UNIT 2:

MODELING AND EVALUATION & BASICS OF FEATURE ENGINEERING

Unit-2

MODELLING AND EVALUATION & BASICS OF FEATURE ENGINEERING

Part-1

INTRODUCTION

The basic learning process, irrespective of the fact that the learner is a human or a machine, can be divided into three parts:

- Data Input
- Abstraction
- Generalization

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.

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 from the 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.

But that is not possible in reality.

The number of criminals in the database and 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.

The same thing can be done using machine learning too.

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 to decide 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 summarized and 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**.

Generalization searches through the huge set of abstracted knowledge to come up with a small and manageable set of key findings.

It is not possible to do an exhaustive search by reviewing each of the abstracted findings one-by-one.

A heuristic search is employed, an approach which is also used for human learning (often termed as ‘gut-feel’).

It is quite obvious that the heuristics sometimes result in erroneous result. If the outcome is systematically incorrect, the learning is said to have a **bias**.

• SELECTING A MODEL

An association between potential causes of disturbance and criminal incidents has 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 or dependent variable).

Input variables can be denoted by X, while individual input variables are represented as $X_1, X_2, X_3, \ldots, X_n$ 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 frequently tracked 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 model is 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 difference being 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 of a 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.

There are three broad categories of machine learning approaches used for resolving different types of problems.
They are

- 1.**Supervised**
  - Classification
  - Regression
-

2.**Unsupervised**
- Clustering

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. 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.

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.

- ## 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 model attempts 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 of a category or class to which a data instance belongs to. Below are some examples:

- Predicting win/loss in a cricket match
- Predicting whether a transaction is fraud
- Predicting whether a customer may move to another product

The models which are used for prediction of target features of 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 popular classification models include *k*-Nearest Neighbor (kNN), Naïve Bayes, and Decision Tree.

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

- Prediction of revenue growth in the succeeding year
- Prediction of rainfall amount in the coming monsoon
- 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.

• 2.Descriptive models

Models for unsupervised learning or descriptive models are used to describe a data set or gain insight from a data set.

There is no target feature or single feature of interest in case of unsupervised 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 of clustering include

- Customer grouping or segmentation based on social, demographic, ethnic, etc. factors
- Grouping of music based on different aspects like genre, language, time-period, etc.
- 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.

3. Holdout method

In case of supervised learning, a model is trained using the labelled input data. 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 sure that the data in both the buckets are similar in nature, the division is done randomly. Random numbers are used to assign data 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 data for validating the trained model is known as holdout method.

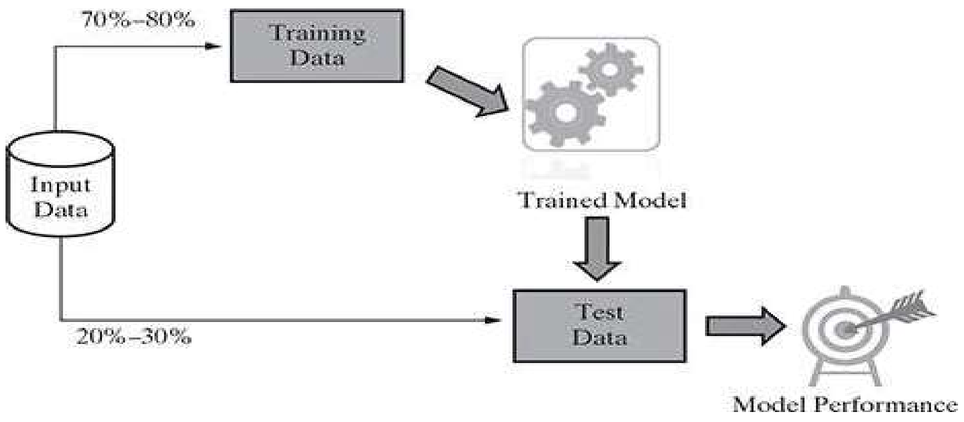


FIG. 3.1 Holdout method

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.

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 the model 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.

- ***4.K*-fold Cross-validation method**

Holdout method employing stratified random sampling approach still heads into issues in certain specific situations..

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 is drawn) 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 any number. However, there are two approaches which are extremely popular:

- 10-fold cross-validation (10-fold CV)
- 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*-fold cross-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., the records in a fold are drawn by using random sampling technique.

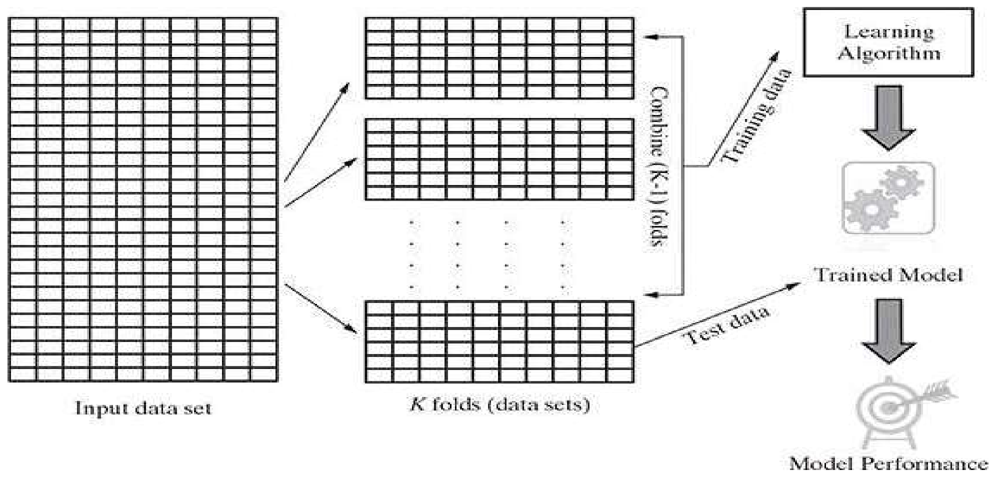


FIG. 3.2 Overall approach for *K*-fold cross-validation

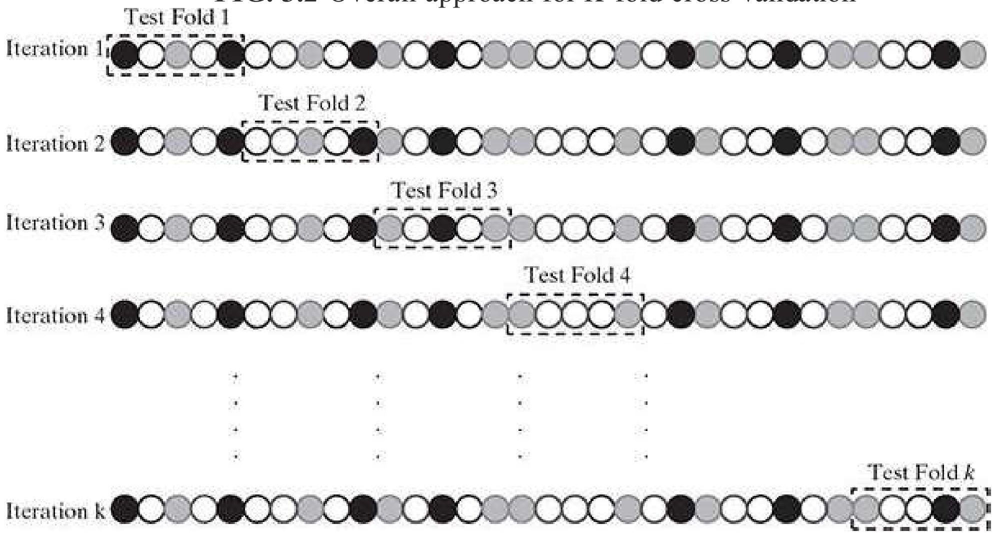


FIG. 3.3 Detailed approach for fold selection

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.

