_2, …, F_m) of F_i (F_1, F_2, …, F_n), where $m < n$, such that F_j is most meaningful and gets the best result for a machine learning problem. We will discuss these concepts in detail in the next section.

4.2 FEATURE TRANSFORMATION

Engineering a good feature space is a crucial prerequisite for the success of any machine learning model. However, often it is not clear which feature is more important. For that reason, all available attributes of the data set are used as features and the problem of identifying the important features is left to the learning model. This is definitely not a feasible approach, particularly for certain domains e.g. medical image classification, text categorization, etc. In case a model has to be trained to classify a document as spam or non-spam, we canrepresent a document as a bag of words. Then the feature space will contain all unique words occurring across all documents. This will easily be a feature space of a few hundred thousand features. If we start including bigrams or trigrams along with words, the count of features will run in millions. To deal with this problem, feature transformation comes into play. Feature transformation is used as an effectivetool for dimensionality reduction and hence for boosting learning model performance. Broadly, there are two distinct goals of feature transformation:

- Achieving best reconstruction of the original features in the data setAchieving
- highest efficiency in the learning task

4.2.1 Feature construction

Feature construction involves transforming a given set of inputfeatures to generate a new set of more powerful features. To understand more clearly, let's take the example of a real estatedata set having details of all apartments sold in a specific region.

The data set has three features – apartment length, apartment breadth, and price of the apartment. If it is used as an input to a regression problem, such data can be training datafor the regression model. So given the training data, the model should be able to predict the price of an apartment whose priceis not known or which has just come up for sale. However, instead of using length and breadth of the apartment as a predictor, it is much convenient and makes more sense to use the area of the apartment, which is not an existing feature of the data set. So such a feature, namely apartment area, can be added to the data set. In other words, we transform the three- dimensional data set to a four-dimensional data set, with the newly 'discovered' feature apartment area being added to the original data set. This is depicted in Figure 4.2.

apartment_ length	apartment_ breadth	apartment_ price
80	59	23,60,000
54	45	12,15,000
78	56	21,84,000
63	63	19,84,000
83	74	30,71,000
92	86	39,56,000

apartment_ length	apartment_ breadth	apartment_ area	apartment_ price
80	59	4,720	23,60,000
54	45	2,430	12,15,000
78	56	4,368	21,84,000
63	63	3,969	19,84,500
83	74	6,142	30,71,000
92	86	7,912	39,56,000

FIG. 4.2 Feature construction (example 1)

Note: Though for the sake of simplicity the features apartment length and apartment breadth have been retained inFigure 4.2, in reality, it makes more sense to exclude these features when building the model.

There are certain situations where feature construction is an essential activity before we can start with the machine learningtask. These situations are

- when features have categorical value and machine learning needs numericvalue inputs
- when features having numeric (continuous) values and need to be convertedto ordinal values
- when text-specific feature construction needs to be done

4.2.1.1 *Encoding categorical (nominal) variables*

Let's take the example of another data set on athletes, as presented in Figure 4.3a. Say the data set has features age, cityof origin, parents athlete (i.e. indicate whether any one of the parents was an athlete) and Chance of Win. The feature chanceof a win is a class variable while the others are predictor variables. We know that any machine learning algorithm, whether it's a classification algorithm (like *k*NN) or a regression algorithm, requires numerical figures to learn from.So there are three features – City of origin, Parents athlete, and

Chance of win, which are categorical in nature and cannot beused by any machine learning task.

In this case, feature construction can be used to create new dummy features which are usable by machine learning algorithms. Since the feature 'City of origin' has three unique values namely City A, City B, and City C, three dummy features namely origin_ city_A, origin_city_B, and origin_city_C is created. In the same way, dummy features parents_athlete_Y and parents_athlete_N are created for feature 'Parents athlete' and win_chance_Y and win_chance_N are created for feature 'Chance of win'. The dummy features have value 0 or 1 based on the categorical value for the original feature in that row. For example, the second row had a categorical value 'City B' for the feature 'City of origin'. So, the newly created features in place of 'City of origin', i.e. origin_city_A, origin_city_B and origin_city_C will have values 0, 1 and 0, respectively. In thesame way, parents_athlete_Y and parents_athlete_N will havevalues 0 and 1, respectively in row 2 as the original feature 'Parents athlete' had a categorical value 'No' in row 2. The entire set of transformation for athletes' data set is shown in Figure 4.3b.

Age (Years)	City of origin	Parents athlete	Chance of win
18	City A	Yes	Y
20	City B	No	Y
23	City B	Yes	Y
19	City A	No	N
18	City C	Yes	N
22	City B	Yes	Y

(a)

Age (Years)	origin_ city_A	origin_ city_B	origin_ city_C	parents_ athlete_Y	parents_ athlete_N	win_ chance_Y	win_ chance_N
18	1	0	0	1	0	1	0
20	0	1	0	0	1	1	0
23	0	1	0	1	0	1	0
19	1	0	0	0	1	0	1
18	0	0	1	1	0	0	1
22	0	1	0	1	0	1	0

(b)

Age (Years)	origin_city_A	origin_city_B	origin_city_C	parents_athlete_Y	win_chance_Y
18	1	0	0	1	1
20	0	1	0	0	1
23	0	1	0	1	1
19	1	0	0	0	0
18	0	0	1	1	0
22	0	1	0	1	1

(c)

FIG. 4.C Feature construction (encoding nominal variables)

However, examining closely, we see that the features ‘Parents athlete’ and ‘Chance of win’ in the original data set can have two values only. So creating two features from them is a kind of duplication, since the value of one feature can be decided from the value of the other. To avoid this duplication, we can just leave one feature and eliminate the other, as shownin Figure 4.3c.

4.2.1.2 *Encoding categorical (ordinal) variables*

Let's take an example of a student data set. Let's assume thatthere are three variable – science marks, maths marks and grade as shown in Figure 4.4a. As we can see, the grade is anordinal variable with values A, B, C, and D. To transform thisvariable to a numeric variable, we can create a feature num_grade mapping a numeric value against each ordinal value. In the context of the current example, grades A, B, C, and D in Figure 4.4a is mapped to values 1, 2, 3, and 4 in the transformed variable shown in Figure 4.4b.

marks_science	marks_maths	Grade
78	75	B
56	62	C
87	90	A
91	95	A
45	42	D
62	57	B

(a)

marks_science	marks_maths	num_grade
78	75	2
56	62	3
87	90	1
91	95	1
45	42	4
62	57	2

(b)

FIG. 4.4 Feature construction (encoding ordinal variables)

4.2.1.3 *Transforming numeric (continuous) features tocategorical features*

Sometimes there is a need of transforming a continuous numerical variable into a categorical variable. For example, wemay want to treat the real estate price prediction problem, which is a regression problem, as a real estate price category prediction, which is a classification problem. In that case, we can 'bin' the numerical data into multiple categories based on the data range. In the context of the real estate price prediction example, the original data set has a numerical feature apartment_price as shown in Figure 4.5a. It can be

transformed to a categorical variable price-grade either asshown in Figure 4.5b or as shown in Figure 4.5c.

4.2.1.4 *Text-specific feature construction*

In the current world, text is arguably the most predominant medium of communication. Whether we think about social networks like Facebook or micro-blogging channels like Twitter or emails or short messaging services such as Whatsapp, text plays a major role in the flow of information. Hence, text mining is an important area of research – not only for technology practitioners but also for industry practitioners. However, making sense of text data, due to the inherent unstructured nature of the data, is not so straightforward. In thefirst place, the text data chunks that we can think about do not have readily available features, like structured data sets, on which machine learning tasks can be executed. All machine learning models need numerical data as input. So the text data in the data sets need to be transformed into numerical features.

apartment_ area	apartment_ price
4,720	23,60,000
2,430	12,15,000
4,368	21,84,000
3,969	19,84,500
6,142	30,71,000
7,912	39,56,000

(a)

apartment_ area	apartment_ grade
4,720	Medium
2,430	Low
4,368	Medium
3,969	Low
6,142	High
7,912	High

(b)

apartment_ area	apartment_ grade
4,720	2
2,430	1
4,368	2
3,969	1
6,142	3
7,912	3

(c)

FIG. 4.5 Feature construction (numeric to categorical)

Text data, or corpus which is the more popular keyword, is converted to a numerical representation following a process isknown as vectorization. In this process, word occurrences in all documents belonging to the corpus are consolidated in the form of bag-of-words. There are three major steps that are followed:

1. tokenize
2. count
3. normalize

In order to tokenize a corpus, the blank spaces and punctuations are used as delimiters to separate out the words,or tokens. Then the number of occurrences of each token is counted, for each document. Lastly, tokens are weighted with

reducing importance when they occur in the majority of the documents. A matrix is then formed with each token representing a column and a specific document of the corpus representing each row. Each cell contains the count of occurrence of the token in a specific document. This matrix isknown as a document-term matrix (also known as a term- document matrix). Figure 4.6 represents a typical document- term matrix which forms an input to a machine learning model.

This	House	Build	Feeling	Well	Theatre	Movie	Good	Lonely	...
2	1	1	0	0	1	1	1	0	
0	0	0	1	1	0	0	0	0	
1	0	0	2	1	1	0	0	1	
0	0	0	0	1	0	1	1	0	
.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	
.	.	.	.	.	.	.	.	.	

FIG. 4.6 Feature construction (text-specific)

4.2.2 Feature extraction

In feature extraction, new features are created from a combination of original features. Some of the commonly usedoperators for combining the original features include

1. For Boolean features: Conjunctions, Disjunctions, Negation, etc.
2. For nominal features: Cartesian product, M of N, etc.
3. For numerical features: Min, Max, Addition, Subtraction, Multiplication, Division, Average, Equivalence, Inequality, etc.

Let's take an example and try to understand. Say, we have adata set with a feature set F_i (F_1, F_2, …, F_n). After feature extraction using a mapping function f (F_1, F_2, …, F_n) say, we

will have a set of features $\acute{F}_i(\acute{F}_1, \acute{F}_2, \ldots, \acute{F}_m)$ such that $\acute{F}_i = f(F_i)$

and $m < n$. For example, $\acute{F}_1 = k_1F_1 + k_2F_2$. This is depicted inFigure 4.7.

$Feat_A$	$Feat_B$	$Feat_C$	$Feat_D$
34	34.5	23	233
44	45.56	11	3.44
78	22.59	21	4.5
22	65.22	11	322.3
22	33.8	355	45.2
11	122.32	63	23.2

→

$Feat_1$	$Feat_2$
41.25	185.80
54.20	53.12
43.73	35.79
65.30	264.10
37.02	238.42
113.39	167.74

$$Feat_1 = 0.3 \times Feat_A + 0.9 \times Feat_A$$
$$Feat_2 = Feat_A + 0.5\ Feat_B + 0.6 \times Feat_C$$

FIG. 4.7 Feature extraction

Let's discuss the most popular feature extraction algorithmsused in machine learning:

4.2.2.1 *Principal Component Analysis*

Every data set, as we have seen, has multiple attributes or dimensions – many of which might have similarity with each other. For example, the height and weight of a person, in general, are quite related. If the height is more, generally weight is more and vice versa. So if a data set has height and weight as two of the attributes, obviously they are expected tobe having quite a bit of similarity. In general, any machine learning algorithm performs better as the number of related attributes or features reduced. In other words, a key to the

success of machine learning lies in the fact that the features areless in number as well as the similarity between each other is very less. This is the main guiding philosophy of principal component analysis (PCA) technique of feature extraction.

In PCA, a new set of features are extracted from the originalfeatures which are quite dissimilar in nature. So an *n*- dimensional feature space gets transformed to an *m*- dimensional feature space, where the dimensions are orthogonal to each other, i.e. completely independent of each other. To understand the concept of orthogonality, we have to step back and do a bit of dip dive into vector space concept in linear algebra.

We all know that a vector is a quantity having both magnitude and direction and hence can determine the position of a point relative to another point in the Euclidean space (i.e. a two or three or 'n' dimensional space). A vector space is a set of vectors. Vector spaces have a property that they can be represented as a linear combination of a smaller set of vectors,called basis vectors. So, any vector 'v' in a vector space can berepresented as

$$v = \sum_{i=1}^{n} a_i u_i$$

where, a_i represents '*n*' scalars and u_i represents the basisvectors. Basis vectors are orthogonal to each other.
Orthogonality of vectors in *n*-dimensional vector space can bethought of an extension of the vectors being perpendicular in atwo-dimensional vector space. Two orthogonal vectors are completely unrelated or independent of each other. So the transformation of a set of vectors to the corresponding set of basis vectors such that each vector in the original set can beexpressed as a linear combination of basis vectors helps in decomposing the vectors to a number of independent components.

Now, let's extend this notion to the feature space of a data set. The feature vector can be transformed to a vector space ofthe basis vectors which are termed as principal components.
These principal components, just like the basis vectors, are orthogonal to each other. So a set of feature vectors which mayhave similarity with each other is transformed to a set of principal components which are completely unrelated.
However, the principal components capture the variability ofthe original feature space. Also, the number of principal component derived, much like the basis vectors, is much smaller than the original set of features.

The objective of PCA is to make the transformation in sucha way that

1. The new features are distinct, i.e. the covariance between the newfeatures, i.e. the principal components is 0.
2. The principal components are generated in order of the variability in thedata that it captures. Hence, the first principal component should capture the maximum

variability, the second principal component should capture the next highest variability etc.

3. The sum of variance of the new features or the principal componentsshould be equal to the sum of variance of the original features.

PCA works based on a process called eigenvalue decomposition of a covariance matrix of a data set. Below arethe steps to be followed:

1. First, calculate the covariance matrix of a data set.
2. Then, calculate the eigenvalues of the covariance matrix.
3. The eigenvector having highest eigenvalue represents the direction in which there is the highest variance. So this will help in identifying the first principal component.
4. The eigenvector having the next highest eigenvalue represents the direction in which data has the highest remaining variance and also orthogonal to the first direction. So this helps in identifying the secondprincipal component.
5. Like this, identify the top '*k*' eigenvectors having top '*k*' eigenvalues soas to get the '*k*' principal components.

4.2.2.2 *Singular value decomposition*

Singular value decomposition (SVD) is a matrix factorizationtechnique commonly used in linear algebra. SVD of a matrixA ($m \times n$) is a factorization of the form:

$$A = U \sum V$$

where, U and V are orthonormal matrices, U is an $m \times m$ unitary matrix, V is an $n \times n$ unitary matrix and Σ is an $m \times n$rectangular diagonal matrix. The diagonal entries of Σ are known as singular values of matrix A. The columns of U and$V$ are called the left-singular and right-singular vectors of matrix A, respectively.

SVD is generally used in PCA, once the mean of each variable has been removed. Since it is not always advisable toremove the mean of a data attribute, especially when the data set is sparse (as in case of text data), SVD is a good choice fordimensionality reduction in those situations.

SVD of a data matrix is expected to have the propertieshighlighted below:

1. Patterns in the attributes are captured by the right-singular vectors, i.e.the columns of *V*.
2. Patterns among the instances are captured by the left-singular, i.e. thecolumns of *U*.

3. Larger a singular value, larger is the part of the matrix A that it accountsfor and its associated vectors.
4. New data matrix with '*k*' attributes is obtained using the equation

$$D' = D \times [v_1, v_2, \ldots, v_k]$$

Thus, the dimensionality gets reduced to *k*
SVD is often used in the context of text data.

4.2.2.3 *Linear Discriminant Analysis*

Linear discriminant analysis (LDA) is another commonly usedfeature extraction technique like PCA or SVD. The objective of LDA is similar to the sense that it intends to transform a data set into a lower dimensional feature space. However, unlike PCA, the focus of LDA is not to capture the data set variability. Instead, LDA focuses on class separability, i.e. separating the features based on class separability so as to avoid over-fitting of the machine learning model.

Unlike PCA that calculates eigenvalues of the covariancematrix of the data set, LDA calculates eigenvalues and eigenvectors within a class and inter-class scatter matrices. Below are the steps to be followed:

1. Calculate the mean vectors for the individual classes.
2. Calculate intra-class and inter-class scatter matrices.
3. Calculate eigenvalues and eigenvectors for S_W^{-1} and S_B, where S_W is the intra-class scatter matrix and S_B is the inter-class scatter matrix

$$S_W = \sum_{i=1}^{c} S_i;$$

$$S_i = \sum_{x \in D_i}^{n} (x - m_i)(x - m_i)^T$$

where, m_i is the mean vector of the *i*-th class

$$S_B = \sum_{i=1}^{c} N_i (m_i - m)(m_i - m)^T$$

where, mi is the sample mean for each class, m is the overall mean ofthe data set, *Ni* is the sample size of each class

4. Identify the top '*k*' eigenvectors having top '*k*' eigenvalues

4.3 FEATURE SUBSET SELECTION

Feature selection is arguably the most critical pre-processing activity in any machine learning project. It intends to select a subset of system attributes or features which makes a most meaningful contribution in a machine learning activity. Let's quickly discuss a practical example to understand the philosophy behind feature selection. Say we are trying to predict the weight of students based on past information aboutsimilar students, which is captured in a 'student weight' data set. The student weight data set has features such as Roll Number, Age, Height, and Weight. We can well understand that roll number can have no bearing, whatsoever, in predicting student weight. So we can eliminate the feature rollnumber and build a feature subset to be considered in this machine learning problem. The subset of features is expected to give better results than the full set. The same has been **depicted i**n Figure 4.8.

Roll Number	Age	Height	Weight
12	12	1.1	23
14	11	1.05	21.6
19	13	1.2	24.7
32	11	1.07	21.3
38	14	1.24	25.2
45	12	1.12	23.4

→

Age	Height	Weight
12	1.1	23
11	1.05	21.6
13	1.2	24.7
11	1.07	21.3
14	1.24	25.2
12	1.12	23.4

FIG. 4.8 Feature selection

But before we go forward with more detailed discussion onfeature selection, let's try to understand the issues which have

made feature selection such a relevant problem to be solved.

4.3.1 Issues in high-dimensional data

With the rapid innovations in the digital space, the volume ofdata generated has increased to an unbelievable extent. At thesame time, breakthroughs in the storage technology area have made storage of large quantity of data quite cheap. This has further motivated the storage and mining of very large and high-dimensionality data sets.

Alongside, two new application domains have seen drastic development. One is that of biomedical research, which includes gene selection from microarray data. The other one istext categorization which deals with huge volumes of text datafrom social networking sites, emails, etc. The first domain, i.e.biomedical research generates data sets having a number of features in the range of a few tens of thousands. The text data generated from different sources also have extremely high dimensions. In a large document corpus having few thousand documents embedded, the number of unique word tokens

which represent the feature of the text data set, can also be in the range of a few tens of thousands. To get insight from such high-dimensional data may be a big challenge for any machinelearning algorithm. On one hand, very high quantity of computational resources and high amount of time will be required. On the other hand the performance of the model – both for supervised and unsupervised machine learning task, also degrades sharply due to unnecessary noise in the data.
Also, a model built on an extremely high number of features may be very difficult to understand. For this reason, it is necessary to take a subset of the features instead of the full set.

The objective of feature selection is three-fold:

- Having faster and more cost-effective (i.e. less need for computationalresources) learning model
- Improving the efficiency of the learning model
- Having a better understanding of the underlying model that generated thedata

4.3.2 Key drivers of feature selection – feature relevanceand redundancy

4.3.2.1 Feature relevance

In supervised learning, the input data set which is the training data set, has a class label attached. A model is inducted based on the training data set – so that the inducted model can assignclass labels to new, unlabelled data. Each of the predictor variables, is expected to contribute information to decide the value of the class label. In case a variable is not contributing any information, it is said to be irrelevant. In case the information contribution for prediction is very little, the variable is said to be weakly relevant. Remaining variables, which make a significant contribution to the prediction task are said to be strongly relevant variables.

In unsupervised learning, there is no training data set or labelled data. Grouping of similar data instances are done and similarity of data instances are evaluated based on the value of different variables. Certain variables do not contribute any useful information for deciding the similarity of dissimilarity of data instances. Hence, those variables make no significant information contribution in the grouping process. These variables are marked as irrelevant variables in the context of the unsupervised machine learning task.

To get a perspective, we can think of the simple example ofthe student data set that we discussed at the beginning of this section. Roll number of a student doesn't contribute any significant information in predicting what the Weight of a student would be. Similarly, if we are trying to group togetherstudents with similar academic capabilities, Roll number can really not contribute any information whatsoever. So, in context of the supervised task of predicting student Weight orthe unsupervised task of grouping students with similar academic merit, the variable Roll number is quite irrelevant.

Any feature which is irrelevant in the context of a machine learning task is a candidate for rejection when we are selectinga subset of features. We can consider whether the weakly relevant features are to be rejected or not on a case-to-case basis.

4.3.2.2 Feature redundancy

A feature may contribute information which is similar to theinformation contributed by one or more other features. For example, in the weight prediction problem referred earlier inthe section, both the features Age and Height contribute similar information. This is because with an increase in Age,

Weight is expected to increase. Similarly, with the increase of Height also Weight is expected to increase. Also, Age and Height increase with each other. So, in context of the Weight prediction problem, Age and Height contribute similar information. In other words, irrespective of whether the featureheight is present as a part of the feature subset, the learning model will give almost same results. In the same way, without age being part of the predictor variables, the outcome of the learning model will be more or less same. In this kind of a situation when one feature is similar to another feature, the feature is said to be potentially redundant in the context of the learning problem.

All features having potential redundancy are candidates forrejection in the final feature subset. Only a small number of representative features out of a set of potentially redundant features are considered for being a part of the final feature subset.

So, in a nutshell, the main objective of feature selection is toremove all features which are irrelevant and take a representative subset of the features which are potentially redundant. This leads to a meaningful feature subset in contextof a specific learning task.

Now, the question is how to find out which of the features are irrelevant or which features have potential redundancy. Forthat multiple measures are being used, some of which have been covered in the next sub-section.

4.3.3 Measures of feature relevance and redundancy

4.3.3.1 Measures of feature relevance

As mentioned earlier, feature relevance is to be gauged by the amount of information contributed by a feature. For supervisedlearning, mutual information is considered as a good measure of information contribution of a feature to decide the value of the class label. That's why it is a good indicator of the relevance of a feature with respect to the class variable. Higher the value of mutual information of a feature, more relevant is that feature. Mutual information can be calculated as follows:

$$MI(C, f) = H(C) + H(f) - H(C, f)$$

where, marginal entropy of the class, H(C) =

$$-\sum_{i=1}^{k} p(C_i) \log_2 p(C_i)$$

marginal entropy of the feature '*x*', $H(f)$ =

$$-\sum_{c} p(f = x) \log_2 p(f = x)$$

and K = number of classes, C = class variable, f = feature setthat take discrete values.

In case of unsupervised learning, there is no class variable. Hence, feature-to-class mutual information cannot be used to measure the information contribution of the features. In case of unsupervised learning, the entropy of the set of features without one feature at a time is

calculated for all the features.

Then, the features are ranked in a descending order of

information gain from a feature and top ‘β’ percentage (valueof ‘β’ is a design parameter of the algorithm) of features are selected as relevant features. The entropy of a feature f is calculated using Shannon’s formula below:

$$H(f) = -\sum_x p(f = x)\log_2 p(f = x)$$

$\sum_x$ is used only for features that take discrete values. For

continuous features, it should be replaced by discretization performed first to estimate probabilities $p(f = x)$.

4.3.3.2 *Measures of Feature redundancy*

Feature redundancy, as we have already discussed, is based onsimilar information contribution by multiple features. There are multiple measures of similarity of information contribution, salient ones being

1. Correlation-based measures
2. Distance-based measures, and
3. Other coefficient-based measure

1. Correlation-based similarity measure

Correlation is a measure of linear dependency between two random variables. Pearson’s product moment correlation coefficient is one of the most popular and accepted measures of correlation between two random variables. For two randomfeature variables F_1 and F_2, Pearson correlation coefficient is defined as:

$$\alpha = \frac{cov(F_1, F_2)}{\sqrt{var(F_1).var(F_2)}}$$

$$cov(F_1, F_2) = \sum (F_{1_i} - \overline{F_1}).(F_{2_i} - \overline{F_2})$$

$$var(F_1) = \sum (F_{1_i} - \overline{F_1})^2, \text{where } \overline{F_1} = \frac{1}{n}.\sum F_{1_i}$$

$$var(F_2) = \sum (F_{2_i} - \overline{F_2})^2, \text{where } \overline{F_2} = \frac{1}{n}.\sum F_{2_i}$$

Correlation values range between +1 and –1. A correlation of 1 (+ / –) indicates perfect correlation, i.e. the two features having a perfect linear relationship. In case the correlation is 0, then the features seem to have no linear relationship.
Generally, for all feature selection problems, a threshold valueis adopted to decide whether two features have adequate similarity or not.

2. Distance-based similarity measure

The most common distance measure is the **Euclideandistance**, which, between two features F_1 and F_2 are calculated as:

$$d(F_1, F_2) = \sqrt{\sum_{i=1}^{n} (F_{1_i} - F_{2_i})^2}$$

where F_1 and F_2 are features of an n-dimensional data set. Refer to the Figure 4.9. The data set has two features, aptitude(F_1) and communication (F_2) under consideration. The Euclidean distance between the features has been calculated using the formula provided above.

Aptitude (F_1)	Communication (F_2)	(F_1 – F_2)	(F_1 – F_2)^2
2	6	–4	16
3	5.5	–2.5	6.25
6	4	2	4
7	2.5	4.5	20.25
8	3	5	25
6	5.5	0.5	0.25
6	7	–1	1
7	6	1	1
8	6	2	4
9	7	2	4
			81.75

FIG. 4.9 Distance calculation between features

A more generalized form of the Euclidean distance is the **Minkowski distance**, measured as

$$d(F_1, F_2) = \sqrt{\sum_{i=1}^{n} (F_{1_i} - F_{2_i})^r}$$

Minkowski distance takes the form of Euclidean distance(also called $\mathbf{L_2}$ **norm**) when $r = 2$.

At $r = 1$, it takes the form of **Manhattan distance** (alsocalled $\mathbf{L_1}$ **norm**), as shown below:

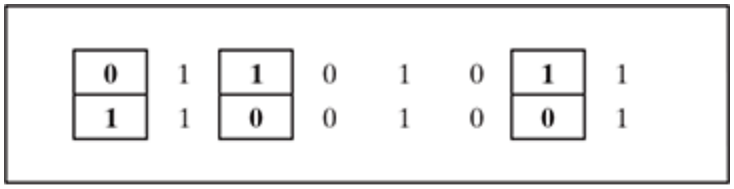
$$d(F_1, F_2) = \sum_{i=1}^{n} |F_{1_i} - F_{2_i}|$$

A specific example of Manhattan distance, used more frequently to calculate the distance

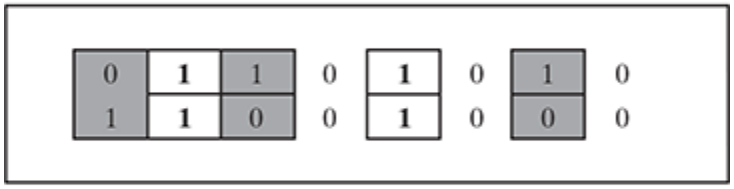
between binary vectors isthe **Hamming distance**. For example, the Hamming distance between two vectors 01101011 and 11001001 is 3, asillustrated in Figure 4.10a.

3. Other similarity measures

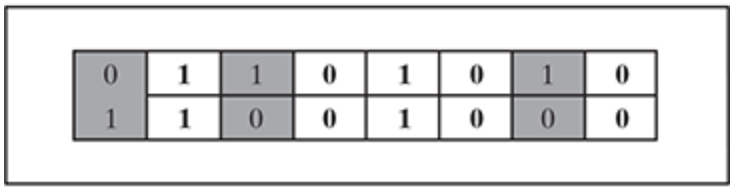
Jaccard index/coefficient is used as a measure of similaritybetween two features. The **Jaccard distance**, a measure of dissimilarity between two features, is complementary of Jaccard index.



(a) Hamming distance measurement



(b) Jaccard coefficient measurement



(c) SMC measurement

FIG. 4.1O Distance measures between features

For two features having binary values, Jaccard index ismeasured as

$$J = \frac{n_{11}}{n_{01} + n_{10} + n_{11}}$$

where, n_{11} = number of cases where both the features havevalue 1

n_{01} = number of cases where the feature 1 has value 0 andfeature 2 has value 1

n_{10} = number of cases where the feature 1 has value 1 andfeature 2 has value 0

Jaccard distance, $d_J = 1 - J$

Let's consider two features F_1 and F_2 having values (0, 1, 1,0, 1, 0, 1, 0) and (1, 1, 0, 0, 1, 0, 0, 0). Figure 4.10b shows the identification of the values of n_{11}, n_{01} and n_{10}. As shown, the cases where both the values are 0 have been left out without border – as an indication of the fact that they will be excluded in the calculation of Jaccard coefficient.

Jaccard coefficient of F_1 and F_2, J =

$$\frac{n_{11}}{n_{01} + n_{10} + n_{11}} = \frac{2}{1 + 2 + 2} = \frac{2}{5} \text{ or } 0.4.$$

$\therefore$ Jaccard distance between F_1 and F_2, $d_J = 1 - J = \frac{1}{2}$ or 0.6.

Simple matching coefficient (SMC) is almost same as Jaccard coeficient except the fact that it includes a number ofcases where both the features have a value of 0.

$$SMC = \frac{n_{11} + n_{00}}{n_{00} + n_{01} + n_{10} + n_{11}}$$

where, n_{11} = number of cases where both the features havevalue 1

n_{01} = number of cases where the feature 1 has value 0 andfeature 2 has value 1

n_{10} = number of cases where the feature 1 has value 1 andfeature 2 has value 0

n_{00} = number of cases where both the features have value 0 Quite understandably, the total

count of rows, $n = n_{00} + n_{01}$

$+ n_{10} + n_{11}$. As shown in Figure 4.10c, all values have been included in the calculation of SMC.

$$\therefore \text{SMC of } F_1 \text{ and } F_2 = \frac{n_{11} + n_{00}}{n_{00} + n_{01} + n_{10} + n_{11}} = \frac{2 + 3}{3 + 1 + 2 + 2} = \frac{1}{2} \text{ or } 0.5.$$

One more measure of similarity using similarity coefficient calculation is **Cosine Similarity**. Let's take the example of a typical text classification problem. The text corpus needs to befirst transformed into features with a word token being a feature and the number of times the word occurs in a document comes as a value in each row. There are thousands of features in such a text data set. However, the data set is sparse in nature as only a few words do appear in a document,and hence in a row of the data set. So each row has very few non-zero

values. However, the non-zero values can be anything integer value as the same word may occur any number of times. Also, considering the sparsity of the data set,the 0-0 matches (which obviously is going to be pretty high) need to be ignored. Cosine similarity which is one of the mostpopular measures in text classification is calculated as:

$$cos\,(x,\ y) = \frac{x.y}{\|x\|.\|y\|}$$

where, $x.y$ = vector dot product of x and y = $\sum_{i=1}^{n} x_i y_i$

$$\|x\| = \sqrt{\sum_{i=1}^{n} x_i^2} \text{ and } \|y\| = \sqrt{\sum_{i=1}^{n} y_i^2}$$

Let's calculate the cosine similarity of x and y, where x = (2,4, 0, 0, 2, 1, 3, 0, 0) and y = (2, 1, 0, 0, 3, 2, 1, 0, 1).

In this case, $x.y$ = 2*2 + 4*1 + 0*0 + 0*0 + 2*3 + 1*2 + 3*1 +0*0 + 0*1 = 19

$$\|x\| = \sqrt{2^2 + 4^2 + 0^2 + 0^2 + 2^2 + 1^2 + 3^2 + 0^2 + 0^2} = \sqrt{34} = 5.83$$

$$\|y\| = \sqrt{2^2 + 1^2 + 0^2 + 0^2 + 3^2 + 2^2 + 1^2 + 0^2 + 1^2} = \sqrt{20} = 4.47$$

$$\therefore cos\,(x, y) = \frac{19}{5.83*4.47} = 0.729$$

Cosine similarity actually measures the angle (refer to Fig. 4.11) between x and y vectors. Hence, if cosine similarity has avalue 1, the angle between x and y is 0° which means x and y are same except for the magnitude. If cosine similarity is 0, theangle between x and y is 90°. Hence, they do not share any similarity (in case of text data, no term/word is common). In the above example, the angle comes to be 43.2°.

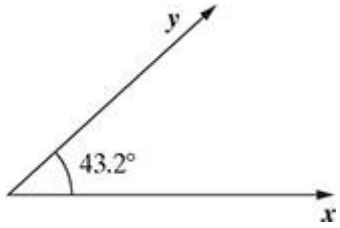


FIG. 4.11 Cosine similarity

4.3.4 Overall feature selection process

Feature selection is the process of selecting a subset of featuresin a data set. As depicted in Figure 4.12, a typical feature selection process consists of four steps:

1. generation of possible subsets
2. subset evaluation
3. stop searching based on some stopping criterion
4. validation of the result

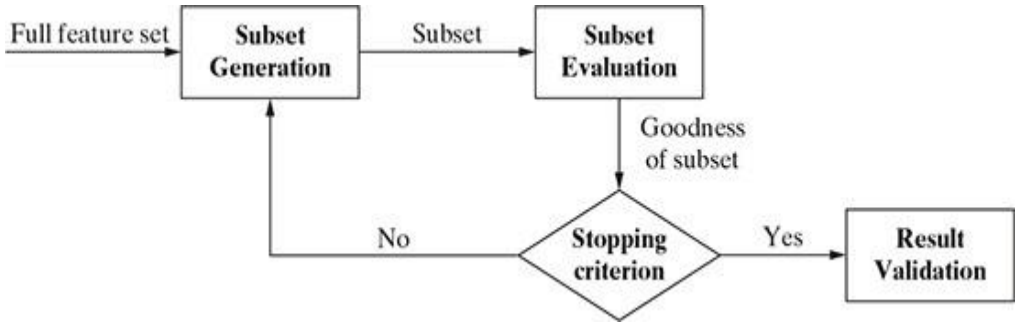


FIG. 4.12 Feature selection process

Subset generation, which is the first step of any feature selection algorithm, is a search procedure which ideally shouldproduce all possible candidate subsets. However, for an *n*-dimensional data set, 2^n subsets can be generated. So, as the value of '*n*' becomes high, finding an optimal subset from all the 2^n candidate subsets becomes intractable. For that reason,

different approximate search strategies are employed to find candidate subsets for evaluation. On one hand, the search maystart with an empty set and keep adding features. This search strategy is termed as a sequential forward selection. On the other hand, a search may start with a full set and successively remove features. This strategy is termed as sequential backward elimination. In certain cases, search start with both ends and add and remove features simultaneously. This strategy is termed as a bi-directional selection.

Each candidate subset is then evaluated and compared withthe previous best performing subset based on certain **evaluation criterion**. If the new subset performs better, it replaces the previous one.

This cycle of subset generation and evaluation continues till a pre-defined **stopping criterion** is fulfilled. Some commonlyused stopping criteria are

1. the search completes
2. some given bound (e.g. a specified number of iterations) is reached
3. subsequent addition (or deletion) of the feature is not producing a bettersubset
4. a sufficiently good subset (e.g. a subset having better classification accuracy than the existing benchmark) is selected

Then the selected best subset is **validated** either against prior benchmarks or by experiments using real-life or syntheticbut authentic data sets. In case of supervised learning, the accuracy of the learning model may be the performance parameter considered for validation. The accuracy of the model using the subset derived is compared against the model accuracy of the subset derived using some other benchmark algorithm. In case of unsupervised, the cluster quality may be the parameter for validation.

4.3.5 Feature selection approaches

There are four types of approach for feature selection:

1. Filter approach
2. Wrapper approach
3. Hybrid approach
4. Embedded approach

In the **filter approach** (as depicted in Fig. 4.13), the featuresubset is selected based on statistical measures done to assess the merits of the features from the data perspective. No learning algorithm is employed to evaluate the goodness of thefeature selected. Some of the common statistical tests conducted on features as a part of filter approach are – Pearson's correlation, information gain, Fisher score, analysis of variance (ANOVA), Chi-Square, etc.

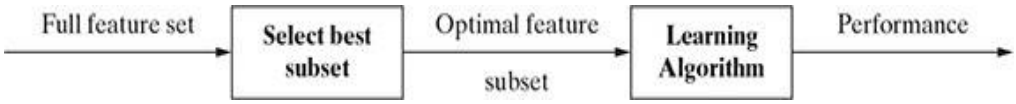


FIG. 4.1C Filter approach

In the **wrapper approach** (as depicted in Fig. 4.14), identification of best feature subset is done using the inductionalgorithm as a black box. The feature selection algorithm searches for a good feature subset using the induction algorithm itself as a part of the evaluation function. Since for every candidate subset, the learning model is trained and the result is evaluated by running the learning algorithm, wrapper approach is computationally very expensive. However, the performance is generally superior compared to filter approach.

