Machine Learning: what is it and what are its components? -- some preliminary observations[1]

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Abstract

This article focuses on conceptualizing machine learning (ML) concepts. The general topics covered are supervised learning based on regression and classification, unsupervised learning based on clustering and dimensionality reduction, and reinforcement learning. The article begins with an overview of ML, including the types of ML and their components. Then, for background, basic concepts associated with ML are addressed. From there on the discussion turns to ML algorithms, by topic. Although insurance applications of ML are not pursued in this version of the article, at the end of each section is a reference to an insurance article that applies the ML algorithm discussed in the section. The article ends with a commentary.

[1] The support of the Risk Management Research Center at the Penn State University is gratefully acknowledged.

1 Introduction

In the preface to Foundations of modern analysis, Dieudonné (1969) writes that he makes “no appeal whatsoever to ‘geometrical intuition’... which [he] emphasised by deliberately abstaining from introducing any diagram in the book.”

Now, if you are a mathematician of the caliber of Dieudonné, you might be of the same mind. For many, however, forgoing the intuition provided by diagrams and pictures is problematic. This is a particular concern when dealing with machine learning (ML), where many of the algorithms are computerized, and it is easy for users to have only a vague notion of the underlying characteristics of the model they are using.

The current version of this article provides a response to this concern in that it focuses on conceptualizing machine learning concepts. The final version will expand on notions included in this draft, and include more details with respect to the underlying mathematics of ML and a broader overview of insurance applications of ML.

The article begins with an overview of ML, including the types of ML and their components. Then, for background, basic concepts associated with ML are addressed. From there on the discussion turns to ML algorithms by type, including supervised learning based on regression, supervised learning based on classification, unsupervised learning based on clustering, unsupervised learning based on dimensionality reduction, and reinforcement learning. In each instance, the emphasis is on conceptualization. Although insurance applications of ML are not pursued in this version of the article, at the end of each section is a reference to an insurance article that applies the ML algorithm discussed in the section. The article ends with a commentary.

2 Machine Learning[2]

Arthur Samuel (1959), who first conceptualized the notion of machine learning (ML), is often quoted as defining it as "a field of study that gives computers the ability to learn without being explicitly programmed."[3] This notion is captured in Figure 1[4], in which traditional programming and machine learning are juxtaposed, to emphasize the difference between the two:

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[2] References for this section include Abellera and Bulusu (2018), Akerkar (2019), Hao (2019), Joshi (2020), KPMG (2018), Lee (2019), Samuel (1959) and Weng (2015).

[3] This definition should more appropriately be attributed to Samuel because it does not actually appear in the article, although the sentiment does.

[4] Adapted from Lee (2019) Figures 1.1 and 1.2.

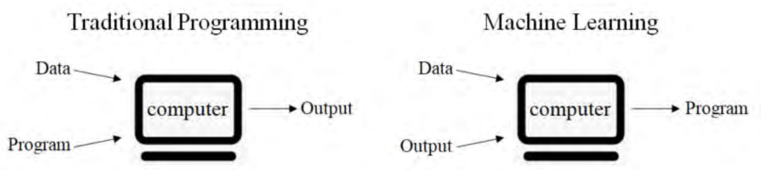

Figure 1: Traditional programming v. ML

As indicated, in traditional programming, the data and the program are the inputs that the computer uses to produce the output. In contrast, under ML, the data and the output are the inputs to the computer, which uses them to develop a program to interrelate the two.

2.1 Types of ML

ML is a subset of artificial intelligence (AI). In Figure 2[5] we address the topic of whether the AI topic under consideration is ML, and, if so, the type of ML.

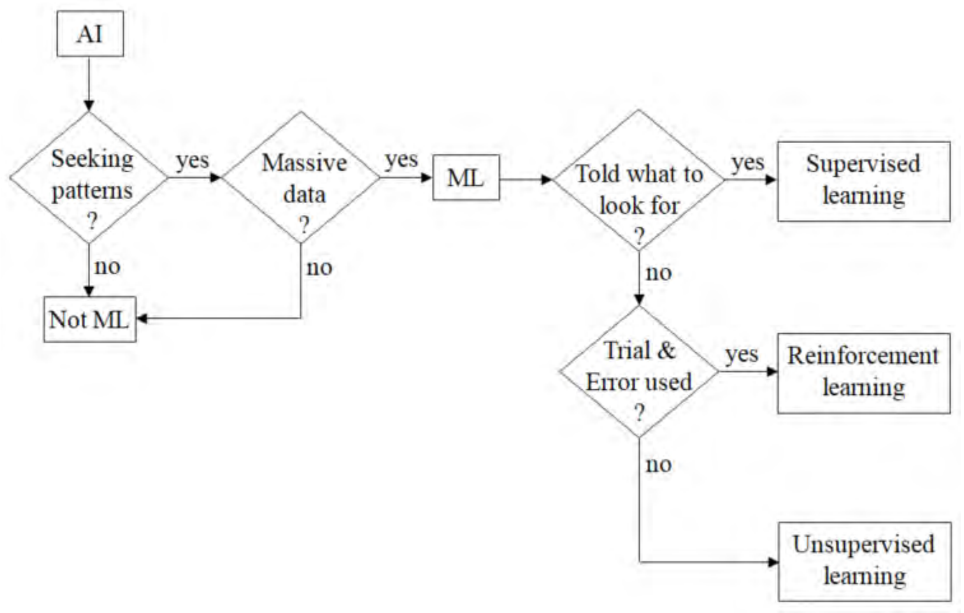

Figure 2: Is it Machine Learning (ML) and, if so, what type?

As indicated, to qualify as ML, it must be seeking a pattern and there must be considerable data involved. If this is the situation,

(1) It is supervised learning if it is told what to look for, that is, it is task driven. The computer is trained to apply a label to data.

(2) It is reinforcement learning if trial and error are involved, in which case, the algorithm learns to react to the environment. The goal is to discover the best sequence of actions that will generate the optimal outcome.

[5] Adapted from Hao (2019).

(3) It is unsupervised learning if it is ML but not supervised or reinforcement learning, in which case, it is data driven. It discovers patterns or hidden structures in unlabeled data.

3 Algorithms of ML

Figure 3 displays the ML algorithms, by type and subcategory that are discussed in this article, the details of which are presented in the following pages. The coverage is not exhaustive, in the sense that not all ML algorithms are addressed, but, hopefully, it is sufficient to provide an insight into the nature of this area.