• 5.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 data sets of small size, i.e. having very less number of data instances.

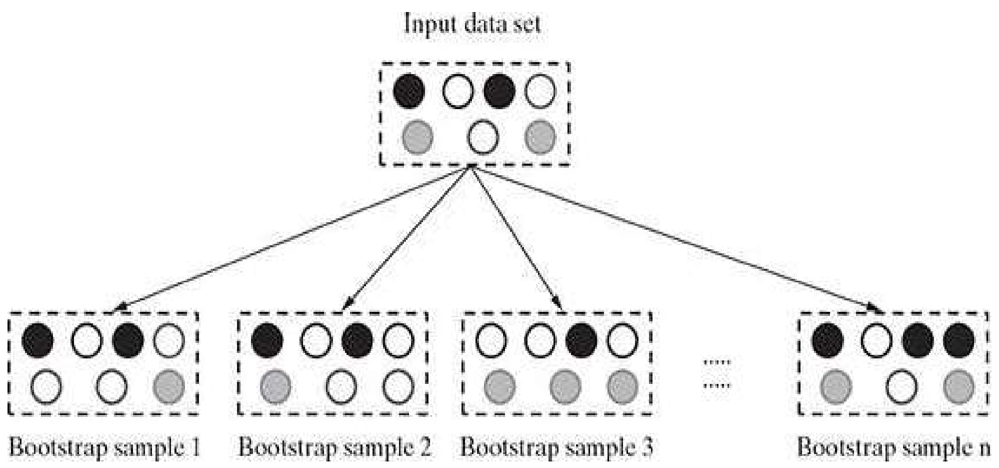
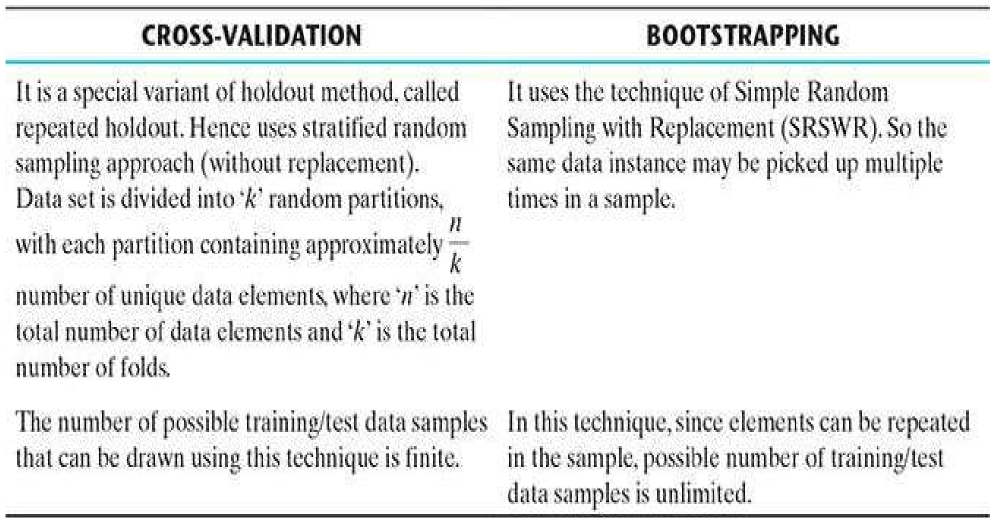


FIG. 3.4 Bootstrap sampling



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.

• Lazy vs. Eager learner

Eager learning follows the general principles of machine learning – it tries to construct a generalized, input-independent target 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 of the 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 learners take more time in the learning phase than the lazy learners.

Some of the algorithms which adopt eager learning approach include Decision Tree, Support Vector Machine, Neural Network, etc.

Lazy learning, on the other hand, completely skips the abstraction and generalization processes, 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 instance learning. They are also called non-parametric learning.

Lazy learners take very little time in training because not much of training actually happens.

One of the most popular algorithm for lazy learning is *k*-nearest neighbor.

MODEL REPRESENTATION AND INTERPRETABILITY

- **1.Underfitting**

If the target function is kept too simple, it may not be able to capture the essential nuances and represent the underlying data well.

A typical case of underfitting may occur when trying to represent a non-linear data with a linear model as demonstrated by both cases of underfitting shown in figure
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 generalization to test data. Underfitting can be avoided by

- using more training data
- reducing features by effective feature selection

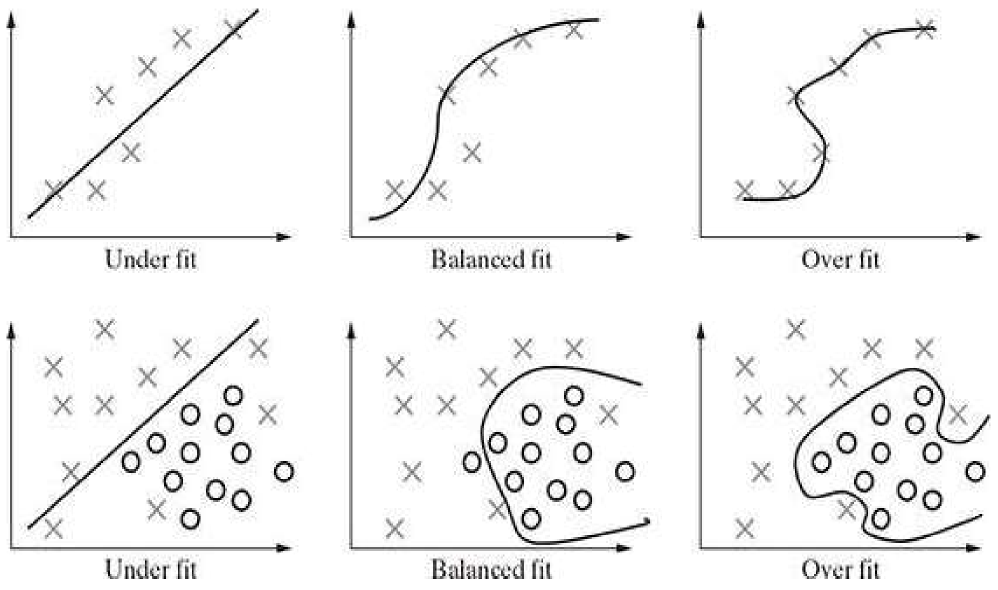


FIG. 3.5 Underfitting and Overfitting of models

- **2.Overfitting**

Overfitting refers to a situation where the model has been designed in such a way that it emulates the training data too closely.

In such a case, any specific deviation in the training data, like noise or outliers, gets embedded in the model.

It adversely impacts the performance of the model on the test data.

Overfitting, in many cases, occur as a result of trying to fit an excessively complex model to closely match the training data. This is represented with a sample data set in figure 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 test data set. Overfitting can be avoided by

- using re-sampling techniques like *k*-fold cross validation
- hold back of a validation data set
- remove the nodes which have little or no predictive power for the given machine learning problem.