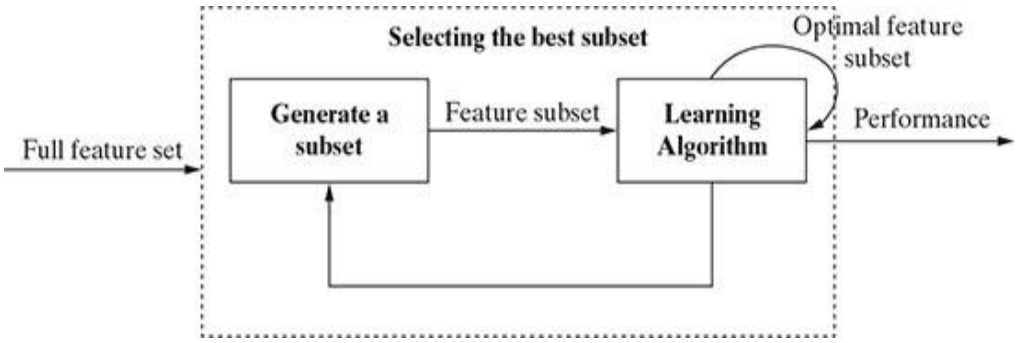


FIG. 4.14 Wrapper approach

Hybrid approach takes the advantage of both filter and wrapper approaches. A typical hybrid algorithm makes use of both the statistical tests as used in filter approach to decide the best subsets for a given cardinality and a learning algorithm toselect the final best subset among the best subsets across different cardinalities.

Embedded approach (as depicted in Fig. 4.15) is quite similar to wrapper approach as it also uses and inductive algorithm to evaluate the generated feature subsets. However, the difference is it performs feature selection and classificationsimultaneously.

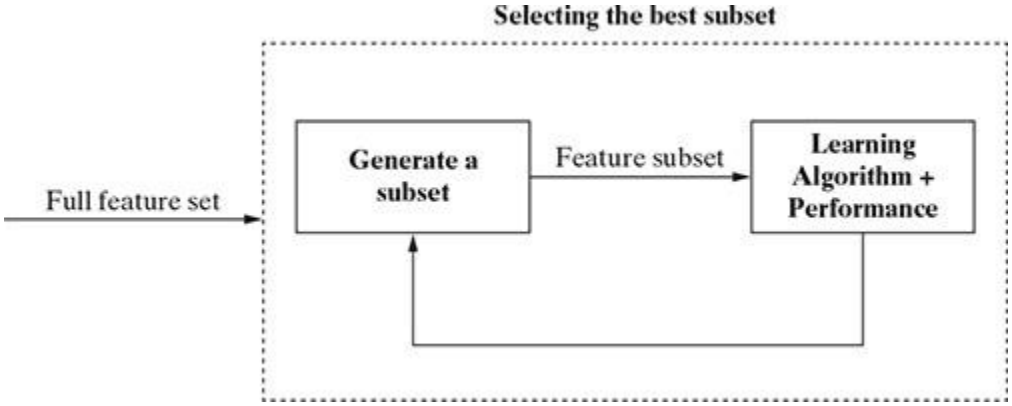


FIG. 4.15 Embedded approach

UNIT-III

Bayesian Concept Learning

INTRODUCTION

In the last chapter, we discussed the rules of probability and possible uses of probability, distribution functions, and hypothesis testing principles in the machine learning domain.In this chapter, we will discuss the details of the Bayesian theorem and how it provides the basis for machine learning

concepts. The technique was derived from the work of the 18th century mathematician Thomas Bayes. He developed the foundational mathematical principles, known as Bayesian methods, which describe the probability of events, and more importantly, how probabilities should be revised when there isadditional information available.

WHY BAYESIAN METHODS ARE IMPORTANT?

Bayesian learning algorithms, like the naive Bayes classifier,are highly practical approaches to certain types of learning problems as they can calculate explicit probabilities for hypotheses. In many cases, they are equally competitive or even outperform the other learning algorithms, including decision tree and neural network algorithms.

Bayesian classifiers use a simple idea that the training data are utilized to calculate an observed probability of each class based on feature values. When the same classifier is used later for unclassified data, it uses the observed probabilities to predict the most likely class for the new features. The application of the observations from the training data can also be thought of as applying our prior knowledge or prior belief to the probability of an outcome, so that it has higher probability of meeting the actual or real-life outcome. This simple concept is used in Bayes' rule and applied for training amachine in machine learning terms. Some of the real-life uses of Bayesian classifiers are as follows:

- Text-based classification such as spam or junk mail filtering, author identification, or topic categorization
- Medical diagnosis such as given the presence of a set of observed symptomsduring a disease, identifying the probability of new patients having the disease
- Network security such as detecting illegal intrusion or anomaly in computernetworks

One of the strengths of Bayesian classifiers is that they utilize all available parameters to subtly change the predictions, while many other algorithms tend to ignore the features that have weak effects. Bayesian classifiers assume that even if few individual parameters have small effect on theoutcome, the collective effect of those parameters could be quite large. For such learning tasks, the naive Bayes classifier is most effective.

Some of the features of Bayesian learning methods thathave made them popular are as follows:

- Prior knowledge of the candidate hypothesis is combined with the observeddata for arriving at the final probability of a hypothesis. So, two important components are the prior probability of each candidate hypothesis and the probability distribution over the observed data set for each possible hypothesis.
- The Bayesian approach to learning is more flexible than the other approachesbecause each observed training pattern can influence the outcome of the hypothesis by increasing or decreasing the estimated probability about the hypothesis, whereas most of the other algorithms tend to eliminate a hypothesis if that is inconsistent with the single training pattern.

- Bayesian methods can perform better than the other methods while validating the hypotheses that make probabilistic predictions. For example, when starting a new software project, on the basis of the demographics of the project, we can predict the probability of encountering challenges during execution of the project.
- Through the easy approach of Bayesian methods, it is possible to classify new instances by combining the predictions of multiple hypotheses, weighted by their respective probabilities.
- In some cases, when Bayesian methods cannot compute the outcome deterministically, they can be used to create a standard for the optimal decision against which the performance of other methods can be measured.

As we discussed above, the success of the Bayesian method largely depends on the availability of initial knowledge about the probabilities of the hypothesis set. So, if these probabilities are not known to us in advance, we have to use some background knowledge, previous data or assumptions about the data set, and the related probability distribution functions

to apply this method. Moreover, it normally involves high computational cost to arrive at the optimal Bayes hypothesis.

BAYES' THEOREM

Before we discuss Bayes' theorem and its application in concept learning, we should be clear about what is **concept learning**. Let us take an example of how a child starts to learn meaning of new words, e.g. 'ball'. The child is provided with positive examples of 'objects' which are 'ball'. At first, the child may be confused with many different colours, shapes and sizes of the balls and may also get confused with some objects which look similar to ball, like a balloon or a globe. The child's parent continuously feeds her positive examples like 'that is a ball', 'this is a green ball', 'bring me that small ball', etc. Seldom there are negative examples used for such concept teaching, like 'this is a non-ball', but the parent may clear the confusion of the child when it points to a balloon and says it is a ball by saying 'that is not a ball'. But it is observed that the learning is most influenced through positive examples rather than through negative examples, and the expectation is that the child will be able to identify the object 'ball' from a wide variety of objects and different types of balls kept together once the concept of a ball is clear to her. We can extend

this example to explain how we can expect machines to learn

through the feeding of positive examples, which forms the basis for concept learning.

To relate the above-mentioned learning concept with the mathematical model of Bayes, we can correlate the learning process of 'meaning of a word' as equivalent to learning, a concept using binary classification. Let us define a concept set C and a corresponding function $f(k)$. We also define $f(k) = 1$, when k is within the set C and $f(k) = 0$ otherwise. Our aim is to learn the indicator function f that defines which elements are

within the set *C*. So, by using the function *f*, we will be able to classify the element either inside or outside our concept set. In Bayes' theorem, we will learn how to use standard probability calculus to determine the uncertainty about the function *f*, and we can validate the classification by feeding positive examples.

There are few notations that will be introduced before going into the details of Bayes' theorem. In Chapter 5, we already discussed Bayes' probability rule as given below:

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

where *A* and *B* are conditionally related events and $p(A|B)$ denotes the probability of event *A* occurring when event *B* has already occurred.

Let us assume that we have a training data set *D* where we have noted some observed data. Our task is to determine the best hypothesis in space *H* by using the knowledge of *D*.

Prior

The prior knowledge or belief about the probabilities of various hypotheses in *H* is called Prior in context of Bayes' theorem. For example, if we have to determine whether a particular type of tumour is malignant for a patient, the prior knowledge of such tumours becoming malignant can be used to validate our current hypothesis and is a prior probability or simply called Prior.

Let us introduce few notations to explain the concepts. We will assume that $P(h)$ is the initial probability of a hypothesis '*h*' that the patient has a malignant tumour based only on the malignancy test, without considering the prior knowledge of the correctness of the test process or the so-called training data. Similarly, $P(T)$ is the prior probability that the training data will be observed or, in this case, the probability of positive malignancy test results. We will denote $P(T|h)$ as the probability of observing data *T* in a space where '*h*' holds true, which means the probability of the test results showing a positive value when the tumour is actually malignant.

Posterior

The probability that a particular hypothesis holds for a data set based on the Prior is called the posterior probability or simply Posterior. In the above example, the probability of the hypothesis that the patient has a malignant tumour considering the Prior of correctness of the malignancy test is a posterior probability. In our notation, we will say that we are interested in finding out $P(h|T)$, which means whether the hypothesis holds true given the observed training data *T*. This is called the posterior probability or simply Posterior in machine learning language. So, the prior probability $P(h)$, which represents the probability of the hypothesis independent of the training data (Prior), now gets refined with the introduction of influence of the training data as $P(h|T)$.

According to Bayes' theorem

$$P(h|T) = \frac{P(T|h)P(h)}{P(T)}$$

combines the prior and posterior probabilities together.

From the above equation, we can deduce that $P(h|T)$ increases as $P(h)$ and $P(T|h)$ increases and also as $P(T)$ decreases. The simple explanation is that when there is more probability that T can occur independently of h then it is less probable that h can get support from T in its occurrence.

It is a common question in machine learning problems to find out the maximum probable hypothesis h from a set of hypotheses H ($h \in H$) given the observed training data T. This maximally probable hypothesis is called the **maximum a posteriori (MAP)** hypothesis. By using Bayes' theorem, we can identify the MAP hypothesis from the posterior probability of each candidate hypothesis:

$$h_{\text{MAP}} = \text{argmax}_{h \in H} P(h|T)$$
$$= \text{argmax}_{h \in H} \frac{P(T|h)P(h)}{P(T)}$$

and as $P(T)$ is a constant independent of h, in this case, wecan write

$$= \text{argmax}_{h \in H} P(T|h)P(h) \qquad (6.1)$$

Likelihood

In certain machine learning problems, we can further simplify equation 6.1 if every hypothesis in H has equal probable priorias $P(h_i) = P(h_j)$, and then, we can determine $P(h|T)$ from the probability $P(T|h)$ only. Thus, $P(T|h)$ is called the likelihood ofdata T given h, and any hypothesis that maximizes $P(T|h)$ is

called the maximum likelihood (ML) hypothesis, h_{ML}. See figure 6.1 and 6.2 for the conceptual and mathematical representation of Bayes theorem and the relationship of Prior, Posterior and Likelihood.

$$h_{\text{ML}} = \text{argmax}_{h \in H} P(T|h) \qquad (6.2)$$

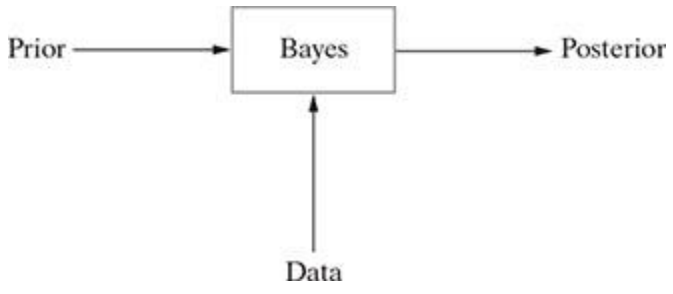


FIG. 6.1
Bayes' theorem

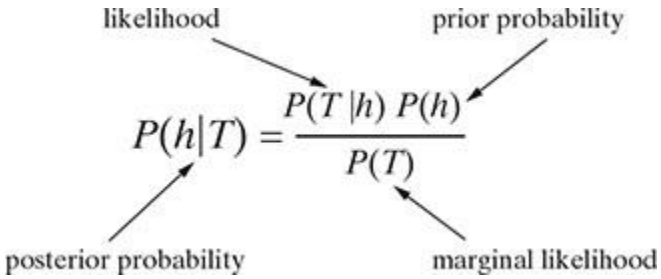


FIG. 6.2
Concept of prior, posterior, and likelihood

Example. Let us take the example of malignancy identification in a particular patient's tumour as an application for Bayes rule. We will calculate how the prior knowledge of the percentage of cancer cases in a sample population and probability of the test result being correct influence the probability outcome of the correct diagnosis. We have two alternative hypotheses: (1) a particular tumour is of malignant type and (2) a particular tumour is non-malignant type. The priori available are—1. only 0.5% of the population has this kind of tumour which is malignant, 2. the laboratory report has some amount of incorrectness as it could detect the malignancy was present only with 98% accuracy whereas could show the malignancy was not present correctly only in 97% of cases. This means the test predicted malignancy was present which actually was a false alarm in 2% of the cases, and also missed detecting the real malignant tumour in 3% of the cases.

Solution: Let us denote Malignant Tumour = MT, Positive Lab Test = PT, Negative Lab Test = NT

h_1 = the particular tumour is of malignant type = MT in ourexample

h_2 = the particular tumour is not malignant type = !MT inour example

P(MT) = 0.005 P(!MT) = 0.995
P(PT|MT) = 0.98 P(PT|!MT) = 0.02
P(NT|!MT) = 0.97 P(NT|MT) = 0.03

So, for the new patient, if the laboratory test report shows positive result, let us see if we should declare this as the malignancy case or not:

$$\begin{aligned} P(h_1|\text{PT}) &= \frac{P(\text{PT}|h_1).P(h_1)}{P(\text{PT})} \\ &= P(\text{PT}|\text{MT})P(\text{MT}) \\ &= 0.98 \times 0.005 \\ &= 0.0049 \\ &= 0.49\% \end{aligned}$$

$$\begin{aligned} P(h_2|\text{PT}) &= \frac{P(\text{PT}|h_2).P(h_2)}{P(\text{PT})} \\ &= P(\text{PT}|!\text{MT})P(!\text{MT}) \\ &= 0.02 \times 0.995 \\ &= 0.0199 \\ &= 1.99\% \end{aligned}$$

As $P(h_2|\text{PT})$ is higher than $P(h_1|\text{PT})$, it is clear that the hypothesis h_2 has more probability of being true. So, $h\text{MAP} = h2 = !\text{MT}$.

This indicates that even if the posterior probability of malignancy is significantly higher than that of non- malignancy, the probability of this patient not having malignancy is still higher on the basis of the prior knowledge. Also, it should be noted that through Bayes' theorem, we identified the probability of one hypothesis being higher than the other hypothesis, and we did not completely accept or reject the hypothesis by this theorem. Furthermore, there is very high dependency on the availability of the prior data for successful application of Bayes' theorem.

BAYES' THEOREM AND CONCEPT LEARNING

One simplistic view of concept learning can be that if we feed the machine with the training data, then it can calculate the posterior probability of the hypotheses and outputs the most probable hypothesis. This is also called brute-force Bayesian learning algorithm, and it is also observed that consistency in providing the right probable hypothesis by this algorithm is very comparable to the other algorithms.

Brute-force Bayesian algorithm

We will now discuss how to use the MAP hypothesis output to design a simple learning algorithm called brute-force map learning algorithm. Let us assume that the learner considers a finite hypothesis space H in which the learner will try to learn some target concept $c{:}X \rightarrow \{0,1\}$ where X is the instance space corresponding to H. The sequence of training examples is $\{(x_1, t_1), (x_2, t_2), \ldots, (x_m, t_m)\}$, where x_i is the instance of X and t_i is the target concept of x_i defined as $t_i = c(x_i)$. Without impacting the efficiency of the algorithm, we can assume that the sequence of instances of x $\{x_1, \ldots, x_m\}$ is held fixed, and then, the sequence of target values becomes $T = \{t_1, \ldots, t_m\}$.

For calculating the highest posterior probability, we can use Bayes' theorem as discussed earlier in this chapter:

Calculate the posterior probability of each hypothesis h in H:

$$P(h|T) = \frac{P(T|h)P(h)}{P(T)}$$

Identify the h_{MAP} with the highest posterior probability

$$h_{MAP} = \text{argmax}_{h \in H} P(h|T)$$

Please note that calculating the posterior probability for each hypothesis requires a very high volume of computation, and for a large volume of hypothesis space, this may be difficult to achieve.

Let us try to connect the concept learning problem with the problem of identifying the h_{MAP}. On the basis of the probability distribution of $P(h)$ and $P(T|h)$, we can derive the prior knowledge of the learning task. There are few important assumptions to be made as follows:

1. The training data or target sequence T is noise free, which means that it is a direct function of X only (i.e. $t_i = c(x_i)$)
2. The concept c lies within the hypothesis space H
3. Each hypothesis is equally probable and independent of each other

On the basis of assumption 3, we can say that each hypothesis h within the space H has equal prior probability, and also because of assumption 2, we can say that these prior probabilities sum up to 1. So, we can write

$$P(h) = \frac{1}{|H|} \text{ for all } h \text{ within } H \qquad (6.3)$$

$P(T|h)$ is the probability of observing the target values t_i in the fixed set of instances $\{x_i, \ldots, x_m\}$ in the space where h holds true and describes the concept c correctly. Using assumption 1 mentioned above, we can say that if T is consistent with h,

then the probability of data T given the hypothesis h is 1 and is0 otherwise:

$$P(T|h) = \begin{cases} 1 & \text{if } t_i = h(x_i) \text{ for all } t_i \text{ within } T \\ 0 & \text{otherwise} \end{cases} \tag{6.4}$$

Using Bayes' theorem to identify the posterior probability

$$P(h|T) = \frac{P(T|h)P(h)}{P(T)} \tag{6.5}$$

For the cases when h is inconsistent with the training data T,using 6.5 we get

$$P(h|T) = \frac{0 \times P(h)}{P(T)} = 0, \text{ when } h \text{ is inconsistent with } T,$$

and when h is consistent with T

$$P(h|T) = \frac{1 \times \frac{1}{|H|}}{P(T)} = \frac{1}{|H|P(T)} \tag{6.6}$$

Now, if we define a subset of the hypothesis H which is consistent with T as H_D, then by using the total probabilityequation, we get

$$\begin{aligned} P(T) &= \sum_{h_i \in H_D} P(T|h_i)P(h_i) \\ &= \sum_{h_i \in H_D} 1.\frac{1}{|H|} + \sum_{h_i \notin H_D} 0.\frac{1}{|H|} \\ &= \sum_{h_i \in H_D} 1.\frac{1}{|H|} \\ &= \frac{|H_D|}{|H|} \end{aligned}$$

This makes 6.5 as

$$P(h|T) = \frac{1}{|H|.\frac{|H_D|}{|H|}}$$
$$= \frac{1}{|H_D|}$$

So, with our set of assumptions about $P(h)$ and $P(T|h)$, we get the posterior probability $P(h|T)$ as

$$P(h|T) = \begin{cases} \frac{1}{|H_D|} & \text{if } h \text{ is consistent with } T \\ 0 & \text{otherwise} \end{cases} \quad (6.7)$$

where H_D is the number of hypotheses from the space H which are consistent with target data set T. The interpretation of this evaluation is that initially, each hypothesis has equal probability and, as we introduce the training data, the posterior probability of inconsistent hypotheses becomes zero and the total probability that sums up to 1 is distributed equally amongthe consistent hypotheses in the set. So, under this condition,

each consistent hypothesis is a MAP hypothesis with posteriorprobability $\frac{1}{|H_D|}$.

Concept of consistent learners

From the above discussion, we understand the behaviour of the general class of learner whom we call as consistent learners. So, the group of learners who commit zero error over the training data and output the hypothesis are called *consistent learners*. If the training data is noise free and deterministic (i.e. $P(D|h) = 1$ if D and h are consistent and 0 otherwise) and if there is uniform prior probability distribution over H (so, $P(h_m) = P(h_n)$ for all m, n), then every consistent learner outputs the MAP hypothesis. An important application of this conclusion is that Bayes' theorem can characterize the behaviour of learning algorithms even when the algorithm does not explicitly manipulate the probability. As it can help toidentify the optimal distributions of $P(h)$ and $P(T|h)$ under which the algorithm outputs the MAP hypothesis, the knowledge can be used to characterize the assumptions under which the algorithms behave optimally.

Though we discussed in this section a special case of Bayesian output which corresponds to the noise-free training data and deterministic predictions of hypotheses where $P(T|h)$takes on value of either 1 or 0, the theorem can be used with the same effectiveness for noisy training data and additional assumptions about the probability distribution governing the noise.

Bayes optimal classifier

In this section, we will discuss the use of the MAP hypothesis to answer the question what is the most probable classification of the new instance given the training data. To illustrate the concept, let us assume three hypotheses h_1, h_2, and h_3 in the hypothesis space H. Let the posterior probability of these hypotheses be 0.4, 0.3, and 0.3, respectively. There is a new instance x, which is classified as true by h_1, but false by h_2 andh_3.

Then the most probable classification of the new instance

(x) can be obtained by combining the predictions of all hypotheses weighed by their corresponding posterior probabilities. By denoting the possible classification of the new instance as c_i from the set C, the probability $P(c_i|T)$ that the correct classification for the new instance is c_i is

$$P(c_i|T) = \sum_{h_i \in H} P(c_i|h_i)P(h_i|T)$$

The optimal classification is for which $P(c_i|T)$ is maximum
is

$$\text{Bayes optimal classifier} = \underset{c_i \in C}{\text{argmax}} \sum_{h_i \in H} P(c_i|h_i)P(h_i|T)$$

So, extending the above example,

The set of possible outcomes for the new instance x is within the set C = {True, False} and

$P(h_1 \mid T) = 0.4$, $P(\text{False} \mid h_1) = 0$, $P(\text{True} \mid h_1) = 1$
$P(h_2 \mid T) = 0.3$, $P(\text{False} \mid h_2) = 1$, $P(\text{True} \mid h_2) = 0$
$P(h_3 \mid T) = 0.3$, $P(\text{False} \mid h_3) = 1$, $P(\text{True} \mid h_3) = 0$

Then,

$$\sum_{h_i \in H} P(\text{True}|h_i)P(h_i|T) = 0.4$$

$$\sum_{h_i \in H} P(\text{False}|h_i)P(h_i|T) = 0.6$$

and

$$\underset{c_i \in \{\text{True, False}\}}{\text{argmax}} \sum_{h_i \in H} P(c_i|h_i)P(h_i|T) = \text{False}$$

This method maximizes the probability that the new instance is classified correctly when the available training data, hypothesis space and the prior probabilities of the hypotheses are known. This is thus also called Bayes optimalclassifier.

Naïve Bayes classifier

Naïve Bayes is a simple technique for building classifiers: models that assign class labels to problem instances. The basic idea of Bayes rule is that the outcome of a hypothesis can be predicted on the basis of some evidence (*E*) that can be observed.

From Bayes rule, we observed that

1. A prior probability of hypothesis *h* or *P*(*h*): This is the probability of an event or hypothesis before the evidence is observed.
2. A posterior probability of *h* or *P*(*h*|*D*): This is the probability of an event after the evidence is observed within the population *D*.

$$\textbf{Posterior probability} = \frac{\textbf{(Prior probability} \times \textbf{Conditional Probability)}}{\textbf{Evidence}}$$

Posterior Probability is of the format 'What is the probability that a particular object belongs to class i given its observed feature values?'

For example, a person has height and weight of 182 cm and 68 kg, respectively. What is the probability that this person belongs to the class 'basketball player'? This can be predicted using the Naïve Bayes classifier. This is known as probabilistic classifications.

In machine learning, a probabilistic classifier is a classifier that can be foreseen, given a perception or information (input), a likelihood calculation over a set of classes, instead of just yielding (outputting) the most likely class that the perception (observation) should belong to. Parameter estimation for Naïve Bayes models uses the method of ML.

Bayes' theorem is used when new information can be used to revise previously determined probabilities. Depending on the particular nature of the probability model, Naïve Bayes classifiers can be trained very professionally in a supervised learning setting.

Let us see the basis of deriving the principles of Naïve Bayes classifiers. We take a learning task where each instance *x* has some attributes and the target function ($f(x)$) can take any value from the finite set of classification values *C*. We also have a set of training examples for target function, and the set of attributes $\{a_1, a_2, \ldots, a_n\}$ for the new instance are known to us. Our task is to predict the classification of the new instance.

According to the approach in Bayes' theorem, the classification of the new instance is performed by assigning the most probable target classification C_{MAP} on the basis of the attribute values of the new instance $\{a_1, a_2, \ldots, a_n\}$. So,

$$C_{\text{MAP}} = \underset{c_i \in C}{\text{argmax}} \sum_{h_i \in H} P\left(c_i | a_1, a_2, \ldots, a_n\right)$$

which can be rewritten using Bayes' theorem as

$$C_{\text{MAP}} = \underset{c_i \in C}{\text{argmax}} \sum_{h_i \in H} \frac{P(a_1, a_2, \ldots, a_n | c_i) P\left(c_i\right)}{P\left(a_1, \ldots a_n\right)}$$

As combined probability of the attributes defining the newinstance fully is always 1

$$C_{\text{MAP}} = \underset{c_i \in C}{\text{argmax}} \sum_{h_i \in H} P(a_1, a_2, \ldots, a_n | c_i) P(c_i) \qquad (6.8)$$

So, to get the most probable classifier, we have to evaluate the two terms $P(a_1, a_2, \text{c}, a_n|c_i)$ and $P(ci)$. In a practical scenario, it is possible to calculate $P(ci)$ by calculating the frequency of each target value c_i in the training data set. But the $P(a_1, a_2, \text{c}, a_n|c_i)$ cannot be estimated easily and needs a very high effort of calculation. The reason is that the number of these terms is equal to the product of number of possible instances and the number of possible target values, and thus, each instance in the instance space needs to be visited many times to arrive at the estimate of the occurrence. Thus, the Naïve Bayes classifier makes a simple assumption that the attribute values are conditionally independent of each other forthe target value. So, applying this simplification, we can now say that for a target value of an instance, the probability of observing the combination a_1,a_2,…, a_n is the product of probabilities of individual attributes $P(a_i|c_j)$.

$$P(a_1, a_2, ..., a_n|c_j) = \prod_i P(a_i|c_j)$$

Then, from equation 6.7, we get the approach for the NaïveBayes classifier as

$$C_{\text{NB}} = \underset{c_i \in C}{\text{argmax}} \sum_{h_i \in H} P(c_i) \prod_i P(a_i|c_j) \qquad (6.9)$$

Here, we will be able to compute $P(a_i|c_j)$ as we have to calculate this only for the number of distinct attributes values(a_i) times the number of distinct target values (c_j), which is much smaller set than the product of both the sets. The most

important reason for the popularity of the Naïve Bayes classifier approach is that it is not required to search the wholehypothesis space for this algorithm, but rather we can arrive atthe target classifier by simply counting the frequencies of various data combinations within the training example.

To summarize, a Naïve Bayes classifier is a primary probabilistic classifier based on a view of applying Bayes' theorem (from Bayesian inference with strong naive) independence assumptions. The prior probabilities in Bayes'theorem that are changed with the help of newly available information are classified as posterior probabilities.

A key benefit of the naive Bayes classifier is that it requires only a little bit of training information (data) to gauge the parameters (mean and differences of the variables) essential for the classification (arrangement). In the Naïve Bayes classifier, independent variables are always assumed, and only the changes (variances) of the factors/variables for each class should be determined and not the whole covariance matrix.
Because of the rather naïve assumption that all features of thedataset are equally important and independent, this is called Naïve Bayes classifier.

Naïve Bayes classifiers are direct linear classifiers that are known for being the straightforward, yet extremely proficient result. The modified version of Naïve Bayes classifier originates from the assumption that information collection (data set) is commonly autonomous (mutually independent). In most of the practical scenarios, the 'independence' assumption is regularly violated. However, Naïve Bayes classifiers still tend to perform

exceptionally well.

Some of the key strengths and weaknesses of Naïve Bayes classifiers are described in Table 6.1.

Table 6.1 *Strengths and Weaknesses of Bayes Classifiers*

Strengths	Weakness
Simple and fast in calculation but yet effective in result	The basis assumption of equal importance and independence often does not hold true
In situations where there are noisy and missing data, it performs well	If the target dataset contains large numbers of numeric features, then the reliability of the outcome becomes limited
Works equally well when smaller number of data is present for training as well as very large number of training data is available	Though the predicted classes have a high reliability, estimated probabilities have relatively lower reliability
Easy and straightforward way to obtain the estimated probability of a prediction	

Example. Let us assume that we want to predict the outcome of a football world cup match on the basis of the past performance data of the playing teams. We have training data available (refer Fig. 6.3) for actual match outcome, while four parameters are considered – Weather Condition (Rainy, Overcast, or Sunny), how many matches won were by this team out of the lastthree matches (one match, two matches, or three matches), Humidity Condition (High or Normal), and whether they won the toss (True or False). Using Naïve Bayesian, you need to classify the conditions when this team wins and then predict the probability of this team winning a particular match when Weather Conditions = Rainy, they won two of the last three matches, Humidity = Normal and they won the toss in the particular match.

Weather Condition	Wins in last 3 matches	Humidity	Win toss	Won match?
Rainy	3 wins	High	FALSE	No
Rainy	3 wins	High	TRUE	No
OverCast	3 wins	High	FALSE	Yes
Sunny	2 wins	High	FALSE	Yes
Sunny	1 win	Normal	FALSE	Yes
Sunny	1 win	Normal	TRUE	No
OverCast	1 win	Normal	TRUE	Yes
Rainy	2 wins	High	FALSE	No
Rainy	1 win	Normal	FALSE	Yes
Sunny	2 wins	Normal	FALSE	Yes
Rainy	2 wins	Normal	TRUE	Yes
OverCast	2 wins	High	TRUE	Yes
OverCast	3 wins	Normal	FALSE	Yes
Sunny	2 wins	High	TRUE	No

FIG. 6.C Training data for the Naïve Bayesian method

Naïve Bayes classifier steps

Step 1: First construct a frequency table. A frequency table is drawn for each attribute against the target outcome. For example, in Figure 6.3, the various attributes are (1) Weather Condition, (2) How many matches won by this teamin last three matches, (3) Humidity Condition, and (4) whether they won the toss and the target outcome is will they win the match or not?

Step 2: Identify the cumulative probability for 'Won match = Yes' and the probability for 'Won match = No' on the basis of all the attributes. Otherwise, simply multiply probabilities of all favourable conditions to derive 'YES' condition. Multiply probabilities of all non-favourable conditions to derive 'No' condition.

Step C: Calculate probability through normalization by applying the belowformula

$$P(\text{Yes}) = \frac{P(\text{Yes})}{P(\text{Yes}) + P(\text{No})}$$

$$P(\text{No}) = \frac{P(\text{No})}{P(\text{Yes}) + P(\text{No})}$$

P(Yes) will give the overall probability of favourablecondition in the given scenario.

P(No) will give the overall probability of non-favourablecondition in the given scenario.

Solving the above problem with Naive Bayes

Step 1: Construct a frequency table. The posterior probability can be easily derived by

constructing a frequency table for each attribute against the target. For example, frequency of Weather Condition variable with values 'Sunny' when the target value Won match is 'Yes', is, 3/(3+4+2) = 3/9.

Figure 6.4 shows the frequency table thus constructed.

Step 2:

To predict whether the team will win for given weather conditions (a_1) = Rainy, Wins in last three matches (a_2) = 2 wins, Humidity (a_3) = Normal and Win toss (a_4) = True, we need to choose 'Yes' from the above table for the given conditions.

From Bayes' theorem, we get

$$P(\text{Win match}|a_1 \cap a_2 \cap a_3 \cap a_4) = \frac{P(a_1 \cap a_2 \cap a_3 \cap a_4|\text{Win match})P(\text{Win match})}{P(a_1 \cap a_2 \cap a_3 \cap a_4)}$$

This equation becomes much easier to resolve if we recall that Naïve Bayes classifier assumes independence among events. This is specifically true for class-conditional independence, which means that the events are independent so long as they are conditioned on the same class value. Also, we know that if

the events are independent, then the probability rule says, $P(A \cap B) = P(A)P(B)$, which helps in simplifying the above equation significantly as

$P(\text{Win match}|a_1 \cap a_2 \cap a_3 \cap a_4)$

$$= \frac{P(a_1|\text{Win match})P(a_2|\text{Win match})P(a_3|\text{Win match})P(a_4|\text{Win match})P(\text{Win match})}{P(a_1)P(a_2)P(a_3)P(a_4)}$$

$$= 2/9*4/9*6/9*9/14$$

$$= 0.014109347$$

This should be compared with

$P(!\text{Win match}|a_1 \cap a_2 \cap a_3 \cap a_4)$

$$= \frac{P(a_1|!\text{Win match})P(a_2|!\text{Win match})P(a_3|!\text{Win match})P(a_4|!\text{Win match})P(!\text{Win match})}{P(a_1)P(a_2)P(a_3)P(a_4)}$$

$$= 3/5*2/5*1/5*5/14$$

$$= 0.010285714$$

	Won Match			Won Match	
Weather condition	Yes	No	**Humidity**	Yes	No
Sunny	3	2	High	3	4
OverCast	4	0	Normal	6	1
Rainy	2	3			
Total	9	5	Total	9	5

	Won Match			Won Match	
Wins in last 3 matches	Yes	No	Win toss	Yes	No
3 wins	2	2	FALSE	6	2
1 win	4	2	TRUE	3	3
2 wins	3	1			
Total	9	5	Total	9	5

FIG. 6.4 Construct frequency table

Step C: by normalizing the above two probabilities, we can ensure that the sumof these two probabilities is 1.

$$P(\textbf{Win match}) = \frac{P(\textbf{Win match})}{P(\textbf{Win match}) + P(\textbf{!Win match})}$$
$$= \frac{0.014109347}{0.014109347 + 0.010285714}$$
$$= 0.578368999$$

$$P(\textbf{!Win match}) = \frac{P(\textbf{!Win match})}{P(\textbf{Win match}) + P(\textbf{!Win match})}$$
$$= \frac{0.010285714}{0.014109347 + 0.010285714}$$
$$= 0.421631001$$

Conclusion: This shows that there is 58% probability that the team will win if the above conditions become true for that particular day. Thus, Naïve Bayes classifier provides a simple yet powerful way to consider the influence of multiple attributes on the target outcome and refine the uncertainty of the event on the basis of the prior knowledge because it is able to simplify the calculation through independence assumption.

Applications of Naïve Bayes classifier

Text classification: Naïve Bayes classifier is among the most successful known algorithms for learning to classify text documents. It classifies the document where the probability of

classifying the text is more. It uses the above algorithm to check the permutation and combination of the probability of classifying a document under a particular 'Title'. It has variousapplications in document categorization, language detection, and sentiment detection, which are very useful for traditional retailers, e-retailors, and other businesses on judging the sentiments of their clients on the basis of keywords in feedback forms, social media comments, etc.

Spam filtering: Spam filtering is the best known use of Naïve Bayesian text classification. Presently, almost all the email providers have this as a built-in functionality, which makes use of a Naïve Bayes classifier to identify spam email on the basis of certain conditions and also the probability of classifying an email as 'Spam'. Naïve Bayesian spam sifting has turned into a mainstream mechanism to recognize illegitimate a spam email from an honest-to-goodness email (sometimes called 'ham'). Users can also install separate email filtering programmes. Server-side email filters such as DSPAM, Spam Assassin, Spam Bayes, and ASSP make use of Bayesian spam filtering techniques, and the functionality is sometimes embedded within the mail server software itself.

Hybrid Recommender System: It uses Naïve Bayes classifier and collaborative filtering. Recommender systems (used by e- retailors like eBay, Alibaba, Target, Flipkart, etc.) apply machine learning and data mining techniques for filtering unseen information and can predict whether a user would like a given resource. For example, when we log in to these retailer websites, on the basis of the usage of texts used by the login and the historical data of purchase, it automatically recommends the product for the particular login persona. One of the algorithms is combining a Naïve Bayes classification approach with collaborative filtering, and experimental results show that this algorithm provides better performance regarding accuracy and coverage than other algorithms.

Online Sentiment Analysis: The online applications use supervised machine learning (Naïve Bayes) and useful computing. In the case of sentiment analysis, let us assume there are three sentiments such as nice, nasty, or neutral, and Naïve Bayes classifier is used to distinguish between them. Simple emotion modelling combines a statistically based

classifier with a dynamical model. The Naïve Bayes classifier employs 'single words' and 'word pairs' like features and determines the sentiments of the users. It allocates user utterances into nice, nasty, and neutral classes, labelled as +1,

−1, and 0, respectively. This binary output drives a simple

first-order dynamical system, whose emotional state representsthe simulated emotional state of the experiment's personification.

Handling Continuous Numeric Features in NaïveBayes Classifier

In the above example, we saw that the Naïve Bayes classifier model uses a frequency table of the training data for its calculation. Thus, each attribute data should be categorical in nature so that the combination of class and feature values can be created. But this is not possible in the case of continuous numeric data as it does not have the categories of data.

The workaround that is applied in these cases is discretizing the continuous data on the basis of some data range. This is also called binning as the individual categories are termed as bins. For example, let us assume we want to market a certain credit card to all the customers who are visiting a particular bank. We have to classify the persons who are visiting a bank as either interested candidate for taking a new card or non- interested candidate for a new card, and on the basis of this classification, the representative will approach the customer for sale. In this case, the customers visit the bank continuouslyduring banking hours and have different values for the attributes we want to evaluate before classifying them into the interested/non-interested categories.

If we plot the number of customers visiting the bank during the 8 hours of banking time, the distribution graph will be a continuous graph. But if we introduce a logic to categorize the customers according to their time of entering the bank, then we will be able to put the customers in 'bins' or buckets for our analysis. We can then try to assess what time range is best suited for targeting the customers who will have interest in the new credit card. The bins created by categorizing the customers by their time of entry looks like Figure 6.5.