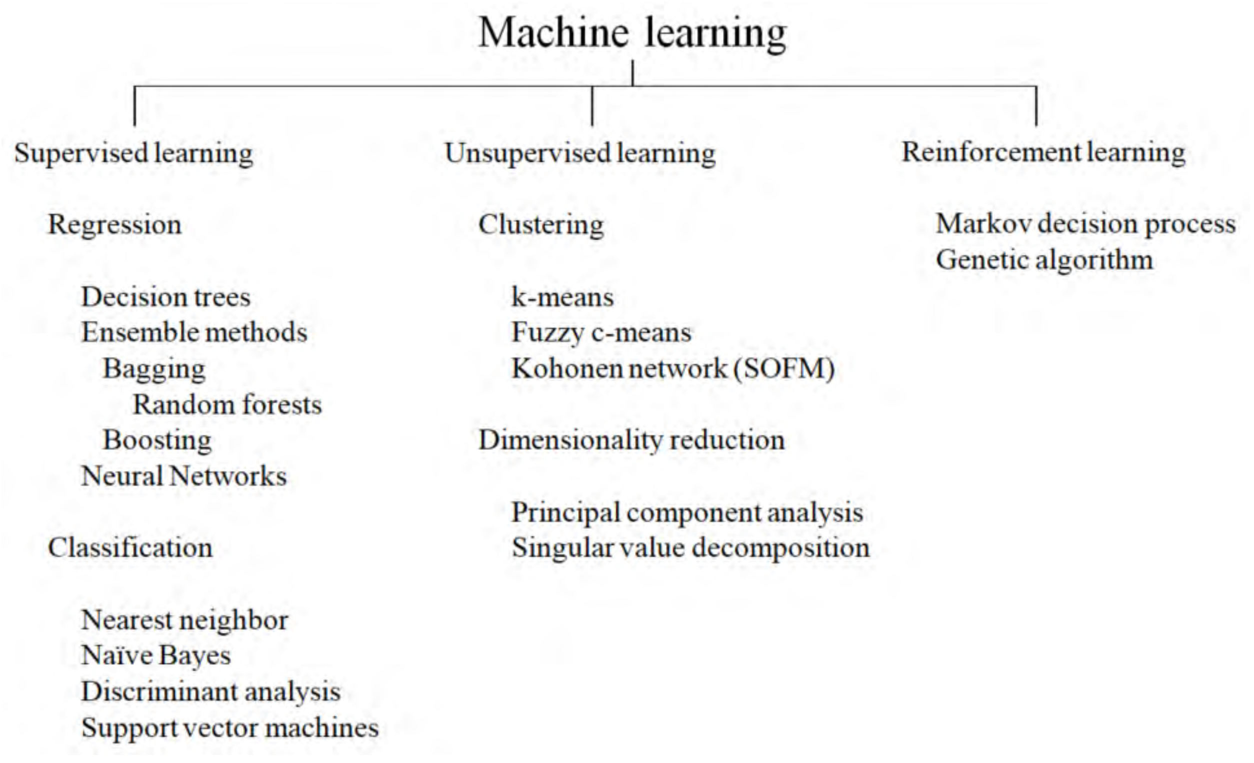

Figure 3: ML components

4 Basic concepts associated with ML[6]

In the following sections, we focus on an explanation of the details of the forgoing ML algorithms. Before doing that, however, as background, we review two basic concepts associated with ML: classifier error and bootstrapping.

[6] References for this section include Abellera and Bulusu (2018), Efron (1979), Efron and Tibshirani (1993), Gareth et al (2013), Knox (2018) and Winston (2010).

4.1 Classifier error functions

The classification error of a ML algorithm depends on the number of samples incorrectly classified, including both false positives plus false negatives. In this regard, Figure 4 shows a representation of a classifier error function.[7]

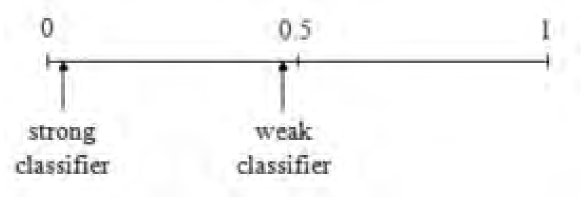

Figure 4: Classifier error function

As indicated, the error rate ranges from 0, which is associated with a strong classifier, to 1, which is associated with a failed classifier. An important part of the error range is that portion labeled weak classifier, where the error rate is just under 50%. A classifier that falls into this category performs better than random guessing, but still performs poorly at classifying objects.

As discussed in §5.2, strong classifiers can be constructed by combining weak classifiers.

4.2 Bootstrapping

Given a dataset and its distribution, the purpose of the bootstrap technique is to generate additional datasets with similar distributions. It does this by randomly sampling the dataset with replacement.

The nature of the bootstrap technique can be explained as follows. Let:

$x = (x_1, x_2, \cdots, x_n)$ be n independent data points
$x_j^* = (\hat{x}_{j1}, \hat{x}_{j2}, \cdots, \hat{x}_{jn})$ be the j-th bootstrap sample of size n

Figure 5 provides a representation of the bootstrap process.[8]

[7] Adapted from Winston (2010).

[8] Adapted from Efron & Tibshirani (1993: 13)

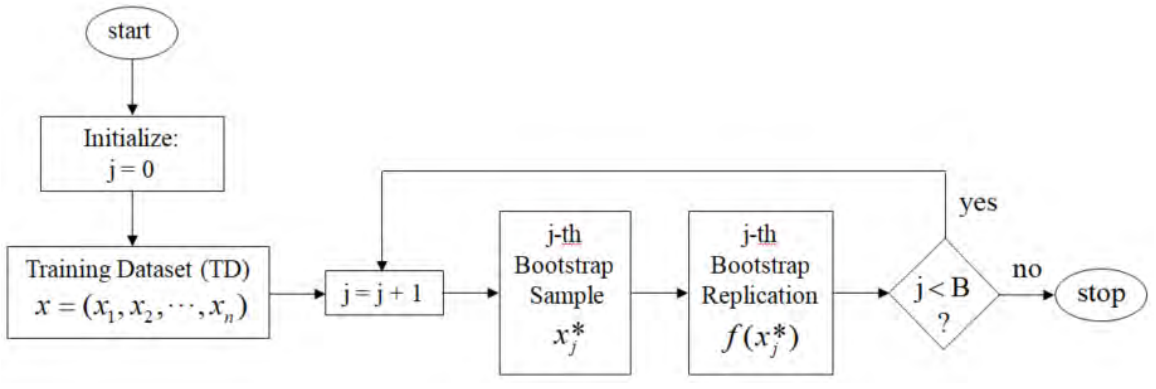
start
Initialize: j = 0
Training Dataset (TD) $x = (x_1, x_2, \cdots, x_n)$
j = j + 1
j-th Bootstrap Sample x_j^*
j-th Bootstrap Replication $f(x_j^*)$
j < B ?
yes
no
stop

Figure 5: The Bootstrap Process

Given the training dataset, $x_1, x_2, \cdots, x_n$, the bootstrap algorithm begins by randomly generating, with replacement, a large number of independent samples, $x_j^* = (\hat{x}_{j1}, \hat{x}_{j2}, \cdots, \hat{x}_{jn})$, each of size n.[9] Here, the number of bootstrap samples is B. Moreover, as indicated, corresponding to each bootstrap sample, j, is a bootstrap replication of the function being investigated, $f(x_j^*)$.

5 Supervised learning based on regression[10]

This section focuses on the regression algorithms of supervised machine learning, which model dependencies and relationships between input features and target outputs. The topics covered are decision trees or CART, ensemble methods, and neural networks.

5.1 Decision Trees or CART[11]

> "The tree methodology ... is a child of the computer age. Unlike many other statistical procedures which were moved from pencil and paper to calculators and then to computers, this use of trees was unthinkable before computers." [Breiman et al (1984: Preface)]

Decision trees, or Classification and Regression Trees (CART)[12], as they are now commonly referred to, are decision tree algorithms that are used to resolve classification or regression predictive modeling problems. These decision trees generally are represented in an upside-down manner, with their leaves pointed down. Observations pass from the root of the tree through a

[9] If, for example, n=5, a random sample, with replacement, might take the form $x^* = (x_2, x_4, x_1, x_1, x_2)$.

[10] References for this section include Abellera and Bulusu (2018), Bhatis (2017) and Joshi (2020).

[11] References for this subsection include Bisong (2019), Breiman et al (1984), Brownlee (2016), Gareth et al (2013), Lan (2017), Loh (2014) and Moisen (2008).

[12] This term is attributed to Breiman et al (1984).

series of nodes, or queries, which, based on the value of an explanatory variables, determine the subsequent direction of the flow. This process continues until a terminal node or leaf is reached, at which time a prediction is made. The process is instinctive and easy to understand.

A representation of a feature space and its associated decision tree are depicted in Figure 6(a) and (b), respectively,[13] where a feature space is the set of possible values associated with features of a database.