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

• 3.Bias – variance trade-off

In supervised learning, the class value assigned by the learning model built based on the training data may differ from the actual class value.

This error in learning can be of two types –errors due to ‘bias’ and error due to ‘variance’. Let’s try to understand each of them in details.

- ## *1.**Errors due to ‘Bias’***

Errors due to bias arise from simplifying assumptions made by the model to make the target function less complex or easier to learn.

In short, it is due to underfitting of the model.

Parametric models generally have high bias making them easier to understand/interpret and faster to learn.

These algorithms have a poor performance on data sets, which are complex in nature and do not align with the simplifying assumptions made by the algorithm. Underfitting results in high bias.

- ## ***2.Errors due to ‘Variance’***

Errors due to variance occur from difference in training data sets used to train the model. Different training data sets (randomly sampled from the input data set) are used to train
the model.

Ideally the difference in the data sets should not be significant and the model trained using different training data sets should not be too different.

 However, in case of overfitting, since the model closely matches the training data, even a small difference in training data gets magnified in
the model.

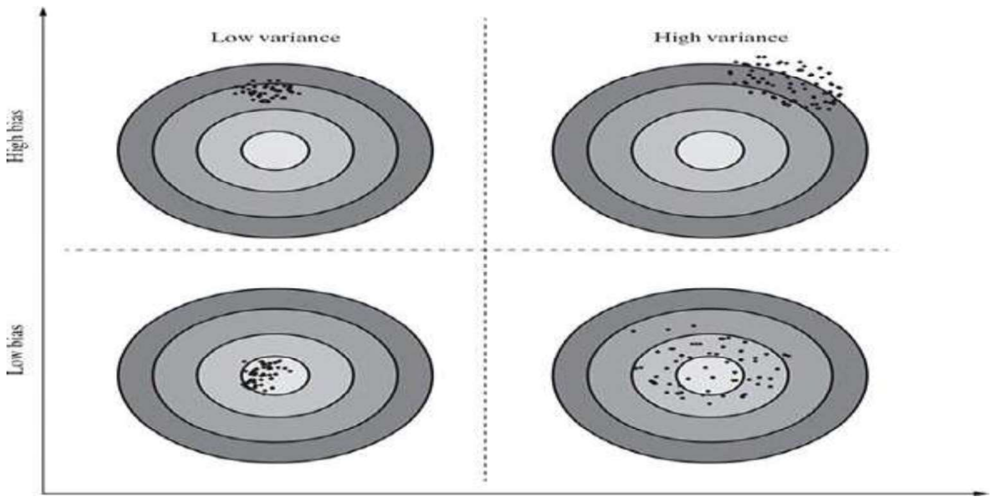


FIG. 3.6 Bias-variance trade-off

So, the problems in training a model can either happen because either (a) the model is too simple and hence fails to interpret the data grossly or

(b) the model is extremely complex and magnifies even small differences in the training data.i.e.,

Increasing the bias will decrease the variance, and Increasing the variance will decrease the bias

On one hand, parametric algorithms are generally seen to demonstrate high bias but low variance.

On the other hand, non-parametric algorithms demonstrate low bias and high variance.

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.

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.

• EVALUATING PERFORMANCE OF A MODEL

• 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 predictor features.

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.

To evaluate the performance of the model, the number 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 classifications or predictions made by a model, the accuracy of the model is calculated. If 99 out of 100 times the model has classified correctly, then the model accuracy is said to be 99%.

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 match win/loss prediction:

- the model predicted win and the team won
- the model predicted win and the team lost
- the model predicted loss and the team won
- 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 as True Positive (TP) cases.

The second case, i.e. the model predicted win and the team lost 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 not the class of interest.
These cases are referred as False Negative (FN) cases.

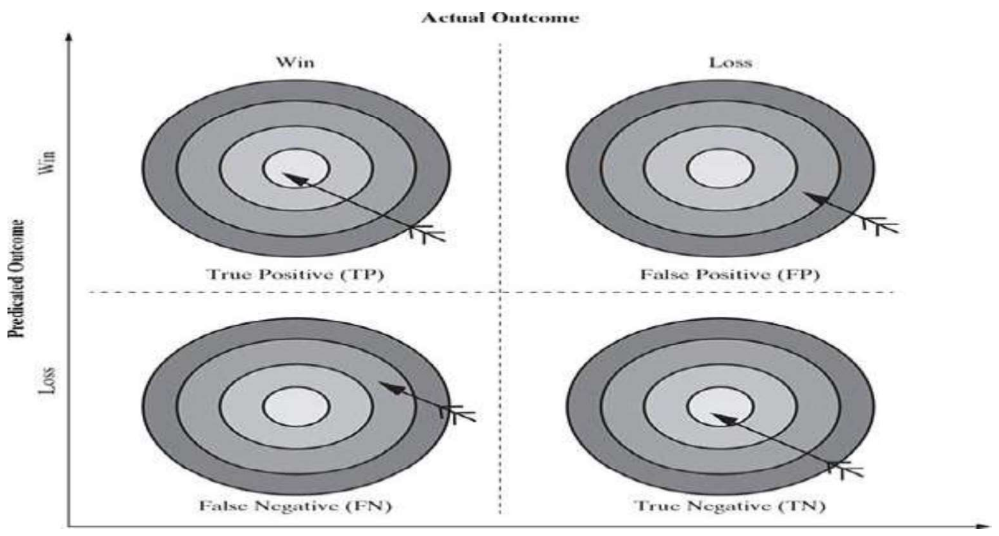


FIG. 3.7 Details of model classification

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.

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

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 problem involving three classes, the confusion matrix would be 3 × 3, etc.

Let’s assume the confusion matrix of the win/loss prediction of 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.

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

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

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

In context of the above confusion matrix,

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

Sometimes, correct prediction, both TPs as well as TNs, may happen by mere coincidence.

Kappa value of a model indicates the adjusted the model accuracy. It is calculated using the formula below:

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

$$P(a) = \text{Proportion of observed agreement between actual and predicted in overall data set}$$

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

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

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

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.

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

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

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

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

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

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

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

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

Sensitivity measure gives the proportion of tumours which are actually malignant and have been predicted as malignant. 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.

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

A higher value of specificity will indicate a better model performance.

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 a class 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 for the 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 precision is 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 the total wins were predicted correctly.

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

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

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

- ***F-measure***

F-measure is another measure of model performance which combines the precision and recall. It takes the harmonic mean of 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 cricket match 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.

- ***Receiver operating characteristic (ROC) curves***

Receiver Operating Characteristic (ROC) curve helps in visualizing the performance of a classification model.

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

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

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.

The area under curve (AUC) value, as shown in figure 3.8a , is the area of the two-dimensional space under the curve extending from (0, 0) to (1, 1). 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 is better than classifier 2.