This creates eight natural bins for us (or we may change the number of bins by changing our categorizing criteria), which can now be used for Bayes analysis.

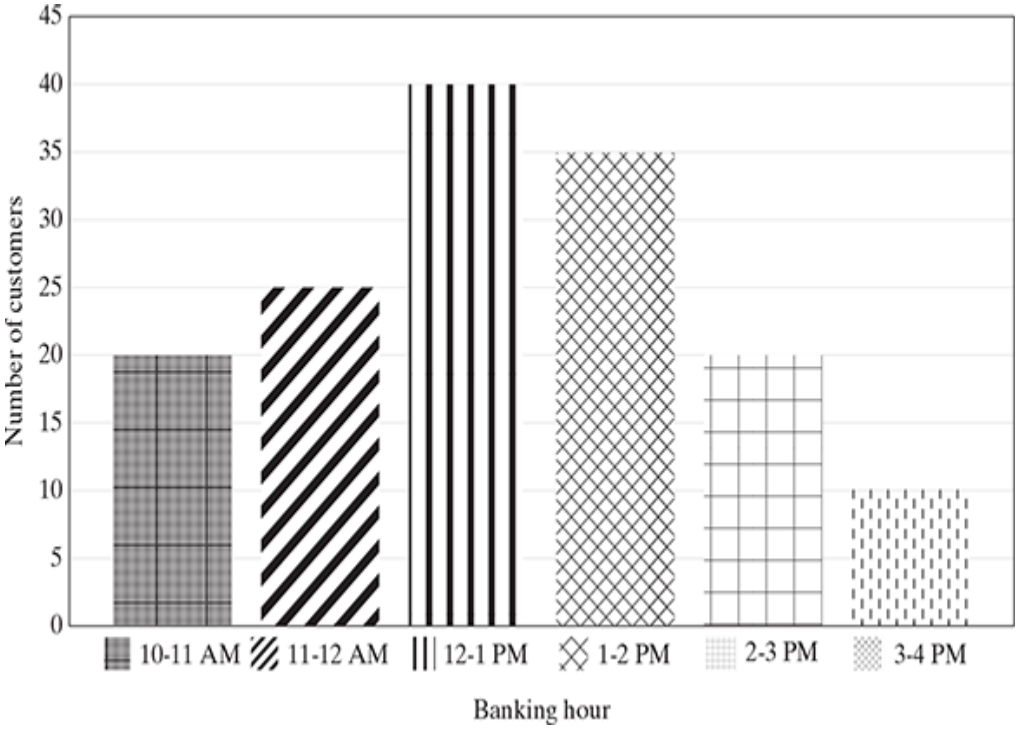


FIG. 6.5 The distribution of bins based on the time of entry of customers in the bank

BAYESIAN BELIEF NETWORK

We must have noted that a significant assumption in the Naïve Bayes classifier was that the attribute values a_1, a_2,…, a_n are conditionally independent for a target value. The Naïve Bayes classifier generates optimal output when this condition is met. Though this assumption significantly reduces the complexity of computation, in many practical scenarios, this requirement of conditional independence becomes a difficult constraint for the application of this algorithm. So, in this section, we will discuss the approach of Bayesian Belief network, which assumes that within the set of attributes, the probability distribution can have conditional probability relationship as well as conditional independence assumptions. This is different from the Naïve Bayes assumption of conditional independence of all the attributes as the belief network provides the flexibility of declaring a subset of the attributes as conditionally dependent while leaving rest of the attributes to hold the assumptions of conditional independence. The prior knowledge or belief about the influence of one attribute over the other is handled through joint probabilities as discussed later in this section.

Let us refresh our mind on the concept of conditional probability. If an uncertain event A is conditional on a knowledge or belief K, then the degree of belief in A with the assumption that K is known is expressed as $P(A|K)$.
Traditionally, conditional probability is expressed by joint probability as follows:

$$P(A|K) = \frac{P(A, K)}{P(K)} \tag{6.10}$$

Rearranging (6.9), we get the product rule
$P(A, K) = P(A|K)P(K)$

This can be extended for three variables or attributes as

$P(A, K, C) = P(A|K, C)P(K, C) = P(A|K, C)P(K|C)P(C)$

For a set of n attributes, the generalized form of the productrule becomes

$P(A_1, A_2, \ldots, A_n) = P(A_1|A_2, \ldots, A_n)P(A_2|A_3, \ldots, A_n)P(A_n\text{-}1|A_n)P(A_n)$ (6.10)

This generalized version of the product rule is called theChain Rule.

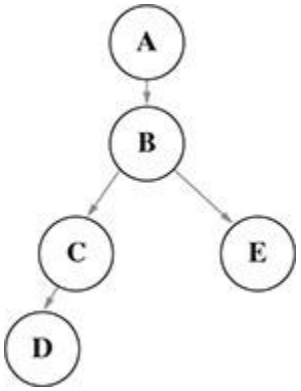


FIG. 6.6 Chain rule

Let us understand the chain rule by using the diagram in Figure 6.6. From the joint probability formula 6.10, we canwrite

$P(A, B, C, D, E) = P(A|B, C, D, E)P(B|C, D, E)P(C|D, E)P(D|E)P(E)$

But from Figure 6.6, it is evident that *E* is not related to *C* and *D*, which means that the probabilities of variables *C* and *D* are not influenced by *E* and vice versa. Similarly, *A* is directly influenced only by *B*. By applying this knowledge of independence, we can simplify the above equation as

$$P(A, B, C, D, E) = P(A|B)P(B|C, D)P(C|D)P(D)P(E)$$

Let us discuss this concept of independence and conditional independence in detail in the next section.

Independence and conditional independence

We represent the conditional probability of *A* with knowledge of *K* as $P(A|K)$. The variables *A* and *K* are said to be independent if $P(A|K) = P(A)$, which means that there is no influence of *K* on the uncertainty of *A*. Similarly, the joint probability can be written as $P(A,K) = P(A)P(K)$.

Extending this concept, the variables *A* and *K* are said to be conditionally independent given *C* if $P(A|C) = P(A|K, C)$.

This concept of conditional independence can also be extended to a set of attributes. We can say that the set of variables $A_1, A_2,\ldots, A_n$ is conditionally independent of the set of variables $B_1, B_2,\ldots, B_m$ given the set of variables $C_1, C_2,\ldots,C_l$ if

$$P(A_1, A_2,\ldots, A_n|B_1, B_2,\ldots, Bm, C_1, C_2,\ldots, C_1) = P(A_1, A_2,\ldots, A_n|C_1, C_2,\ldots, C_l)$$

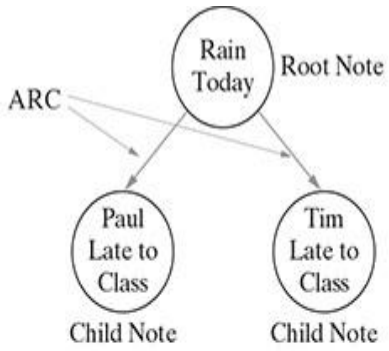
If we compare this definition with our assumption in the Naïve Bayes classifier, we see that the Naïve Bayes classifier assumes that the instance attribute A_1 is conditionally independent of the instance attribute A_2, given the target value *V*, which can be written using the general product rule and application of conditional independence formula as

$$P(A_1, A_2|V) = P(A_1|A_2, V)P(A_2, V) = P(A_1, V)P(A_2, V)$$

A Bayesian Belief network describes the joint probability distribution of a set of attributes in their joint space. In Figure 6.7, a Bayesian Belief network is presented. The diagram consists of nodes and arcs. The nodes represent the discrete or continuous variables for which we are interested to calculate the conditional probabilities. The arc represents the causal relationship of the variables.

The two important information points we get from this network graph are used for the determining the joint probability of the variables. First, the arcs assert that the node variables are conditionally independent of its non-descendants in the network given its immediate predecessors in the network. If two variables *A* and *B* are connected through a directed path, then *B* is called the descendent of *A*. Second, the conditional probability table for each variable provides the probability distribution of that variable given the values of its immediate predecessors. We can use Bayesian probability to calculate different behaviours of the

variables in Figure 6.7.



Rain Today (Root Node) Probability	
True	0.1
False	0.9

Node Conditional probability	Rain Today		
		True	False
Paul Late to Class	True	0.6	0.5
	False	0.4	0.5

Node Conditional probability	Rain Today		
		True	False
Tim Late to Class	True	0.8	0.1
	False	0.2	0.9

FIG. 6.7 Bayesian belief network

1. The unconditional probability that Tim is late to class –
   P(Tim is late to class)
   = *P*(Tim late|Rain Today)*P*(Rain Today) + *P*(Tim late|No Rain Today)*P*(No Rain Today)
   = (0.8 × 0.1) × (0.1 × 0.9)
   = 0.17
   From this unconditional probability, the most important use of the Bayesian Belief network is to find out the revised probability on the basis of the prior knowledge. If we assume that there was rain today,then the probability table can quickly provide us the information about the probability of Paul being late to class or the probability of Tim being late to class from the probability distribution table itself. But if we donot know whether there was rain today or not, but we only know thatTim is late to class today, then we can arrive at the following probabilities –
2. The revised probability that there was rain today –

$$P(\text{Rain Today}|\text{Tim late to class}) = \frac{P(\text{Tim late}|\text{Rain today})\,P(\text{Rain today})}{P(\text{Tim late})}$$
$$= \frac{(0.8 \times 0.1)}{0.17}$$
$$= 0.47$$
$$= P(\text{Rain Today}) \text{as Tim late to class is already known}$$

3. The revised probability that Paul will be late to class today –
   P(Paul late to class today)

= *P*(Paul late|Rain today)*P*(Rain today) + *P*(Paul late|No raintoday)*P*(No rain today)
= (0.6 × 0.47) + (0.5 × (1-0.47))
= 0.55

Here, we used the concept of hard evidence and soft evidence. Hard evidence (instantiation) of a node is evidence that the state of the variable is definitely as a particular value. In our above example, we had hard evidence that 'Tim is late to class'. If a particular node is instantiated, then it will block propagation of evidence further down to its child nodes. Soft evidence for a node is the evidence that provides the prior probability values for the node. The node 'Paul is late to class' is soft evidenced with the prior knowledge that 'Tim is late to class'.

The Bayesian Belief network can represent much more complex scenarios with dependence and independence concepts. There are three types of connections possible in a Bayesian Belief network.

Diverging Connection: In this type of connection, the evidence can be transmitted between two child nodes of the same parent provided that theparent is not instantiated. In Figure 6.7, we already saw the behaviour of diverging connection.

Serial Connection: In this type of connection, any evidence entered at the beginning of the connection can be transmitted through the directed path provided that no intermediate node on the path is instantiated (see Fig. 6.8 forillustration).

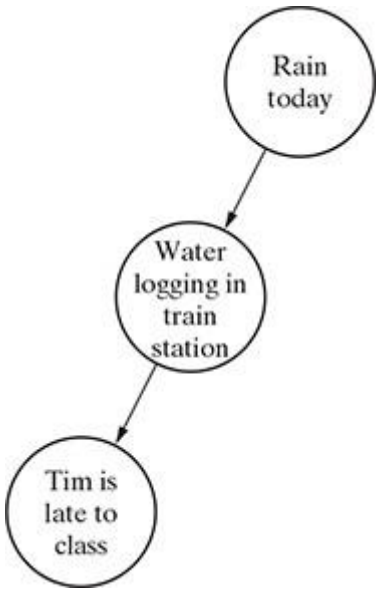


FIG. 6.8 Serial connection

Converging Connection: In this type of connection, the evidence can only be transmitted between two parents when the child (converging) node has received some evidence and that evidence can be soft or hard (see Fig. 6.9 for illustration).

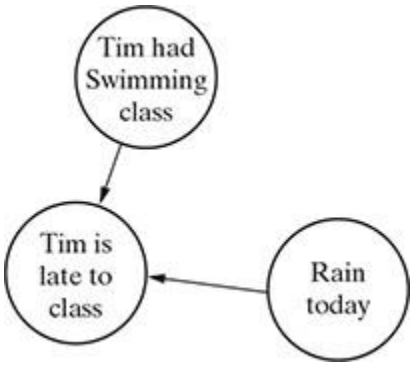


FIG. 6.9 Convergent connection

As discussed above, by using the Bayesian network, we would like to infer the value of a target variable on the basis ofthe observed values of some other variables. Please note that it will not be possible to infer a single value in the case of random variables we are dealing with, but our intention is to

infer the probability distribution of the target variable given the observed values of other variables. In general, the Bayesian network can be used to compute the probability distribution of any subset of node variables given the values ordistribution of the remaining variables.

Use of the Bayesian Belief network in machinelearning

We have seen that the Bayesian network creates a complete model for the variables and their relationships and thus can beused to answer probabilistic queries about them. A common use of the network is to find out the updated knowledge aboutthe state of a subset of variables, while the state of the other subset (known as the evidence variables) is observed. This concept, often known as probabilistic inference process of computing the posterior distribution of variables, given some evidences, provides a universal sufficient statistic for applications related to detections. Thus if one wants to choose the values for a subset of variables in order to minimize some expected loss functions or decision errors, then this method is quiet effective. In other words, the Bayesian network is a mechanism for automatically applying Bayes' theorem to complex problems. Bayesian networks are used for modelling beliefs in domains like computational biology and bioinformatics such as protein structure and gene regulatory networks, medicines, forensics, document classification, information retrieval, image processing, decision support systems, sports betting and gaming, property market analysis and various other fields.

Supervised Learning: Classification

INTRODUCTION

In the last chapter on Bayesian Concept Learning, you were introduced to an important supervised learning algorithm – the Naïve Bayes algorithm. As we have seen, it is a very simple but powerful classifier based on Bayes' theorem of conditional probability. However, other than the Naïve Bayes classifier, there are more algorithms for classification. This chapter will focus on other classification algorithms.

The first algorithm we will delve into in this chapter is *k*-Nearest Neighbour (*k*NN), which tries to classify unlabelled data instances based on the similarity with thelabelled instances in the training data.

Then, another critical classifier, named as decision tree, will be explained in detail. Decision tree, as the name suggests, is a classifier based on a series of logical decisions, which resembles a tree with branches.

EXAMPLE OF SUPERVISED LEARNING

In supervised learning, the labelled training data provide the basis for learning. According to the definition of machine learning, this labelled training data is the experience or prior knowledge or belief. It is called supervised learning because the process of learning from the training data by a machine can be related to a teacher supervising the learning process of a student who is new to the subject. Here, the teacher is the training data.

Training data is the past information with known value of class field or '**label**'. Hence, we say that the '**training data islabelled**' in the case of supervised learning (refer Fig. 7.1). Contrary to this, there is no labelled training data for unsupervised learning. Semi-supervised learning, as depictedin Figure 7.1, uses a small amount of labelled data along withunlabelled data for training.

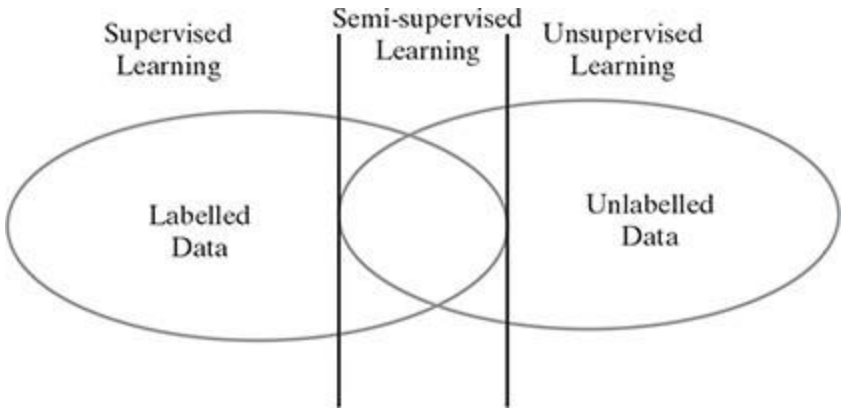


FIG. 7.1 Supervised learning vs. unsupervised learning

In a hospital, many patients are treated in the general wards.In comparison, the number of beds in the Intensive Care Unit (ICU) is much less. So, it is always a cause of worry for the hospital management that if the health condition of a number of patients in the general ward suddenly aggravates and they would have to be moved to ICU. Without previous planning and preparations, such a spike in demand becomes difficult forthe hospital to manage. This problem can be addressed in a much better way if it is possible to predict which of the patients in the normal wards have a possibility of their health condition deteriorating and thus need to be moved to ICU.

This kind of prediction problem comes under the purview ofsupervised learning or, more specifically, under classification. The hospital already has all past patient records. The records of the patients whose health condition aggravated in the past and had to be moved to ICU can form the training data for this prediction problem. Test results of newly admitted patients areused to classify them as high-risk or low-risk patients.

Some more examples of supervised learning are as follows:

- Prediction of results of a game based on the past analysis of results
- Predicting whether a tumour is malignant or benign on the basis of the analysis of data
- Price prediction in domains such as real estate, stocks, etc.

7.1 CLASSIFICATION MODEL

Let us consider two examples, say 'predicting whether a tumour is malignant or benign' and 'price prediction in the domain of real estate'. Are these two problems same in nature?

The answer is 'no'. It is true that both of them are problems related to prediction. However, for tumour prediction, we are trying to predict which category or class, i.e. 'malignant' or 'benign', an unknown input data related to tumour belongs to. In the other case, that is, for price prediction, we are trying to predict an absolute value and not a class.

When we are trying to predict a categorical or nominal variable, the problem is known as a classification problem. A classification problem is one where the output variable is a category such as 'red' or 'blue' or 'malignant tumour' or 'benign tumour', etc.

Whereas when we are trying to predict a numerical variable such as 'price', 'weight', etc. the problem falls under the category of regression.

We can observe that in classification, the whole problem centres around assigning a label or category or class to a test data on the basis of the label or category or class information that is imparted by the training data. Because the target objective is to assign a class label, we call this type of problem as a classification problem. Figure 7.2 depicts the typical process of classification where a classification model is obtained from the labelled training data by a classifier algorithm. On the basis of the model, a class label (e.g. 'Intel' as in the case of the test data referred in Fig. 7.2) is assigned to the test data.

A critical classification problem in the context of the banking domain is identifying potentially fraudulent transactions. Because there are millions of transactions which have to be scrutinized to identify whether a particular transaction might be a fraud transaction, it is not possible for any human being to carry out this task. Machine learning is leveraged efficiently to do this task, and this is a classic case of classification. On the basis of the past transaction data, especially the ones labelled as fraudulent, all new incoming transactions are marked or labelled as usual or suspicious. The suspicious transactions are subsequently segregated for a closer review.

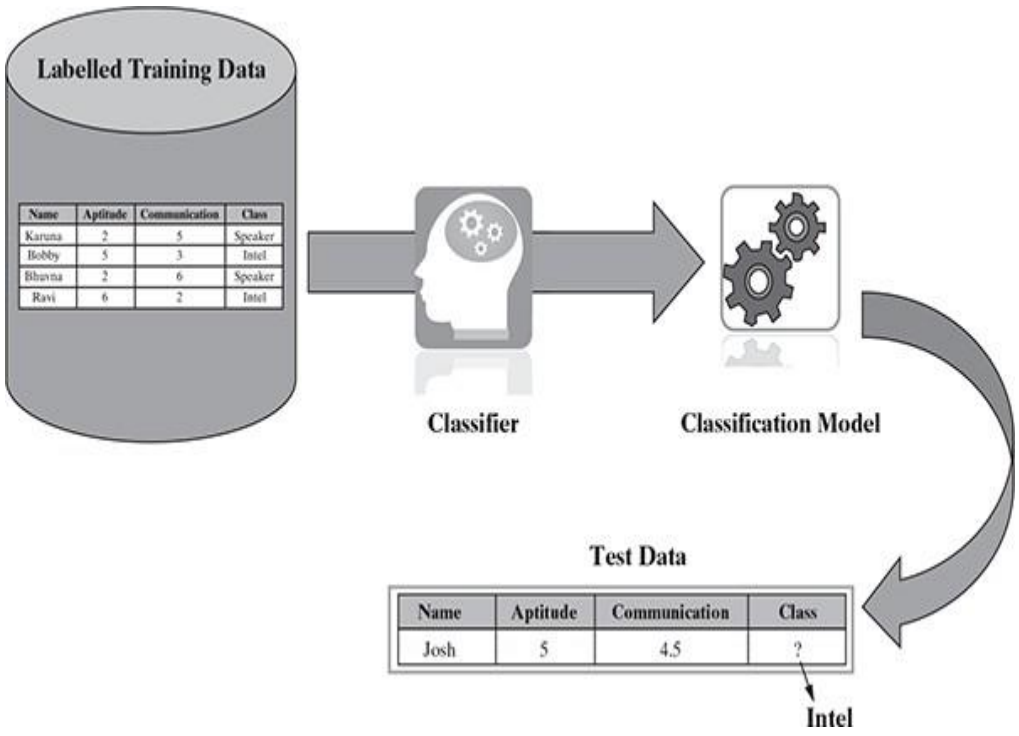


FIG. 7.2 Classification model

In summary, classification is a type of supervised learning where a target feature, which is of categorical type, is predicted for test data on the basis of the information impartedby the training data. The target categorical feature is known as**class** .

Some typical classification problems include the following:

- Image classification Disease
- prediction
- Win–loss prediction of games
- Prediction of natural calamity such as earthquake, flood, etc. Handwriting
- recognition :

CLASSIFICATION LEARNING STEPS

First, there is a problem which is to be solved, and then, the required data (related to the problem, which is already stored in the system) is evaluated and pre-processed based on the algorithm. Algorithm selection is a critical point in supervised learning. The result after iterative training rounds is a classifierfor the problem in hand (refer Fig. 7.3).

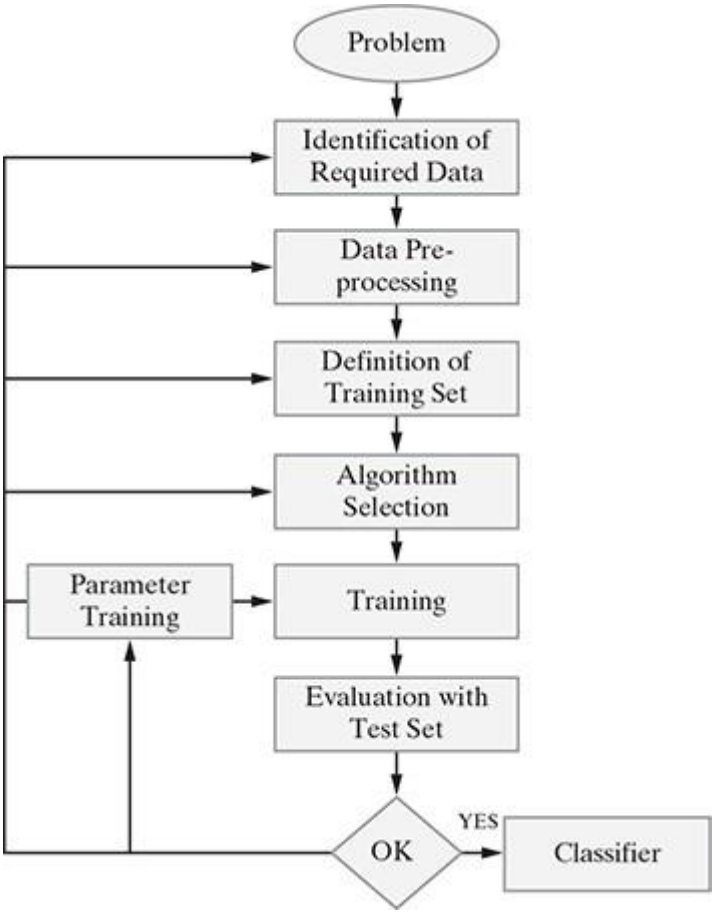


FIG. 7.C Classification model steps

Problem Identification: Identifying the problem is the first step in the supervised learning model. The problem needs to be a well-formed problem,i.e. a problem with well-defined goals and benefit, which has a long-term impact.

Identification of Required Data: On the basis of the problem identified above, the required data set that precisely represents the identified problem needs to be identified/evaluated. For example: If the problem is to predict whether a tumour is malignant or benign, then the corresponding patient data sets related to malignant tumour and benign tumours are to be identified.

Data Pre-processing: This is related to the cleaning/transforming the data set. This step ensures that all the unnecessary/irrelevant data elements are removed. Data pre-processing refers to the transformations applied to the identified data before feeding the same into the algorithm.

Because the data is gathered from different sources, it is usually collected in a raw format and is not ready for immediate analysis. This step ensures that the data is ready to be fed into the machine learning algorithm.

Definition of Training Data Set: Before starting the analysis, the user should decide what kind of data set is to be used as a training set. In the case of signature analysis, for example, the training data set might be a single handwritten alphabet, an entire handwritten word (i.e. a group of the alphabets) or an entire line of handwriting (i.e. sentences or a group of words). Thus, a set of 'input meta-objects' and corresponding 'output meta-objects' are also gathered. The training set needs to be actively representative of the real-world use of the given scenario. Thus, a set of data input (X) and corresponding outputs (Y) is gathered either from human experts or experiments.

Algorithm Selection: This involves determining the structureof the learning function and the corresponding learning algorithm. This is the most critical step of supervised learningmodel. On the basis of various parameters, the best algorithmfor a given problem is chosen.

Training: The learning algorithm identified in the previous step is run on the gathered training set for further fine tuning. Some supervised learning algorithms require the user to determine specific control parameters (which are given as inputs to the algorithm). These parameters (inputs given to algorithm) may also be adjusted by optimizing performance ona subset (called as validation set) of the training set.

Evaluation with the Test Data Set: Training data is run on the algorithm, and its performance is measured here. If a suitable result is not obtained, further training of parametersmay be required.

COMMON CLASSIFICATION ALGORITHMS

Let us now delve into some common classification algorithms. Following are the most common classification algorithms, outof which we have already learnt about the Naïve Bayes classifier in Chapter 6. We will cover details of the other algorithms in this chapter.

1. *k*-Nearest Neighbour (*k*NN)
2. Decision tree
3. Random forest
4. Support Vector Machine (SVM)
5. Naïve Bayes classifier

k -Nearest Neighbour (*k*NN)

The *k*NN algorithm is a simple but extremely powerful classification algorithm. The name of the algorithm originates from the underlying philosophy of *k*NN – i.e. people having similar background or mindset tend to stay close to each other.In other words, neighbours in a locality have a similar background. In the same way, as a part of the *k*NN algorithm, the unknown and unlabelled data which comes for a prediction problem is judged on the basis of the training data set elements which are similar to the unknown element. So, the class label of the unknown element is assigned on the basis of the class labels of the similar training data set elements (metaphorically

can be considered as neighbours of the unknown element). Let us try to understand the algorithm with a simple data set.

How kNN works

Let us consider a very simple Student data set as depicted in Figure 7.4. It consists of 15 students studying in a class. Eachof the students has been assigned a score on a scale of 10 on two performance parameters – 'Aptitude' and 'Communication'. Also, a class value is assigned to each student based on the following criteria:

1. Students having good communication skills as well as a good level of aptitude have been classified as 'Leader'
2. Students having good communication skills but not so good level of aptitude have been classified as 'Speaker'
3. Students having not so good communication skill but a good level of aptitude have been classified as 'Intel'

Name	Aptitude	Communication	Class
Karuna	2	5	Speaker
Bhuvna	2	6	Speaker
Gaurav	7	6	Leader
Parul	7	2.5	Intel
Dinesh	8	6	Leader
Jani	4	7	Speaker
Bobby	5	3	Intel
Parimal	3	5.5	Speaker
Govind	8	3	Intel
Susant	6	5.5	Leader
Gouri	6	4	Intel
Bharat	6	7	Leader
Ravi	6	2	Intel
Pradeep	9	7	Leader
Josh	5	4.5	Intel

FIG. 7.4 Student data set

As we have already discussed, in the *k*NN algorithm, the class label of the test data elements is decided by the class label of the training data elements which are neighbouring, i.e.similar in nature. But there are two challenges:

1. What is the basis of this similarity or when can we say that two data elements are similar?
2. How many similar elements should be considered for deciding the class label of each test data element?

To answer the first question, though there are many measures of similarity, the most common approach adopted by *k*NN to measure similarity between two data elements is Euclidean distance. Considering a very simple data set having two features (say f_1 and f_2), Euclidean distance between two data elements d_1 and d_2 can be measured by

$$\text{Euclidean distance} = \sqrt{(f_{11} - f_{12})^2 + (f_{21} - f_{22})^2}$$

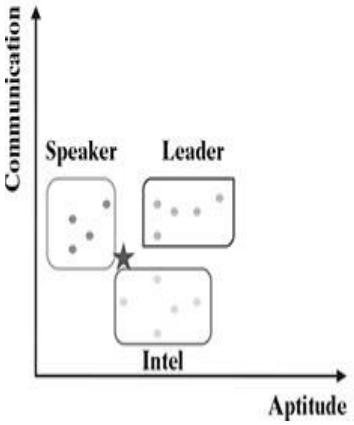
where f_{11} = value of feature f_1 for data element $d_1 f_{12}$ = value of feature f_1 for data element d_2

f_{21} = value of feature f_2 for data element $d_1 f_{22}$ = value of feature f_2 for data element d_2

	Name	Aptitude	Communication	Class
Training Data	Karuna	2	5	Speaker
	Bhuvna	2	6	Speaker
	Gaurav	7	6	Leader
	Parul	7	2.5	Intel
	Dinesh	8	6	Leader
	Jani	4	7	Speaker
	Bobby	5	3	Intel
	Parimal	3	5.5	Speaker
	Govind	8	3	Intel
	Susant	6	5.5	Leader
	Gouri	6	4	Intel
	Bharat	6	7	Leader
	Ravi	6	2	Intel
	Pradeep	9	7	Leader
Test Data →	Josh	5	4.5	Intel

FIG. 7.5 Segregated student data set

So, as depicted in Figure 7.6, the training data points of the Student data set considering only the features 'Aptitude' and 'Communication' can be represented as dots in a two-dimensional feature space. As shown in the figure, the training data points having the same class value are coming close to each other. The reason for considering two-dimensional data space is that we are considering just the two features of the Student data set, i.e. 'Aptitude' and 'Communication', for doing the classification. The feature 'Name' is ignored because, as we can understand, it has no role to play in deciding the class value. The test data point for student Josh is represented as an asterisk in the same space. To find out the closest or nearest neighbours of the test data point, Euclidean distance of the different dots need to be calculated from the asterisk. Then, the class value of the closest neighbours helps in assigning the class value of the test data element.



Name	Aptitude	Communication	Class
Karuna	2	5	Speaker
Bhuvna	2	6	Speaker
Gaurav	7	6	Leader
Parul	7	2.5	Intel
Dinesh	8	6	Leader
Jani	4	7	Speaker
Bobby	5	3	Intel
Parimal	3	5.5	Speaker
Govind	8	3	Intel
Susant	6	5.5	Leader
Gouri	6	4	Intel
Bharat	6	7	Leader
Ravi	6	2	Intel
Pradeep	9	7	Leader
Josh	5	4.5	???

FIG. 7.6 2-D representation of the student data set

Now, let us try to find the answer to the second question, i.e. how many similar elements should be considered. The answer lies in the value of '*k*' which is a user-defined parameter given

as an input to the algorithm. In the *k*NN algorithm, the value of '*k*' indicates the number of neighbours that need to be considered. For example, if the value of *k* is 3, only three nearest neighbours or three training data elements closest to the test data element are considered. Out of the three data elements, the class which is predominant is considered as the class label to be assigned to the test data. In case the value of *k*is 1, only the closest training data element is considered. The class label of that data element is directly assigned to the test data element. This is depicted in Figure 7.7.

Name	Aptitude	Communication	Class	Distance	*k* = 1	*k* = 2	*k* = 3
Karuna	2	5	Speaker	3.041			
Bhuvna	2	6	Speaker	3.354			
Parimal	3	5.5	Speaker	2.236			
Jani	4	7	Speaker	2.693			
Bobby	5	3	Intel	1.500			1.500
Ravi	6	2	Intel	2.693			
Gouri	6	4	Intel	1.118	1.118	1.118	1.118
Parul	7	2.5	Intel	2.828			
Govind	8	3	Intel	3.354			
Susant	6	5.5	Leader	1.414			
Bharat	6	7	Leader	2.693			
Gaurav	7	6	Leader	2.500			
Dinesh	8	6	Leader	3.354			
Pradeep	9	7	Leader	4.717			
Josh	5	4.5	???				

FIG. 7.7 Distance calculation between test and training points

Let us now try to find out the outcome of the algorithm forthe Student data set we have. In other words, we want to see what class value *k*NN will assign for the test data for student Josh. Again, let us refer back to Figure 7.7. As is evident, when the value of *k* is taken as 1, only one training data pointneeds to be considered. The training record for student Gouri comes as the closest one to test record of Josh, with a distance value of 1.118. Gouri has class value 'Intel'. So, the test data point is also assigned a class label value 'Intel'. When the value of *k* is assumed as 3, the closest neighbours of Josh in the training data set are Gouri, Susant, and Bobby with distances being 1.118, 1.414, and 1.5, respectively. Gouri and Bobby have class value 'Intel', while Susant has class value 'Leader'. In this case, the class value of Josh is decided by majority voting. Because the class value of 'Intel' is formed bythe majority of the neighbours, the class value of Josh is assigned as 'Intel'. This same process can be extended for any value of *k*.

But it is often a tricky decision to decide the value of *k*. Thereasons are as follows:

- If the value of *k* is very large (in the extreme case equal to the total number of records in the training data), the class label of the majority class of the training data set will be assigned to the test data regardless of the class labelsof the neighbours nearest to the test data.
- If the value of *k* is very small (in the extreme case equal to 1), the class valueof a noisy data or outlier in the training data set which is the nearest neighbour to the test

data will be assigned to the test data.

The best *k* value is somewhere between these two extremes.

Few strategies, highlighted below, are adopted by machine learning practitioners to arrive at a value for *k*.

- One common practice is to set *k* equal to the square root of the number of training records.
- An alternative approach is to test several *k* values on a variety of test datasets and choose the one that delivers the best performance.
- Another interesting approach is to choose a larger value of *k*, but apply a weighted voting process in which the vote of close neighbours is consideredmore influential than the vote of distant neighbours.

kNN algorithm

Input: Training data set, test data set (or data points), value of '*k*' (i.e. number of nearest neighbours to be considered)

Steps:

Do for all test data points

Calculate the distance (usually Euclidean distance) of the test data point from the different training data points.
Find the closest '*k*' training data points, i.e. training data points whosedistances are least from the test data point.

If *k* = 1

Then assign class label of the training data point to the test data point

Else

Whichever class label is predominantly present in the training data points,assign that class label to the test data point

End do

Why the kNN algorithm is called a lazy learner?

We have already discussed in Chapter 3 that eager learners follow the general steps of machine learning, i.e. perform an abstraction of the information obtained from the input data andthen follow it through by a generalization step. However, as we have seen in the case of the kNN algorithm, these steps arecompletely skipped. It stores the training data and directly applies the philosophy of nearest neighbourhood finding to arrive at the classification. So, for *k*NN, there is no learning happening in the real sense. Therefore, *k*NN falls under the category of lazy learner.

Strengths of the kNN algorithm

- Extremely simple algorithm – easy to understand
- Very effective in certain situations, e.g. for recommender system design Very
- fast or almost no time required for the training phase

Weaknesses of the kNN algorithm

- Does not learn anything in the real sense. Classification is done completely on the basis of the training data. So, it has a heavy reliance on the training data. If the training data does not represent the problem domain comprehensively, the algorithm fails to make an effective classification.
- Because there is no model trained in real sense and the classification is done completely on the basis of the training data, the classification process is very slow.
- Also, a large amount of computational space is required to load the training data for classification.

Application of the kNN algorithm

One of the most popular areas in machine learning where the *k*NN algorithm is widely adopted is recommender systems. As we know, recommender systems recommend users different items which are similar to a particular item that the user seems to like. The liking pattern may be revealed from past purchases or browsing history and the similar items are identified using the *k*NN algorithm.

Another area where there is widespread adoption of *k*NN issearching documents/ contents similar to a given document/content. This is a core area under information retrieval and is known as concept search.

Decision tree

Decision tree learning is one of the most widely adopted algorithms for classification. As the name indicates, it builds a model in the form of a tree structure. Its grouping exactness is focused with different strategies, and it is exceptionally productive.

A decision tree is used for multi-dimensional analysis with multiple classes. It is characterized by fast execution time and

ease in the interpretation of the rules. The goal of decision tree learning is to create a model (based on the past data called past vector) that predicts the value of the output variable based on the input variables in the feature vector.

Each node (or decision node) of a decision tree corresponds to one of the feature vector. From every node, there are edges to children, wherein there is an edge for each of the possible values (or range of values) of the feature associated with the node. The tree terminates at different leaf nodes (or terminal nodes) where each leaf node represents a possible value for theoutput variable. The output variable is determined by following a path that starts at the root and is guided by the values of the input variables.

A decision tree is usually represented in the format depictedin Figure 7.8.