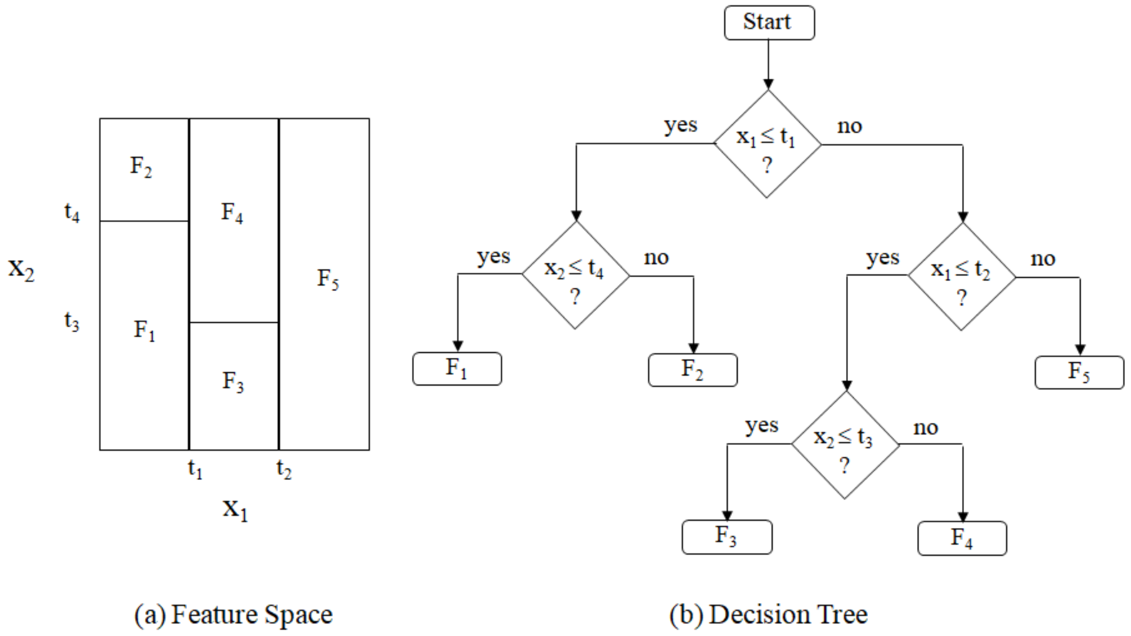

Figure 6: Feature space and associated decision tree

Here, the feature space, X_1 and X_2, is divided into the distinct and non-overlapping regions, F_1, F_2, . . . , F_5. Observations that are contained in the latter are assigned the mean of all the response values of the region. The Xs are considered to be ordered variables if they are represented by numerical values that have an intrinsic ordering, and categorical variables otherwise. As indicated, the nodes of the decision tree (the diamond-shaped icons) represent decision points while the branches, which are binary[14] (yes or no, true or false, etc.) correspond to possible paths between the nodes.

The allocation of a predicted value to the terminal nodes depends on the type of supervised learning involved. For regression trees, the terminal node values are allocated based on the mean for that node. In contrast, for classification trees, the terminal node values are assigned the class that represents the most cases in that node.

An informative reference for this topic is Loh (2014).

[13] Adapted from Bisong (2019)

[14] The parent node will always split into exactly two child nodes.

5.2 Ensemble methods

Ensemble, or committee, methods help improve machine learning outcomes by merging machine learning techniques into a single predictive model. Potential benefits of the method include such things as decreasing variances and reducing bias. In this subsection, three ensemble methods are discussed: bagging, random forest and boosting.

5.2.1 Bagging[15]

Bagging, is a portmanteau[16] word denoting "**b**ootstrap **agg**regat**ing**." One of the simpler ensemble method, its essential characteristic is that samples are taken with replacement, passed through a classification criterion, and the results thereof are used for prediction. It was first discussed by Breiman (1996), who envisioned it as a variance reduction technique. The logic being that the variance of an average is smaller than the variance of the elements of the average.

Figure 7[17] provides a conceptual representation of the bagging technique.

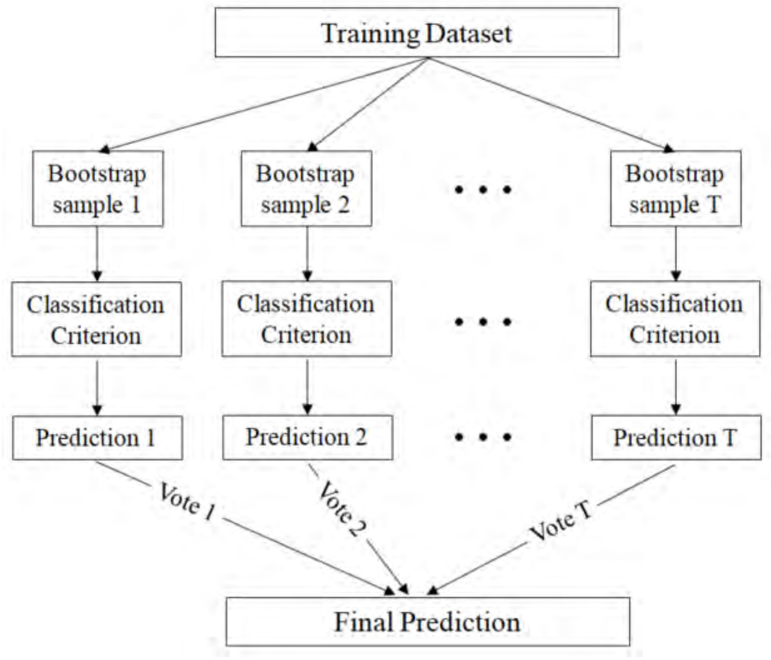

Figure 7: Bagging flowchart

[15] References for this subsection include Breiman (1996), Bühlmann (2012), Bühlmann and Yu (2002), Diana et al (2019), Knox (2018), Li et al (2018), Winston (2010) and Yuan et al (2018).

[16] Portmanteau is a literary device in which two or more words are joined together to coin a new word, which refers to a single concept. https://literarydevices.net/portmanteau/

[17] Adapted from Winston (2010) and Yuan et al (2018: 4-5).

The specific steps can be described as follows:

(1) Use the method of bootstrap to re-sample, and randomly produce T training sets.
(2) Create the corresponding classification criterion for each training set.
(3) For the sample of testing sets, using each classification criterion to test, obtain the T predictions.
(4) Based on the method of voting, the prediction with the highest number of votes becomes the final prediction.

At its inception, Breiman (1996) gave only heuristic arguments as to why bagging worked. Subsequently, Bühlmann and Yu (2002) verified that bagging is a smoothing operation that improves the predictive performance of regression or classification trees, and confirmed Breiman's intuition that bagging is a variance reduction technique.

5.2.1.1 Bagging applications in insurance

Li et al (2018) provides an example of a bagging application in insurance.

5.2.2 Random Forests[18]

> "Random Forests Algorithm [is] identical to bagging in every way, except: each time a tree is fit, at each node, censor some of the predictor variables." [Breiman (2011: 12)]

The essential idea behind the random forest concept is that it adds the random selection of features to the bagging algorithm. The idea was conceived by Ho (1995)[19], who called it "random decision forest," and described its essence as being "to build multiple trees in randomly selected subspaces of the feature space." Breiman (2001), who renamed the concept "random forest" and provided an algorithm for its implementation, is often cited as the originator of the idea.

Figure 8[20] provides a conceptual representation of the random forest technique.

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[18] References for this subsection include Breiman (2011), Derrig and Francis (2005), Diana et al (2019), Ho (1995), Li et al (2018), Winston (2010) and Yiu (2019).

[19] Apparently, Amit and Geman (1997) also independently conceived the idea.

[20] Adapted from Winston (2010).

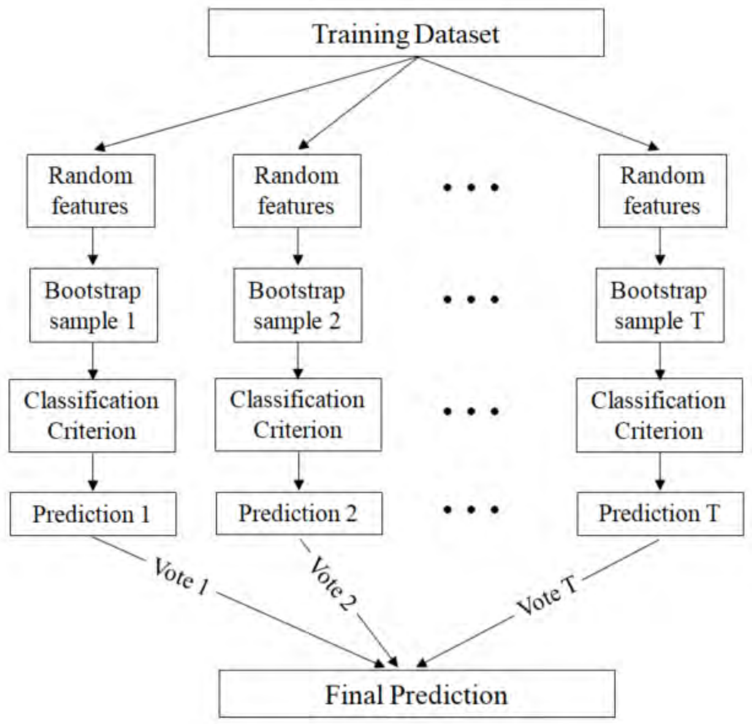


Figure 8: Random forest flowchart

As indicated, the essential modification to the bagging algorithm depicted in Figure 7, and discussed in the subsequent text, is that only a random subset (without replacement) of the features are used for each tree.