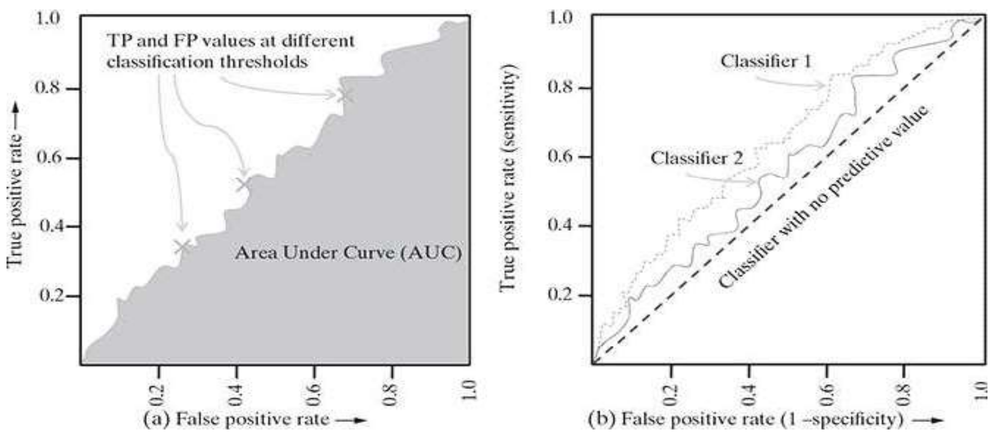


FIG. 3.8 ROC curve

A quick indicative interpretation of the predictive values from 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

• Supervised learning – regression

A regression model which ensures that the difference between predicted and actual values is 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 the predictor variable (say x) and 'value' is the target variable (say y), the linear regression model can be represented in the form:

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

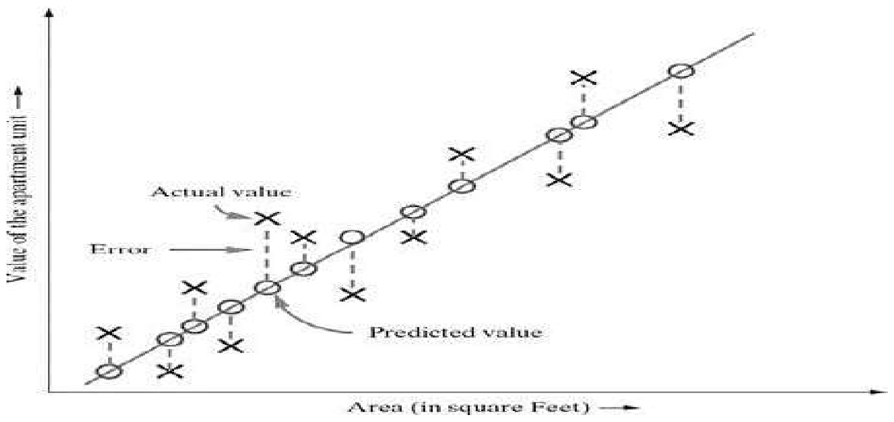


FIG. 3.9 Error – Predicted vs. actual value

For a certain value of *x*, say x̂, 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 ȳ is the mean.

Sum of Squared Errors (SSE) (of prediction) = sum of the

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

- **Unsupervised learning - clustering**

Clustering algorithms try to reveal natural groupings amongst the data sets.

Even if the number of clusters is given, the same number of clusters can be formed with different groups of data instances.

A clustering algorithm is successful if the clusters identified using the algorithm is able to achieve the right results in the overall problem domain.

There are couple of popular approaches which are adopted for cluster quality evaluation.

- *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,

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

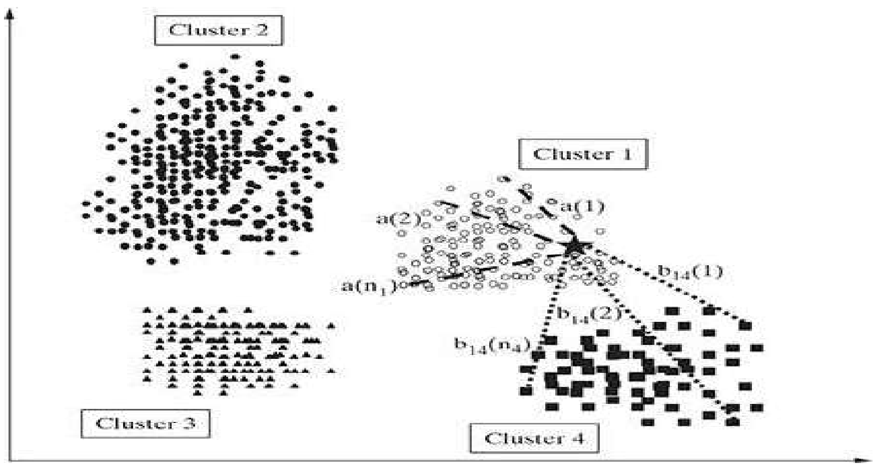


FIG. 3.1O Silhouette width calculation

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 4 and take an average of all those distances. Hence,

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

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

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

- *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 data used 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:

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

• IMPROVING PERFORMANCE OF A MODEL

Model selection is done one several aspects:

- Type of learning the task in hand, i.e. supervised or unsupervised

- Type of the data, i.e. categorical or numeric
- Sometimes on the problem domain
- Above all, experience in working with different models to solve problems of diverse domains

So, assuming that the model selection is done, what are the different 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, in the popular classification model *k*-Nearest Neighbour (*k*NN), using different values of '*k*' or the number of nearest neighbours to be considered, the model can be tuned.
In the same way, a number of hidden layers can be adjusted to tune the 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.
This approach of combining different models with diverse strengths is 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 as usual 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 be used to generate unique training data sets.

Alternatively, the same training data may be used but the models combined are quite varying, e.g, SVM, neural network, *k*NN, etc.
The outputs from the different models are combined using a combination function.

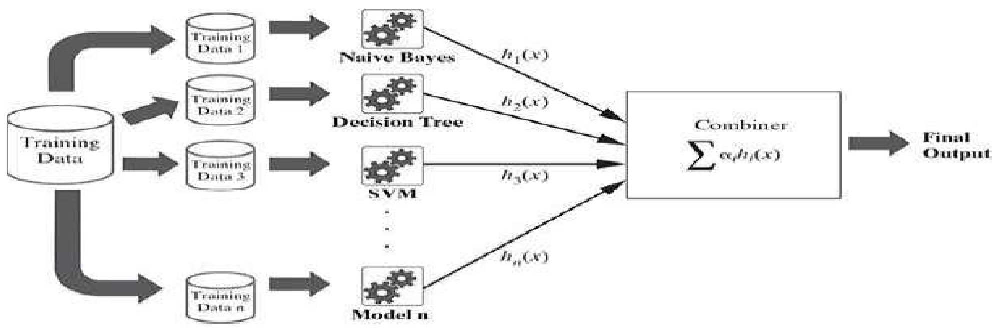


FIG. 3.11 Ensemble

One of the earliest and most popular ensemble models is **bootstrap aggregating** or **bagging**.

Bagging uses bootstrap sampling method 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 a very simple ensemble technique which can perform really well for unstable learners like a decision tree

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 of different models.

Adaptive boosting or **AdaBoost** is a special variant of boosting algorithm. It is based on the idea of generating weak learners and slowly learning

Random forest is another ensemble-based technique. It is an ensemble of decision trees – hence the name random forest to indicate a forest of decision trees.

•

Part-2

Basics of Feature Engineering

- **INTRODUCTION**

Modelling alone doesn’t help us to realize the effectiveness of machine learning as a problem- solving tool. So we also learnt how to measure the effectiveness of machine learning models in solving problems.