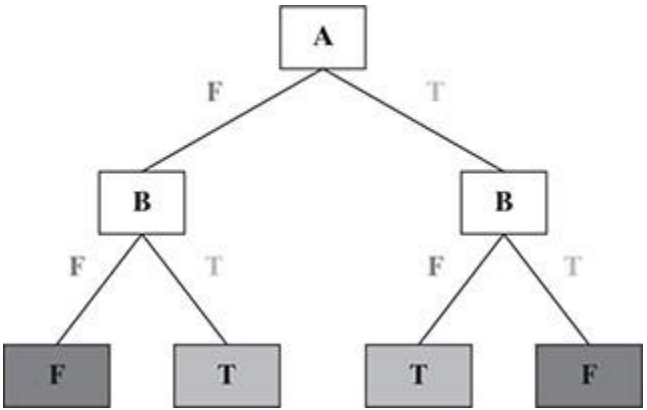


FIG. 7.8 Decision tree structure

Each internal node (represented by boxes) tests an attribute (represented as 'A'/'B' within the boxes). Each branch corresponds to an attribute value (T/F) in the above case. Each leaf node assigns a classification. The first node is called as 'Root' Node. Branches from the root node are called as 'Leaf'

Nodes where 'A' is the Root Node (first node). 'B' is the Branch Node. 'T' & 'F' are Leaf Nodes.

Thus, a decision tree consists of three types of nodes:

- Root Node
- Branch Node
- Leaf Node

Figure 7.9 shows an example decision tree for a car driving

— the decision to be taken is whether to 'Keep Going' or to 'Stop', which depends on various situations as depicted in the figure. If the signal is RED in colour, then the car should be stopped. If there is not enough gas (petrol) in the car, the car should be stopped at the next available gas station.

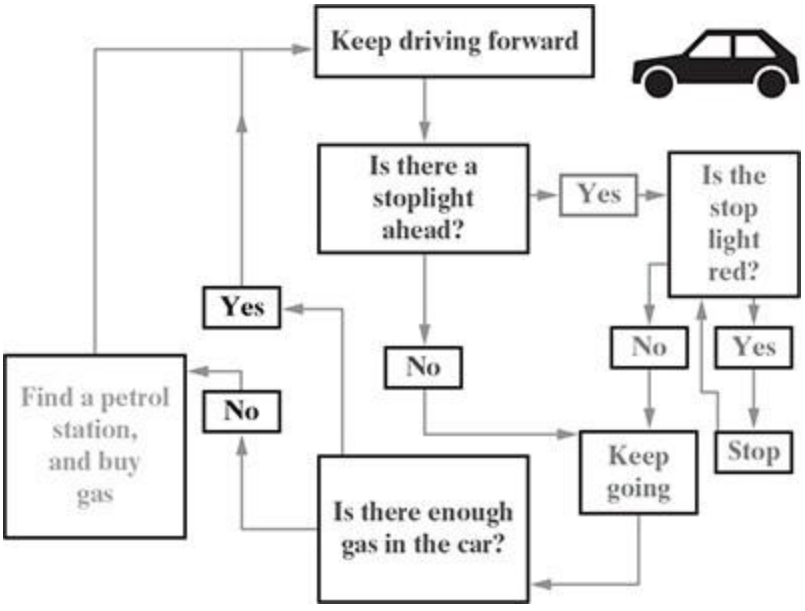


FIG. 7.9 Decision tree example

Building a decision tree

Decision trees are built corresponding to the training data following an approach called recursive partitioning. The

approach splits the data into multiple subsets on the basis of the feature values. It starts from the root node, which is nothing but the entire data set. It first selects the feature whichpredicts the target class in the strongest way. The decision tree splits the data set into multiple partitions, with data in each partition having a distinct value for the feature based on whichthe partitioning has happened. This is the first set of branches.Likewise, the algorithm continues splitting the nodes on the basis of the feature which helps in the best partition. This continues till a stopping criterion is reached. The usual stopping criteria are –

1. All or most of the examples at a particular node have the same class
2. All features have been used up in the partitioning
3. The tree has grown to a pre-defined threshold limit

Let us try to understand this in the context of an example. Global Technology Solutions (GTS), a leading provider of IT solutions, is coming to College of Engineering and Management (CEM) for hiring B.Tech. students. Last year during campus recruitment, they had shortlisted 18 students for the final interview. Being a company of international repute, they follow a stringent interview process to select only the best of the students. The information related to the interview evaluation results of shortlisted students (hiding the names) on the basis of different evaluation parameters is available for reference in Figure 7.10. Chandra, a student of CEM, wants to find out if he may be offered a job in GTS. His CGPA is quite high. His self-evaluation on the other parameters is as follows:

Communication – Bad; Aptitude – High; Programming skills – Bad

CGPA	Communication	Aptitude	Programming Skill	Job offered?
High	Good	High	Good	Yes
Medium	Good	High	Good	Yes
Low	Bad	Low	Good	No
Low	Good	Low	Bad	No
High	Good	High	Bad	Yes
High	Good	High	Good	Yes
Medium	Bad	Low	Bad	No
Medium	Bad	Low	Good	No
High	Bad	High	Good	Yes
Medium	Good	High	Good	Yes
Low	Bad	High	Bad	No
Low	Bad	High	Bad	No
Medium	Good	High	Bad	Yes
Low	Good	Low	Good	No
High	Bad	Low	Bad	No
Medium	Bad	High	Good	No
High	Bad	Low	Bad	No
Medium	Good	High	Bad	Yes

FIG. 7.1O Training data for GTS recruitment

Let us try to solve this problem, i.e. predicting whether Chandra will get a job offer, by using the decision tree model. First, we need to draw the decision tree corresponding to the training data given in Figure 7.10. According to the table, job offer condition (i.e. the outcome) is FALSE for all the cases where **Aptitude = Low**, irrespective of other conditions. So, the feature Aptitude can be taken up as the first node of the decision tree.

For **Aptitude = High**, job offer condition is TRUE for all the cases where **Communication = Good**. For cases where **Communication = Bad**, job offer condition is TRUE for allthe cases where **CGPA = High**.

Figure 7.11 depicts the complete decision tree diagram forthe table given in Figure 7.10.

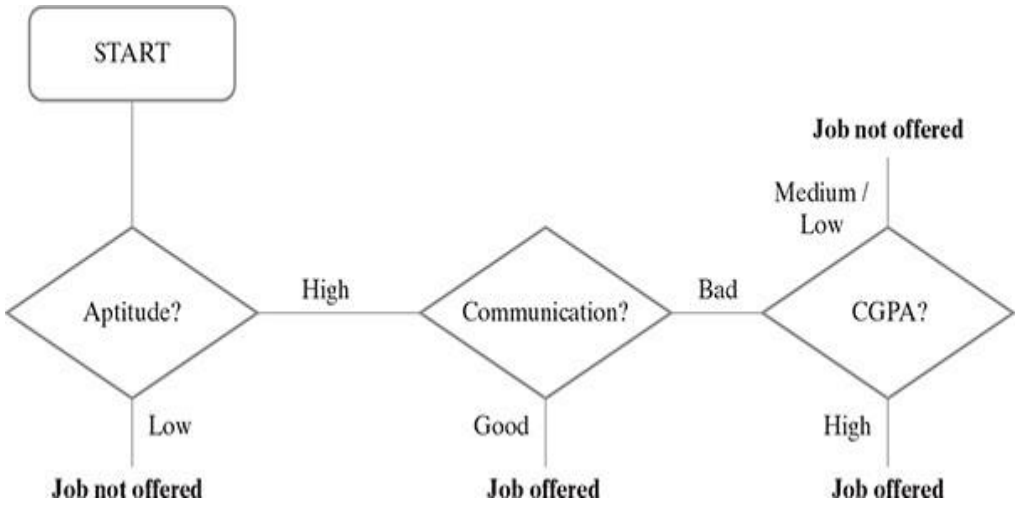


FIG. 7.11 Decision tree based on the training data

Searching a decision tree

By using the above decision tree depicted in Figure 7.11, we need to predict whether Chandra might get a job offer for the given parameter values: CGPA = **High**, Communication = **Bad**, Aptitude = **High**, Programming skills = **Bad**. There are multiple ways to search through the trained decision tree for asolution to the given prediction problem.

Exhaustive search

1. Place the item in the first group (class). Recursively examine solutions with the item in the first group (class).
2. Place the item in the second group (class). Recursively examine solutions with the item in the second group (class).
3. Repeat the above steps until the solution is reached.

Exhaustive search travels through the decision tree exhaustively, but it will take much time when the decision treeis big with multiple leaves and multiple attribute values.

Branch and bound search

Branch and bound uses an existing best solution to sidestep searching of the entire decision

tree in full. When the algorithm starts, the best solution is well defined to have the worst possible value; thus, any solution it finds out is an improvement. This makes the algorithm initially run down to the left-most branch of the tree, even though that is unlikely toproduce a realistic result. In the partitioning problem, that solution corresponds to putting every item in one group, and itis an unacceptable solution. A programme can speed up the process by using a fast heuristic to find an initial solution. Thiscan be used as an input for branch and bound. If the heuristic is right, the savings can be substantial.

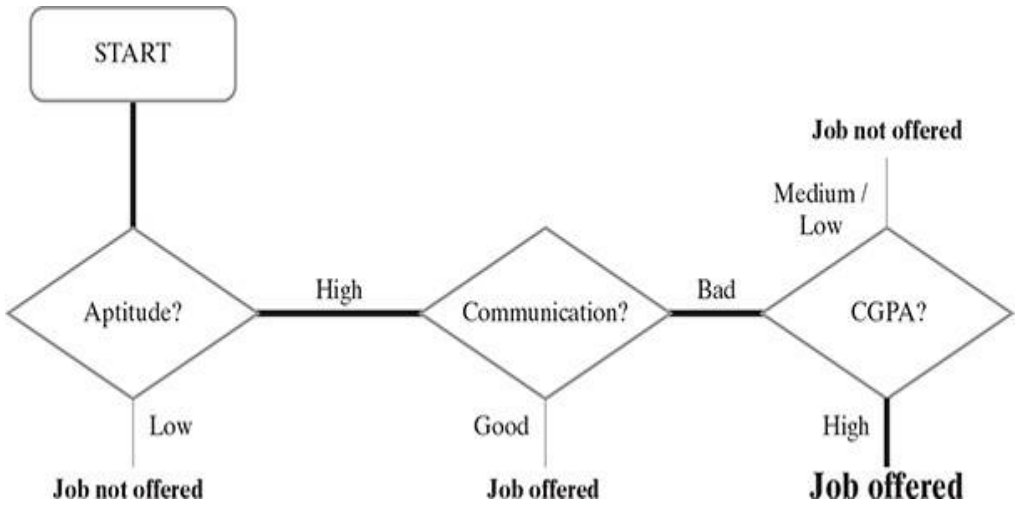


FIG. 7.12 Decision tree based on the training data (depicting a sample path)

Figure 7.12 depicts a sample path (thick line) for the conditions CGPA = **High**, Communication = Bad, Aptitude = High and Programming skills = Bad. According to the above decision tree, the prediction can be made as Chandra **will getthe job offer**.

There are many implementations of decision tree, the most prominent ones being C5.0, CART (Classification and Regression Tree), CHAID (Chi-square Automatic Interaction Detector) and ID3 (Iterative Dichotomiser 3) algorithms. The biggest challenge of a decision tree algorithm is to find out which feature to split upon. The main driver for identifying the feature is that the data should be split in such a way that the partitions created by the split should contain examples belonging to a single class. If that happens, the partitions are considered to be **pure**. Entropy is a measure of impurity of an attribute or feature adopted by many algorithms such as ID3 and C5.0. The information gain is calculated on the basis of the decrease in entropy (S) after a data set is split according to a particular attribute (A). Constructing a decision tree is all about finding an attribute that returns the highest information gain (i.e. the most homogeneous branches).

Entropy of a decision tree

Let us say S is the sample set of training examples. Then, Entropy (S) measuring the impurity of S is defined as

$$\textbf{Entropy}(S) = \sum_{i=1}^{c} - p_i \log_2 p_i$$

where c is the number of different class labels and p refers to the proportion of values falling into the *i*-th class label.

For example, with respect to the training data in Figure 7.10, we have two values for the target class 'Job Offered?' – Yes and No. The value of p_i for class value 'Yes' is 0.44 (i.e. 8/18) and that for class value 'No' is 0.56 (i.e. 10/18). So, we can calculate the entropy as

$$\textbf{Entropy}(S) = -0.44 \log_2(0.44) - 0.56 \log_2(0.56) = 0.99.$$

Information gain of a decision tree

The information gain is created on the basis of the decrease in entropy (*S*) after a data set is split according to a particular attribute (*A*). Constructing a decision tree is all about finding an attribute that returns the highest information gain (i.e. the most homogeneous branches). If the information gain is 0, it means that there is no reduction in entropy due to split of the data set according to that particular feature. On the other hand, the maximum amount of information gain which may happen is the entropy of the data set before the split.

Information gain for a particular feature A is calculated by the difference in entropy before a split (or S_{bs}) with the entropy after the split (S_{as}).

$$\textbf{Information Gain (S, A) = Entropy } (S_{bs}) - \textbf{Entropy } (S_{as})$$

For calculating the entropy after split, entropy for all partitions needs to be considered. Then, the weighted summation of the entropy for each partition can be taken as the total entropy after split. For performing weighted summation, the proportion of examples falling into each partition is used as weight.

$$\textbf{Entropy}(S_{as}) = \sum_{i=1}^{n} w_i \text{ Entropy } (p_i)$$

Let us examine the value of information gain for the training data set shown in Figure 7.10. We will find the value of entropy at the beginning before any split happens and then again after the split happens. We will compare the values for all the cases –

1. when the feature 'CGPA' is used for the split
2. when the feature 'Communication' is used for the split
3. when the feature 'Aptitude' is used for the split
4. when the feature 'Programming Skills' is used for the split

Figure 7.13a gives the entropy values for the first level split for each of the cases mentioned above.

As calculated, entropy of the data set before split (i.e. Entropy (S_{bs})) = 0.99, and entropy of the data set after split(i.e. Entropy (S_{as})) is

- 0.69 when the feature 'CGPA' is used for split
- 0.63 when the feature 'Communication' is used for split
- 0.52 when the feature 'Aptitude' is used for split
- 0.95 when the feature 'Programming skill' is used for split

(a) Original data set:

	Yes	No	Total
Count	8	10	18
pi	0.44	0.56	
-pi*log(pi)	0.52	0.47	0.99

Total Entropy = 0.99

(b) Splitted data set (based on the feature 'CGPA'):

CGPA = High

	Yes	No	Total
Count	4	2	6
pi	0.67	0.33	
-pi*log(pi)	0.39	0.53	0.92

Total Entropy = 0.69

CGPA = Medium

	Yes	No	Total
Count	4	3	7
pi	0.57	0.43	
-pi*log(pi)	0.46	0.52	0.99

Information Gain = 0.30

CGPA = Low

	Yes	No	Total
Count	0	5	5
pi	0.00	1.00	
-pi*log(pi)	0.00	0.00	0.00

(c) Splitted data set (based on the feature 'Communication'):

Communication = Good

	Yes	No	Total
Count	7	2	9
pi	0.78	0.22	
-pi*log(pi)	0.28	0.48	0.76

Total Entropy = 0.63

Communication = Bad

	Yes	No	Total
Count	1	8	9
pi	0.11	0.89	
-pi*log(pi)	0.35	0.15	0.50

Information Gain = 0.36

(d) Splitted data set (based on the feature 'Aptitude'):

Aptitude = High

	Yes	No	Total
Count	8	3	11
pi	0.73	0.27	
-pi*log(pi)	0.33	0.51	0.85

Total Entropy = 0.52

Aptitude = Low

	Yes	No	Total
Count	0	7	7
pi	0.00	1.00	
-pi*log(pi)	0.00	0.00	0.00

Information Gain = 0.47

(e) Splitted data set (based on the feature 'Programming Skill'):

Programming Skill = Good

Programming Skill = Bad

	Yes	No	Total
Count	5	4	9
pi	0.56	0.44	
-pi*log(pi)	0.47	0.52	0.99

Total Entropy = 0.95

	Yes	No	Total
Count	3	6	9
pi	0.33	0.67	
-pi*log(pi)	0.53	0.39	092

Information Gain = 0.04

FIG. 7.1CA Entropy and information gain calculation (Level 1)

Therefore, the information gain from the feature 'CGPA' = 0.99 − 0.69 = 0.3, whereas the information gain from the feature 'Communication' = 0.99 − 0.63 = 0.36. Likewise, theinformation gain for 'Aptitude' and 'Programming skills' is 0.47 and 0.04, respectively.

Hence, it is quite evident that among all the features, 'Aptitude' results in the best information gain when adopted for the split. So, at the first level, a split will be applied according to the value of 'Aptitude' or in other words, 'Aptitude' will be the first node of the decision tree formed. One important point to be noted here is that for **Aptitude = Low**, entropy is 0, which indicates that always the result willbe the same irrespective of the values of the other features.
Hence, the branch towards Aptitude = Low will not continueany further.

As a part of level 2, we will thus have only one branch tonavigate in this case – the one for **Aptitude = High**. Figure 7.13b presents calculations for level 2. As can be seen fromthe figure, the entropy value is as follows:

- 0.85 before the split
- 0.33 when the feature 'CGPA' is used for split
- 0.30 when the feature 'Communication' is used for split
- 0.80 when the feature 'Programming skill' is used for split

Hence, the information gain after split with the features CGPA, Communication and Programming Skill is 0.52, 0.55 and 0.05, respectively. Hence, the feature Communication should be used for this split as it results in the highest information gain. So, at the second level, a split will be applied on the basis of the value of 'Communication'. Again, the point to be noted here is that for **Communication = Good**, entropy is 0, which indicates that always the result will be the same irrespective of the values of the other features. Hence, the branch towards Communication = Good will not continue any further.

Aptitude = High

CGPA	Communication	Programming Skill	Job offered?
High	Good	Good	Yes
Medium	Good	Good	Yes
High	Good	Bad	Yes
High	Good	Good	Yes
High	Bad	Good	Yes
Medium	Good	Good	Yes
Low	Bad	Bad	No
Low	Bad	Bad	No
Medium	Good	Bad	Yes
Medium	Bad	Good	No
Medium	Good	Bad	Yes

(a) Level 2 starting set:

	Yes	No	Total
Count	8	3	11
pi	0.73	0.27	
-pi*log(pi)	0.33	0.51	0.85

Total Entropy = 0.85

(b) Splitted data set (based on the feature 'CGPA'):

CGPA = High **CGPA = Medium** **CGPA = Low**

	Yes	No	Total
Count	4	0	4
pi	1.00	0.00	
-pi*log(pi)	0.00	0.00	0.00

	Yes	No	Total
Count	4	1	5
pi	0.80	0.20	
-pi*log(pi)	0.26	0.46	0.72

	Yes	No	Total
Count	0	2	2
pi	0.00	1.00	
-pi*log(pi)	0.00	0.00	0.00

Total Entropy = 0.33 Information Gain = 0.52

(c) Splitted data set (based on the feature 'Communication'):

Communication = Good Communication = Bad

	Yes	No	Total
Count	7	0	7
pi	1.00	0.00	
-pi*log(pi)	0.00	0.00	0.00

	Yes	No	Total
Count	1	3	4
pi	0.25	0.75	
-pi*log(pi)	0.50	0.31	0.81

Total Entropy = 0.30 Information Gain = 0.55

(d) Spitted data set (based on the feature 'Programming Skill'):

Programming Skill = Good Programming Skill = Bad

	Yes	No	Total
Count	5	1	6
pi	0.83	0.17	
-pi*log(pi)	0.22	0.43	0.65

	Yes	No	Total
Count	3	2	5
pi	0.60	0.40	
-pi*log(pi)	0.44	0.53	0.97

Total Entropy = 0.80 Information Gain = 0.05

FIG. 7.1CB Entropy and information gain calculation (Level 2)

As a part of level 3, we will thus have only one branch to navigate in this case – the one for **Communication = Bad**. Figure 7.13c presents calculations for level 3. As can be seen from the figure, the entropy value is as follows:

- 0.81 before the split
- 0 when the feature 'CGPA' is used for split

- 0.50 when the feature 'Programming Skill' is used for split

Aptitude = High & Communication = Bad

CGPA	Programming Skill	Job offered?
High	Good	Yes
Low	Bad	No
Low	Bad	No
Medium	Good	No

(a) Level 2 starting set:

	Yes	No	Total
Count	1	3	4
pi	0.25	0.75	
-pi*log(pi)	0.50	0.31	0.81

Total Entropy = 0.81

(b) Splitted data set (based on the feature 'CGPA'):

CGPA = High

	Yes	No	Total
Count	1	0	1
pi	1.00	0.00	
-pi*log(pi)	0.00	0.00	0.00

Total Entropy = 0.00

CGPA = Medium

	Yes	No	Total
Count	0	1	1
pi	0.00	1.00	
-pi*log(pi)	0.00	0.00	0.00

Information Gain = 0.81

CGPA = Low

	Yes	No	Total
Count	0	2	2
pi	0.00	1.00	
-pi*log(pi)	0.00	0.00	0.00

(c) Splitted data set (based on the feature 'Programming Skill'):

Programming Skill = Good

	Yes	No	Total
Count	1	1	2
pi	0.50	0.50	
-pi*log(pi)	0.50	0.50	1.00

Total Entropy = 0.50

Programming Skill = Bad

	Yes	No	Total
Count	0	2	2
pi	0.00	1.00	
-pi*log(pi)	0.00	0.00	0.00

Information Gain = 0.31

FIG. 7.1CC Entropy and information gain calculation (Level 3)

Hence, the information gain after split with the feature CGPA is 0.81, which is the maximum possible information gain (as the entropy before split was 0.81). Hence, as obvious, a split will be applied on the basis of the value of 'CGPA'.
Because the maximum information gain is already achieved, the tree will not continue any further.

Algorithm for decision tree

Input: Training data set, test data set (or data points)

Steps:

Do for all attributes

Calculate the entropy E_i of the attribute F_i

if $E_i < E_{\min}$

then $E_{\min} = E_i$ and $F_{\min} = F_i$

end if

End do

Split the data set into subsets using the attribute $F_{\min}$

Draw a decision tree node containing the attribute $F_{\min}$ and split the data set into subsets
Repeat the above steps until the full tree is drawn covering all the attributes of the original table.

Avoiding overfitting in decision tree – pruning

The decision tree algorithm, unless a stopping criterion is applied, may keep growing indefinitely – splitting for every feature and dividing into smaller partitions till the point that the data is perfectly classified. This, as is quite evident, results in overfitting problem. To prevent a decision tree getting overfitted to the training data, pruning of the decision tree is essential. Pruning a decision tree reduces the size of the tree

such that the model is more generalized and can classify unknown and unlabelled data in a better way.

There are two approaches of pruning:

- Pre-pruning: Stop growing the tree before it reaches perfection.
- Post-pruning: Allow the tree to grow entirely and then post-prune some of the branches from it.

In the case of pre-pruning, the tree is stopped from further growing once it reaches a certain number of decision nodes or decisions. Hence, in this strategy, the algorithm avoids overfitting as well as optimizes computational cost. However, it also stands a chance to ignore important information contributed by a feature which was skipped, thereby resulting in miss out of certain patterns in the data.

On the other hand, in the case of post-pruning, the tree is allowed to grow to the full extent. Then, by using certain pruning criterion, e.g. error rates at the nodes, the size of the tree is reduced. This is a more effective approach in terms of classification accuracy as it considers all minute information available from the training data. However, the computational cost is obviously more than that of pre-pruning.

Strengths of decision tree

- It produces very simple understandable rules. For smaller trees, not much mathematical and computational knowledge is required to understand this model.
- Works well for most of the problems.
- It can handle both numerical and categorical variables. Can
- work well both with small and large training data sets.
- Decision trees provide a definite clue of which features are more useful for classification.

Weaknesses of decision tree

- Decision tree models are often biased towards features having more number of possible values, i.e. levels.
- This model gets overfitted or underfitted quite easily.
- Decision trees are prone to errors in classification problems with many classes and relatively small number of training examples.
- A decision tree can be computationally expensive to train. Large
- trees are complex to understand.

Application of decision tree

Decision tree can be applied in a data set in which there is a finite list of attributes and each data instance stores a value forthat attribute (e.g. 'High' for the attribute CGPA). When each attribute has a small number of distinct values (e.g. 'High', 'Medium', 'Low'), it is easier/quicker for the decision tree to suggest (or choose) an effective solution. This algorithm can be extended to handle real-value attributes (e.g. a floating point temperature).

The most straightforward case exists when there are only two possible values for an attribute (Boolean classification). Example: Communication has only two values as 'Good' or'Bad'. It is also easy to extend the decision tree to create a target function with more than two possible output values.
Example: CGPA can take one of the values from 'High', 'Medium', and 'Low'. Irrespective of whether it is a binary value/ multiple values, it is discrete in nature. For example, Aptitude can take the value of either 'High' or 'Low'. It is not possible to assign the value of both 'High' and 'Low' to the attribute Aptitude to draw a decision tree.

There should be no infinite loops on taking a decision. As we move from the root node to the next level node, it should move step-by-step towards the decision node. Otherwise, the algorithm may not give the final result for a given data. If a set
of code goes in a loop, it would repeat itself forever, unless thesystem crashes.

A decision tree can be used even for some instances with missing attributes and instances with errors in the classification of examples or in the attribute values describing those examples; such instances are handled well by decision trees, thereby making them a robust learning method.

Random forest model

Random forest is an ensemble classifier, i.e. a combining classifier that uses and combines many decision tree classifiers. Ensembling is usually done using the concept of bagging with different feature sets. The reason for using large number of trees in random forest is to train the trees enough such that contribution from each feature comes in a number of models. After the random forest is generated by combining thetrees, majority vote is applied to combine the

output of the different trees. A simplified random forest model is depicted in Figure 7.14. The result from the ensemble model is usually better than that from the individual decision tree models.

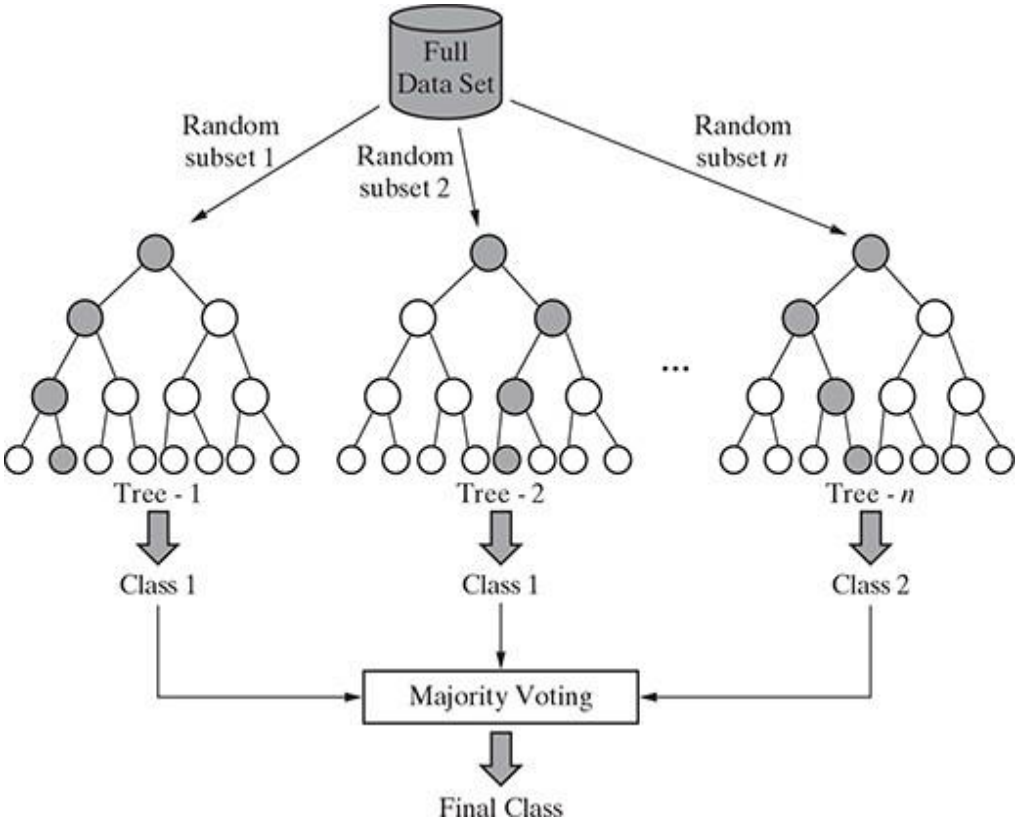


FIG. 7.14 Random forest model

How does random forest work?

The random forest algorithm works as follows:

1. If there are *N* variables or features in the input data set, select a subsetof '*m*' (*m* < *N*) features at random out of the *N* features. Also, the observations or data instances should be picked randomly.
2. Use the best split principle on these '*m*' features to calculate the number of nodes '*d*'.
3. Keep splitting the nodes to child nodes till the tree is grown to the maximum possible extent.
4. Select a different subset of the training data 'with replacement' to train another decision tree following steps (1) to (3). Repeat this to build and train '*n*' decision trees.
5. Final class assignment is done on the basis of the majority votes from the '*n*' trees.

Out-of-bag (OOB) error in random forest

In random forests, we have seen, that each tree is constructed using a different bootstrap sample from the original data. The samples left out of the bootstrap and not used in the construction of the i-th tree can be used to measure the performance of the model. At the end of the run, predictions for each such sample evaluated each time are tallied, and the final prediction for that sample is obtained by taking a vote.
The total error rate of predictions for such samples is termedas out-of-bag (OOB) error rate.

The error rate shown in the confusion matrix reflects the OOB error rate. Because of this reason, the error rate displayedis often surprisingly high.

Strengths of random forest

- It runs efficiently on large and expansive data sets.
- It has a robust method for estimating missing data and maintains precision when a large proportion of the data is absent.
- It has powerful techniques for balancing errors in a class population ofunbalanced data sets.
- It gives estimates (or assessments) about which features are the mostimportant ones in the overall classification.
- It generates an internal unbiased estimate (gauge) of the generalization error as the forest generation progresses.
- Generated forests can be saved for future use on other data.
- Lastly, the random forest algorithm can be used to solve both classification and regression problems.

Weaknesses of random forest

- This model, because it combines a number of decision tree models, is not as easy to understand as a decision tree model.
- It is computationally much more expensive than a simple model like decisiontree.

Application of random forest

Random forest is a very powerful classifier which combines the versatility of many decision tree models into a single model. Because of the superior results, this ensemble model isgaining wide adoption and popularity amongst the machine learning practitioners to solve a wide range of classification problems.

Support vector machines

SVM is a model, which can do linear classification as well as regression. SVM is based on the concept of a surface, called ahyperplane, which draws a boundary between data instances plotted in the multi-dimensional feature space. The output prediction of an SVM is one of two conceivable classes whichare already defined in the training data. In summary, the SVM algorithm builds an N-dimensional hyperplane model that assigns future instances into one of the two possible output classes.

Classification using hyperplanes

In SVM, a model is built to discriminate the data instances belonging to different classes. Let us assume for the sake of simplicity that the data instances are linearly separable. In this case, when mapped in a two-dimensional space, the data instances belonging to different classes fall in different sides of a straight line drawn in the two-dimensional space as depicted in Figure 7.15a. If the same concept is extended to a multi- dimensional feature space, the straight line dividing data instances belonging to different classes transforms to a hyperplane as depicted in Figure 7.15b.

Thus, an SVM model is a representation of the input instances as points in the feature space, which are mapped so that an apparent gap between them divides the instances of the separate classes. In other words, the goal of the SVM analysis is to find a plane, or rather a hyperplane, which separates the instances on the basis of their classes. New examples (i.e. newinstances) are then mapped into that same space and predicted to belong to a class on the basis of which side of the gap the new instance will fall on. In summary, in the overall training process, the SVM algorithm analyses input data and identifies a surface in the multi-dimensional feature space called the hyperplane. There may be many possible hyperplanes, and oneof the challenges with the SVM model is to find the optimal hyperplane.

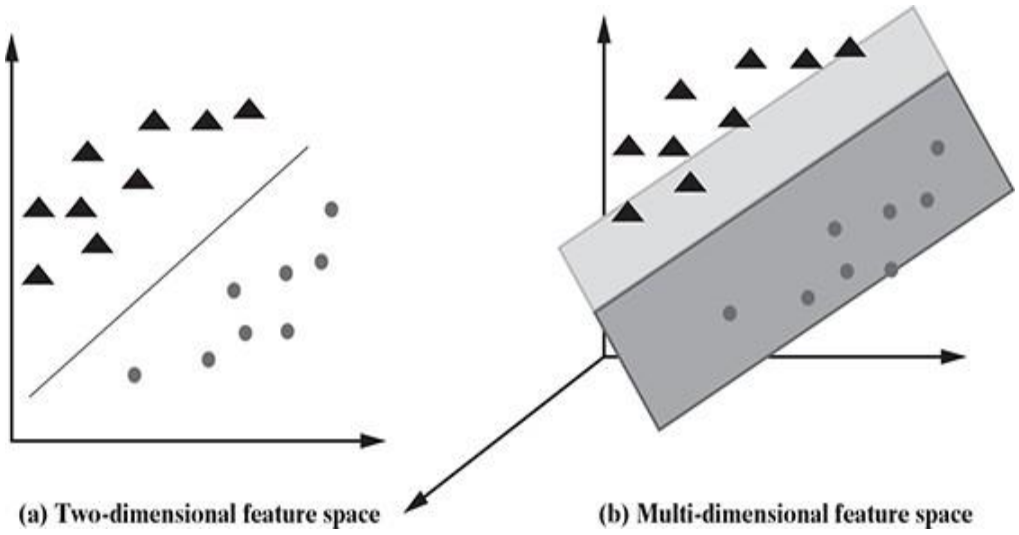


FIG. 7.15 Linearly separable data instances

Training data sets which have a substantial grouping periphery will function well with SVM. Generalization error in terms of SVM is the measure of how accurately and precisely this SVM model can predict values for previously unseen data (new data). A hard margin in terms of SVM means that an SVM model is inflexible in classification and tries to work exceptionally fit in the training set, thereby causing overfitting.

Support Vectors: Support vectors are the data points (representing classes), the critical component in a data set, which are near the identified set of lines (hyperplane). If support vectors are removed, they will alter the position of thedividing hyperplane.

Hyperplane and Margin: For an N-dimensional feature space, hyperplane is a flat subspace of dimension $(N-1)$ thatseparates and classifies a set of data. For example, if we consider a two-dimensional feature space (which is nothing but a data set having two features and a class variable), a hyperplane will be a one-dimensional subspace or a straight

line. In the same way, for a three-dimensional feature space (data set having three features and a class variable), hyperplane is a two-dimensional subspace or a simple plane. However, quite understandably, it is difficult to visualize a feature space greater than three dimensions, much like for a subspace or hyperplane having more than three dimensions.

Mathematically, in a two-dimensional space, hyperplane canbe defined by the equation:

$c_0 + c_1X_1 + c_2X_2 = 0$, which is nothing but an equation of astraight line.

Extending this concept to an *N*-dimensional space,hyperplane can be defined by the equation:

$c_0 + c_1X_1 + c_2X_2 + \ldots + c_NX_N = 0$ which, in short, can berepresented as follows:

$$\vec{c}.\vec{X} + c_0 = 0$$

Spontaneously, the further (or more distance) from the hyperplane the data points lie, the more confident we can be about correct categorization. So, when a new testing data point/data set is added, the side of the hyperplane it lands on will decide the class that we assign to it. The distance between hyperplane and data points is known as **margin**.

7.5.4.1 *Identifying the correct hyperplane in SVM*

As we have already discussed, there may be multiple options for hyperplanes dividing the data instances belonging to the different classes. We need to identify which one will result in the best classification. Let us examine a few scenarios before

arriving to that conclusion. For the sake of simplicity of visualization, the hyperplanes have been shown as straightlines in most of the diagrams.

Scenario 1

As depicted in Figure 7.16, in this scenario, we have three hyperplanes: A, B, and C. Now, we need to identify the correcthyperplane which better segregates the two classes representedby the triangles and circles. As we can see, hyperplane ‘A’ hasperformed this task quite well.

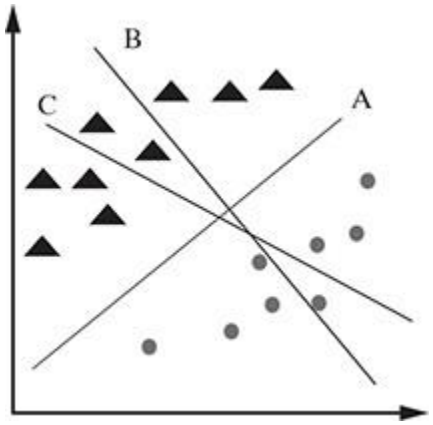


FIG. 7.16 Support vector machine: Scenario 1

Scenario 2

As depicted in Figure 7.17, we have three hyperplanes: A, B,and C. We have to identify the correct hyperplane which classifies the triangles and circles in the best possible way.
Here, maximizing the distances between the nearest data points of both the classes and hyperplane will help us decidethe correct hyperplane. This distance is called as **margin**.

In Figure 7.17b, you can see that the margin for hyperplane A is high as compared to those for both B and C. Hence, hyperplane A is the correct hyperplane. Another quick reason for selecting the hyperplane with higher margin (distance) is robustness. If we select a hyperplane having a lower margin (distance), then there is a high probability of misclassification.