5.2.2.1 Insurance applications of random forest

Derrig and Francis (2006) provides an example of a random forest application in insurance.

5.2.3 Boosting[21]

Boosting is an enhancement of the bagging algorithm that endeavors to improve the learning process by focusing on areas where the system is underperforming. Under this approach, the first decision tree is trained on a random sample of data, and the areas that were misclassified are noted. Then, during the training of the second decision tree, extra weight is given to those samples where the misclassification occurred. This same sequential procedure continues for the third and subsequent decision trees, until a stopping criterion is met.

Figure 9 depicts a boosting flowchart.

[21] References for this subsection include Bühlmann (2012), Joshi (2020), Kim (2015) and Udacity (2016).

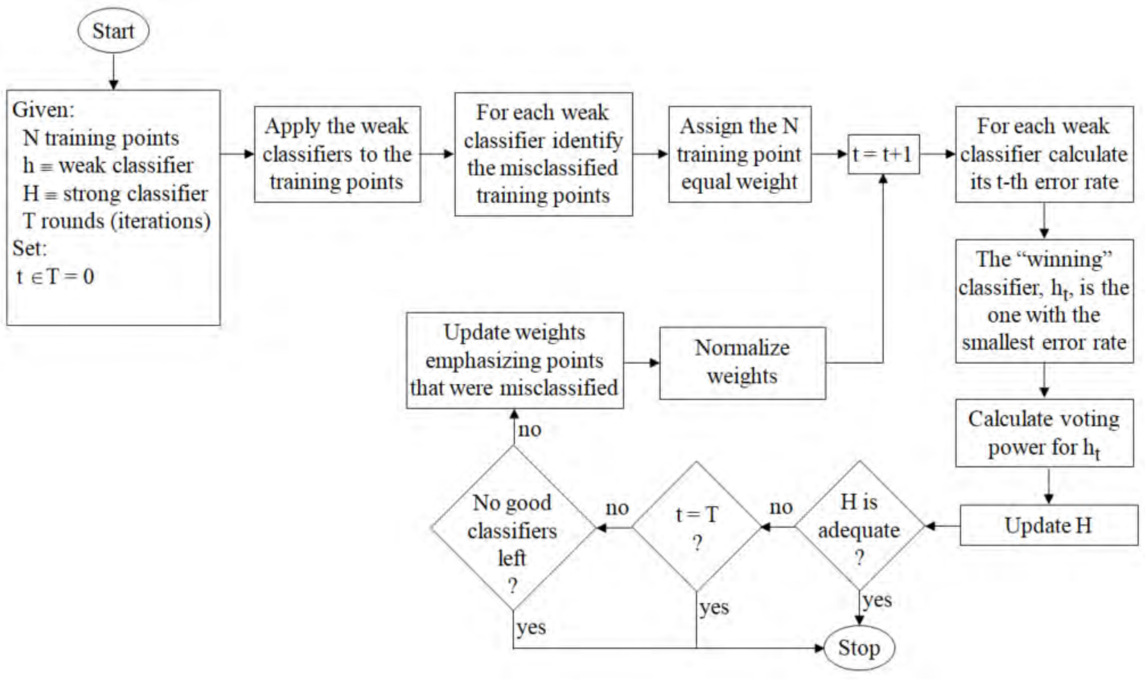

Start
Given:
N training points
h ≡ weak classifier
H ≡ strong classifier
T rounds (iterations)
Set:
t ∈ T = 0
Apply the weak classifiers to the training points
For each weak classifier identify the misclassified training points
Assign the N training point equal weight
t = t+1
For each weak classifier calculate its t-th error rate
The "winning" classifier, h_t, is the one with the smallest error rate
Calculate voting power for h_t
Update H
H is adequate ?
t = T ?
No good classifiers left ?
Update weights emphasizing points that were misclassified
Normalize weights
no
no
no
yes
yes
yes
Stop

Figure 9: Boosting flowchart

As indicated, we start with the training points (dataset), the weak classifiers, a strong classifier function, whose initial value is zero, and the potential number of iterations. The weak classifiers, which are given equal weight to start, are applied to the training points, the points that are misclassified are documented, and the error rate of the classifier is determined. The classifiers are assigned a value of 1 or -1 accordingly as the data points that they are applied to are correctly or incorrectly labeled. The weak classifier with the smallest error rate is the winner for that iteration, and its voting power, which is a function of its error rate, is calculated. Then, the strong classifier function is updated by appending the product of the voting power and the sign of the winning weak classifier to its previous value.

If the strong classifier is adequate, in the sense that it correctly classifies all the samples, or the iterations have reached their maximum number, or there are no good classifiers left, the algorithm stops. If that is not the case, the weights are updated, with more emphasizing on the points that were misclassified, the sum of the weights is normalized, and the next iteration takes place.

5.2.3.1 Comments

Joshi (2020: 62) notes that because of the unavailability of parallel computation, the training of boosted trees is significantly slower than training trees using bagging and random forest. This computational disadvantage notwithstanding, he claims boosting is often preferred over other techniques due to its superior performance in most cases.

Bühlmann (2012: 2), on the other hand, remarked that from the perspective of prediction, random forests is about as good as boosting, and often superior to bagging.

5.2.3.2 Insurance Applications of Boosting

Guelman (2012) provides an example of a boosting application in insurance.

5.3 Neural Networks[22]

> "The traditional approach of capturing first-order behavior has represented a very important step toward capturing complex behavior. Now, the use of neural networks that can go into the data without any kind of assumption and begin to quantify interactions represents the next phase of picking up the higher order terms." [Shapiro (2000: 205)]

Neural networks (NNs) are software programs that emulate the biological structure of the human brain and its associated neural complex and are used for pattern classification, prediction and analysis, and control and optimization.

An example of a three layer NN is depicted in Figure 10(a).[23] Here, the first layer, the input layer, has three neurons[24], the second layer, the hidden processing layer,[25] has three neurons, and the third layer, the output layer, has one neuron. If the flow of information through the network is from the input to the output, it is known as a feed forward network. Moreover, if the process involves supervised learning, in the sense that inadequacies in the output are fed back through the network so that the algorithm can be improved, the NN is said to involve backpropagation.

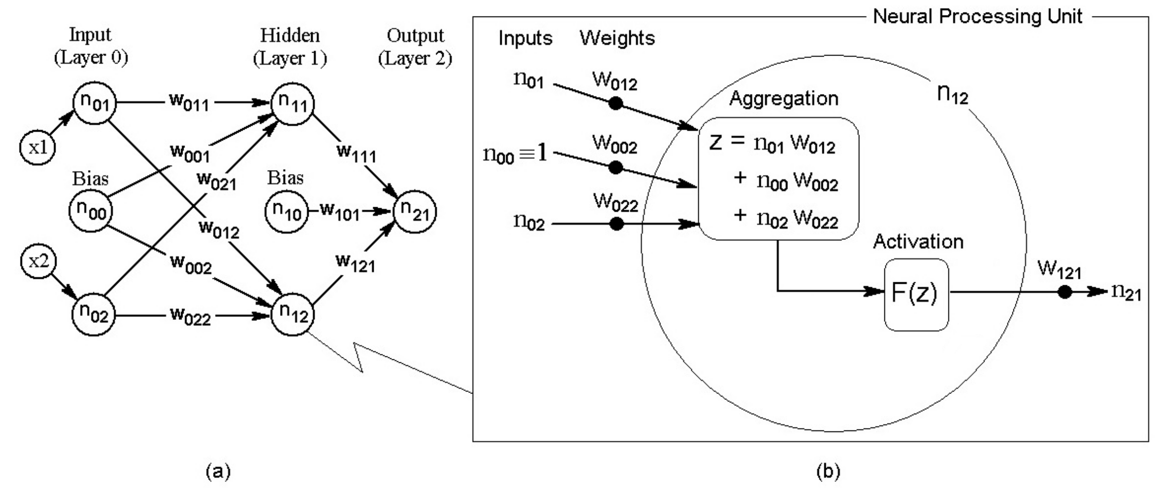


Figure 10: A 3-layer NN

[22] References for this subsection include Brockett et. al. (1994) and Shapiro (1998, 1999, 2000 and 2002).