We need to touch upon another key aspect which plays a critical role in solving any machine learning problem – feature engineering.

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.

- What is a feature?

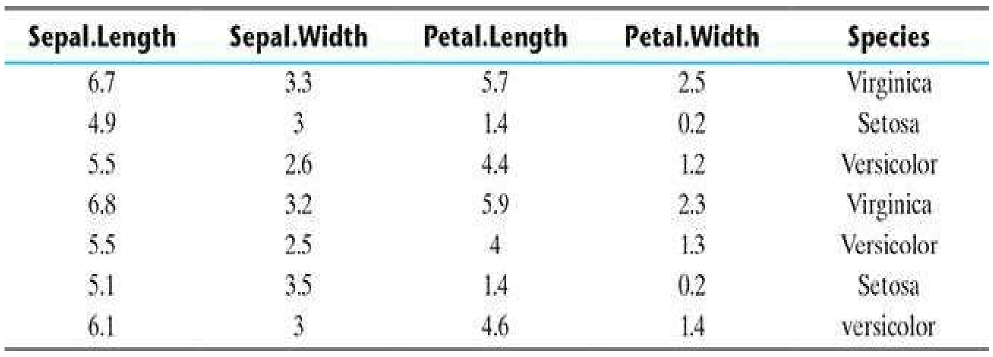
A feature is an attribute of a data set that is used in a machine learning process.

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 attributes or 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

- What is feature engineering?

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

Feature engineering is an important pre-processing step for machine learning. It has two major elements:

- feature transformation
- 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:

- feature construction
- 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 $(F_1, F_2, \ldots, F_m)$ of F_i $(F_1, F_2, \ldots, F_n)$, where $m < n$, such that F_j is most meaningful and gets the best result for a machine learning problem.

- **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.

To deal with this problem, feature transformation comes into play. Feature transformation is used as an effective tool 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 set Achieving highest efficiency in the learning task

- **1.Feature construction**

Feature construction involves transforming a given set of input features to generate a new set of more powerful features.

let’s take the example of a real estate data set having details of all apartments sold in a specific region.

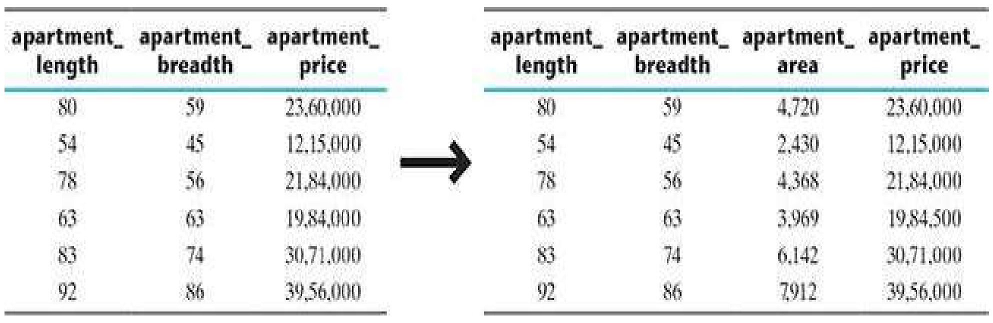
The data set has three features – apartment length, apartment breadth, and price of the apartment. If it is used as an input to a regression problem, such data can be training data for the regression model.

So given the training data, the model should be able to predict the price of an apartment whose price is 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

$\rightarrow$

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	7912	39,56,000

FIG. 4.2 Feature construction (example 1)

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

when features have categorical value and machine learning needs numeric value inputs
when features having numeric (continuous) values and need to be converted to ordinal values

when text-specific feature construction needs to be done

- *2.Encoding categorical (nominal) variables*

Let's take the example of another data set on athletes, as presented in Figure 4.3a.

The data set has features age, city of origin, parents athlete (i.e. indicate whether any one of the parents was an athlete) and Chance of Win.

The feature chance of a win is a class variable while the others are predictor variables.

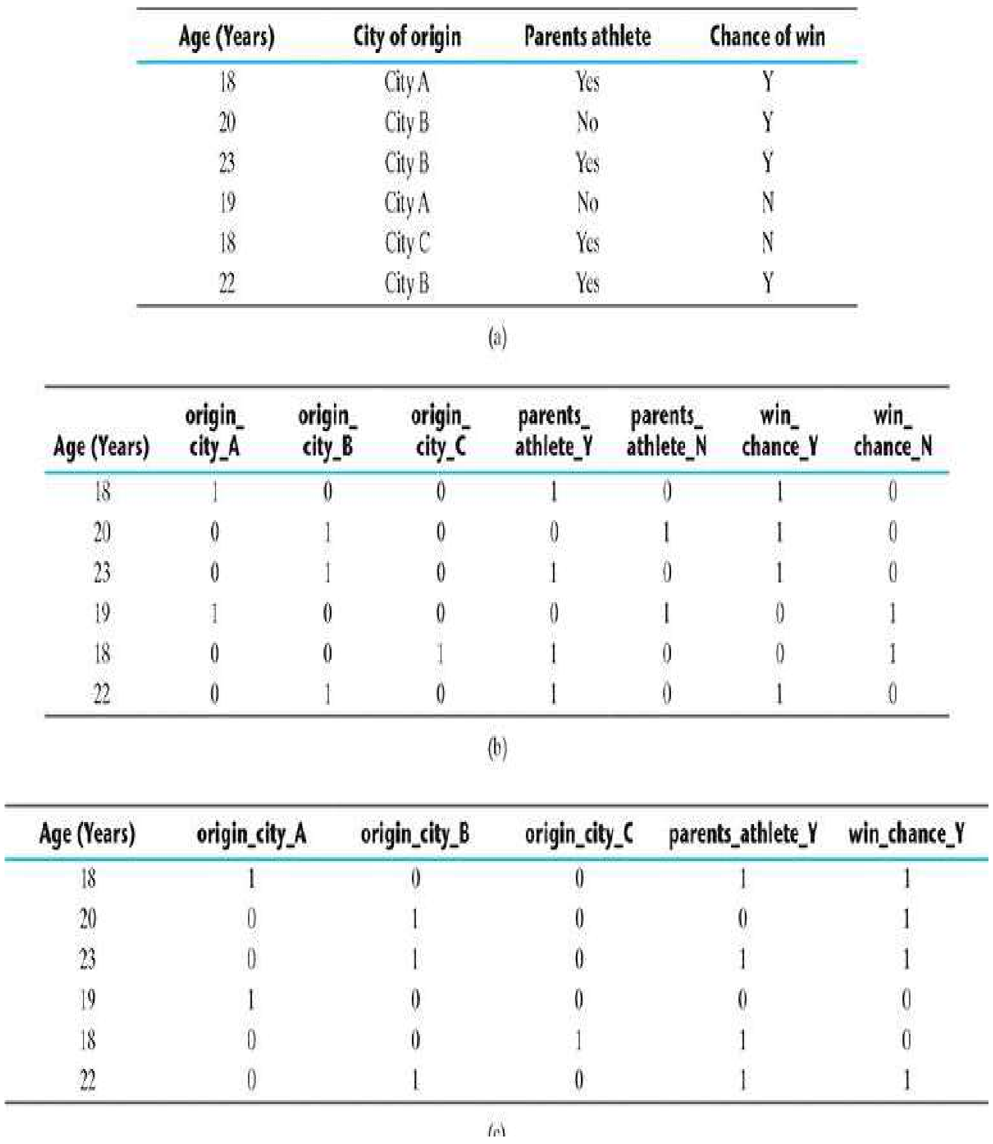
Any machine learning algorithm, whether it's a classification algorithm (like *k*NN) or a regression algorithm, requires numerical figures to learn from.