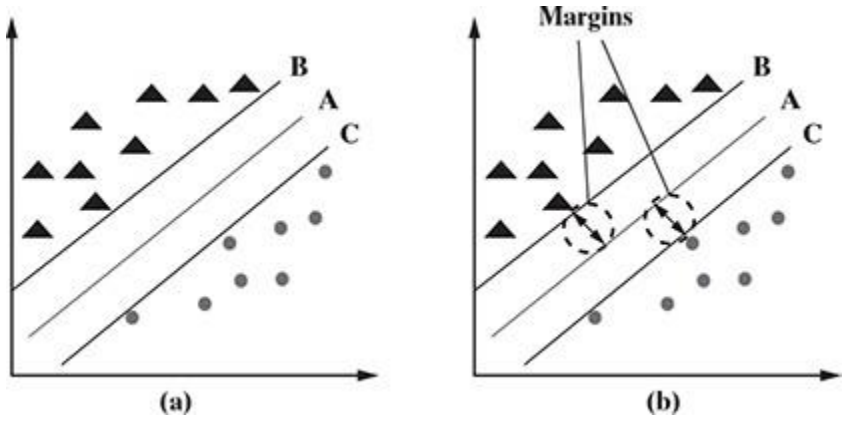


FIG. 7.17 Support vector machine: Scenario 2

Scenario 3

Use the rules as discussed in the previous section to identify the correct hyperplane in the scenario shown in Figure 7.18. Some of you might have selected hyperplane B as it has a higher margin (distance from the class) than A. But, here is thecatch; SVM selects the hyperplane which classifies the classesaccurately before maximizing the margin. Here, hyperplane B has a classification error, and A has classified all data instances correctly. Therefore, A is the correct hyperplane.

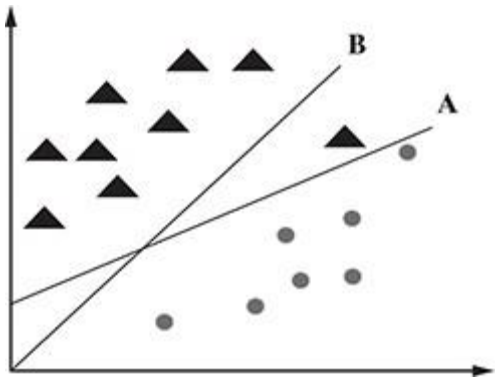


FIG. 7.18 Support vector machine: Scenario 3

Scenario 4

In this scenario, as shown in Figure 7.19a, it is not possible to distinctly segregate the two classes by using a straight line, as one data instance belonging to one of the classes (triangle) liesin the territory of the other class (circle) as an outlier.

One triangle at the other end is like an outlier for the triangle class. SVM has a feature to ignore outliers and find the hyperplane that has the maximum margin (hyperplane A, as shown in Fig. 7.19b). Hence, we can say that SVM is robustto outliers.

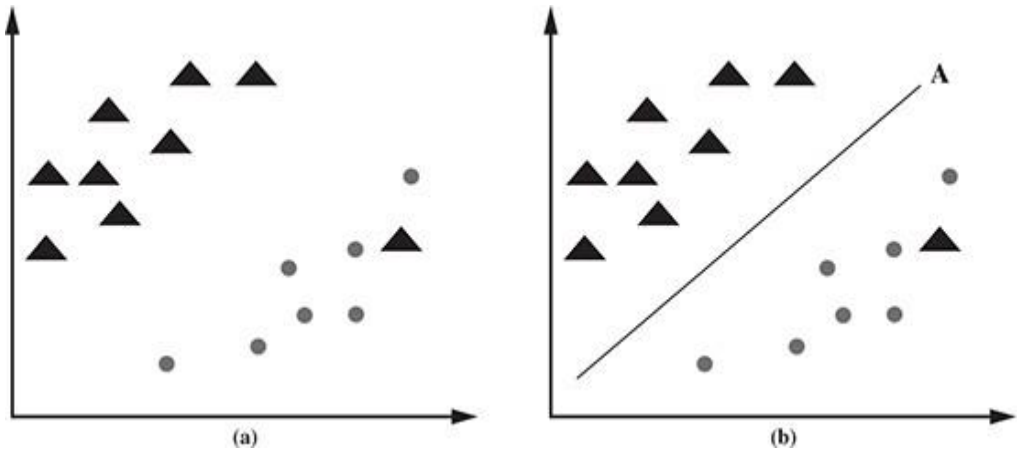


FIG. 7.19 Support vector machine: Scenario 4

So, by summarizing the observations from the differentscenarios, we can say that

1. The hyperplane should segregate the data instances belonging to the twoclasses in the best possible way.
2. It should maximize the distances between the nearest data points of boththe classes, i.e. maximize the margin.
3. If there is a need to prioritize between higher margin and lesser misclassification, the hyperplane should try to reduce misclassifications.

Our next focus is to find out a way to identify a hyperplanewhich maximizes the margin.

Maximum margin hyperplane

Finding the Maximum Margin Hyperplane (MMH) is nothing but identifying the hyperplane which has the largest separation with the data instances of the two classes. Though any set of three hyperplanes can do the correct classification, why do we need to search for the set of hyperplanes causing the largest separation? The answer is that doing so helps us in achieving more generalization and hence less number of issues in the classification of unknown data.

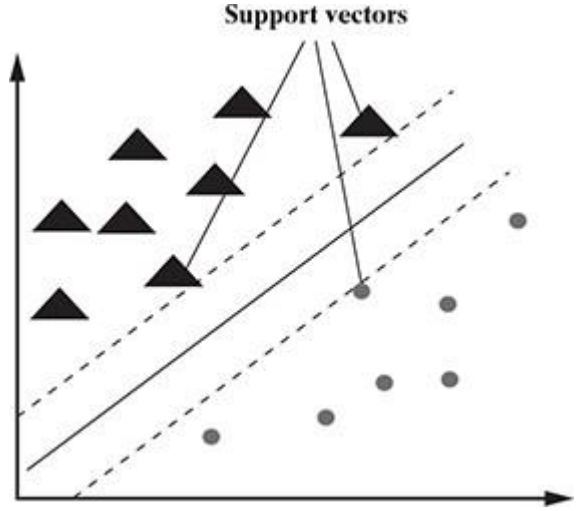


FIG. 7.2O Support vectors

Support vectors, as can be observed in Figure 7.20, are data instances from the two classes which are closest to the MMH. Quite understandably, there should be at least one support vector from each class. The identification of support vectors requires intense mathematical formulation, which is out of scope of this book. However, it is fairly intuitive to understand that modelling a problem using SVM is nothing but identifying the support vectors and MMH corresponding to the problem space.

Identifying the MMH for linearly separable data

Finding out the MMH is relatively straightforward for the data that is linearly separable. In this case, an outer boundary needs to be drawn for the data instances belonging to the different classes. These outer boundaries are known as convex hull, as depicted in Figure 7.21. The MMH can be drawn as the perpendicular bisector of the shortest line (i.e. the connecting line having the shortest length) between the convex hulls.

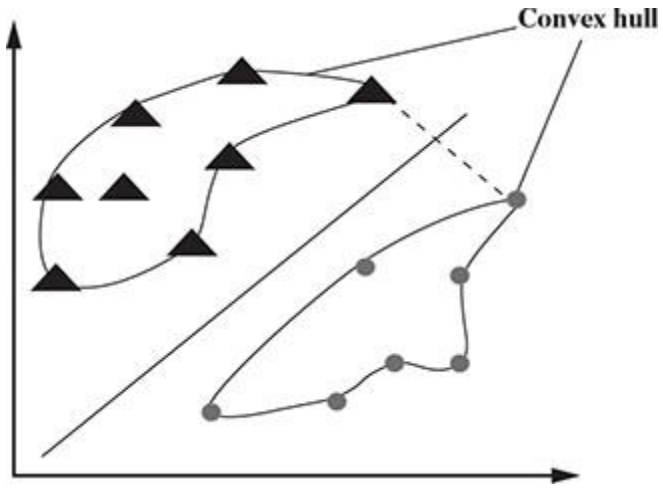


FIG. 7.21 Drawing the MMH for linearly separable data

We have already seen earlier that a hyperplane in the N- dimensional feature space can be represented by the equation:

$$\vec{c}.\vec{X} + c_0 = 0$$

Using this equation, the objective is to find a set of values for the vector such that two hyperplanes, represented by theequations below, can be specified.

$\vec{c}$

$$\vec{c}.\vec{X} + c_0 \geq +1$$
$$\vec{c}.\vec{X} + c_0 \leq -1$$

This is to ensure that all the data instances that belong to one class falls above one hyperplane and all the data instancesbelonging to the other class falls below another hyperplane.

According to vector geometry, the distance of these planes

should be $\frac{2}{\vec{c}}$. It is quite obvious that in order to maximize the

distance between hyperplanes, the value of should be

$\vec{c}$

minimized. So, in summary, the task of SVM is to solve theoptimization problem:

$$\min\left(\frac{1}{2}\vec{c}\right)$$

Identifying the MMH for non-linearly separable data

Now that we have a clear understanding of how to identify theMMH for a linearly separable data set, let us do some study about how non-linearly separable data needs to be handled by SVM. For this, we have to use a slack variable ξ, which provides some soft margin for data instances in one class that fall on the wrong side of the hyperplane. As depicted in Figure7.22, a data instance belonging to the circle class falls on the side of the hyperplane designated for the data instances belonging to the triangle class. The same issue also happens for a data instance belonging to the triangle class.

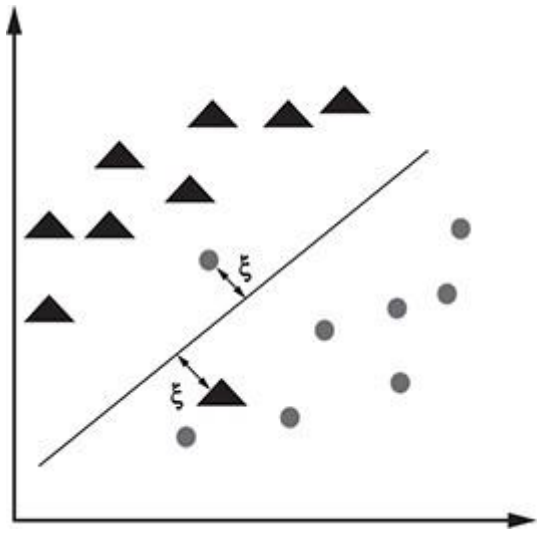


FIG. 7.22 Drawing the MMH for non-linearly separable data

A cost value '*C*' is imposed on all such data instances that fall on the wrong side of the hyperplane. The task of SVM isnow to minimize the total cost due to such data instances in order to solve the revised optimization problem:

$$\min\left(\frac{1}{2}\vec{c}^2\right) + C\sum_{i=1}^{N}\xi_i$$

Kernel trick

As we have seen in the last section, one way to deal with non- linearly separable data is by using a slack variable and an optimization function to minimize the cost value. However, this is not the only way to use SVM to solve machine learning problems involving non-linearly separable data sets. SVM has a technique called the **kernel trick** to deal with non-linearly separable data. As shown in Figure 7.23, these are functions which can transform lower dimensional input space to a higherdimensional space. In the process, it converts linearly non-

separable data to a linearly separable data. These functions arecalled **kernels**.

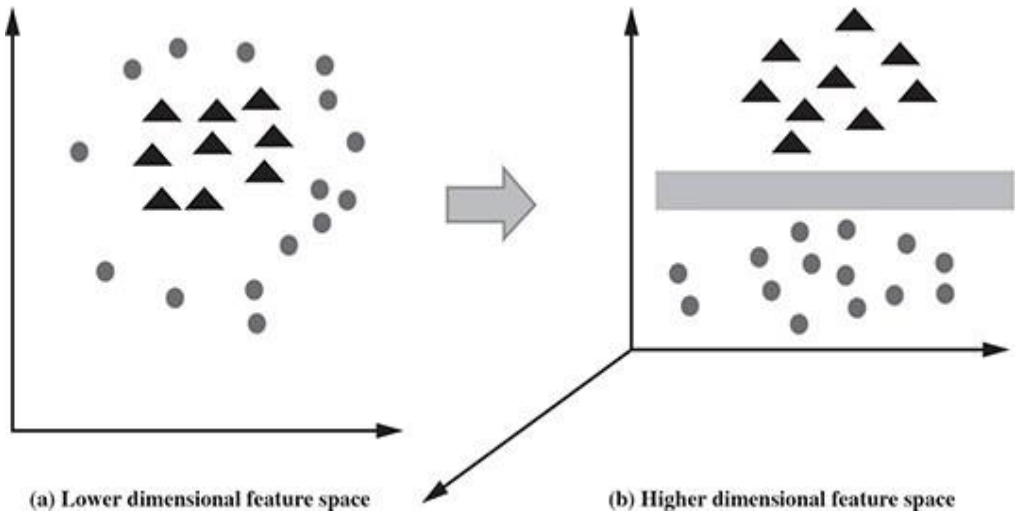


FIG. 7.2C Kernel trick in SVM

Some of the common kernel functions for transforming from a lower dimension '*i*' to a higher dimension '*j*' used bydifferent SVM implementations are as follows:

- Linear kernel: It is in the form $K(\vec{x_i}, \vec{x_j}) = \vec{x_i}.\vec{x_j}$
- Polynomial kernel: It is in the form $K(\vec{x_i}, \vec{x_j}) = (\vec{x_i}.\vec{x_j} + 1)^d$ Sigmoid
- kernel: It is in the form $K(\vec{x_i}, \vec{x_j}) = \tan h(k\vec{x_i}.\vec{x_j} - \partial)$
- Gaussian RBF kernel: It is in the form $K(\vec{x_i}, \vec{x_j}) = e\frac{-\vec{x_i} - \vec{x_j}^2}{2\sigma^2}$

When data instances of the classes are closer to each other, this method can be used. The effectiveness of SVM depends both on the

- selection of the kernel function
- adoption of values for the kernel parameters

Strengths of SVM

- SVM can be used for both classification and regression.
- It is robust, i.e. not much impacted by data with noise or outliers. The prediction results using this model are very promising.

Weaknesses of SVM

- SVM is applicable only for binary classification, i.e. when there are only two classes in the problem domain.
- The SVM model is very complex – almost like a black box when it deals with a high-dimensional data set. Hence, it is very difficult and close to impossible to understand the model in such cases.
- It is slow for a large dataset, i.e. a data set with either a large number of features or a large number of instances.
- It is quite memory-intensive.

Application of SVM

SVM is most effective when it is used for binary classification,
i.e. for solving a machine learning problem with two classes. One common problem on which SVM can be applied is in the field of bioinformatics – more specifically, in detecting cancer and other genetic disorders. It can also be used in detecting the image of a face by binary classification of images into face and non-face components. More such applications can be described.

UNIT-IV

Supervised Learning: Regression

EXAMPLE OF REGRESSION

We have mentioned many times that real estate price prediction is a problem that can be solved by supervised learning or, more specifically, by regression. So, what this problem really is? Let us delve a little deeper into the problem.

New City is the primary hub of the commercial activities inthe country. In the last couple of decades, with increasing globalization, commercial activities have intensified in New City. Together with that, a large number of people have come and settled in the city with a dream to achieve professional growth in their lives. As an obvious fall-out, a large number ofhousing projects have started in every nook and corner of the city. But the demand for apartments has still outgrown the supply. To get benefit from this boom in real estate business, Karen has started a digital market agency for buying and selling real estates (including apartments, independent houses, town houses, etc.). Initially, when the business was small, she used to interact with buyers and sellers personally and help them arrive at a price quote – either for selling a property (for

a seller) or for buying a property (for a buyer). Her long experience in real estate business helped her develop an intuition on what the correct price quote of a property could be

— given the value of certain standard parameters such as area (sq. m.) of the property, location, floor, number of years since purchase, amenities available, etc. However, with the huge surge in the business, she is facing a big challenge. She is not able to manage personal interactions as well as setting the correct price quote for the properties all alone. She hired an assistant for managing customer interactions. But the assistant, being new in the real estate business, is struggling with price quotations. How can Karen solve this problem?

Fortunately, Karen has a friend, Frank, who is a data scientist with in-depth knowledge in machine learning models. Frank comes up with a solution to Karen's problem. He builds a model which can predict the correct value of a real estate if ithas certain standard inputs such as area (sq. m.) of the property, location, floor, number of years since purchase, amenities available, etc. Wow, that sounds to be like Karen herself doing the job! Curious to know what model Frank has used? Yes, you guessed it right. He used a regression model tosolve Karen's real estate price prediction problem.

So, we just discussed about one problem which can be solved using regression. In the same way, a bunch of other problems related to prediction of numerical value can be solved using the regression model. In the context of regression, dependent variable (Y) is the one whose value is tobe predicted, e.g. the price quote of the real estate in the context of Karen's problem. This variable is presumed to be functionally related to one (say, X) or more independent variables called predictors. In the context of Karen's problem,Frank used area of the property, location, floor, etc. as

predictors of the model that he built. In other words, the dependent variable depends on independent variable(s) or predictor(s). Regression is essentially finding a relationship (or) association between the dependent variable (*Y*) and the independent variable(s) (*X*), i.e. to find the function '*f* ' for theassociation *Y* = *f* (*X*).

COMMON REGRESSION ALGORITHMS

The most common regression algorithms are

- Simple linear regression
- Multiple linear regression
- Polynomial regression
- Multivariate adaptive regression splines Logistic
- regression
- Maximum likelihood estimation (least squares)

Simple Linear Regression

As the name indicates, simple linear regression is the simplest regression model which involves only one predictor. This model assumes a linear relationship between the dependent variable and the predictor variable as shown in Figure 8.1.

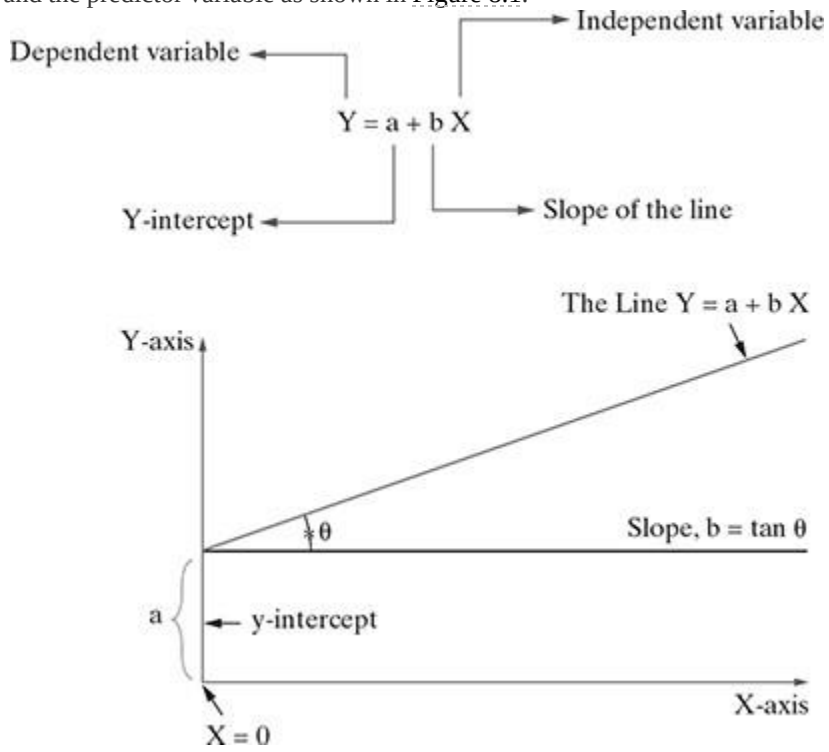


FIG. 8.1 Simple linear regression

In the context of Karen's problem, if we take Price of a Property as the dependent variable and the Area of the Property (in sq. m.) as the predictor variable, we can build a model using simple linear regression.

$\text{Price}_{\text{Property}} = f(\text{Area}_{\text{Property}})$

Assuming a linear association, we can reformulate themodel as

$$\text{Price}_{\text{Property}} = a + b.\ \text{Area}_{\text{Property}}$$

where '*a*' and '*b*' are intercept and slope of the straight line,respectively.

Just to recall, straight lines can be defined in a slope– intercept form $Y = (a + bX)$, where a = intercept and b = slopeof the straight line. The value of intercept indicates the value of Y when $X = 0$. It is known as 'the intercept or Y intercept' because it specifies where the straight line crosses the verticalor Y-axis (refer to Fig. 8.1).

Slope of the simple linear regression model

Slope of a straight line represents how much the line in a graphchanges in the vertical direction (Y-axis) over a change in the horizontal direction (X-axis) as shown in Figure 8.2.

Slope = Change in Y/Change in X

Rise is the change in Y-axis ($Y_2 - Y_1$) and Run is the changein X-axis ($X_2 - X_1$). So, slope is represented as given below:

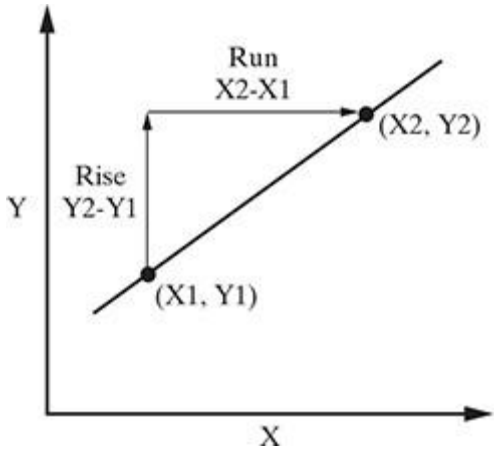


FIG. 8.2 Rise and run representation

$$\text{Slope} = \frac{\text{Rise}}{\text{Run}} = \frac{Y2 - Y1}{X2 - X1}$$

Example of slope

Let us find the slope of the graph where the lower point on theline is represented as (−3, −2) and the higher point on the line is represented as (2, 2).

$(X_1, Y_1) = (-3, -2)$ and $(X_2, Y_2) = (2, 2)$

Rise = $(Y_2 - Y_1) = (2 - (-2)) = 2 + 2 = 4$

Run = $(X_2 - X_1) = (2 - (-3)) = 2 + 3 = 5$

Slope = Rise/Run = 4/5 = 0.8

There can be two types of slopes in a linear regression model: positive slope and negative slope. Different types ofregression lines based on the type of slope include

- Linear positive slope Curve
- linear positive slope Linear
- negative slope Curve linear
- negative slope

Linear positive slope

A positive slope always moves upward on a graph from left toright (refer to Fig. 8.3).

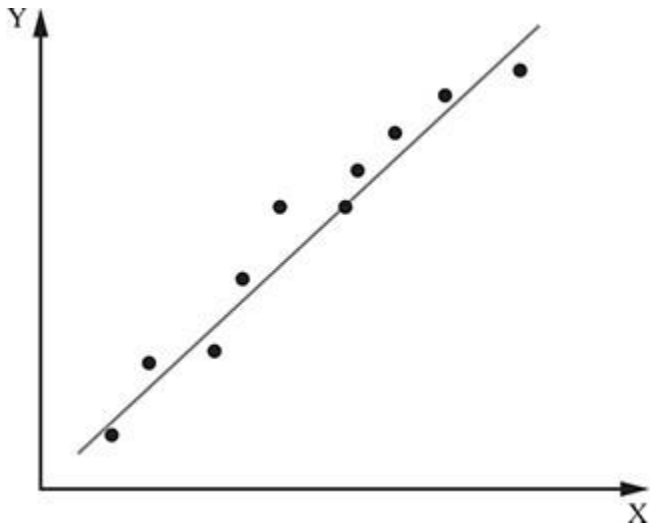


FIG. 8.C Linear positive slope

Slope = Rise/Run = $(Y_2 - Y_1) / (X_2 - X_1)$ = Delta (Y) / Delta(X)

- Scenario 1 for positive slope: Delta (Y) is positive and Delta (X) is positive Scenario
- 2 for positive slope: Delta (Y) is negative and Delta (X) is negative

Curve linear positive slope

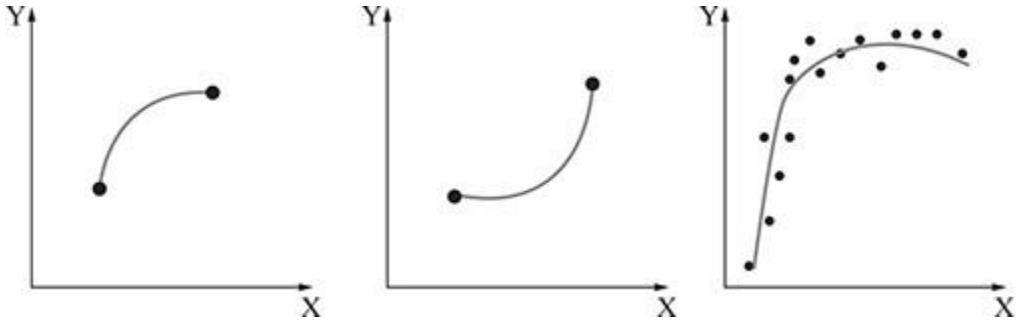


FIG. 8.4 Curve linear positive slope

Curves in these graphs (refer to Fig. 8.4) slope upward fromleft to right.

Slope = $(Y_2 - Y_1) / (X_2 - X_1)$ = Delta (Y) / Delta(X)

Slope for a variable (X) may vary between two graphs, but itwill always be positive; hence, the above graphs are called as graphs with curve linear positive slope.

Linear negative slope

A negative slope always moves downward on a graph fromleft to right. As X value (on X-axis) increases, Y value decreases (refer to Fig. 8.5).

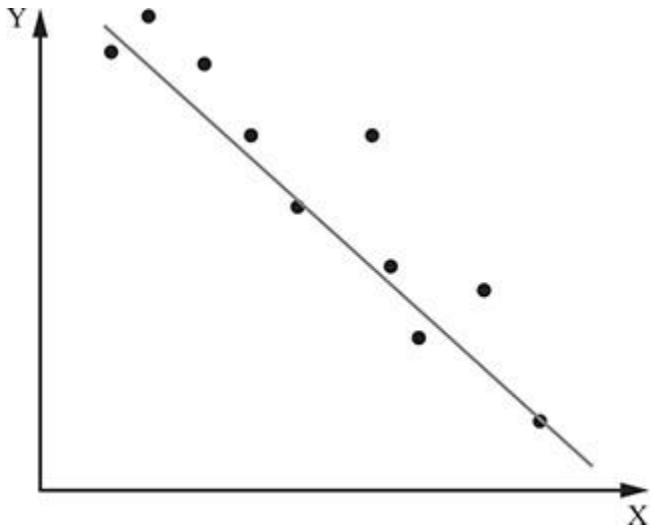


FIG. 8.5 Linear negative slope

Slope = Rise/Run = $(Y_2 - Y_1) / (X_2 - X_1)$ = Delta (Y) / Delta(X)

- Scenario 1 for negative slope: Delta (Y) is positive and Delta (X) is negative
- Scenario 2 for negative slope: Delta (Y) is negative and Delta (X) is positive

Curve linear negative slope

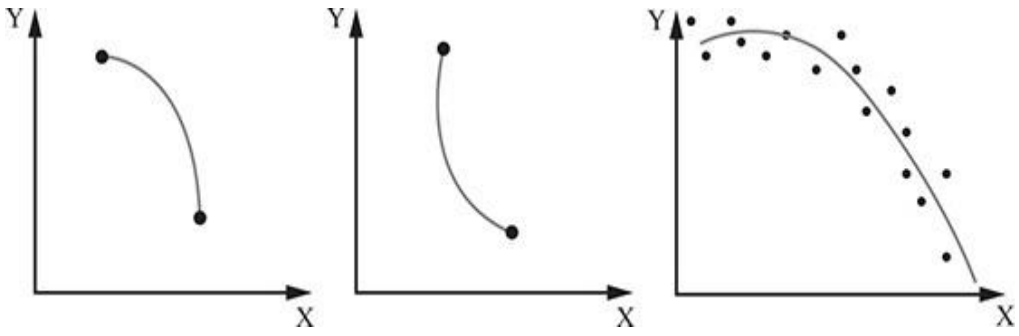


FIG. 8.6 Curve linear negative slope

Curves in these graphs (refer to Fig. 8.6) slope downwardfrom left to right.

Slope = $(Y_2 - Y_1) / (X_2 - X_1)$ = Delta (Y) / Delta(X)

Slope for a variable (X) may vary between two graphs, but it will always be negative; hence, the above graphs are called as graphs with curve linear negative slope.

No relationship graph

Scatter graph shown in Figure 8.7 indicates 'no relationship' curve as it is very difficult to conclude whether the relationship between X and Y is positive or negative.

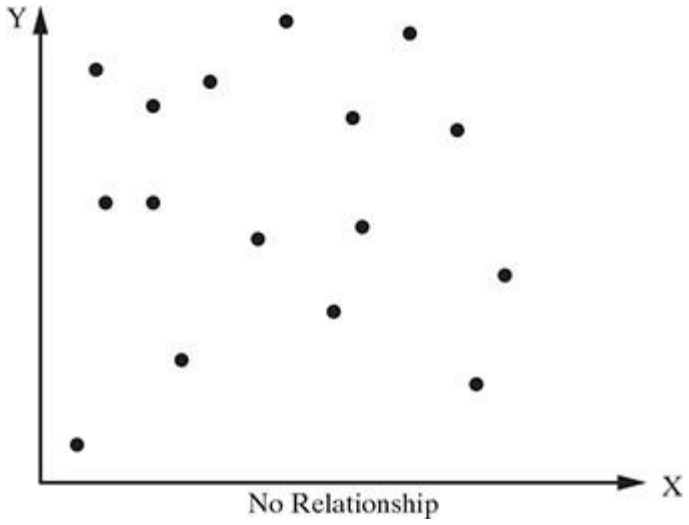


FIG. 8.7 No relationship graph

Error in simple regression

The regression equation model in machine learning uses the above slope–intercept format in algorithms. X and Y values are provided to the machine, and it identifies the values of a (intercept) and b (slope) by relating the values of X and Y. However, identifying the exact match of values for a and b is not always possible. There will be some error value (ε) associated with it. This error is called marginal or residual error.

$Y = (a + bX) + \varepsilon$

Now that we have some context of the simple regression model, let us try to explore an example to understand clearly how to decide the parameters of the model (i.e. values of a and b) for a given problem.

Example of simple regression

A college professor believes that if the grade for internal examination is high in a class, the grade for external examination will also be high. A random sample of 15 students in that class

was selected, and the data is given below:

Internal Exam	15	23	18	23	24	22	22	19	19	16	24	11	24	16	23
External Exam	49	63	58	60	58	61	60	63	60	52	62	30	59	49	68

A scatter plot was drawn to explore the relationship between the independent variable (internal marks) mapped to *X*-axis and dependent variable (external marks) mapped to *Y*-axis as depicted in Figure 8.8.

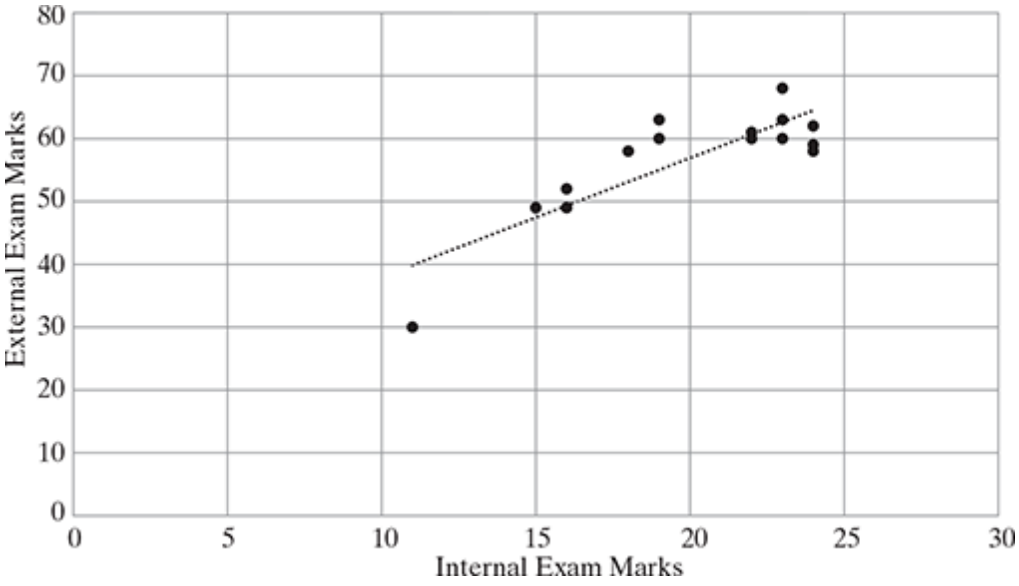
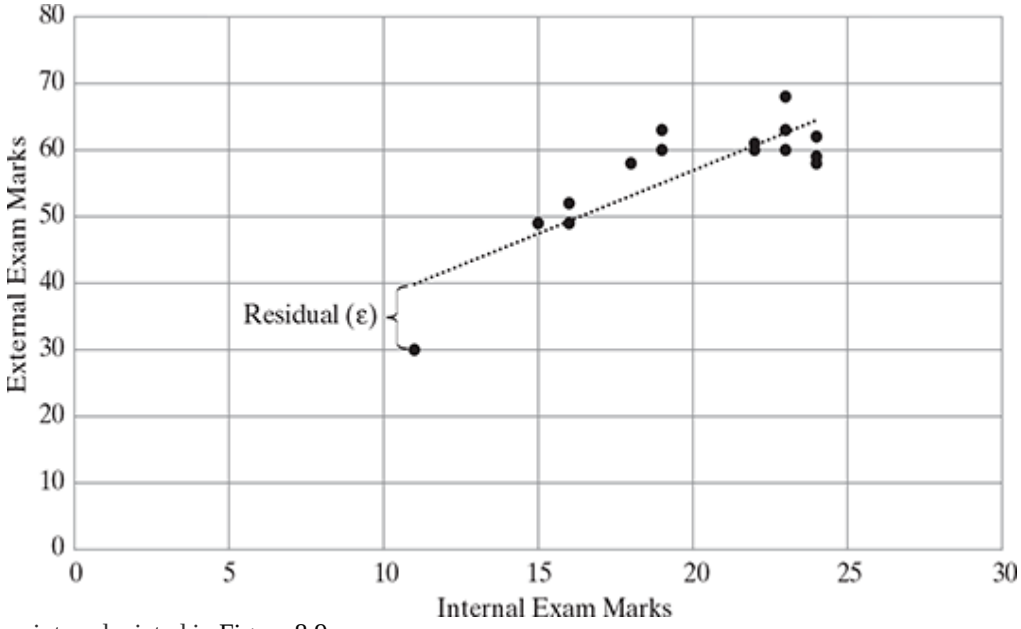


FIG. 8.8 Scatter plot and regression line

As you can observe from the above graph, the line (i.e. the regression line) does not predict the data exactly (refer to Fig. 8.8). Instead, it just cuts through the data. Some predictions

are lower than expected, while some others are higher thanexpected.

Residual is the distance between the predicted point (on theregression line) and the actual



point as depicted in Figure 8.9.

FIG. 8.9 Residual error

As we know, in simple linear regression, the line is drawnusing the regression formula.

$$Y = (a + bX) + \varepsilon$$

If we know the values of '*a*' and '*b*', then it is easy to predict the value of *Y* for any given *X* by using the above formula. But the question is how to calculate the values of '*a*'and '*b*' for a given set of *X* and *Y* values?

A straight line is drawn as close as possible over the pointson the scatter plot. Ordinary Least Squares (OLS) is the technique used to estimate a line that will minimize the error (ε), which is the difference between the predicted and the actual values of *Y*. This means summing the errors of each prediction or, more appropriately, the Sum of the Squares of

the Errors (SSE) $\left(\text{i.e. } \sum_i \varepsilon_i^2\right)$.

It is observed that the SSE is least when b takes the value

$$b = \frac{\Sigma_i (X_i - \overline{X})(Y_i - \overline{Y})}{\Sigma_i (X_i - \overline{X})^2} = \frac{\text{cov}(X, Y)}{\text{Var}(X)}$$

The corresponding value of '*a*' calculated using the abovevalue of '*b*' is

$$a = \overline{Y} - b\overline{X}$$

So, let us calculate the value of a and b for the given example. For detailed calculation, refer to Figure 8.10.