[23] Adapted from Shapiro (2002).

[24] A neuron is a mathematical function that is meant to model the functioning of a biological neuron.

[25] In essence, as observed by Brockett et. al. (1994), p. 408, the "hidden" layers in the model are conceptually similar to nonorthogonal latent factors in a factor analysis, providing a mutually depend summarization of the pertinent commonalities in the input data.

The core of a NN is the neural processing unit, an example of which is shown in Figure 10(b). As indicated, the inputs to the neuron, $n_{j,}$ are multiplied by their respective weights, w_j, and aggregated. The weight w_0 serves the same function as the intercept in a regression formula.[26] The weighted sum is then passed through an activation function, F, to produce the output of the unit. In the past, the activation function often took the form of a logistic function, $F(z)=(1+e^{-z})^{-1}$, where, as indicated in the figure, $z = \sum_j w_j \, x_j$. Recently, especially where complex hidden layers are involved, as is the case in deep learning, the Rectified Linear Unit (ReLU), F(z) = max(0,z), is being used.

The neurons are connected by the weights w_{ijk}, where the subscripts i, j, and k refer to the i-th layer, the j-th node of the i-th layer, and the k-th node of the (i+l)st layer, respectively. Thus, for example, w_{021} is the weight connecting node 2 of the input layer (layer 0) to node 1 of the hidden layer (layer 1). It follows that the aggregation in the neural processing associated with the hidden neuron n_{11} results in $z = n_{00}\, w_{001} + n_{01}\, w_{011} + n_{02}\, w_{021}$, which is the input to the activation function.

A measure of the prediction error in this simple example could be $(T\text{-}O)^2$, where T is the targeted value and O is the output of a given iteration through the network.[27] Now, the weights of the network serve as its memory and the network "learns" when its weights are updated. To this end, the prediction error, adjusted by a learning rule, is propagated back through the network so that the weights can be improved.

5.3.1.1 Insurance Applications of NNs

Brockett et al (1994) provides an early example of a neural network application in insurance.

6 Supervised Learning based on Classification[28]

This section addresses the problem of supervised learning when the range of the unknown function is a discrete, unordered set of labels.

Classification is a classic example of supervised learning in insurance. Suppose we have measured 5 different properties (blood pressure, smoking status, cholesterol ratios, build, and family history of cancer)[29] of 3 different types of insurance applicants (standard, substandard, and superstandard). We have measurements for say 1000 different examples of each type of

[26] Anders (1996) investigates neural networks as a generalization of nonlinear regression models.

[27] The prediction error can be measured in a number of ways. See, for example, Anders (1996, p. 973) and Shepherd (1997, p 5)

[28] References for this section include Abellera and Bulusu (2018) and Knox (2018).

[29] See Justman (2007) for a discussion of these factors.

applicant. This data would then serve as training data where we have the inputs (the 5 measured properties) and corresponding outputs (the type of applicant) available for training the model. Then a suitable ML model can be trained in a supervised manner. Once the model is trained, we can then classify any applicant (between the three known types) based on the property measurements.[30]

6.1 K-nearest-neighbor (KNN)[31]

The essential feature of the k-nearest neighbor algorithm is that it classifies objects on the basis of their proximity to training examples in the feature space. The underlying logic being that objects in the immediate vicinity are likely to have similar predictive qualities. As one would anticipate, and as noted by Akerkar (2019: 24), the method is highly effective when confronted with noisy or missing training data.

As far as its history, Cover and Hart (1967) are often cited as the early source of the k-NN algorithm, largely because of their description of how they discovered it. However, the rule was mentioned by Sebestyen (1962), who labeled it the “proximity algorithm” and by Nilsson (1965) who labeled it the “minimum distance classifier.” Moreover, as discussed in Pelillo (2014), the nearest neighbor concept can be traced at least as far back as Alhazen's (1030) Book of Optics.

Figure 11 provides a simple example of a 3-nearest neighbor technique.

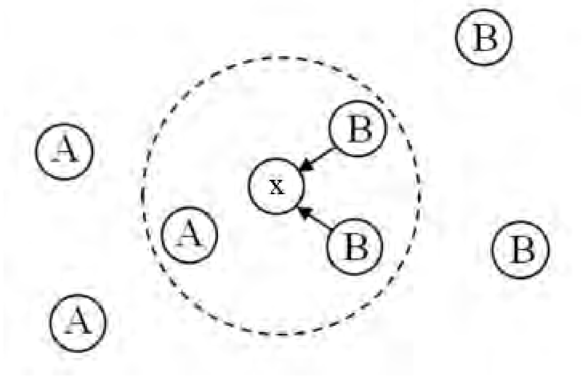


Figure 11: 3-nearest neighbor example

In this case, given the 7 data points, comprising two classes, A and B, and a new point x, the 3-nearest-neighbor (3NN) algorithm classifies x as belonging to the most frequent class of the 3 nearest training data, class B.

Thus, in general, given the training data (x_1, y_1),…, (x_n, y_n) and a new point (x, y), the k-nearest-neighbor (KNN) algorithm classifies (x, y) as belonging to the most frequent class of the k nearest training data.

[30] Adapted from Joshi (2020: 10).

[31] References for this subsection include Akerkar (2019), Cover and Hart (1967), Knox (2018), Nilsson (1965), Pelillo (2014), Sebestyen (1962).

6.1.1 Insurance applications of k-nearest-neighbor

Dittmer (2006) provides an example of a k-nearest-neighbor application in insurance.

6.2 Naïve Bayes[32]

Naïve Bayes, an offshoot of Bayes' theorem, finds application in high dimensional training data sets. Its purpose, given the features and classes of a classification problem, is to compute the conditional probability that an object belongs to a particular class. The algorithm is designated as naive because it is based on the assumption that the features are independent.

Explicitly, given the classes C_i, i = 1, 2, …, K, and the features x_j, j = 1, …, n, the goal is to calculate the conditional probability that an object with a feature vector $(x_1, x_2, \dots, x_n)$ is a member of C_i, that is, $P(C_i \mid x_1, x_2, \cdots, x_n)$.
Figure 12[33] depicts a simple example involving the Naïve Bayes approach.

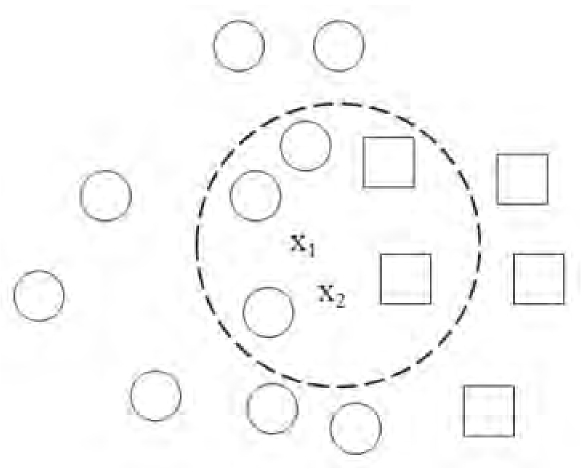


Figure 12: Classify 2 new sample using Naïve Bayes

In this case, there are two classes, C_1, represented by circles, and C_2, represented by squares, and two new samples, x_1 and x_2.

The questions at hand are:

What is the probability that the new samples came from each of the classes?

Which class are the samples most likely from?

[32] References for this section include Balaji and Srivatsa (2012), Global Software Support, Salma et al (2019) and Zakrzewska (2008).

[33] Adapted from the Global Software Support (2018) example at:
https://www.globalsoftwaresupport.com/naive-bayes-classifier-explained-step-step/

Before the new samples, the probability of a circle, P(C_1), and a square, P(C_2), were 10/15= 2/3, and 5/15=1/3, respectively.

Now, considering just the neighborhood of the new samples, the area enclosed by the dashed circle in Figure 12, the probability that the new sample will be a circle or a square will be P(x_i |C_1) = 3/10 and P(x_i |C_2) = 2/5, respectively.