So there are three features – City of origin, Parents athlete, and Chance of win, which are categorical in nature and cannot be used 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 the same way, parents_athlete_Y and parents_athlete_N will have values 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. 4.3 Feature construction (encoding nominal variables)

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 shown in Figure 4.3c.

- ***3.Encoding categorical (ordinal) variables***

Let’s take an example of a student data set. Let’s assume that there are three variable – science marks, maths marks and grade as shown in Figure 4.4a.

As we can see, the grade is an ordinal variable with values A, B, C, and D.

To transform this variable 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.Transforming numeric (continuous) features to categorical features***

Sometimes there is a need of transforming a continuous numerical variable into a categorical variable.

For example, we may 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. The numerical feature apartment_price as shown in Figure 4.5a.

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

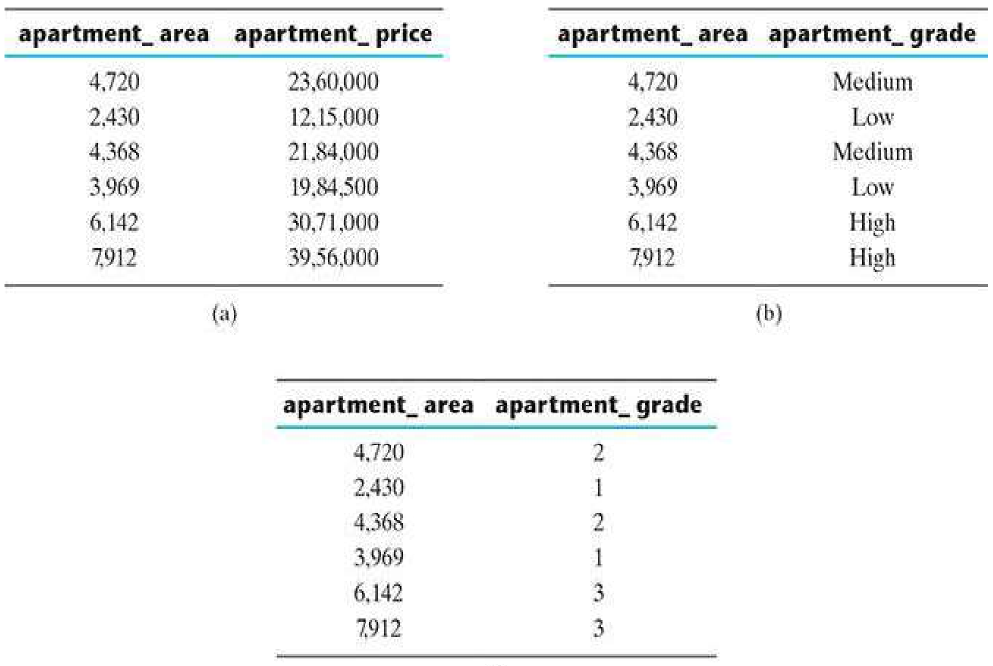
- ***5.Text-specific feature construction***

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.

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 is known 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:

- tokenize
- count
- normalize

In order to tokenize a corpus, the blank spaces and punctuations are used as delimiters to separate out the words, or tokens.

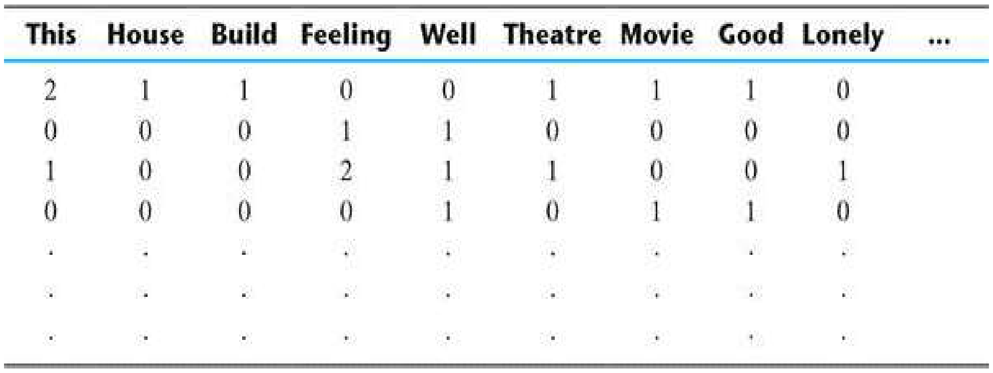
Then the number of occurrences of each token is counted, for each document. Lastly, tokens are weighted with
reducing importance when they occur in the majority of the documents.

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 is known 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)

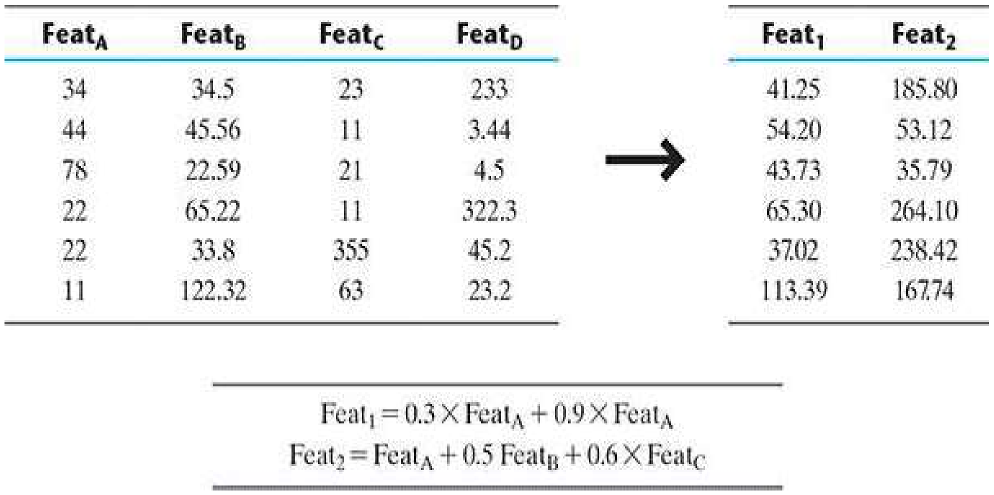
• Feature extraction

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

- For Boolean features: Conjunctions, Disjunctions, Negation, etc.
- For nominal features: Cartesian product, M of N, etc.
- 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 a data 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

$\acute{F}_i(\acute{F}_1, \acute{F}_2, \ldots, \acute{F}_m)\acute{F}_i = f(F_i)$will have a set of features such that and $m < n$. For example, $\acute{F}_1 = k_1F_1 + k_2F_2$. This is depicted in Figure 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

$\rightarrow$

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

$$\text{Feat}_1 = 0.3 \times \text{Feat}_A + 0.9 \times \text{Feat}_A$$
$$\text{Feat}_2 = \text{Feat}_A + 0.5\ \text{Feat}_B + 0.6 \times \text{Feat}_C$$

FIG. 4.7 Feature extraction

The most popular feature extraction algorithms used in machine learning are:

- ***1.Principal Component Analysis***

Every data set, 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.