Calculation summary

Sum of X = 299 Sum of

Y = 852

Mean X, M_X = 19.93 Mean Y,

M_Y = 56.8

Sum of squares (SS_X) = 226.9333 Sum of products

(SP) = 429.8 Regression equation = $\hat{y} = bX + a$

$$b = \frac{SP}{SS_X} = \frac{429.8}{226.93} = 1.89395$$

$a = M_Y - bM_X = 56.8 - (1.89 \times 19.93) = 19.0473$

$\hat{y} = 1.89395X + 19.0473$

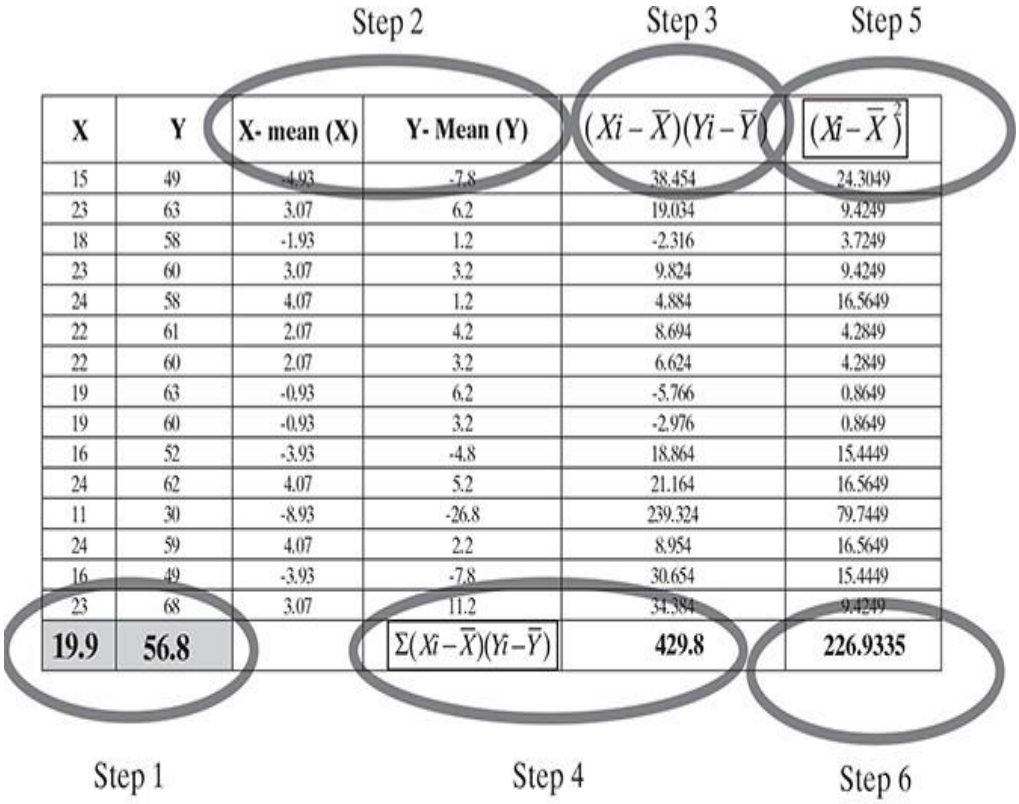
Hence, for the above example, the estimated regression equation is constructed on the basis of the estimated values of a and b:

$$\hat{y} = 1.89395X + 19.0473$$

So, in the context of the given problem, we can say

Marks in external exam = 19.04 + 1.89 × (Marks in internal exam)

or, $M_{Ext} = 19.04 + 1.89 \times M_{Int}$



Step 7: Divide (step4 / step6)

b = 429.28 / 226.93 = 1.89

Step 8: Calculate a using the value of b

$a = \overline{Y} - b\overline{X}$

a = 56.8 – 1.89 × 19.9

a = 19.05

FIG. 8.1O Detailed calculation of regression parameters

The model built above can be represented graphically as

- an extended version (refer to Fig. 8.11) a
- zoom-in version (refer to Fig. 8.12)

Interpretation of the intercept

As we have already seen, the simple linear regression modelbuilt on the data in the example is

$$M_{\mathbf{Ext}} = \mathbf{19.O4} + \mathbf{1.89} \times M_{\mathbf{Int}}$$

The value of the intercept from the above equation is 19.05.However, none of the internal mark is 0. So, intercept = 19.05indicates that 19.05 is the portion of the external examination marks not explained by the internal examination marks.

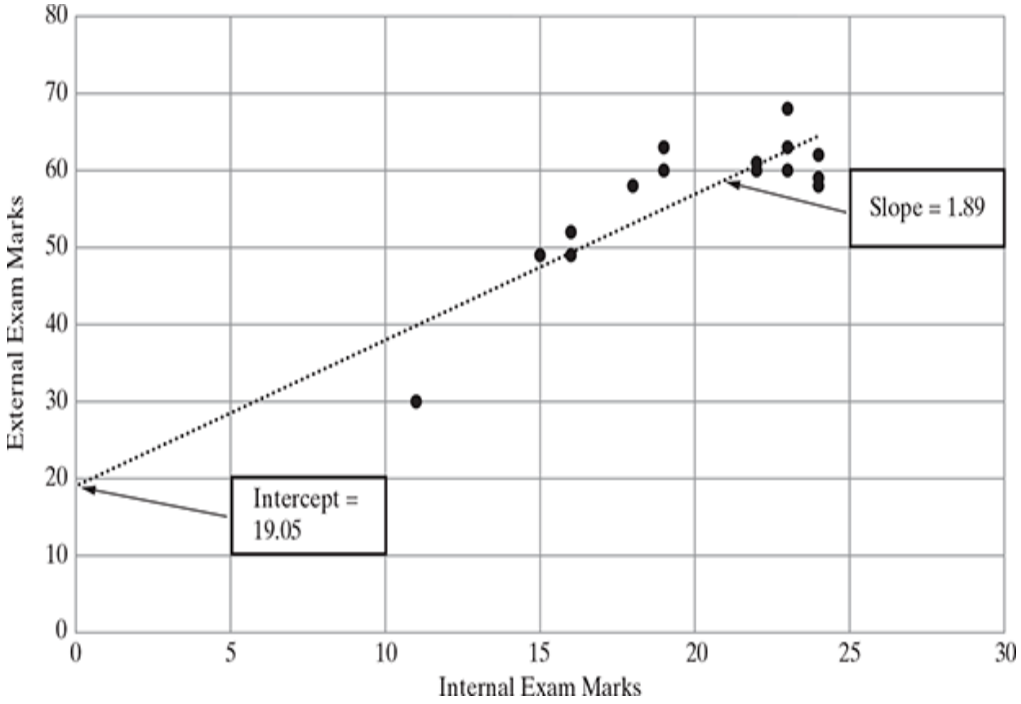


FIG. 8.11 Extended version of the regression graph

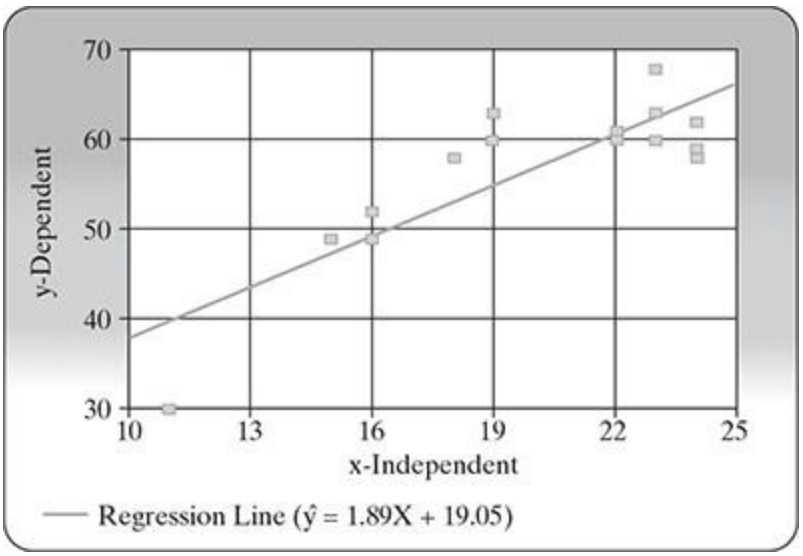


FIG. 8.12 Zoom-in regression line

Slope measures the estimated change in the average value of *Y* as a result of a one-unit change in *X*. Here, slope = 1.89 tells us that the average value of the external examination marks

increases by 1.89 for each additional 1 mark in the internalexamination.

Now that we have a complete understanding of how to build a simple linear regression model for a given problem, it is timeto summarize the algorithm.

OLS algorithm

- Step 1: Calculate the mean of *X* and *Y* Step
- 2: Calculate the errors of *X* and *Y* Step 3:
- Get the product
- Step 4: Get the summation of the productsStep 5:
- Square the difference of *X*
- Step 6: Get the sum of the squared difference
- Step 7: Divide output of step 4 by output of step 6 to calculate '*b*'Step 8:
- Calculate '*a*' using the value of '*b*'

Maximum and minimum point of curves

Maximum (shown in Fig. 8.13) and minimum points (shown in Fig. 8.14) on a graph are found at points where the slope ofthe curve is zero. It becomes zero either from positive or negative value. The maximum point is the point on the curve of the graph with the highest *y*-coordinate and a slope of zero.The minimum point is the point on the curve of the graph with the lowest *y*-coordinate and a slope of zero.

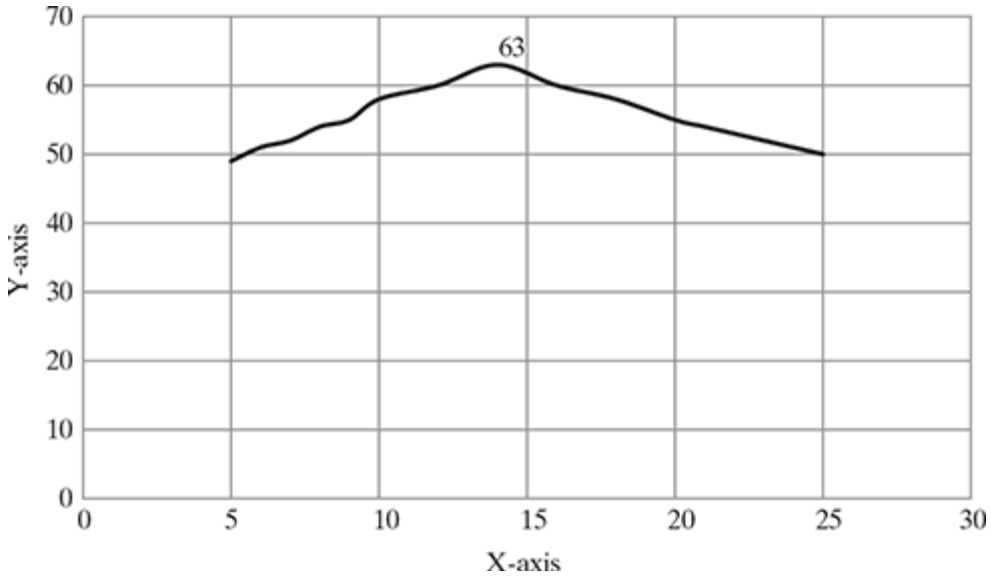


FIG. 8.1C Maximum point of curve

Point 63 is at the maximum point for this curve (refer to Fig. 8.13). Point 63 is at the highest point on this curve. It has a greater *y*-coordinate value than any other point on the curveand has a slope of zero.

Point 40 (marked with an arrow in Fig. 8.14) is the minimum point for this curve. Point 40 is at the lowest point on this curve. It has a lesser *y*-coordinate value than any otherpoint on the curve and has a slope of zero.

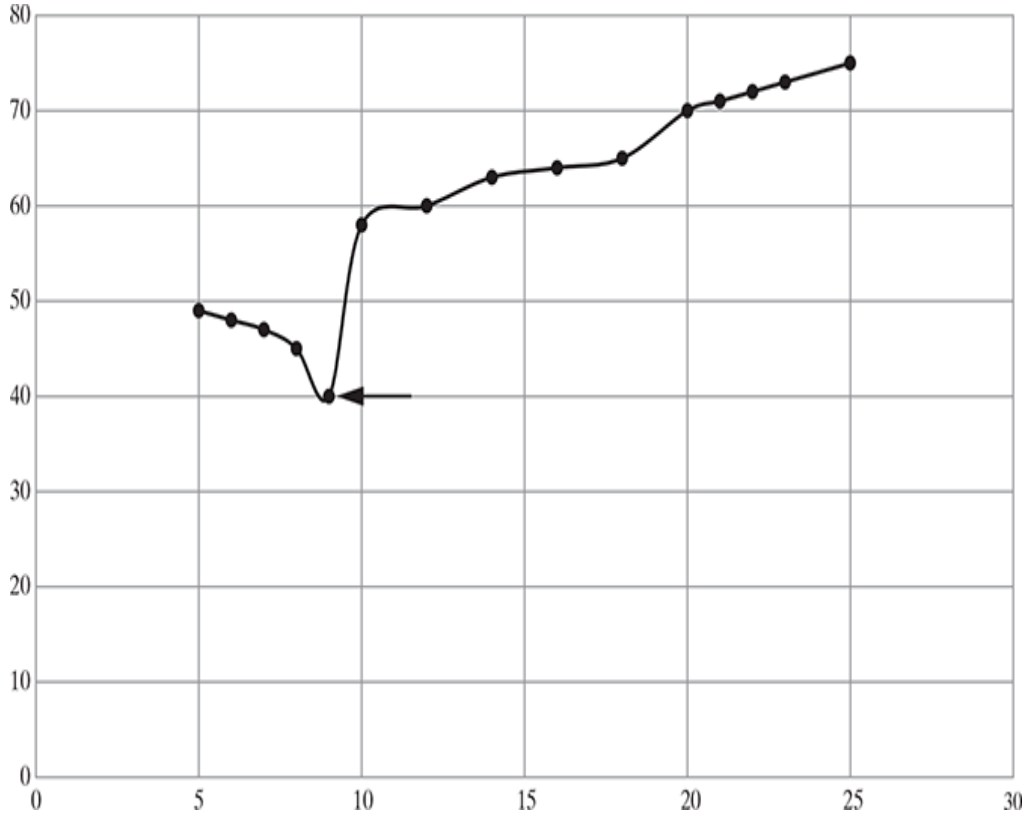


FIG. 8.14 Minimum point of curve

Multiple Linear Regression

In a multiple regression model, two or more independent variables, i.e. predictors are involved in the model. If we think in the context of Karen's problem, in the last section, we came up with a simple linear regression by considering Price of a Property as the dependent variable and the Area of the Property (in sq. m.) as the predictor variable. However, location, floor, number of years since purchase, amenities available, etc. are also important predictors which should not be ignored. Thus, if we consider Price of a Property (in $) as the dependent variable and Area of the Property (in sq. m.), location, floor, number of years since purchase and amenities

available as the independent variables, we can form a multiple regression equation as shown below:

$$\text{Price}_{\text{Property}} = f(\text{Area}_{\text{Property}}, \text{location, floor, Ageing, Amenities})$$

The simple linear regression model and the multiple regression model assume that the dependent variable is continuous.

The following expression describes the equation involving the relationship with two predictor variables, namely X_1 and X_2.

$$Y = a + b_1X_1 + b_2X_2$$

The model describes a plane in the three-dimensional spaceof Y, X_1, and X_2. Parameter 'a' is the intercept of this plane.
Parameters 'b_1' and 'b_2' are referred to as **partial regression coefficients**. Parameter b_1 represents the change in the mean response corresponding to a unit change in X_1 when X_2 is heldconstant. Parameter b_2 represents the change in the mean response corresponding to a unit change in X_2 when X_1 is heldconstant.

Consider the following example of a multiple linear regression model with two predictor variables, namely X_1 andX_2 (refer to Fig. 8.15).

$$Y = 22 + 0.3X_1 + 1.2X_2$$

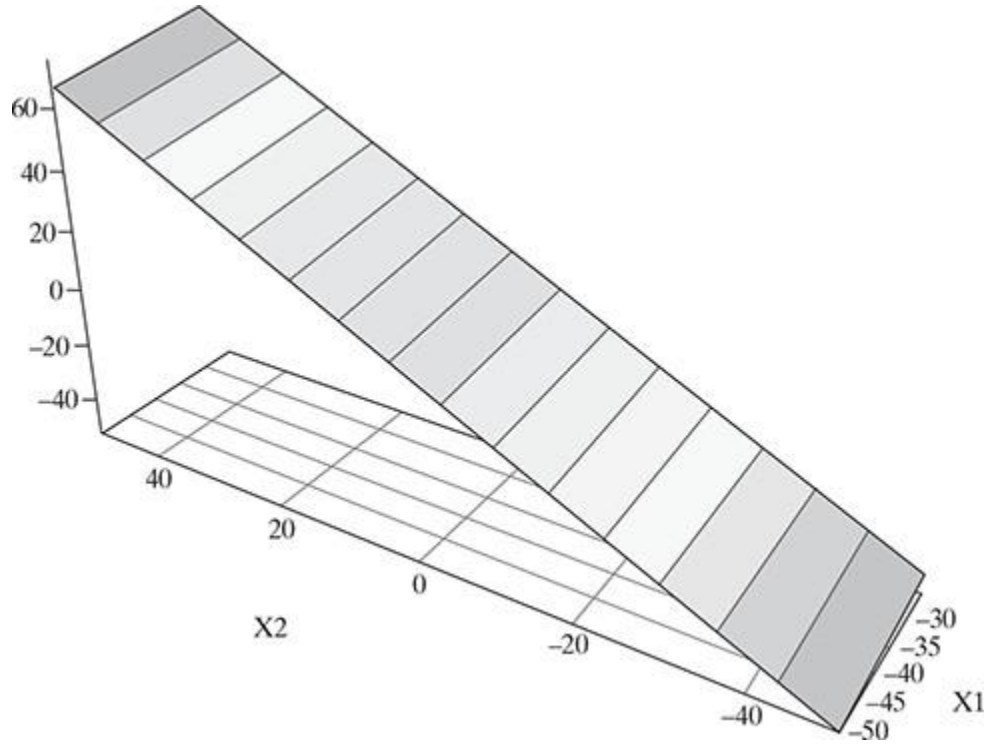


FIG. 8.15 Multiple regression plane

Multiple regression for estimating equation when there are 'n' predictor variables is as follows:

$$Y = a + b_1X_1 + b_2X_2 + b_3X_3 + \ldots + b_nX_n$$

While finding the best fit line, we can fit either a polynomial or curvilinear regression. These are known as polynomial or curvilinear regression, respectively.

Assumptions in Regression Analysis

1. The dependent variable (Y) can be calculated / predicated as a linear function of a specific set of independent variables (X's) plus an error term (ε).
2. The number of observations (n) is greater than the number of parameters (k) to be estimated, i.e. $n > k$.
3. Relationships determined by regression are only relationships of association based on the data set and not necessarily of cause and effect of the defined class.
4. Regression line can be valid only over a limited range of data. If the line is extended (outside the range of extrapolation), it may only lead to wrong predictions.
5. If the business conditions change and the business assumptions underlying the regression model are no longer valid, then the past dataset will no longer be able to predict future trends.
6. Variance is the same for all values of X (homoskedasticity).
7. The error term (ε) is normally distributed. This also means that themean of the error (ε) has an expected value of 0.
8. The values of the error (ε) are independent and are not related to anyvalues of X. This means that there are no relationships between a particular X, Y that are related to another specific value of X, Y.

Given the above assumptions, the OLS estimator is the **BestLinear Unbiased Estimator (BLUE)**, and this is called as **Gauss-Markov Theorem**.

Main Problems in Regression Analysis

In multiple regressions, there are two primary problems: multicollinearity and heteroskedasticity.

Multicollinearity

Two variables are perfectly collinear if there is an exact linear relationship between them. Multicollinearity is the situation in which the degree of correlation is not only between the dependent variable and the independent variable, but there is also a strong correlation within (among) the independent

variables themselves. A multiple regression equation can makegood predictions when there is multicollinearity, but it is difficult for us to determine how the dependent variable will change if each independent variable is changed one at a time.

When multicollinearity is present, it increases the standard errors of the coefficients. By overinflating the standard errors, multicollinearity tries to make some variables statistically insignificant when they actually should be significant (with lower standard errors). One way to gauge multicollinearity is to calculate the Variance Inflation Factor (VIF), which assesses how much the variance of an estimated regression coefficient increases if the predictors are correlated. If no factors are correlated, the VIFs will be equal to 1.

The assumption of no perfect collinearity states that there is no exact linear relationship among the independent variables. This assumption implies two aspects of the data on the independent variables. First, none of the independent variables, other than the variable associated with the interceptterm, can be a constant. Second, variation in the X's is necessary. In general, the more variation in the independent variables, the better will be the OLS estimates in terms of identifying the impacts of the different independent variables on the

dependent variable.

Heteroskedasticity

Heteroskedasticity refers to the changing variance of the errorterm. If the variance of the error term is not constant across data sets, there will be erroneous predictions. In general, for a regression equation to make accurate predictions, the error term should be independent, identically (normally) distributed(iid).

Mathematically, this assumption is written as

$$\text{var}(u_i|X) = \sigma^2 \quad \text{and}$$
$$\text{cov}(u_i u_j|X) = 0 \quad \text{for } i \neq j$$

where 'var' represents the variance, 'cov' represents the covariance, '*u*' represents the error terms, and '*X*' representsthe independent variables.

This assumption is more commonly written as

$$\text{var}(u_i) = \sigma^2 \quad \text{and}$$
$$\text{cov}(u_i u_j) = 0 \quad \text{for } i \neq j.$$

Improving Accuracy of the Linear RegressionModel

Let us understand bias and variance in the regression model before exploring how to improve the same. The concept of bias and variance is similar to accuracy and prediction. Accuracy refers to how close the estimation is near the actual value, whereas prediction refers to continuous estimation of the value.

High bias = low accuracy (not close to real value) High

variance = low prediction (values are scattered)Low bias =

high accuracy (close to real value)

Low variance = high prediction (values are close to each other)

Let us say we have a regression model which is highly accurate and highly predictive; therefore, the overall error ofour model will be low, implying a low bias (high accuracy) and low variance (high prediction). This is highly preferable.Similarly, we can say that if the variance increases (low prediction), the spread of our data points increases, which results in less accurate prediction. As the bias increases (low accuracy), the error between our predicted value and the observed values increases. Therefore, balancing out bias and accuracy is essential in a regression model.

In the linear regression model, it is assumed that the numberof observations (*n*) is greater than the number of parameters

(k) to be estimated, i.e. $n > k$, and in that case, the least squaresestimates tend to have low

variance and hence will perform well on test observations.

However, if observations (n) is not much larger than parameters (k), then there can be high variability in the leastsquares fit, resulting in overfitting and leading to poor predictions.

If $k > n$, then linear regression is not usable. This also indicates infinite variance, and so, the method cannot be usedat all.

Accuracy of linear regression can be improved using thefollowing three methods:

1. Shrinkage Approach
2. Subset Selection
3. Dimensionality (Variable) Reduction

Shrinkage (Regularization) approach

By limiting (shrinking) the estimated coefficients, we can tryto reduce the variance at the cost of a negligible increase in bias. This can in turn lead to substantial improvements in theaccuracy of the model.

Few variables used in the multiple regression model are in fact not associated with the overall response and are called as irrelevant variables; this may lead to unnecessary complexityin the regression model.

This approach involves fitting a model involving all predictors. However, the estimated coefficients are shrunken towards zero relative to the least squares estimates. This shrinkage (also known as regularization) has the effect of reducing the overall variance. Some of the coefficients may also be estimated to be exactly zero, thereby indirectly performing variable selection. The two best-known techniques for shrinking the regression coefficients towards zero are

1. ridge regression
2. lasso (Least Absolute Shrinkage Selector Operator)

Ridge regression performs L2 regularization, i.e. it adds penalty equivalent to square of the magnitude of coefficients

Minimization objective of ridge = LS Obj + a × (sum ofsquare of coefficients)

Ridge regression (include all k predictors in the final model)is very similar to least squares, except that the coefficients are estimated by minimizing a slightly different quantity. If $k > n$, then the least squares estimates do not even have a unique

solution, whereas ridge regression can still perform well by trading off a small increase in bias for a large decrease in variance. Thus, ridge regression works best in situations wherethe least squares estimates have high variance. One disadvantage with ridge regression is that it will include all k predictors in the final model. This may not be a problem for prediction accuracy, but it can create a challenge in model interpretation in settings in which the number of variables k is quite large. Ridge regression will perform better when the response is a function of many predictors, all with coefficientsof roughly equal size.

Lasso regression performs L1 regularization, i.e. it adds penalty equivalent to the absolute value of the magnitude ofcoefficients.

Minimization objective of ridge = LS Obj + a × (absolute value of the magnitude of

coefficients)

The *lasso* overcomes this disadvantage by forcing some of the coefficients to zero value. We can say that the lasso yieldssparse models (involving only subset) that are simpler as well as more interpretable. The lasso can be expected to perform better in a setting where a relatively small number of predictors have substantial coefficients, and the remaining predictors have coefficients that are very small or equal to zero.

Subset selection

Identify a subset of the predictors that is assumed to be related to the response and then fit a model using OLS on the selectedreduced subset of variables. There are two methods in which subset of the regression can be selected:

1. Best subset selection (considers all the possible (2^k))
2. Stepwise subset selection
    1. Forward stepwise selection (0 to *k*)
    2. Backward stepwise selection (*k* to 0)

In best subset selection, we fit a separate least squares regression for each possible subset of the *k* predictors. For computational reasons, best subset selection cannot be applied with very large value of predictors (*k*). The best subset selection procedure considers all the possible (2^k) models containing subsets of the *p* predictors.

The stepwise subset selection method can be applied tochoose the best subset. There are two stepwise subset selection:

1. Forward stepwise selection (0 to *k*)
2. Backward stepwise selection (*k* to 0)

Forward stepwise selection is a computationally efficient alternative to best subset selection. Forward stepwise considers a much smaller set of models, that too step by step, compared to best set selection. Forward stepwise selection begins with a model containing no predictors, and then, predictors are added one by one to the model, until all the *k* predictors are included in the model. In particular, at each step, the variable (*X*) that gives the highest additional improvement to the fit is added.

Backward stepwise selection begins with the least squares model which contains all *k* predictors and then iteratively removes the least useful predictor one by one.

Dimensionality reduction (Variable reduction)

The earlier methods, namely subset selection and shrinkage, control variance either by using a subset of the original variables or by shrinking their coefficients towards zero. In dimensionality reduction, predictors (*X*) are transformed, and the model is set up using the transformed variables after dimensionality reduction. The number of variables is reducedusing the dimensionality reduction method. Principal component analysis is one of the most important dimensionality (variable) reduction techniques.

Polynomial Regression Model

Polynomial regression model is the extension of the simple linear model by adding extra predictors obtained by raising (squaring) each of the original predictors to a power. For example, if there are three variables, *X*, X^2, and X^3 are used as predictors. This approach provides a simple way to yield a non-linear fit to data.

$$f(x) = c_0 + c_1.X^1 + c_2.X^2 + c_3.X^3$$

In the above equation, c_0, c_1, c_2, and c_3 are the coefficients.

Example: Let us use the below data set of (X, Y) for degree3 polynomial.

Internal Exam (X)	15	23	18	23	24	22	22	19	19	16	24	11	24	16	23
External Exam (Y)	49	63	58	60	58	61	60	63	60	52	62	30	59	49	68

As you can observe, the regression line (refer to Fig. 8.16) is slightly curved for polynomial degree 3 with the above 15data points. The regression line will curve further if we increase the polynomial degree (refer to Fig. 8.17). At the extreme value as shown below, the regression line will be overfitting into all the original values of X.

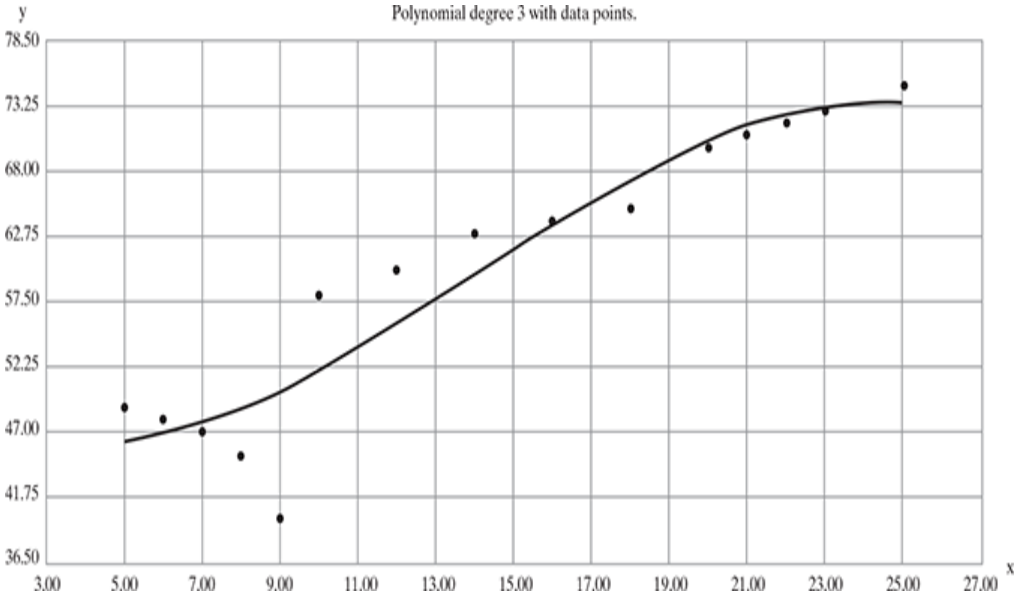


FIG. 8.16 Polynomial regression degree 3

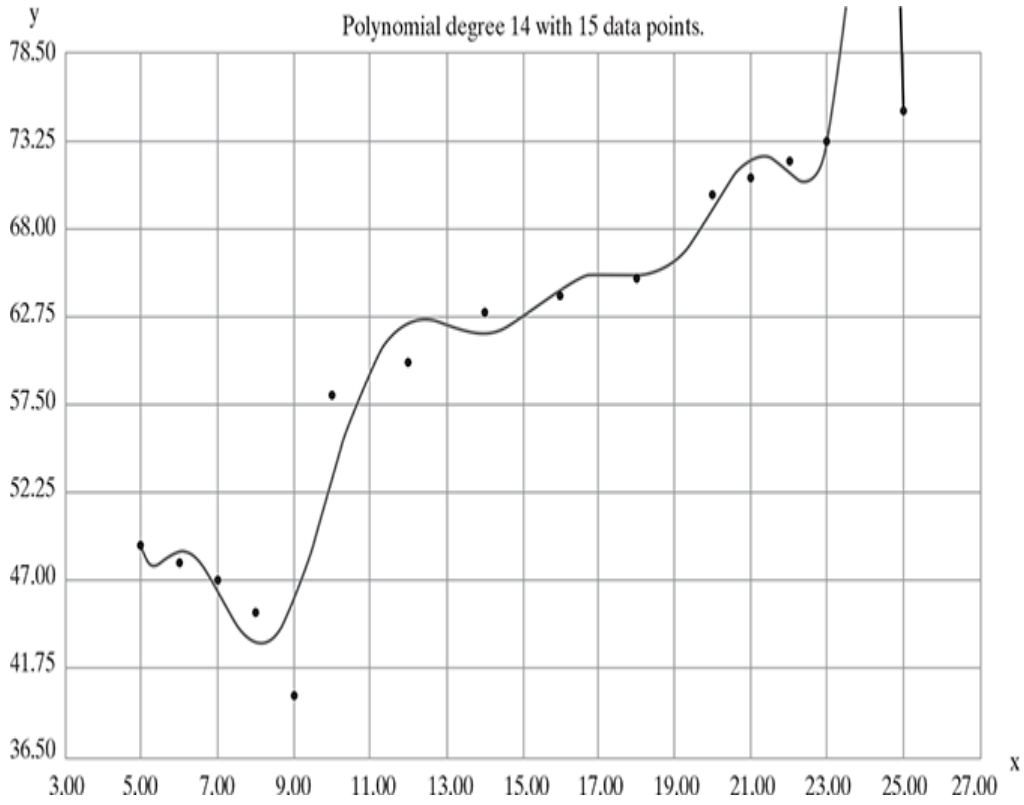


FIG. 8.17 Polynomial regression degree 14

Logistic Regression

Logistic regression is both classification and regression technique depending on the scenario used. Logistic regression(logit regression) is a type of regression analysis used for predicting the outcome of a categorical dependent variable similar to OLS regression. In logistic regression, dependent variable (*Y*) is binary (0,1) and independent variables (*X*) are continuous in nature. The probabilities describing the possibleoutcomes (probability that $Y = 1$) of a single trial are modelledas a logistic function of the predictor variables. In the logistic regression model, there is no R^2 to gauge the fit of the overall model; however, a chi-square test is used to gauge how well the logistic regression model fits the data. The goal of logistic regression is to predict the likelihood that *Y* is equal to 1 (probability that $Y = 1$ rather than 0) given certain values of *X*.That is, if *X* and *Y* have a strong positive linear relationship, the probability that a person will have a score of $Y = 1$ will increase as values of *X* increase. So, we are predicting probabilities rather than the scores of the dependent variable.

For example, we might try to predict whether or not a smallproject will succeed or fail on the basis of the number of yearsof experience of the project manager handling the project. We presume that those project managers who have been managingprojects for many years will be more likely to succeed. This means that as *X* (the number of years of experience of project manager) increases, the probability that *Y* will be equal to 1 (success of the new project) will tend to increase. If we take a hypothetical example in which 60 already executed projects were studied and the years of experience of project managers ranges from 0 to 20 years, we could represent this tendency toincrease the probability that $Y = 1$ with a graph.

To illustrate this, it is convenient to segregate years of experience into categories (i.e. 0–8, 9–16, 17–24, 25–32, 33– 40). If we compute the mean score on Y (averaging the 0s and1s) for each category of years of experience, we will get something like

X	Y
0–8	0.27
9–16	0.5
17–24	0.6
25–32	0.66
33–40	0.93

When the graph is drawn for the above values of X and Y, it appears like the graph in Figure 8.18. As X increases, the probability that $Y = 1$ increases. In other words, when the project manager has more years of experience, a larger percentage of projects succeed. A perfect relationship represents a perfectly curved S rather than a straight line, as was the case in OLS regression. So, to model this relationship, we need some fancy algebra / mathematics that accounts for the bends in the curve.

An explanation of logistic regression begins with an explanation of the logistic function, which always takes values between zero and one. The logistic formulae are stated in terms of the probability that $Y = 1$, which is referred to as P. The probability that Y is 0 is $1 - P$.

$$\ln\left(\frac{P}{1-P}\right) = a + bX$$

$$\ln(p/1-p) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \varepsilon$$

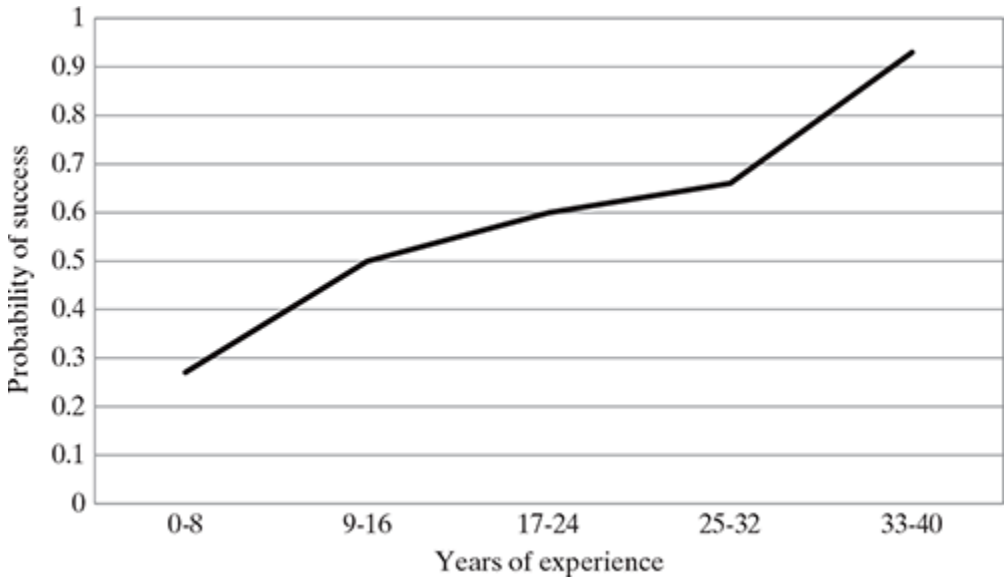


FIG. 8.18 Logistic regression

The 'ln' symbol refers to a natural logarithm and $a + bX$ is the regression line equation. Probability (P) can also be computed from the regression equation. So, if we know the

regression equation, we could, theoretically, calculate the expected probability that $Y = 1$ for a given value of X.

$$P = \frac{\exp(a + bX)}{1 + \exp(a + bx)} = \frac{e^{a+bx}}{1 + e^{a+bx}}$$

'exp' is the exponent function, which is sometimes alsowritten as e.

Let us say we have a model that can predict whether a person is male or female on the basis of their height. Given a

height of 150 cm, we need to predict whether the person ismale or female.

We know that the coefficients of $a = -100$ and $b = 0.6$.
Using the above equation, we can calculate the probability of male given a height of 150 cm or more formally P(male|height

= 150).

$y = e\text{^}(a + b \times X)/(1 + e\text{^}(a + b \times X))$
y = exp (−100 + 0.6 × 150)/(1 + EXP(−100 + 0.6 × *X*)*y* = 0.000046

or a probability of near zero that the person is a male.

Assumptions in logistic regression

The following assumptions must hold when building a logisticregression model:

- There exists a linear relationship between logit function and independentvariables
- The dependent variable Y must be categorical (1/0) and take binary value, e.g. if pass then $Y = 1$; else $Y = 0$
- The data meets the 'iid' criterion, i.e. the error terms, ε, are independent from one another and identically distributed
- The error term follows a binomial distribution [n, p]n = #
  - of records in the data
  - p = probability of success (pass, responder)

Maximum Likelihood Estimation

The coefficients in a logistic regression are estimated using a process called Maximum Likelihood Estimation (MLE). First, let us understand what is likelihood function before moving to

MLE. A fair coin outcome flips equally heads and tails of thesame number of times. If we toss the coin 10 times, it is expected that we get five times Head and five times Tail.

Let us now discuss about the probability of getting onlyHead as an outcome; it is 5/10 = 0.5 in the above case.
Whenever this number (P) is greater than 0.5, it is said to be infavour of Head. Whenever P is lesser than 0.5, it is said to be against the outcome of getting Head.

Let us represent 'n' flips of coin as X_1, X_2, X_3,…, X_n. Now
X_i can take the value of 1 or 0.

X_i = 1 if Head is the outcome

X_i = 0 if Tail is the outcome

When we use the Bernoulli distribution represents each flipof the coin:

$$f(x_i|\theta) = \theta^{x_i}(1-\theta)^{1-x_i}$$

Each observation X_i is independent and also identically distributed (iid), and the joint distribution simplifies to a product of distributions.

$$f(x_1, ..., x_n|\theta)\prod_{i=1}^{n} f(x_i|\theta) = \theta^{x_1}(1-\theta)^{1-x_i} \ldots \theta^{x_n}(1-\theta)^{1-x_n} = \theta^{\#H}(1-\theta)^{n-\#H},$$

where #H is the number of flips that resulted in the expectedoutcome (heads in this case).