Generalizing, and implementing the Naïve Bayes assumption that

$$\mathrm{P}(\mathrm{x}_1, \mathrm{x}_2 \mid \mathrm{C}_i) = \mathrm{P}(\mathrm{x}_1 \mid \mathrm{C}_i)\ \mathrm{P}(\mathrm{x}_2 \mid \mathrm{C}_i)$$

gives

$$P(C_i \mid x_1, x_2) = \frac{P(C_i)}{P(x_1, x_2)} P(x_1 \mid C_i) P(x_2 \mid C_i), \;\; 1 \le i \le K$$

which is the Naïve Bayes version of $P(C_i \mid x_1, x_2)$.

6.2.1.1 **Insurance applications of Naïve Bayes**

Balaji and Srivatsa (2012) provides an example of a Naïve Bayes application in insurance.

6.3 Discriminant Analysis[34]

Discriminant analysis, which is based on the means and variances of sets of samples, was developed to address classification problems where two or more groups or populations are known a priori and new observations are to be classified into one of the known groups or populations. In this context, the term "discriminant" refers to a function of a set of variables that is used as an aid in discriminating between them. There are two types of discriminant analysis: linear discriminant analysis (LDA) and quadratic discriminant analysis (QDA). These are discussed in the two subsections that follow.

6.3.1 Linear Discriminant Analysis[35]

Linear discriminant analysis (LDA), which can be traced to the early work of Fisher (1936), is used for classification involving multidimensional normal distributions with homogeneous variance-covariances. Essentially, given the mean vectors of each class, LDA finds the projection direction that maximizes separation of means, while taking into account the within-class variance.

[34] References for this portion include Ben-Ari and Mondada (2018) and Timm (2002).

[35] References for this subsection include Ben-Ari and Mondada (2018), Knox (2018), Matlab (2018) and Timm (2002).

Figure 13[36] is a representation of a linear discriminant analysis example.

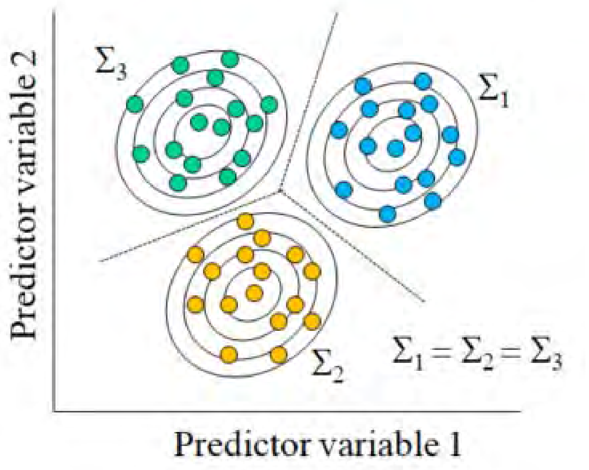


Figure 13: Linear discriminant analysis

As indicated, there are three groups of a priori data. The location of the linear boundaries are determined by treating the observations of each group as samples from a multidimensional normal distribution with homogeneous variance-covariance matrices (i.e., $\Sigma_1 = \Sigma_2 = \Sigma_3$). Given the fitted distributions, the boundary between the groups are the set of points where the probabilities are equal, and new observations are classified based on where they occurred relative to the boundaries.

Discriminants that are linear functions of the variables, as in Figure 13, are called linear discriminant functions.

6.3.2 Quadratic Discriminant Analysis

Quadratic discriminant analysis is used with heterogeneous variance-covariance matrices, which allows the variance-covariance matrices to depend on the population.

Figure 14[37] provides a representation of quadratic discriminant analysis.

[36] Adapted from Matlab (2018)

[37] Adapted from Matlab (2018)

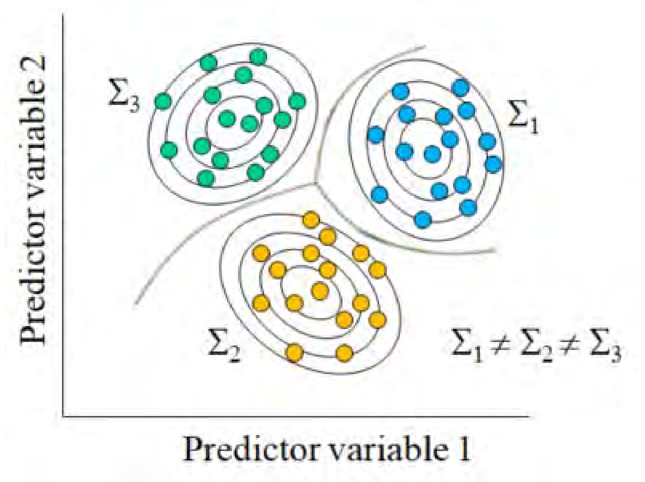


Figure 14: Quadratic discriminant analysis

Here, as in the linear discriminant analysis case, the coefficients of the boundary lines are determined by the mean vectors and covariance matrices of the observed classes. However, since the covariance matrices are not the same for all classes (i.e., $\Sigma_1 \neq \Sigma_2 \neq \Sigma_3$), the boundaries are quadratic.

6.3.3 Comment

Bartlett's test[38] is used to determine if the variance-covariance matrices are homogeneous for all populations involved and, hence, whether to use Linear or Quadratic Discriminant Analysis.

6.3.4 Insurance applications of discriminant analysis

Riashchenko et al (2017) provides an example of a discriminant analysis application in insurance.

6.4 Support Vector Machines (SVM)[39]

Given a dataset with two target classes that are linearly separable, the objective of a support vector machine (SVM) is to find the line that best separates the two classes.

A representation of a SVM is shown in Figure 15, in the case where the dichotomy is between solvent insurance firms and insolvent firms.[40]

[38] See Keating and Leung (2010).

[39] References for this portion include Bisong (2019) and Diepen et al (2017).

[40] Adapted from Diepen et al (2017).

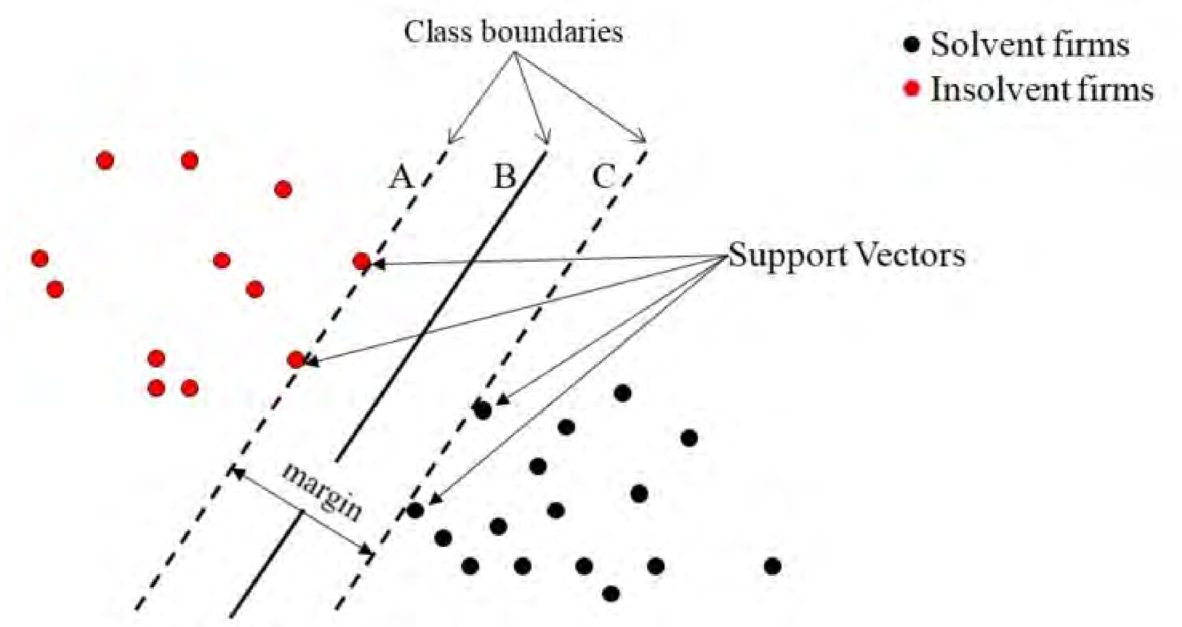


Figure 15: Support vector machine example

In this example, the black and red circles represent solvent firms and insolvent firms, respectively. Any line that keeps the red circles on the left and the black circles on the right is considered a valid boundary line for this classification problem.