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 are less 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 original features 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 be represented as

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

where, a_i represents ‘*n*’ scalars and u_i represents the basis vectors. Basis vectors are orthogonal to each other.
Orthogonality of vectors in *n*-dimensional vector space can be thought of an extension of the vectors being perpendicular in a two-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 be expressed as a linear combination of basis vectors helps in decomposing the vectors to a number of independent components.

The feature vector can be transformed to a vector space of the 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 may have similarity with each other is transformed to a set of principal components which are completely unrelated.

However, the principal components capture the variability of the 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 such a way that

- The new features are distinct, i.e. the covariance between the new features, i.e. the principal components is 0.
- The principal components are generated in order of the variability in the data that it captures. Hence, the first principal component should capture the maximum variability, the second principal component should capture the next highest variability etc.
- The sum of variance of the new features or the principal components should 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 are the steps to be followed:

- First, calculate the covariance matrix of a data set.
- Then, calculate the eigenvalues of the covariance matrix.
- 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.

- 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 second principal component.
- Like this, identify the top ‘*k*’ eigenvectors having top ‘*k*’ eigenvalues so as to get the ‘*k*’ principal components.

• 2.Singular value decomposition

Singular value decomposition (SVD) is a matrix factorization technique commonly used in linear algebra. SVD of a matrix A ($m \times n$) 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 to remove the mean of a data attribute, especially when the data set is sparse (as in case of text data), SVD is a good choice for dimensionality reduction in those situations.

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

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

- Larger a singular value, larger is the part of the matrix A that it accounts for and its associated vectors.
- New data matrix with ‘*k*’ attributes is obtained using the equation

$D' = D \times [v_1, v2, \ldots, vk]$

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

• 3.Linear Discriminant Analysis

Linear discriminant analysis (LDA) is another commonly used feature 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 covariance matrix of the data set, LDA calculates eigenvalues and eigenvectors within a class and inter-class scatter matrices. Below are the steps to be followed:

- Calculate the mean vectors for the individual classes.
- Calculate intra-class and inter-class scatter matrices.
- 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 of the data set, *Ni* is the sample size of each class

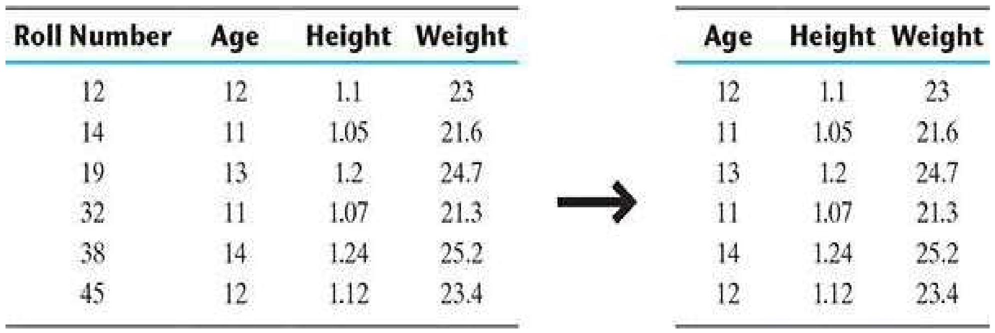
- Identify the top '*k*' eigenvectors having top '*k*' eigenvalues

• 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 about similar 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.
Roll number can have no bearing, whatsoever, in predicting student weight. So we can eliminate the feature roll number 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

$\rightarrow$

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

The issues which have made feature selection such a relevant problem to be solved are

- 1.Issues in high-dimensional data

With the rapid innovations in the digital space, the volume of data generated has increased to an unbelievable extent.

At the same 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 is text categorization which deals with huge volumes of text data from 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 machine learning 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 computational resources) learning model
Improving the efficiency of the learning model
Having a better understanding of the underlying model that generated the data

- **Key drivers of feature selection – feature relevance and redundancy**

  - ***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 assign class 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.

Let take a simple example of the student data set. 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 together students with similar academic capabilities,

Roll number can really not contribute any information whatsoever.

So, in context of the supervised task of predicting student Weight or the 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 selecting a subset of features.

- ***2.Feature redundancy***

A feature may contribute information which is similar to the information contributed by one or more other features.

For example, in the weight prediction, 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.

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 for rejection 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.

The main objective of feature selection is to remove 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 context of a specific learning task.

- **Measures of feature relevance and redundancy**
  - ***1.Measures of feature relevance***

Feature relevance is to be gauged by the amount of information contributed by a feature.

For supervised learning, 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 set that take discrete values.

In case of unsupervised learning, there is no class variable.

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 (value of '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 $p(f = x)$.

• 2.Measures of Feature redundancy

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

- Correlation-based measures
- Distance-based measures, and
- Other coefficient-based measure

• a.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 random feature 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 value is adopted to decide whether two features have adequate similarity or not.

- ***b.Distance-based similarity measure***

The most common distance measure is the **Euclidean distance**, 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

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

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

At $r = 1$, it takes the form of **Manhattan distance** (also called **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 is the **Hamming distance**. For example, the Hamming distance

between two vectors 01101011 and 11001001 is 3, as illustrated in Figure 4.10a.

- ***Other similarity measures***

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

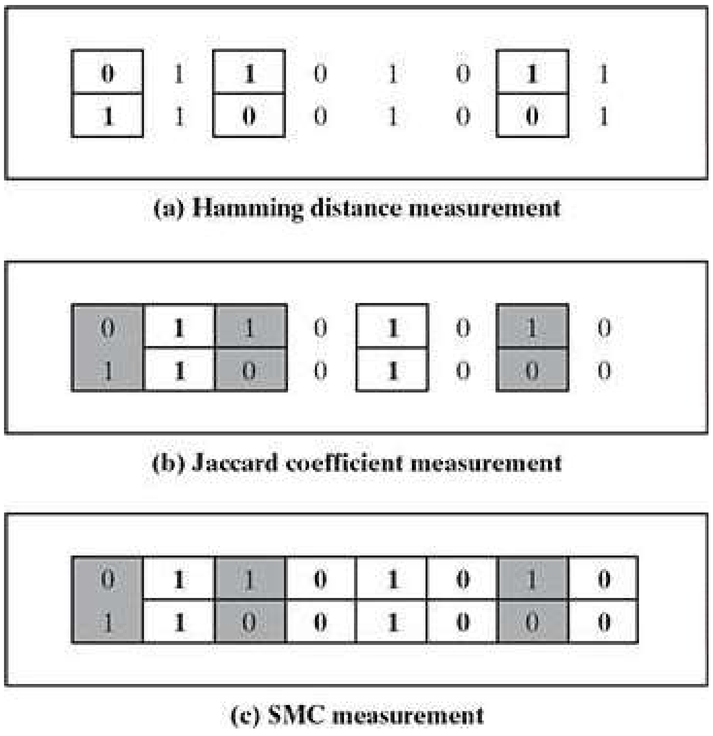

(a) Hamming distance measurement
(b) Jaccard coefficient measurement
(c) SMC measurement

FIG. 4.1O Distance measures between features

For two features having binary values, Jaccard index is measured as

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

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

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

n_{10} = number of cases where the feature 1 has value 1 and feature 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, $J =$

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

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

2.Simple matching coefficient (SMC) is almost same as Jaccard coeficient except the fact that it includes a number of cases 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 have value 1

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

n_{10} = number of cases where the feature 1 has value 1 and feature 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 be first 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.