The likelihood equation is

$$L(\theta|x) = \prod_{i=1}^{n} f(x_i|\theta)$$

But the likelihood function is not a probability. Thelikelihood for some coins may be 0.25 or 0 or 1.

MLE is about predicting the value for the parameters that maximizes the likelihood function.

$$\log L(\theta|x) = \sum_{i=1}^{n} \log f(x_i|\theta)$$

UNIT-V

Unsupervised Learning

INTRODUCTION

Unsupervised learning is a machine learning concept where the unlabelled and unclassified information is analysed to discover hidden knowledge. The algorithms work on the data without any prior training, but they are constructed in such a way that they can identify patterns, groupings, sorting order, and numerous other interesting knowledge from the set of data.

UNSUPERVISED VS SUPERVISED LEARNING

Till now, we have discussed about supervised learning where the aim was to predict the outcome variable Y on the basis of the feature set X_1:X_2:… X_n, and we discussed methods such as *regression* and *classification* for the same. We will now introduce the concept of unsupervised learning where the objective is to observe only the features X_1:X_2:… X_n; we are not going to predict any outcome variable, but rather our intention is to find out the association between the features or their grouping to understand the nature of the data. This analysis may reveal an interesting correlation between the features or a common behaviour within the subgroup of the data, which provides better understanding of the data.

In terms of statistics, a supervised learning algorithm will try to learn the probability of outcome Y for a particular input X, which is called the posterior probability. Unsupervised learning is closely related to density estimation in statistics.
Here, every input and the corresponding targets are concatenated to create a new set of input such as $\{(X_1, Y_1), (X_2, Y_2),\ldots, (X_n, Y_n)\}$, which leads to a better understanding of the correlation of X and Y; this probability notation is called the joint probability.

Let us take an example of how unsupervised learning helps in pushing movie promotions to the correct group of people. Inearlier days, movie promotions were blind push of the same data to all demography, such that everyone used to watch the same posters or trailers irrespective of their choice or preference. So, in most of the cases, the person watching the promotion or trailer would end up ignoring it, which leads to waste of effort and money on the promotion. But with the advent of smart devices and apps, there is now a huge database available to understand what type of movie is liked by what segment of the demography. Machine learning helps to find out the pattern or the repeated behaviour of the smaller groups/clusters within this database to provide the intelligence about liking or disliking of certain types of movies by different groups within the demography. So, by using this intelligence, the smart apps can push only the relevant movie promotions or trailers to the selected groups, which will significantly increase the chance of targeting the right interested person for the movie.

We will discuss two methods in this chapter for explaining the principle underlying unsupervised learning – Clustering and Association Analysis. **Clustering** is a broad class of methods used for discovering unknown subgroups in data, which is the most important concept in unsupervised learning. Another technique is **Association Analysis** which identifies alow-dimensional representation of the observations that can explain the variance and identify the association rule for the explanation.

APPLICATION OF UNSUPERVISED LEARNING

Because of its flexibility that it can work on uncategorized andunlabelled data, there are many domains where unsupervised learning finds its application. Few examples of such applications are as follows:

- Segmentation of target consumer populations by an advertisement consultingagency on the basis of few dimensions such as demography, financial data, purchasing habits, etc. so that the advertisers can reach their target consumers efficiently
- Anomaly or fraud detection in the banking sector by identifying the patternof loan defaulters
- Image processing and image segmentation such as face recognition, expression identification, etc.
- Grouping of important characteristics in genes to identify important influencers in new areas of genetics
- Utilization by data scientists to reduce the dimensionalities in sample data tosimplify modelling
- Document clustering and identifying potential labelling options

Today, unsupervised learning is used in many areas involving Artificial Intelligence (AI) and Machine Learning (ML). Chat bots, self-driven cars, and many more recent innovations are results of the combination of unsupervised andsupervised learning.

So, in this chapter, we will cover two major aspects of unsupervised learning, namely *Clustering* which helps in segmentation of the set of objects into groups of similar objects and *Association Analysis* which is related to the identification of relationships among objects in a data set.

CLUSTERING

Clustering refers to a broad set of techniques for finding subgroups, or clusters, in a data set on the basis of the characteristics of the objects within that data set in such a manner that the objects within the group are similar (or related to each other) but are different from (or unrelated to) the objects from the other groups. The effectiveness of clustering depends on how similar or related the objects within a group are or how different or unrelated the objects in different groups are from each other. It is often domain specific to define whatis meant by two objects to be similar or dissimilar and thus is an important aspect of the unsupervised machine learning task.

As an example, suppose we want to run some advertisements of a new movie for a countrywide promotionalactivity. We have data for the age, location, financial condition, and political stability of the people in different partsof the country. We may want to run a different type of campaign for the different parts grouped according to the data we have. Any logical grouping obtained by analysing the characteristics of the people will help us in driving the campaigns in a more targeted way. Clustering analysis can help in this activity by analysing different ways to group the set of people and arriving at different types of clusters.

There are many different fields where cluster analysis isused effectively, such as

- Text data mining: this includes tasks such as text categorization, text clustering, document summarization, concept extraction, sentiment analysis, and entity relation modelling
- Customer segmentation: creating clusters of customers on the basis of parameters such as demographics, financial conditions, buying habits, etc., which can be used by retailers and advertisers to promote their products inthe correct segment
- Anomaly checking: checking of anomalous behaviours such as fraudulent bank transaction, unauthorized computer intrusion, suspicious movements on a radar

scanner, etc.

- Data mining: simplify the data mining task by grouping a large number offeatures from an extremely large data set to make the analysis manageable

In this section, we will discuss the methods related to the machine learning task of clustering, which involves findingnatural groupings of data. The focus will be on

- how clustering tasks differ from classification tasks and how clustering defines groupsa classic and easy-to-understand clustering algorithm, namely *k*-means,which
- is used for clustering along with the *k*-medoids algorithm application of clustering in real-life scenarios

Clustering as a machine learning task

The primary driver of clustering knowledge is discovery rather than prediction, because we may not even know what we are looking for before starting the clustering analysis. So, clustering is defined as an unsupervised machine learning task that automatically divides the data into **clusters** or groups of similar items. The analysis achieves this without prior knowledge of the types of groups required and thus can provide an insight into the natural groupings within the data set. The primary guideline of clustering task is that the data inside a cluster should be very similar to each other but very different from those outside the cluster. We can assume that the definition of similarity might vary across applications, but the basic idea is always the same, that is, to create the group such that related elements are placed together. Using this principle, whenever a large set of diverse and varied data is presented for analysis, clustering enables to represent the data in a smaller number of groups. It helps to reduce the complexity and provides insight into patterns of relationships to generate meaningful and actionable structures within the data. The effectiveness of clustering is measured by the homogeneity within a group as well as the difference between distinct groups. See Figure 9.1 for reference.

From the above discussion, it may seem that through clustering, we are trying to label the objects with class labels. But clustering is somewhat different from the classification and numeric prediction discussed in supervised learning chapters. In each of these cases, the goal was to create a modelthat relates features to an outcome or to other features and the

model identifies patterns within the data. In contrast, clustering creates new data. Unlabelled objects are given a cluster label which is inferred entirely from the relationship of attributes within the data.

Let us take an example. You were invited to take a session on Machine Learning in a reputed university for induction of their professors on the subject. Before you create the material for the session, you want to know the level of acquaintance of the professors on the subject so that the session is successful. But you do not want to ask the inviting university, but rather do some analysis on your own on the basis of the data available freely. As Machine Learning is the intersection of Statistics and Computer Science, you focused on identifying the professors from these two areas also. So, you searched the list of research publications of these professors from the internet, and by using the machine learning algorithm, you now want to group the papers and thus infer the expertise of the professors into three buckets – Statistics, Computer Science, and Machine Learning.

After plotting the number of publications of these professors in the two core areas, namely Statistics and Computer Science,you obtain a scatter plot as shown in Figure 9.2.

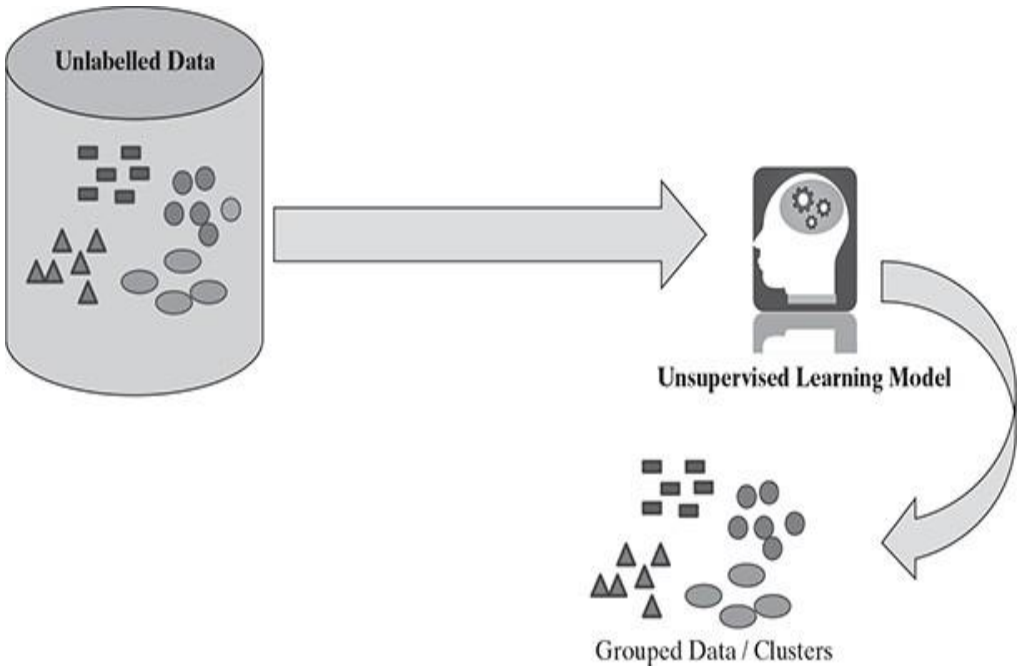


FIG. 9.1 Unsupervised learning – clustering

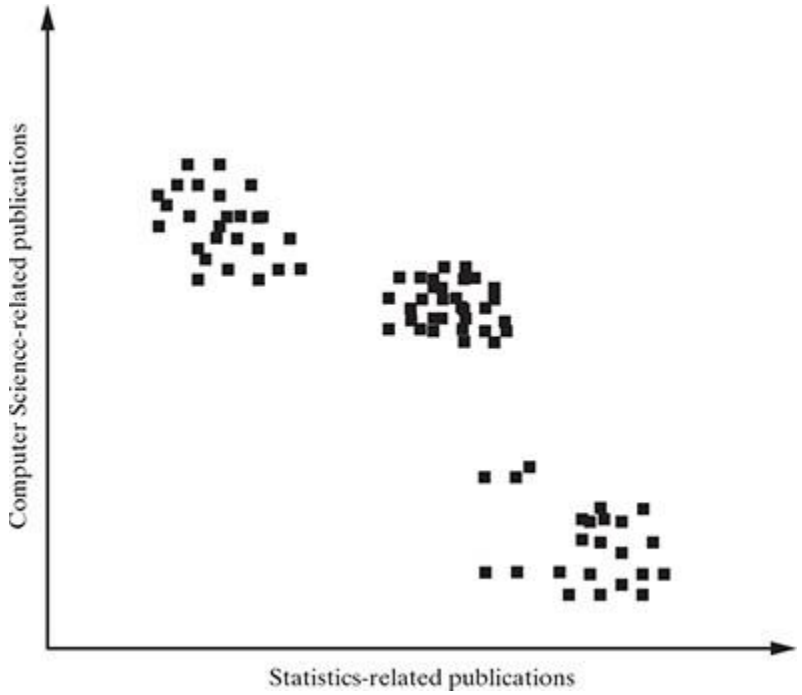


FIG. 9.2 Data set for the conference attendees

Some inferences that can be derived from the pattern analysis of the data is that there seems to be three groups or clusters emerging from the data. The pure statisticians have very less Computer Science-related papers, whereas the pure Computer Science professors have less number of statistics- related papers than Computer Science-related papers. There is a third cluster of professors who have published papers on both these areas and thus can be assumed to be the persons knowledgeable in machine learning concepts, as shown in Figure 9.3.

Thus, in the above problem, we used visual indication of logical grouping of data to identify a pattern or cluster and labelled the data in three different clusters. The main driver for our clustering was the closeness of the points to each other to form a group. The clustering algorithm uses a very similar approach to measure how closely the data points are related and decides whether they can be labelled as a homogeneous group. In the next section, we will discuss few important algorithms for clustering.

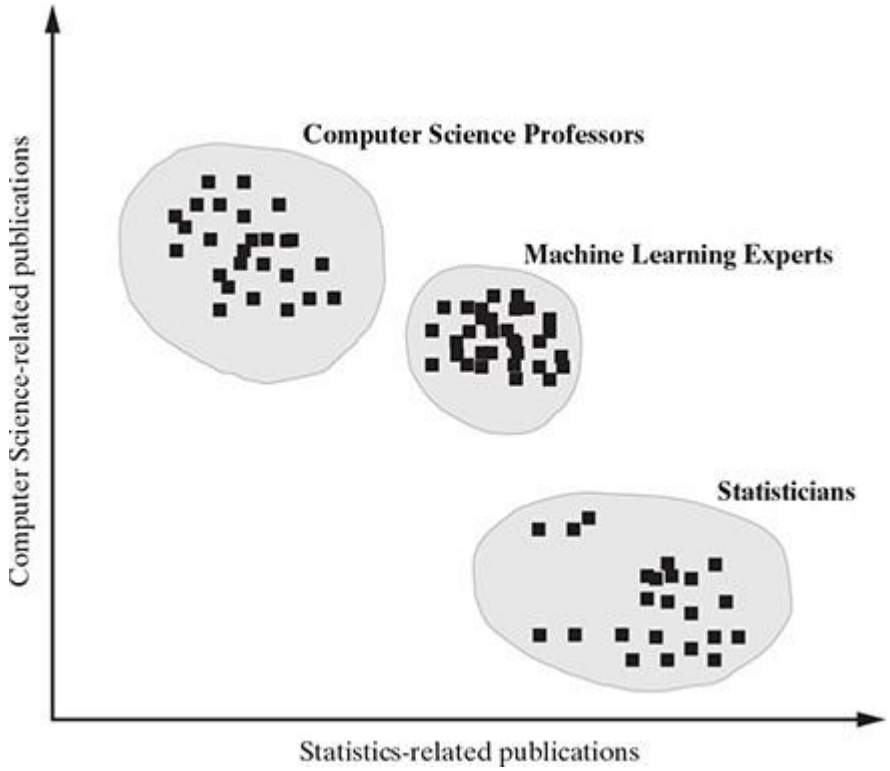


FIG. 9.C Clusters for the conference attendees

Different types of clustering techniques

The major clustering techniques are

- Partitioning methods,
- Hierarchical methods, and
- Density-based methods.

Their approach towards creating the clusters, way to measure the quality of the clusters, and applicability are different. **Table 9.1** summarizes the main characteristics ofeach method for each reference.

Table 9.1 *Different Clustering Methods*

Method	Characteristics
Partitioning methods	• Uses mean or medoid (etc.) to represent cluster centre • Adopts distance-based approach to refine clusters • Finds mutually exclusive clusters of spherical or nearly spherical shape • Effective for data sets of small to medium size
Hierarchical methods	• Creates hierarchical or tree-like structure through decomposition or merger • Uses distance between the nearest or furthest points in neighbouring clusters as a guideline for refinement • Erroneous merges or splits cannot be corrected at subsequent levels
Density-based methods	• Useful for identifying arbitrarily shaped clusters • Guiding principle of cluster creation is the identification of dense regions of objects in space which are separated by low-density regions • May filter out outliers

We will discuss each of these methods and their related techniques in details in the following sections.

Partitioning methods

Two of the most important algorithms for partitioning-based clustering are *k*-means and *k*-medoid. In the *k*-means algorithm, the centroid of the prototype is identified for clustering, which is normally the mean of a group of points. Similarly, the *k*-medoid algorithm identifies the medoid whichis the most representative point for a group of points. We can also infer that in most cases, the centroid does not correspond to an actual data point, whereas medoid is always an actual data point. Let us discuss both these algorithms in detail.

K-means - A centroid-based technique

This is one of the oldest and most popularly used algorithm forclustering. The basic principles used by this algorithm also

serves as the basis for other more sophisticated and complex algorithms. **Table 9.2** provides the strengths and weaknessesof this algorithm.

The principle of the *k*-means algorithm is to assign each of the '*n*' data points to one of the *K* clusters where '*K*' is a user-defined parameter as the number of clusters desired. The objective is to maximize the homogeneity within the clusters and also to maximize the differences between the clusters. Thehomogeneity and differences are measured in terms of the distance between the objects or points in the data set.

Algorithm 9.1 shows the simple algorithm of *K*-means

Step 1: Select *K* points in the data space and mark them as initial centroids

loop

Step 2: Assign each point in the data space to the nearest centroid to form Kclusters

Step C: Measure the distance of each point in the cluster from the centroid

Step 4: Calculate the Sum of Squared Error (SSE) to measure the quality of the clusters *(described later in this chapter)*

Step 5: Identify the new centroid of each cluster on the basis of distancebetween points

Step 6: Repeat Steps 2 to 5 to refine until centroids do not change

end loop

Table 9.2 *Strengths and Weaknesses of K-means*

Strengths	Weaknesses
• The principle used for identifying the clusters is very simple and involves very less complexity of statistical terms • The algorithm is very flexible and thus can be adjusted for most scenarios and complexities • The performance and efficiency are very high and comparable to those of any sophisticated algorithm in term of dividing the data into useful clusters	• The algorithm involves an element of random chance and thus may not find the optimal set of cluster in some cases • The starting point of guessing the number natural clusters within the data requires some experience of the user, so that the final outcome is efficient

Let us understand this algorithm with an example. In Figure9.4, we have certain set of data points, and we will apply the *k*-means algorithm to find out the clusters generated from this data set. Let us fix $K = 4$, implying that we want to create four clusters out of this data set. As the first step, we assign four random points from the data set as the centroids, as represented by the * signs, and we assign the data points to thenearest centroid to create four clusters. In the second step, on the basis of the distance of the points from the corresponding centroids, the centroids are updated and points are reassigned to the updated centroids. After three iterations, we found that the centroids are not moving as there is no scope for refinement, and thus, the *k*-means algorithm will terminate.

This provides us the most logical four groupings or cluster of the data sets where the homogeneity within the groups is highest and difference between the groups is maximum.

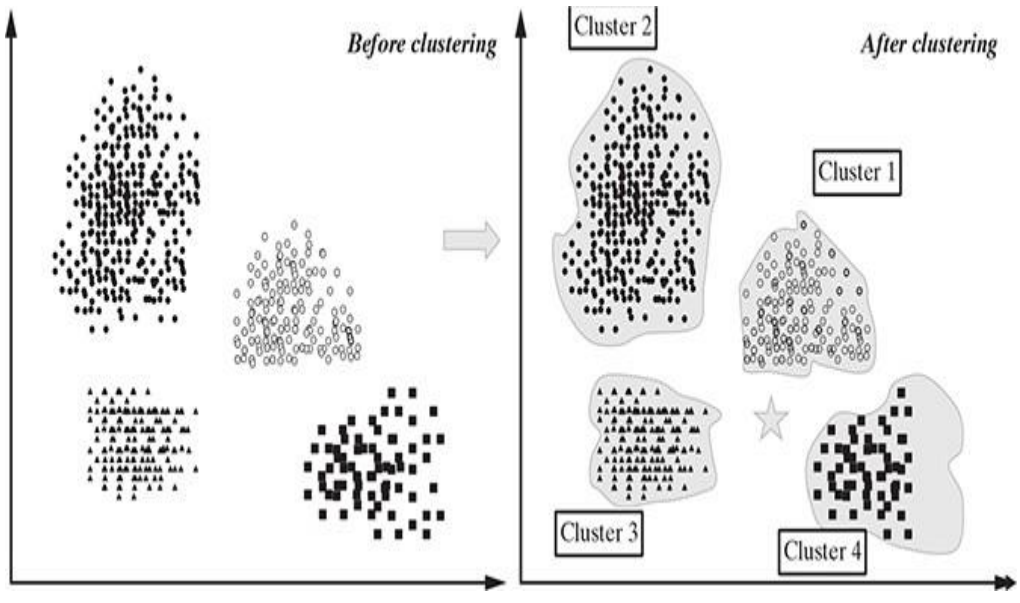


FIG. 9.4 Clustering concept – before and after clustering

Choosing appropriate number of clusters

One of the most important success factors in arriving at correct clustering is to start with the correct number of cluster assumptions. Different numbers of starting cluster lead to completely different types of data split. It will always help if we have some prior knowledge about the number of clusters and we start our *k*-means algorithm with that prior knowledge. For example, if we are clustering the data of the students of a university, it is always better to start with the number of departments in that university. Sometimes, the business needs or resource limitations drive the number of required clusters.
For example, if a movie maker wants to cluster the movies on the basis of combination of two parameters – budget of the movie: high or low, and casting of the movie: star or non-star, then there are 4 possible combinations, and thus, there can be four clusters to split the data.

For a small data set, sometimes a rule of thumb that is followed is

$$K = \sqrt{\frac{n}{2}}$$

which means that K is set as the square root of $n/2$ for a data set of n examples. But unfortunately, this thumb rule does not work well for large data sets. There are several statistical methods to arrive at the suitable number of clusters.

Elbow method

This method tries to measure the homogeneity or heterogeneity within the cluster and for various values of '*K*' and helps in arriving at the optimal '*K*'. From Figure 9.5, we can see the homogeneity will increase or heterogeneity will decrease with increasing '*K*' as the number of data points inside each cluster reduces with this increase. But these iterations take significant computation effort, and after a certain point, the increase in homogeneity benefit is no longer in accordance with the investment required to achieve it, as is evident from the figure. This point is known as the elbow point, and the '*K*' value at this point produces the optimal clustering performance. There are a large number of algorithms to calculate the homogeneity and heterogeneity of the clusters, which are not discussed in this book.

Choosing the initial centroids

Another key step for the *k*-means algorithm is to choose the initial centroids properly. One common practice is to choose random points in the data space on the basis of the number of cluster requirement and refine the points as we move into the iterations. But this often leads to higher squared error in the final clustering, thus resulting in sub-optimal clustering solution. The assumption for selecting random centroids is that

multiple subsequent runs will minimize the SSE and identify the optimal clusters. But this is often not true on the basis of the spread of the data set and the number of clusters sought. So, one effective approach is to employ the hierarchical clustering technique on sample points from the data set and then arrive at sample *K* clusters. The centroids of these initial *K* clusters are used as the initial centroids. This approach is practical when the data set has small number of points and *K* is relatively small compared to the data points. There are procedures such as bisecting *k*-means and use of post- processing to fix initial clustering issues; these procedures can produce better quality initial centroids and thus better SSE for the final clusters.

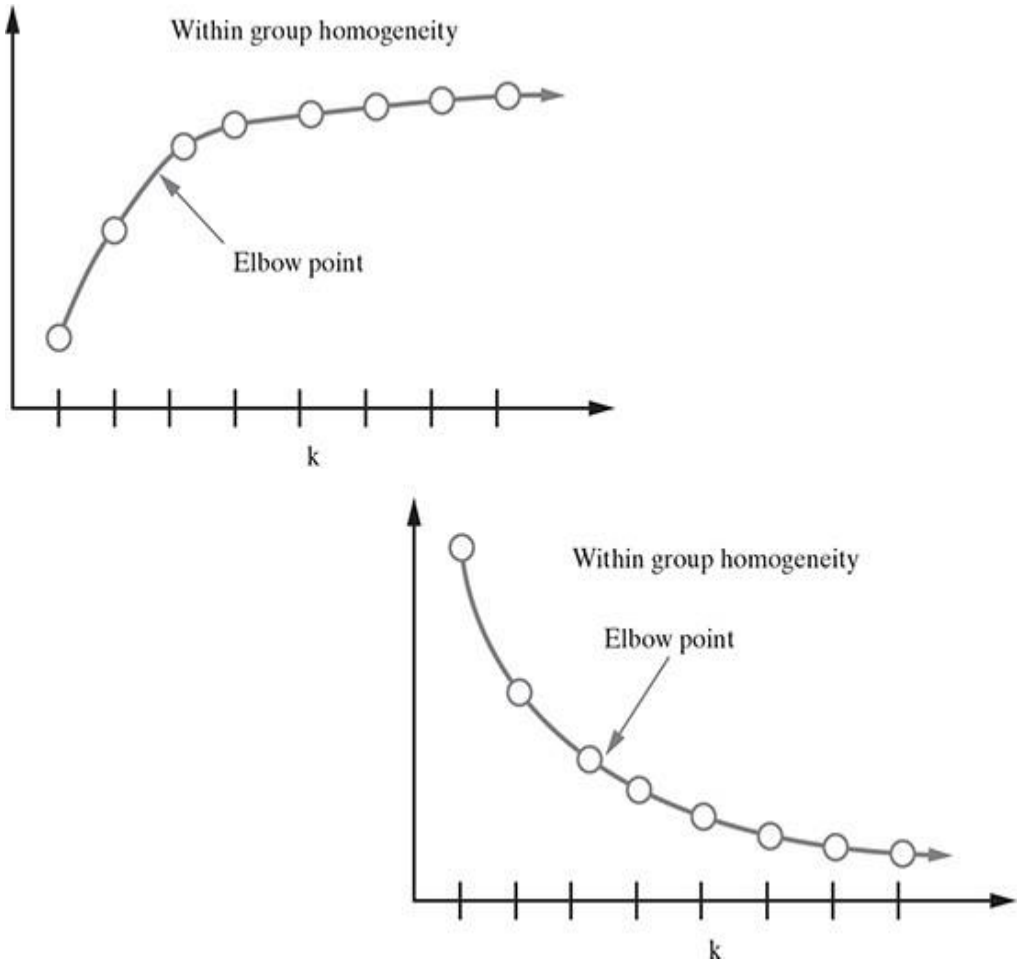


FIG. 9.5 Elbow point to determine the appropriate number of clusters

Recomputing cluster centroids

We discussed in the *k*-means algorithm that the iterative step isto recalculate the centroids of the data set after each iteration. The proximities of the data points from each other within a cluster is measured to minimize the distances. The distance of the data point from its nearest centroid can also be calculated to minimize the distances to arrive at the refined centroid. The Euclidean distance between two data points is measured as follows:

$$\text{dist}(x, y) = \sqrt{\sum_{1}^{n} (x_i - y_i)^2} \qquad (9.1)$$

Using this function, the distance between the example dataand its nearest centroid and the objective is calculated to minimize this distance. The measure of quality of clustering uses the SSE technique. The formula used is as follows:

$$\text{SSE} = \sum_{i=1}^{k} \sum_{x \in C_i} \text{dist}\,(c_i, x)^2 \qquad (9.2)$$

where dist() calculates the Euclidean distance between the centroid c_i of the cluster C_i and the data points x in the cluster.The summation of such distances over all the 'K' clusters gives the total sum of squared error. As you can understand, the lower the SSE for a clustering solution, the better is the representative position of the centroid. Thus, in our clusteringalgorithm in Algorithm 9.1, the recomputation of the
centroid involves calculating the SSE of each new centroid and arriving at the optimal centroid identification. After the centroids are repositioned, the data points nearest to the centroids are assigned to form the refined clusters. It is observed that the centroid that minimizes the SSE of the cluster is its mean. One limitation of the squared error methodis that in the case of presence of outliers in the data set, the squared error can distort the mean value of the clusters.

Let us use this understanding to identify the cluster step for the data set in Figure 9.6. Assume that the number of cluster requirement, $K = 4$. We will randomly select four cluster centroids as indicated by four different colours in Figure 9.7.

Now, on the basis of the proximity of the data points in this data set to the centroids, we partition the data set into four segments as represented by dashed lines in Figure 9.8. This diagram is called **Voronoi diagram** which creates the boundaries of the clusters. We got the initial four clusters, namely C 1 , C 2 , C 3 , and C 4 , created by the dashed lines from the vertex of the clusters, which is the point with the maximal distance from the centre of the clusters. It is now easy to understand the areas covered by each cluster and the data points within each cluster through this representation.

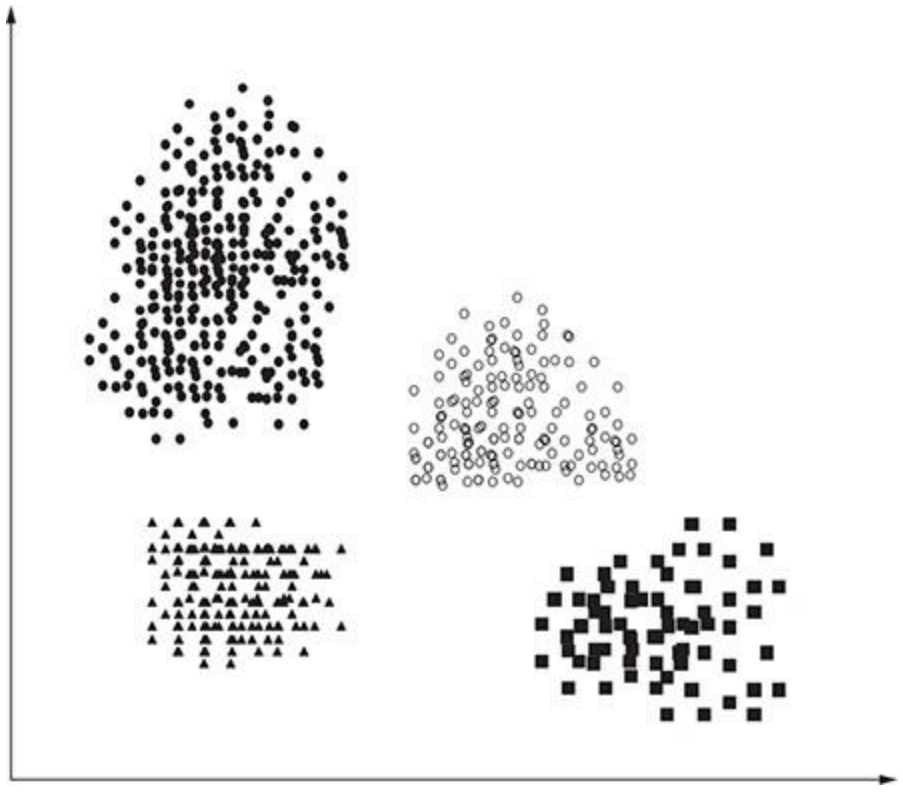


FIG. 9.6 Clustering of data set

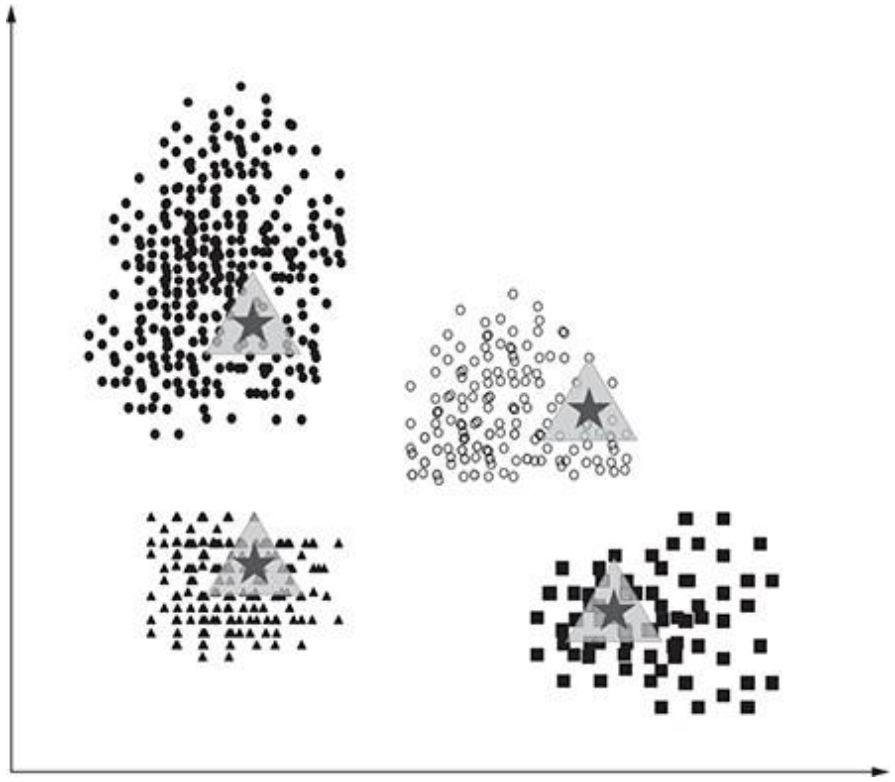


FIG. 9.7 Clustering with initial centroids

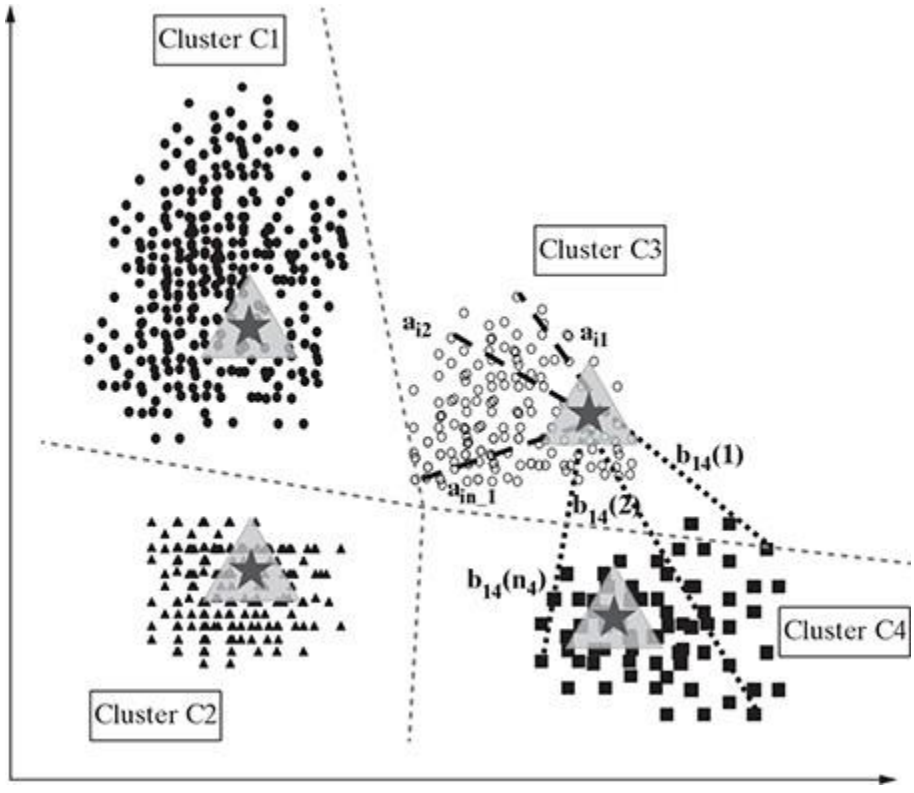


FIG. 9.8 Iteration 1: Four clusters and distance of points from the centroids

The next step is to calculate the SSE of this clustering and update the position of the

centroids. We can also proceed by our understanding that the new centroid should be the mean of the data points in the respective clusters. The distances of the data points currently marked as Cluster C_3 from the centroid of cluster C_3 are marked as a_{i1} , a_{i2} ,…, a_{in} in the figure and those determine the homogeneity within cluster C_3. On the other hand, the distances of data points of cluster C_4 from the centroid of cluster C_3 determine the heterogeneity among these two different clusters. Our aim is to minimize the homogeneity within the clusters and maximize the heterogeneity among the different clusters. So, the revised centroids are as shown in Figure 9.9.

We can also find out that the cluster boundaries are refined on the basis of the new centroids and the identification of the nearest centroids for the data points and reassigning them to the new centroids. The new points reclaimed by each cluster are shown in the diagram.

The *k*-means algorithm continues with the update of the centroid according to the new cluster and reassignment of the points, until no more data points are changed due to the centroid shift. At this point, the algorithm stops. Figure 9.10 shows the final clustering of the data set we used. The complexity of the *k*-means algorithm is *O* (*nKt*), where ‘ *n* ’ is the total number of data points or objects in the data set, *K* is the number of clusters, and ‘ *t* ’ is the number of iterations.

Normally, ‘ *K* ’ and ‘ *t* ’ are kept much smaller than ‘ *n* ’, and thus, the *k*-means method is relatively scalable and efficient in processing large data sets.