The two dashed lines are the parallel separation lines with the largest space between them, while the actual classification boundary, which serves as the solution to this SVM problem, since it maximizes the separation between the two classes, is the solid line exactly in the middle of the two dotted lines.

The term Support Vector Machine derives from the support vectors that are the basis for the dashed lines in the figure. Here, there are four supporting vectors.

6.4.1 LDA and SVM

Although both LDA and SVM are linear discriminant functions, there generally is a clear distinction between them:

> LDA is concerned with maximizing the distance between the means of the two groups while SVM is concerned with maximizing the margin between the two groups.
>
> LDA works best when each of the labeled class data are normally distributed while SVM does not depend on how the data is distributed.

On the other hand, SVM and LDA would produce the same result if the data is normally distributed.

6.4.2 Insurance applications of SVM

Salcedo-Sanz et al (2003) provides an example of a SVM application in insurance.

7 Unsupervised learning based on clustering

The purpose of unsupervised learning based on clustering is to partition a set of observations into separate groups or clusters in such a way that all observations within a group are similar, while observations in different groups are dissimilar. Given this clustering, a new observation can be compared to the clusters and assigned to the one to which they are most closely aligned.

In the rest of this section we discuss three types of clustering: k-means algorithm, fuzzy c-means algorithm and self-organizing feature map.

7.1 k-means[41]

Given a dataset, the purpose of the k-means clustering algorithm is to arrange the data in k clusters such that the total within-cluster variation is minimized.

Figure 16[42] shows a simple example of 3-means clustering.

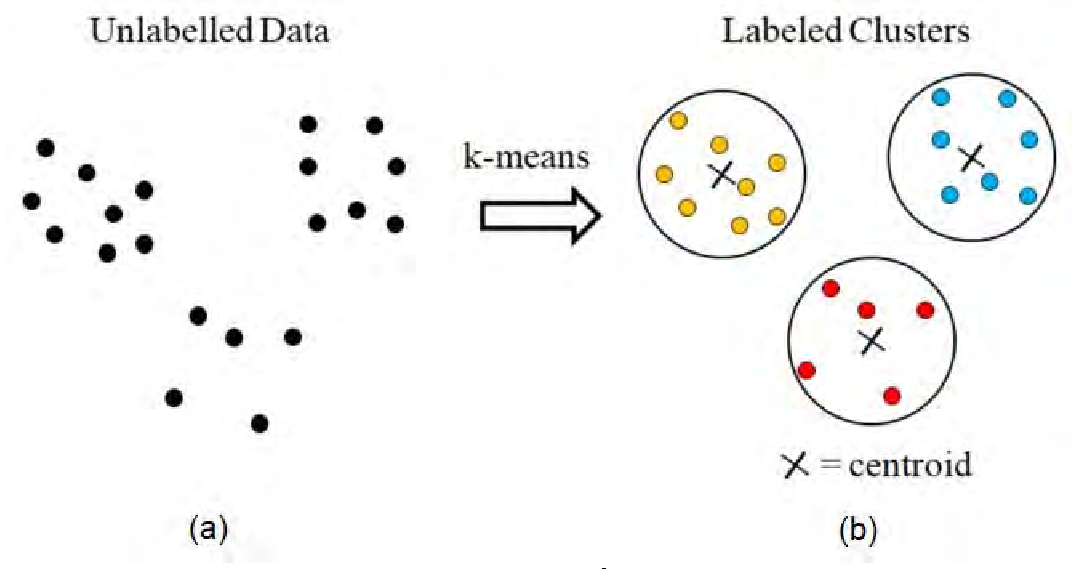


Figure 16 3-means clustering

Starting with the training data in Figure 16(a) and the goal of 3 clusters, 3 points are randomly chosen, the tentative centroids or centers of mass, one for each cluster. Then, as shown in Figure

[41] References for this portion include Dinov (2018), Jeffares (2019) and medium.com.

[42] Adapted from Jeffares (2019)

16(b), each data point is assigned to the cluster that it is closest to. Next, a new centroid is located for each cluster based on the current cluster members. Given the new centroids, the foregoing steps are repeated until convergence occurs, in the sense that the centroids do not change from one iteration to the next.

7.1.1 Insurance applications of k-means

Hainaut (2019) provides an example of a k-means application in insurance.

7.2 Fuzzy c-means[43]

The essence of the c-means algorithm is that it produces reasonable centers for clusters of data, in the sense that the centers capture the essential feature of the cluster, and then groups data vectors around cluster centers that are reasonably close to them.

Figure 17[44] shows a flowchart of the c-means clustering algorithm.

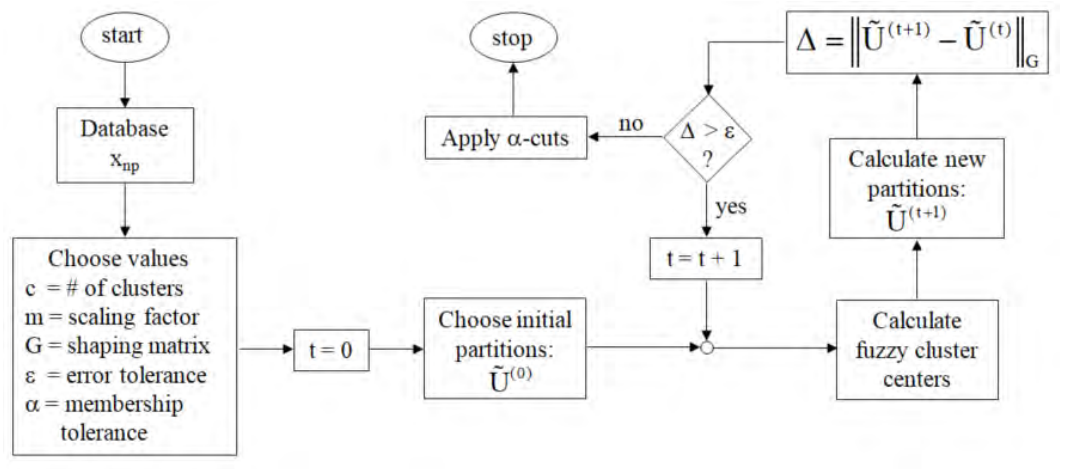

start
Database X_{np}
Choose values
c = # of clusters
m = scaling factor
G = shaping matrix
ε = error tolerance
α = membership tolerance
t = 0
Choose initial partitions: $\tilde{U}^{(0)}$
Calculate fuzzy cluster centers
Calculate new partitions: $\tilde{U}^{(t+1)}$
$\Delta = \left\| \tilde{U}^{(t+1)} - \tilde{U}^{(t)} \right\|_G$
Δ > ε ?
yes
no
t = t + 1
Apply α-cuts
stop

Figure 17: c-means clustering algorithm

As indicated, the database consists of the n×p matrix, X_{np}, where n indicates the number of patterns and p denotes the number of features. The algorithm seeks to segregate these n patterns into c, $2 \leq c \leq n - 1$, clusters, where the within clusters variances are minimized and the between clusters variances are maximized. To this end, the algorithm is initialized by resetting the counter, t, to zero, and choosing: c, the number of clusters; m, the exponential weight, which acts to reduce the influence of noise in the data because it limits the influence of small values of membership functions; G, a symmetric, positive-definite (all its principal minors have strictly positive determinants), p × p shaping matrix, which represents the relative importance of the elements of the data set and the correlation between them, examples of which are the identity and

[43] References for this subsection include Bezdek (1981) and Shapiro (2004)

[44] This figure and related discussion follows Shapiro (2004).

covariance matrixes; ε, the tolerance, which controls the stopping rule; and α, the membership tolerance, which defines the relevant portion of the membership functions.