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 most popular measures in text classification is calculated as:

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

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

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

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.

• 11) between *x* and *y* vectors.

• Hence, if cosine similarity has a value 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, the angle 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°.

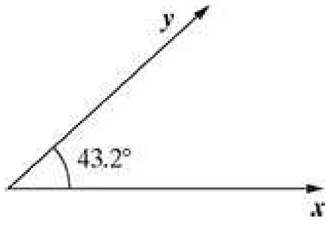


FIG. 4.11 Cosine similarity

• Overall feature selection process

Feature selection is the process of selecting a subset of features in a data set.

As depicted in Figure 4.12, a typical feature selection process consists of four steps:

- generation of possible subsets
- subset evaluation
- stop searching based on some stopping criterion
- validation of the result

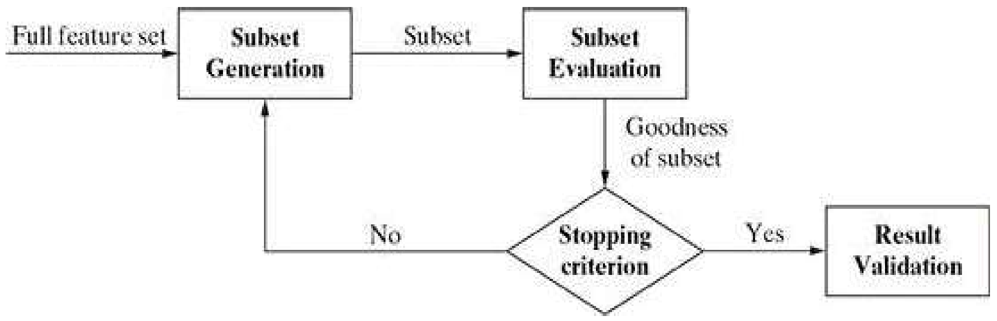


FIG. 4.12 Feature selection process

Subset generation, which is the first step of any feature selection algorithm, is a search procedure which ideally should produce 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 may start 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 with the 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 commonly used stopping criteria are

- the search completes
- some given bound (e.g. a specified number of iterations) is reached
- subsequent addition (or deletion) of the feature is not producing a better subset
- 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 synthetic but 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.

- **Feature selection approaches**

There are four types of approach for feature selection:

- Filter approach
- Wrapper approach
- Hybrid approach
- Embedded approach

In the **filter approach** (as depicted in Fig. 4.13), the feature subset 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 the feature 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.

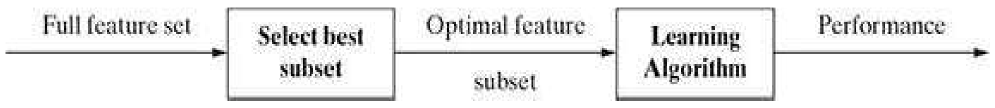


FIG. 4.13 Filter approach

In the **wrapper approach** (as depicted in Fig. 4.14), identification of best feature subset is done using the induction algorithm 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.

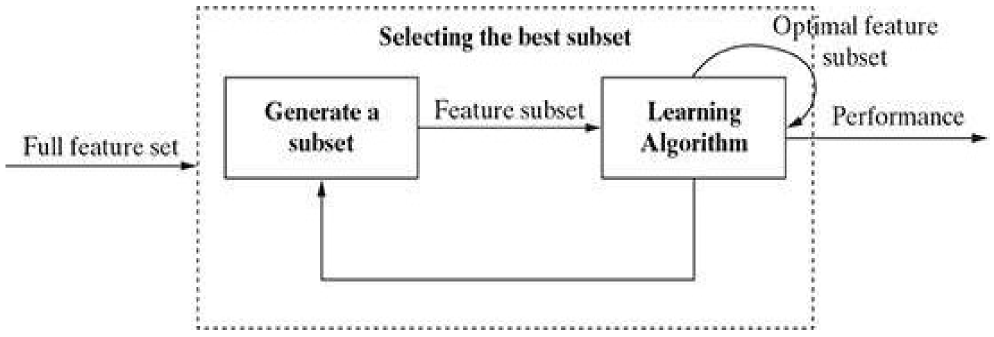


FIG. 4.14 Wrapper approach

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 to select 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 classification simultaneously.

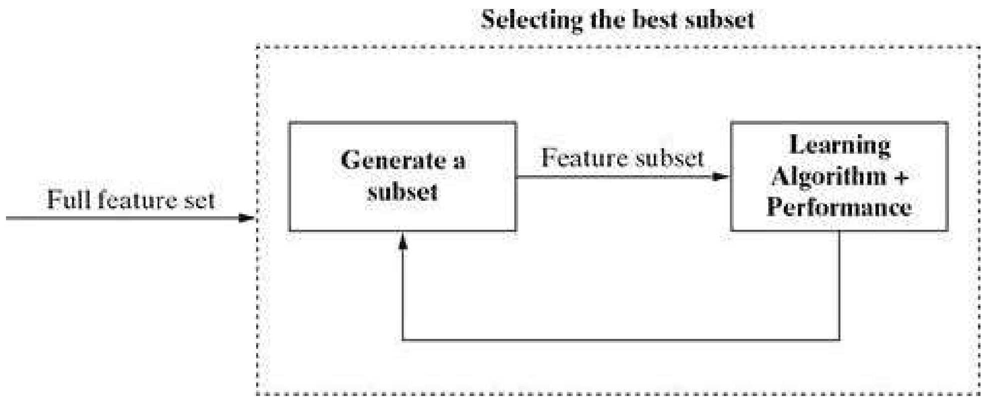


FIG. 4.15 Embedded approach

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-
-
- **Important Points to Remember**

A feature is an attribute of a data set that is used in a machine learning process.
Feature engineering is an important pre-processing step for machine learning, having two major elements:

- feature transformation
- feature subset selection

Feature transformation transforms data into a new set of features which can represent the underlying machine learning problem
There are two variants of feature transformation:

- feature construction
- feature extraction

Feature construction process discovers missing information about the relationships between features and augments the feature space by creating additional features.
Feature extraction is the process of extracting or creating a new set of features from the original set of features using some functional mapping. Some popular feature extraction algorithms used in machine learning:

- Principal Component Analysis (PCA)
- Singular Value Decomposition (SVD)
- Linear Discriminant Analysis (LDA)

Feature subset selection is intended to derive a subset of features from the full feature set. No new feature is generated.
The objective of feature selection is three-fold:

- Having faster and more cost-effective (i.e. less need for computational resources) learning model
- Improving the efficiency of the learning model
- Having a better understanding of the underlying model that generated the data
  Feature selection intends to remove 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 context of a specific learning task.

Feature relevance is indicated by the information gain from a feature measured in terms of relative entropy.
Feature redundancy is based on similar information contributed by multiple features measured by feature-to-feature:

- Correlation
- Distance (Minkowski distances, e.g. Manhattan, Euclidean, etc. used as most popular measures)
- Other coefficient-based (Jaccard, SMC, Cosine similarity, etc.)

Main approaches for feature selection are

- Filter
- Wrapper
- Hybrid
- Embedded

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