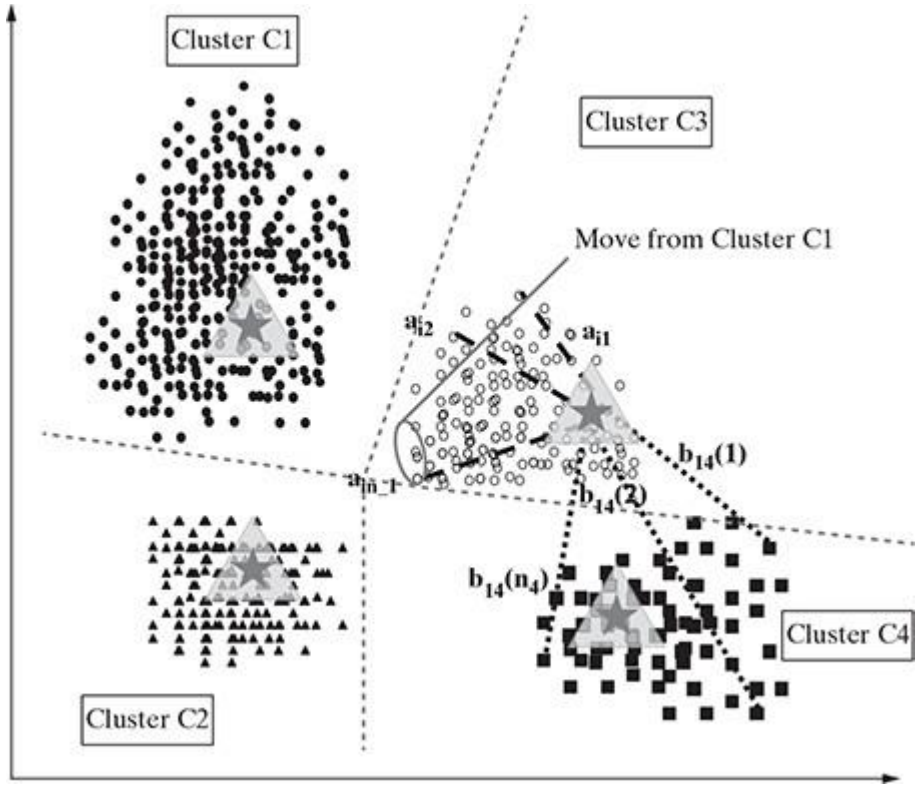


FIG. 9.9 Iteration 2: Centroids recomputed and points redistributed among the clusters according to the nearest centroid

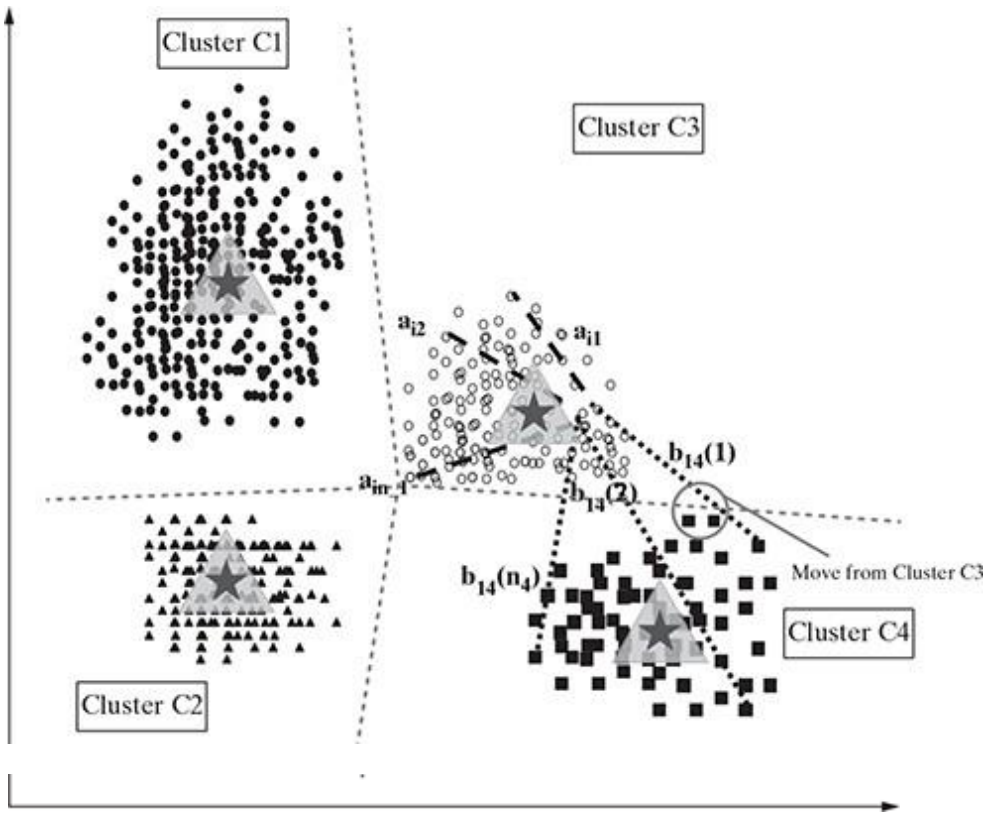


FIG. 9.1O Iteration 3: Final cluster arrangement: Centroids recomputed and points redistributed among the clusters according to the nearest centroid

groups or classes which will make it easy to identify the developer who should be fixing it.

K-Medoids: a representative object-basedtechnique

As discussed earlier, the *k*-means algorithm is sensitive to outliers in the data set and inadvertently produces skewedclusters when the means of the data points are used as centroids. Let us take an example of eight data points, and for simplicity, we can consider them to be 1-D data with values 1,2, 3, 5, 9, 10, 11, and 25. Point 25 is the outlier, and it affects the cluster formation negatively when the mean of the points isconsidered as centroids.

With $K = 2$, the initial clusters we arrived at are {1, 2, 3, 6} and {9, 10, 11, 25}.

The mean of the cluster $\{1, 2, 3, 6\} = \frac{12}{4} = 3,$

and the mean of the cluster $\{9, 10, 12, 25\} = \frac{56}{4} = 14.$ So, the SSE within the clusters is

$$(1-3)^2+(2-3)^2+(3-3)^2+(6-3)^2+(9-14)^2$$
$$+(10-14)^2+(12-14)^2+(25-14)^2=179$$

If we compare this with the cluster {1, 2, 3, 6, 9} and {10, 11, 25},

the mean of the cluster $\{1,2,3,6,9\} = \frac{21}{5} = 4.2$, and the

mean of the cluster

So, the SSE within the clusters is $\{10,12,25\} = \frac{47}{3} = 15.67.$

$$(1-4.2)^2+(2-4.2)^2+(3-4.2)^2+(6-4.2)^2+(9-4.2)^2$$
$$+(10-15.67)^2+(12-15.67)^2+(25-15.67)^2=113.84$$

Because the SSE of the second clustering is lower, *k*-meanstend to put point 9 in the same cluster with 1, 2, 3, and 6 though the point is logically nearer to points 10 and 11. This skewedness is introduced due to the outlier point 25, which shifts the mean away from the centre of the cluster.

k-medoids provides a solution to this problem. Instead of considering the mean of the data points in the cluster, *k*- medoids considers *k* representative data points from the existing points in the data set as the centre of the clusters. It then assigns the data points according to their distance from these centres to form *k* clusters. Note that the medoids in this case are actual data points or objects from the data set and notan imaginary point as in the case when the mean of the data sets within cluster is used as the centroid in the *k*-means technique. The SSE is calculated as

$$\text{SSE} = \sum_{i=1}^{k} \sum_{x \in C_i} \text{dist}\,(o_i, x)^2 \qquad (9.3)$$

where o_i is the representative point or object of cluster C_i.

Thus, the *k*-medoids method groups *n* objects in *k* clusters by minimizing the SSE. Because of the use of medoids fromthe actual representative data points, *k*-medoids is less influenced by the outliers in the data. One of the practical implementation of the *k*-medoids principle is the Partitioning

Around Medoids (PAM) algorithm. Refer to Algorithm 2table:

Algorithm 2: PAM

Step 1: Randomly choose *k* points in the data set as the initial representativepoints

loop

Step 2: Assign each of the remaining points to the cluster which has thenearest representative point

Step C: Randomly select a non-representative point o_r in each cluster

Step 4: Swap the representative point o_j with o_r and compute the new SSE after swapping

Step 5: If SSEnew < SSEold, then swap o_j with o_r to form the new set of *k* representative objects;

Step 6: Refine the *k* clusters on the basis of the nearest representative point. Logic continues until there is no change

end loop

In this algorithm, we replaced the current representative object with a non-representative object and checked if it improves the quality of clustering. In the iterative process, all possible replacements are attempted until the quality of clusters no longer improves.

If $o_1,\ldots, o_k$ are the current set of representative objects or medoids and there is a non-representative object o_r, then to determine whether o_r is a good replacement of o_j ($1 \le j \le k$), the distance of each object x is calculated from its nearest medoid from the set $\{o_1, o_2,\ldots, o_{j-1}, o_r, o_{j+1},\ldots, o_k\}$ and the SSE is calculated. If the SSE after replacing o_j with o_r decreases, it means that o_r represents the cluster better than o_j, and the data points in the set are reassigned according to the nearest medoids now.

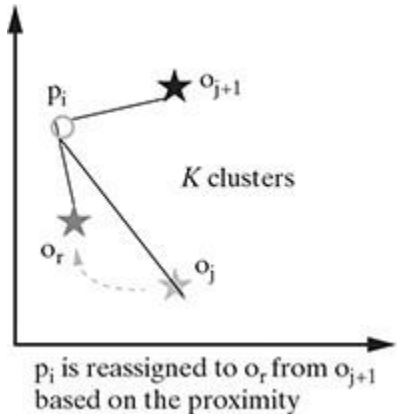


FIG. 9.11 PAM algorithm: Reassignment of points to different clusters

As shown in Figure 9.11, point p_i was belonging to the cluster with medoid o_{j+1} in the first iteration, but after o_j was replaced by o_r, it was found that p_i is nearest to the new random medoid and thus gets assigned to it. In this way, the clusters get refined after each medoid is replaced with a new non-representative medoid. Each time a reassignment is done, the SSE based on the new medoid is calculated. The differencebetween the SSE before and after the swap indicates whether or not the replacement is improving the quality of the clustering by

bringing the most similar points together.Though the *k*-medoids algorithm provides an effective way to eliminate the noise or outliers in the data set, which was the problem in the *k*-means algorithm, it is expensive in terms of calculations. The complexity of each iteration in the *k*-medoidsalgorithm is $O(k(n - k)^2)$. For large value of '*n*' and '*k*', this calculation becomes much costlier than that of the *k*-means algorithm.

Hierarchical clustering

Till now, we have discussed the various methods for partitioning the data into different clusters. But there are situations when the data needs to be partitioned into groups at different levels such as in a hierarchy. The hierarchical clustering methods are used to group the data into hierarchy ortree-like structure. For example, in a machine learning problem of organizing employees of a university in different departments, first the employees are grouped under the different departments in the university, and then within each department, the employees can be grouped according to their roles such as professors, assistant professors, supervisors, lab assistants, etc. This creates a hierarchical structure of the employee data and eases visualization and analysis. Similarly, there may be a data set which has an underlying hierarchy structure that we want to discover and we can use the hierarchical clustering methods to achieve that.

There are two main hierarchical clustering methods:agglomerative clustering and divisive clustering.
Agglomerative clustering is a bottom-up technique which starts with individual objects as clusters and then iteratively merges them to form larger clusters. On the other hand, the divisive method starts with one cluster with all given objects

and then splits it iteratively to form smaller clusters. SeeFigure 9.12.

The agglomerative hierarchical clustering method uses the bottom-up strategy. It starts with each object forming its owncluster and then iteratively merges the clusters according to their similarity to form larger clusters. It terminates either when a certain clustering condition imposed by the user is achieved or all the clusters merge into a single cluster.

The divisive hierarchical clustering method uses a top-downstrategy. The starting point is the largest cluster with all the objects in it, and then, it is split recursively to form smaller and smaller clusters, thus forming the hierarchy. The end of iterations is achieved when the objects in the final clusters are sufficiently homogeneous to each other or the final clusters contain only one object or the user-defined clustering condition is achieved.

In both these cases, it is important to select the split and merger points carefully, because the subsequent splits or mergers will use the result of the previous ones and there is nooption to perform any object swapping between the clusters orrectify the decisions made in previous steps, which may resultin poor clustering quality at the end.

A dendrogram is a commonly used tree structure representation of step-by-step creation of hierarchical clustering. It shows how the clusters are **merged** iteratively (in the case of agglomerative clustering) or **split** iteratively (in thecase of divisive clustering) to arrive at the optimal clustering solution. Figure 9.13 shows a dendro-gram with four levels and how the objects are merged or split at each level to arrive at the hierarchical clustering.

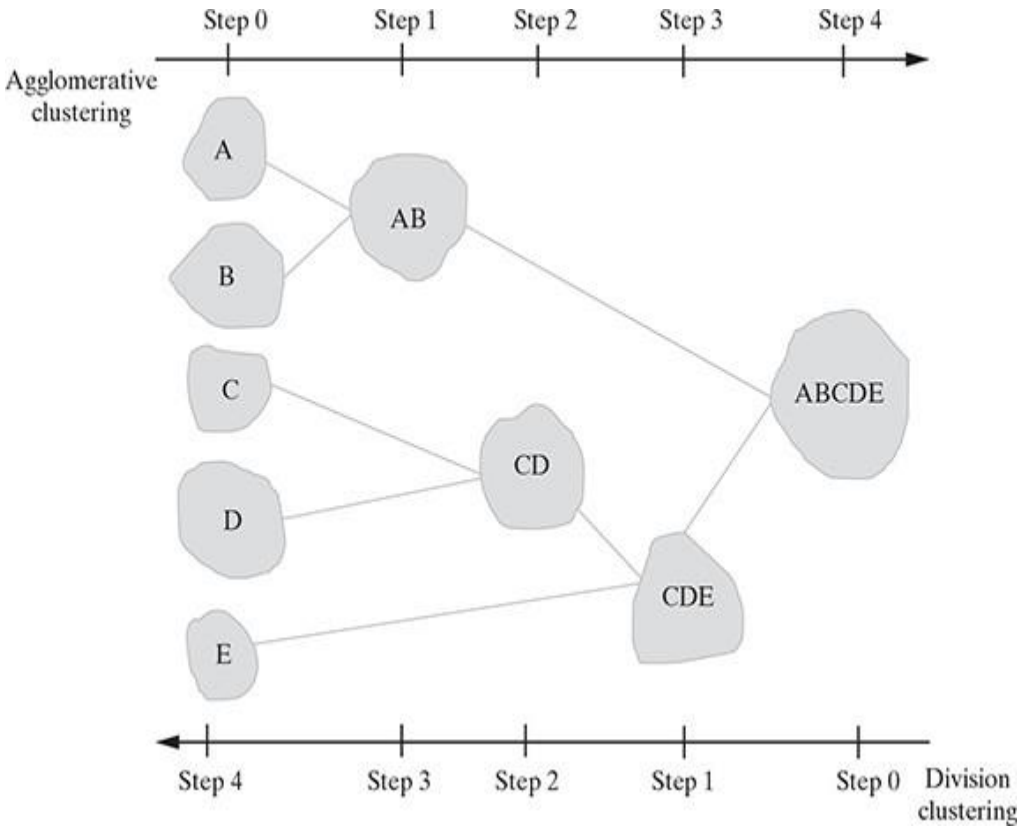


FIG. 9.12 Agglomerative and divisive hierarchical clustering

One of the core measures of proximities between clusters is the distance between them. There are four standard methods tomeasure the distance between clusters:

Let C_i and C_j be the two clusters with n_i and n_j respectively.p_i and p_j represents the points in clusters C_i and C_j respectively. We will denote the mean of cluster C_i as m_i.

$$\text{Minimum distance } D_{\min}(C_i, C_j) = \min_{p_i \in C_i,\ p_j \in C_j} \{|p_i - p_j|\} \tag{9.4}$$

$$\text{Maximum distance } D_{\max}(C_i, C_j) = \max_{p_i \in C_i,\ p_j \in C_j} \{|p_i - p_j|\} \tag{9.5}$$

$$\text{Mean distance } D_{\text{mean}}(C_i, C_j) = \{|m_i - m_j|\} \tag{9.6}$$

$$\text{Average distance } D_{\text{avg}}(C_i, C_j) = \frac{1}{n_i n_j} \sum_{p_i \in C_i,\ p_j \in C_j} |pi - pj| \tag{9.7}$$

Refer to Figure 9.14 for understanding the concept of thesedistances.

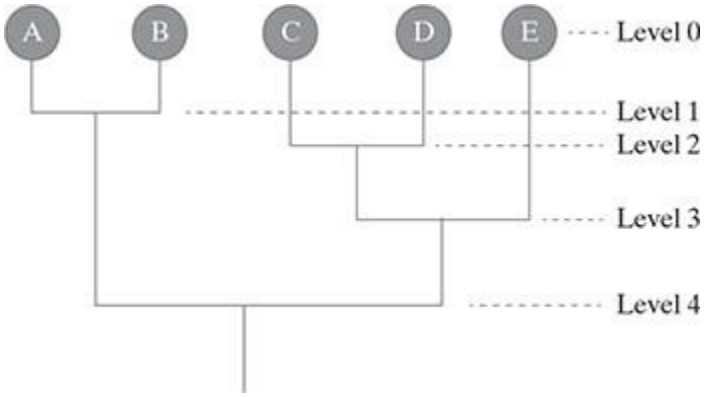


FIG. 9.1C Dendrogram representation of hierarchical clustering

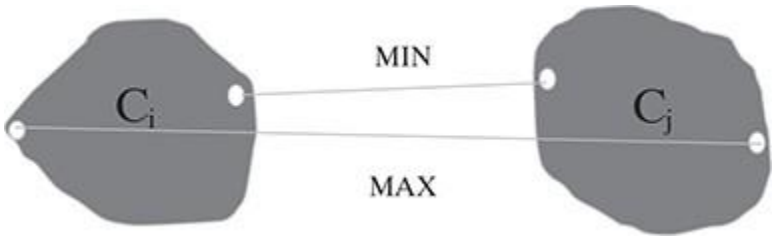


FIG. 9.14 Distance measure in algorithmic methods

Often the distance measure is used to decide when to terminate the clustering algorithm. For example, in an agglomerative clustering, the merging iterations may be

stopped once the MIN distance between two neighbouring clusters becomes less than the user-defined threshold. So, when an algorithm uses the minimum distance D_{min} to measure the distance between the clusters, then it is referred to as nearest neighbour clustering algorithm, and if the decision to stop the algorithm is based on a user-defined limit on D_{min}, then it is called single linkage algorithm.

On the other hand, when an algorithm uses the maximum distance D_{max} to measure the distance between the clusters, then it is referred to as furthest neighbour clustering algorithm, and if the decision to stop the algorithm is based on a user- defined limit on D_{max} then it is called complete linkage algorithm.

As minimum and maximum measures provide two extreme options to measure distance between the clusters, they are prone to the outliers and noisy data. Instead, the use of mean and average distance helps in avoiding such problem and provides more consistent results.

Density-based methods - DBSCAN

You might have noticed that when we used the partitioning and hierarchical clustering methods, the resulting clusters are spherical or nearly spherical in nature. In the case of the other shaped clusters such as S-shaped or uneven shaped clusters, the above two types of method do not provide accurate results. The density-based clustering approach provides a solution to identify clusters of arbitrary shapes. The principle is based on identifying the dense area and sparse area within the data set and then run the clustering algorithm. DBSCAN is one of the popular density-based algorithm which creates clusters by using connected regions with high density.

FINDING PATTERN USING ASSOCIATION RULE

Association rule presents a methodology that is useful for identifying interesting relationships hidden in large data sets. It is also known as **association analysis**, and the discovered relationships can be represented in the form of association rules comprising a set of frequent items. A common application of this analysis is the **Market Basket Analysis** that retailers use for cross-selling of their products. For example, every large grocery store accumulates a large volume of data about the buying pattern of the customers. On the basis of the items purchased together, the retailers can push some cross-selling either by placing the items bought together in adjacent areas or creating some combo offer with those different product types. The below association rule signifies that people who have bought bread and milk have often boughtegg also; so, for the retailer, it makes sense that these items areplaced together for new opportunities for cross-selling.

$$\{\text{Bread, Milk}\} \rightarrow \{\text{Egg}\}$$

The application of association analysis is also widespread in other domains such as bioinformatics, medical diagnosis, scientific data analysis, and web data mining. For example, by discovering the interesting relationship between food habit and patients developing breast cancer, a new cancer prevention mechanism can be found which will benefit thousands of people in the world. In this book, we will mainly illustrate the analysis techniques by using the market basket example, but it can be used more widely across domains to identify association among items in transactional data. The huge pool

of data generated everyday through tracked transactions such as barcode scanner, online purchase, and inventory tracking systems has enabled for machine learning systems to learn from this wealth of data. We will discuss the methods for finding useful associations in large databases by using simple statistical performance measures while managing the peculiarities of working with such transactional data. One significant challenge in working with the large volume of data is that it may be computationally very expensive to discover patterns from such data. Moreover, there may be cases when some of the associations occurred by chance, which can lead to potentially false knowledge. While discussing the association analysis, we will discuss both these points.

We will use the transaction data in the table below for our examples of association analysis. This simplified version of the market basket data will show how the association rules canbe effectively used for the market basket analysis.

Definition of common terms

Let us understand few common terminologies used inassociation analysis.

Itemset

One or more items are grouped together and are surrounded bybrackets to indicate that they form a set, or more specifically, an **itemset** that appears in the data with some regularity. For example, in **Table 9.C**, {Bread, Milk, Egg} can be grouped together to form an itemset as those are frequently bought together. To generalize this concept, if $I = \{i_1, i_2, \ldots, i_n\}$ are the items in a market basket data and $T = \{t_1, t_2, \ldots, t_n\}$ are the set of all the transactions, then each transaction t_i contains a subset of items from I. A collection of zero or more items is

called an itemset. A null itemset is the one which does not contain any item. In the association analysis, an itemset is called *k*-itemset if it contains *k* number of items. Thus, theitemset {Bread, Milk, Egg} is a three-itemset.

Table 9.C *Market Basket Transaction Data*

Transaction Number	Purchased Items
1	{Bread, Milk, Egg, Butter, Salt, Apple}
2	{Bread, Milk, Egg, Apple}
3	{Bread, Milk, Butter, Apple}
4	{Milk, Egg, Butter, Apple}
5	{Bread, Egg, Salt}
6	{Bread, Milk, Egg, Apple}

Support count

Support count denotes the number of transactions in which a particular itemset is present. This is a very important propertyof an itemset as it denotes the frequency of occurrence for theitemset. This is expressed as

$$\sigma(X) = |\{t_i | X \subseteq t_i, t_i \varepsilon T\}|$$

where |{}| denotes the number of elements in a set

In **Table 9.C**, the itemset {Bread, Milk, Egg} occurs together three times and thus have a support count of 3.

Association rule

The result of the market basket analysis is expressed as a set of**association rules** that specify patterns of relationships among items. A typical rule might be expressed as{Bread, Milk} →{Egg}, which denotes that if Bread and Milk are purchased, then Egg is also likely to be purchased. Thus, association rules are learned from subsets of itemsets. For example, the preceding rule was identified from the set of *{Bread, Milk, Egg}*.

It should be noted that an association rule is an expressionof $X \rightarrow Y$ where X and Y are disjoint itemsets, i.e. $X \cap Y = 0$.

Support and confidence are the two concepts that are usedfor measuring the strength of an association rule. Support denotes how often a rule is applicable to a given data set.
Confidence indicates how often the items in Y appear in transactions that contain X in a total transaction of N. Confidence denotes the predictive power or accuracy of the rule. So, the mathematical expressions are

$$\text{Support}, s(X \rightarrow Y) = \frac{\sigma\left(X \bigcup Y\right)}{N} \qquad (9.8)$$

$$\text{Confidence}, c(X \rightarrow Y) = \frac{\sigma\left(X \bigcup Y\right)}{\sigma\left(X\right)} \qquad (9.9)$$

In our data set 9.3, if we consider the association rule {Bread, Milk} → {Egg}, then from the above formula

$$\text{Confidence } c(\{\text{Bread, Milk}\} \rightarrow \{\text{Egg}\}) = \frac{\text{support count of } \{\text{Bread, Milk, Egg}\}}{\text{support count of } \{\text{Bread, Milk}\}}$$
$$= \frac{3}{4}$$
$$= 0.75$$

$$\text{Confidence } c(\{\text{Bread, Milk}\} \rightarrow \{\text{Egg}\}) = \frac{\text{support count of } \{\text{Bread, Milk, Egg}\}}{\text{support count of } \{\text{Bread, Milk}\}}$$
$$= \frac{3}{4}$$
$$= 0.75$$

It is important to understand the role of support and confidence in the association analysis. A low support may indicate that the rule has occurred by chance. Also, from its application perspective, this rule may not be a very attractive business investment as the items are seldom bought together by the customers. Thus, support can provide the intelligence ofidentifying the most interesting rules for analysis.

Similarly, confidence provides the measurement for reliability of the inference of a rule. Higher confidence of arule $X \rightarrow Y$ denotes more likelihood of to be present in transactions that contain X as it is the estimate of the conditional probability of Y given X.

Also, understand that the confidence of X leading to Y is notthe same as the confidence of Y leading to X. In our example, confidence of {Bread, Milk} → {Egg} = 0.75 but confidence of $\{\text{Egg}\} \rightarrow \{\text{Bread, Milk}\} = \frac{3}{5} = 0.6.$ Here, the rule {Bread, Milk} → {Egg} is the strong rule.

Association rules were developed in the context of Big Data and data science and are not used for prediction. They are used for unsupervised knowledge discovery in large databases, unlike the classification and numeric prediction algorithms.
Still we will find that association rule learners are closely related to and share many features of the classification rule learners. As association rule learners are unsupervised, there is no need for the algorithm to be trained; this means that no prior labelling of the data is required. The programme is simply run on a data set in the hope that interesting associations are found.

Obviously, the downside is that there is not an easy way to objectively measure the performance of a rule learner, aside from evaluating them for qualitative usefulness. Also, note that the association rule analysis is used to search for interesting connections among a very large number of variables. Though human beings are capable of such insight quite intuitively, sometimes it requires expert-level knowledge or a great deal of experience to achieve the performance of a rule-learning algorithm. Additionally, some data may be too large or complex for humans to decipher and analyse so easily.

The apriori algorithm for association rule learning

As discussed earlier, the main challenge of discovering an association rule and learning from it is the large volume of transactional data and the related complexity. Because of the variation of features in transactional data, the number of feature sets within a data set usually becomes very large. This leads to the problem of handling a very large number of itemsets, which grows exponentially with the number of features. If there are k items which may or may not be part of an itemset, then there is 2^k ways of creating itemsets with those items. For example, if a seller is dealing with 100 different items, then the learner need to evaluate $2^{100} = 1 \times e^{30}$ itemsets for arriving at the rule, which is computationally impossible. So, it is important to filter out the most important (and thus manageable in size) itemsets and use the resources on those to arrive at the reasonably efficient association rules.

The first step for us is to decide the minimum support and minimum confidence of the association rules. From a set of transaction T, let us assume that we will find out all the rules that have support $\geq \min S$ and confidence $\geq \min C$, where $\min S$ and $\min C$ are the support and confidence thresholds, respectively, for the rules to be considered acceptable. Now, even if we put the $\min S = 20\%$ and $\min C = 50\%$, it is seen that more than 80% of the rules are discarded; this means that a large portion of the computational efforts could have been avoided if the itemsets for consideration were first pruned and the itemsets which cannot generate association rules with reasonable support and confidence were removed. The approach to achieve this goal is discussed below.

Step 1: decouple the support and confidence requirements.
According to formula 9.8, the support of the rule $X \rightarrow Y$ is dependent only on the support of its corresponding itemsets. For example, all the below rules have the same support as their itemsets are the same {Bread, Milk, Egg}:

- {Bread, Milk} → {Egg}
- {Bread, Egg} → {Milk}
- {Egg, Milk} → {Bread}
- {Bread} → {Egg, Milk}
- {Milk} → {Bread, Egg}
- {Egg} → {Bread, Milk}

So, the same treatment can be applied to this association rule on the basis of the frequency of the itemset. In this case, if

the itemset {Bread, Milk, Egg} is rare in the basket transactions, then all these six rules can be discarded withoutcomputing their individual support and confidence values.
This identifies some important strategies for arriving at theassociation rules:

1. **Generate Frequent Itemset:** Once the min*S* is set for a particular assignment, identify all the itemsets that satisfy min*S*. These itemsets are called frequent itemsets.
2. **Generate Rules:** From the frequent itemsets found in the previous step, discover all the high confidence rules. These are called strong rules.

Please note that the computation requirement for identifying frequent itemsets is more intense than the rule generation. So, different techniques have been evolved to optimize the performance for frequent itemset generation as well as rule discovery as discussed in the next section.

Build the apriori principle rules

One of the most widely used algorithm to reduce the number of itemsets to search for the association rule is known as Apriori. It has proven to be successful in simplifying the association rule learning to a great extent. The principle got its name from the fact that the algorithm utilizes a simple prior belief (i.e. *a priori*) about the properties of frequent itemsets:

If an itemset is frequent, then all of its subsets must also befrequent.

This principle significantly restricts the number of itemsets to be searched for rule generation. For example, if in a market basket analysis, it is found that an item like 'Salt' is not so frequently bought along with the breakfast items, then it is fine to remove all the itemsets containing salt for rule generation as

their contribution to the support and confidence of the rule willbe insignificant.

The converse also holds true:

If an itemset is frequent, then all the supersets must befrequent too.

These are very powerful principles which help in pruning the exponential search space based on the support measure andis known as support-based pruning. The key property of the support measure used here is that the support for an itemset never exceeds the support for its subsets. This is also known asthe anti-monotone property of the support measure.

Let us use the transaction data in **Table 9.C** to illustrate the Apriori principle and its use. From the full itemset of six items
{Bread, Milk, Egg, Butter, Salt, Apple}, there are 2^6 ways to create baskets or itemsets (including the null itemset) as shownin Figure 9.15:

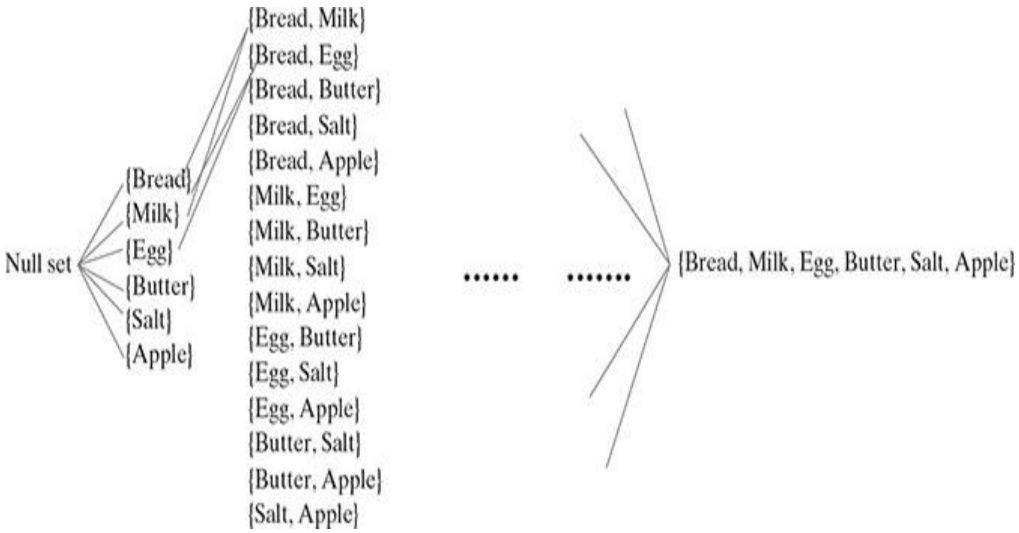


FIG. 9.15 Sixty-four ways to create itemsets from 6 items

Without applying any filtering logic, the brute-force approach would involve calculating the support count for each itemset in Figure 9.16. Thus, by comparing each item in the generated itemset with the actual transactions mentioned in **Table 9.C**, we can determine the support count of the itemset. For example, if {Bread, Milk} is present in any transactions in **Table 9.C**, then its support count will be incremented by 1. As we can understand, this is a very computation heavy activity, and as discussed earlier, many of the computations may get wasted at a later point of time because some itemsets will be found to be infrequent in the transactions. To get an idea of thetotal computations to be done, the number of comparisons to be done is $T \times N \times L$, where T is the number of transactions (6 in our case), N is the number of candidate itemsets (64 in our case), and L is the maximum transaction width (6 in our case).

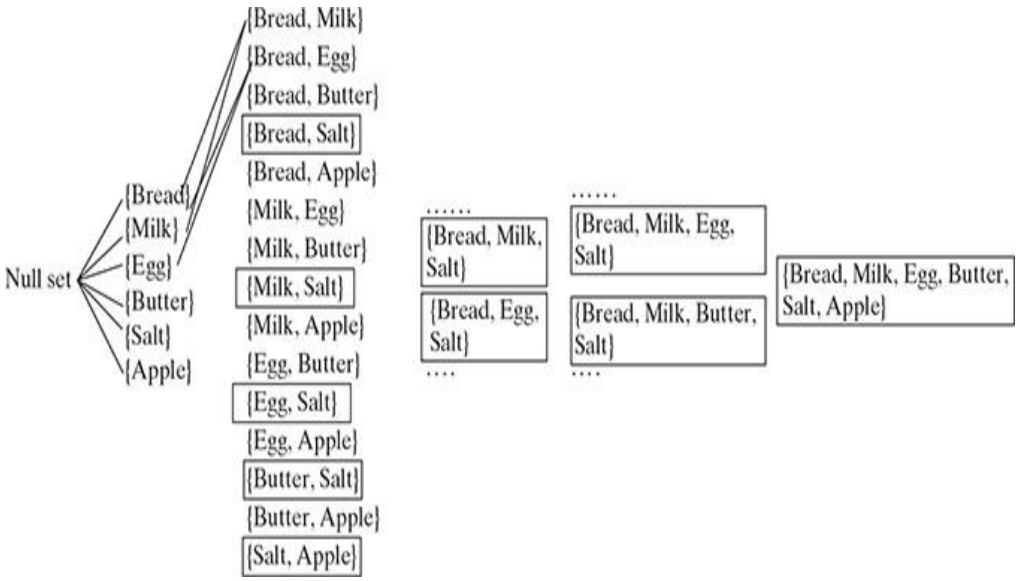


FIG. 9.16 Discarding the itemsets consisting of Salt

Let us apply the Apriori principle on this data set to reduce the number of candidate itemsets (N). We could identify from the transaction **Table 9.C** that Salt is an infrequent item. So, by

applying the Apriori principle, we can say that all the itemsetswhich are superset of Salt will be infrequent and thus can be discarded from comparison to discover the association rule as shown in Figure 9.16.

This approach reduces the computation effort for a good number of itemsets and will make our search process more efficient. Thus, in each such iteration, we can determine the support count of each itemset, and on the basis of the min support value fixed for our analysis, any itemset in the hierarchy that does not meet the min support criteria can be discarded to make the rule generation faster and easier.

To generalize the example in order to build a set of rules with the Apriori principle, we will use the Apriori principle that states that all subsets of a frequent itemset must also be frequent. In other words, if $\{X, Y\}$ is frequent, then both $\{X\}$ and $\{Y\}$ must be frequent. Also by definition, the support metric indicates how frequently an itemset appears in the data.Thus, if we know that $\{X\}$ does not meet a desired support threshold, there is no reason to consider $\{X, Y\}$ or any itemset containing $\{X\}$; it cannot possibly be frequent.

This logic of the Apriori algorithm excludes potential association rules prior to actually evaluating them. The actualprocess of creating rules involves two phases:

- Identifying all itemsets that meet a minimum support threshold set for theanalysis
- Creating rules from these itemsets that meet a minimum confidence threshold which identifies the strong rules

The first phase involves multiple iterations where each successive iteration requires evaluating the support of storing aset of increasingly large itemsets. For instance, iteration 1 evaluates the set of one-item itemsets (one-itemsets), iteration2 involves evaluating the two-itemsets, etc.. The result of eachiteration N is a set of all *N*-itemsets that meet the minimum support threshold. Normally, all the itemsets from iteration *N* are combined in order to generate candidate itemsets for evaluation in iteration $N + 1$, but by applying the Apriori principle, we can eliminate some of them even before the nextiteration starts. If $\{X\}$, $\{Y\}$, and $\{Z\}$ are frequent in iteration 1while $\{W\}$ is not frequent, then iteration 2 will consider only $\{X, Y\}$, $\{X, Z\}$, and $\{Y, Z\}$. We can see that the algorithm needs to evaluate only three itemsets rather than the six that would have been evaluated if sets containing *W* had not beeneliminated by *apriori*.

By continuing with the iterations, let us assume that during iteration 2, it is discovered that $\{X, Y\}$ and $\{Y, Z\}$ are frequent,but $\{X, Z\}$ is not. Although iteration 3 would normally begin by evaluating the support for $\{X, Y, Z\}$, this step need not occur at all. The Apriori principle states that $\{X, Y, Z\}$ cannot be frequent, because the subset $\{X, Z\}$ is not. Therefore, in iteration 3, the algorithm may stop as no new itemset can be generated.

Once we identify the qualifying itemsets for analysis, the second phase of the Apriori algorithm begins. For the given setof frequent itemsets, association rules are generated from all possible subsets. For example, $\{X, Y\}$ would result in candidate rules for $\{X\} \rightarrow \{Y\}$ and $\{Y\} \rightarrow \{X\}$. These rules are evaluated against a minimum confidence threshold, and any rule that does not meet the desired confidence level is eliminated, thus finally yielding the set of strong rules.

Though the Apriori principle is widely used in the market basket analysis and other applications of association rule help

in the discovery of new relationship among objects, there are certain strengths and weaknesses we need to keep in mind before employing it over the target data set:

Strengths	Weaknesses
• Provides reasonable accuracy while working with very large amounts of transactional data • Discovers rules that are easy to understand • Provides valuable insight into the unexpected knowledge in data sets, which is a key aspect of learning	• Not very accurate in the case the data set is small as the smaller occurrences of itemsets may not be due to chance • Some effort is involved to separate the insight from the common sense • In the case of widespread presence of random patterns, the principle can draw spurious conclusions