Given the database and the initialized values, the counter, t, is set to zero. The next step is to choose the initial partition (membership matrix), $\tilde{U}^{(0)}$, which may be based on a best guess or experience. Next, the fuzzy cluster centers are computed, which, in effect, are elements that capture the essential feature of the cluster. Using these fuzzy cluster centers, a new (up-dated) partition, $\tilde{U}^{(t+1)}$, is calculated. The partitions are compared using the matrix norm $\left\|\tilde{U}^{(t+1)} - \tilde{U}^{(t)}\right\|_G$ and if the difference exceeds ε, the counter, t, is increased and the process continues. If the difference does not exceed ε, the process stops. As part of this final step, α-cuts are applied to clarify the results and make interpretation easier, that is, all membership function values less than α are set to zero and the function is renormalized.

7.2.1 Insurance applications of c-means algorithm

Subudhi and Panigrahi (2020) provides an example of a c-means algorithm application in insurance.

7.3 Kohonen network (SOFM)[45]

This section discusses a common unsupervised NN, the Kohonen network (Kohonen,1988), which otherwise is referred to as a self-organizing feature map (SOFM). The purpose of the network is to emulate our understanding of how the brain uses spatial mappings to model complex data structures. Specifically, the learning algorithm develops a mapping from the input patterns to the output units that embodies the features of the input patterns.

In contrast to the supervised network, where the neurons are arranged in layers, in the Kohonen network they are arranged in a planar configuration and the inputs are connected to each unit in the network. This configuration is depicted in Figure 18.[46]

[45] References for this subsection include Kohonen (1988) and Shapiro (2000b).

[46] This figure and related discussion follows Shapiro (2000b).

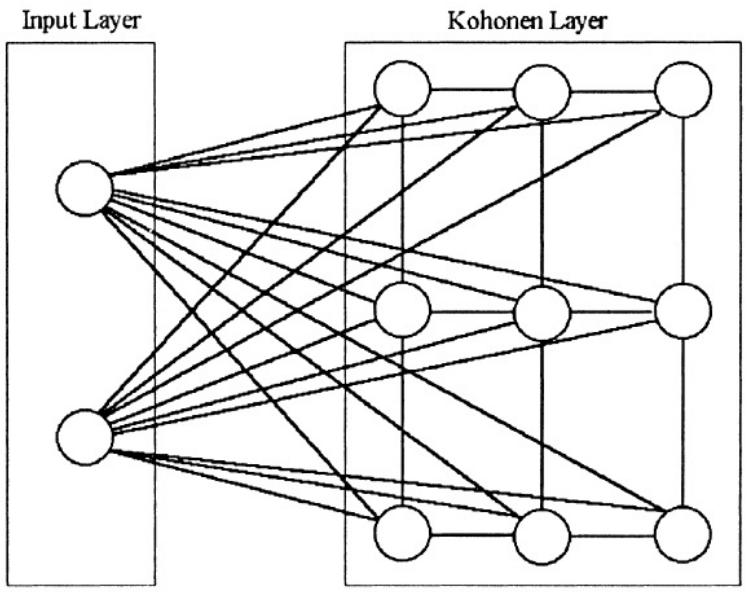


Figure 18: 2-D Kohonen network

As indicated, the Kohonen SOFM is a two-layered network consisting of a set of input units in the input layer and a set of output units arranged in a grid called a Kohonen layer. The input and output layers are totally interconnected and there is a weight associated with each link, which is a measure of the intensity of the link.

The sketch of the operation of a Kohonen network is shown in Figure 19.

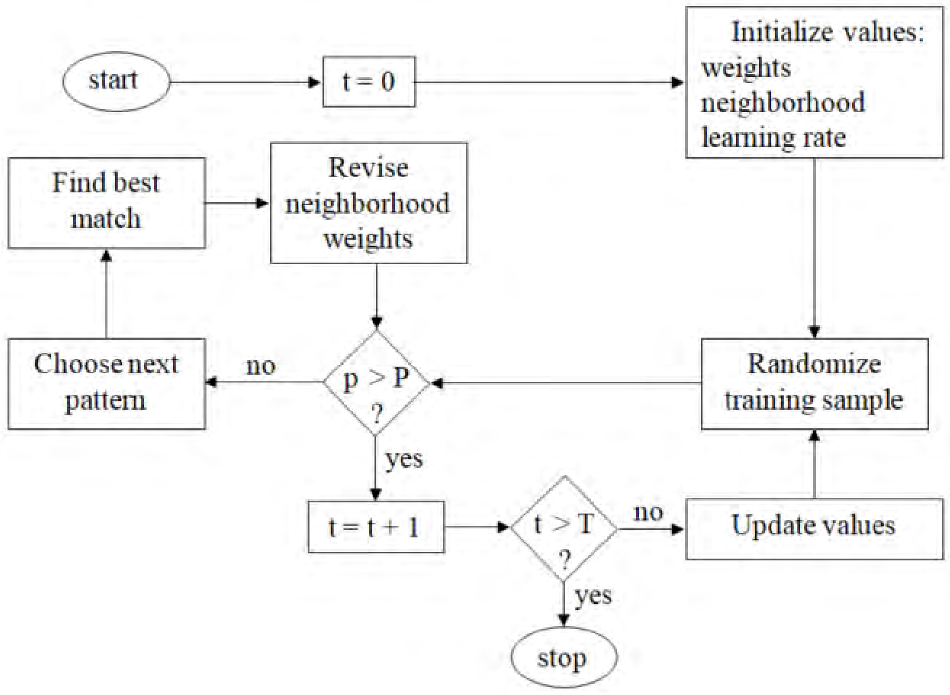

start
t = 0
Initialize values: weights neighborhood learning rate
Find best match
Revise neighborhood weights
Choose next pattern
no
p > P ?
Randomize training sample
yes
t = t + 1
t > T ?
no
Update values
yes
stop

Figure 19: Operation of a Kohonen network

The first step in the process is to initialize the parameters and organize the data. This entails setting the iteration index, t, to 0, the interconnecting weights to small positive random values, and the learning rate to a value smaller than but close to 1. Each unit has a neighborhood of units associated with it and empirical evidence suggests that the best approach is to have the neighborhoods fairly broad initially and then to have them decrease over time. Similarly, the learning rate is a decreasing function of time.

Each iteration begins by randomizing the training sample, which is composed of P patterns, each of which is represented by a numerical vector. For example, the patterns may be composed of solvent and insolvent insurance companies and the input variables may be financial ratios. Until the number of patterns used (p) exceeds the number available ($p > P$), the patterns are presented to the units on the grid, each of which is assigned the Euclidean distance between its connecting weight to the input unit and the value of the input.

The unit which is the best match to the pattern, the winning unit, is used to adjust the weights of the units in its neighborhood. The process continues until the number of iterations exceeds some predetermined value (T).

In the foregoing training process, the winning units in the Kohonen layer develop clusters of neighbors which represent the class types found in the training patterns. As a result, patterns associated with each other in the input space will be mapped on to output units which also are associated with each other. Since the class of each cluster is know, the network can be used to classify the inputs.

7.3.1 Insurance applications of SOFM

Brockett et al (1998) provides an example of a SOFM application in insurance.

8 Unsupervised learning based on Dimensionality Reduction[47]

The purpose of dimensionality reduction is to reduce the dimensions of a dataset while maintaining most of its relevant information. A separate preprocessing step, it reduces the demand on storage space, improves computational efficiency, and, by reducing exposure to the curse of dimensionality[48], it can improve the predictive performance.

In the rest of this section we discuss two types of dimensionality reduction: principal component analysis and singular vector decomposition.

[47] References for this subsection include Alpaydin (2014), Hoang (2016) and Lorraine (2019).

[48] The curse of dimensionality refers to various phenomena that arise when analyzing and organizing data in high-dimensional spaces that do not occur in low-dimensional settings such as the three-dimensional physical space of everyday experience. Wikipedia

8.1 Principal component analysis (PCA)[49]

Principal Component Analysis (PCA) is a feature (dimension) extraction method that seeks to reduce a set of correlated features of a data set to a smaller set of uncorrelated hypothetical features called principal components (PCs). It does this by focusing on directions of maximum variance of the data. The rational for a PCA is that if fewer features can be used to represent a dataset, without significant loss of information, analysis is facilitated.

Figure 20[50] provides a simple example of a PCA application, where x_1 and x_2 represent the features.

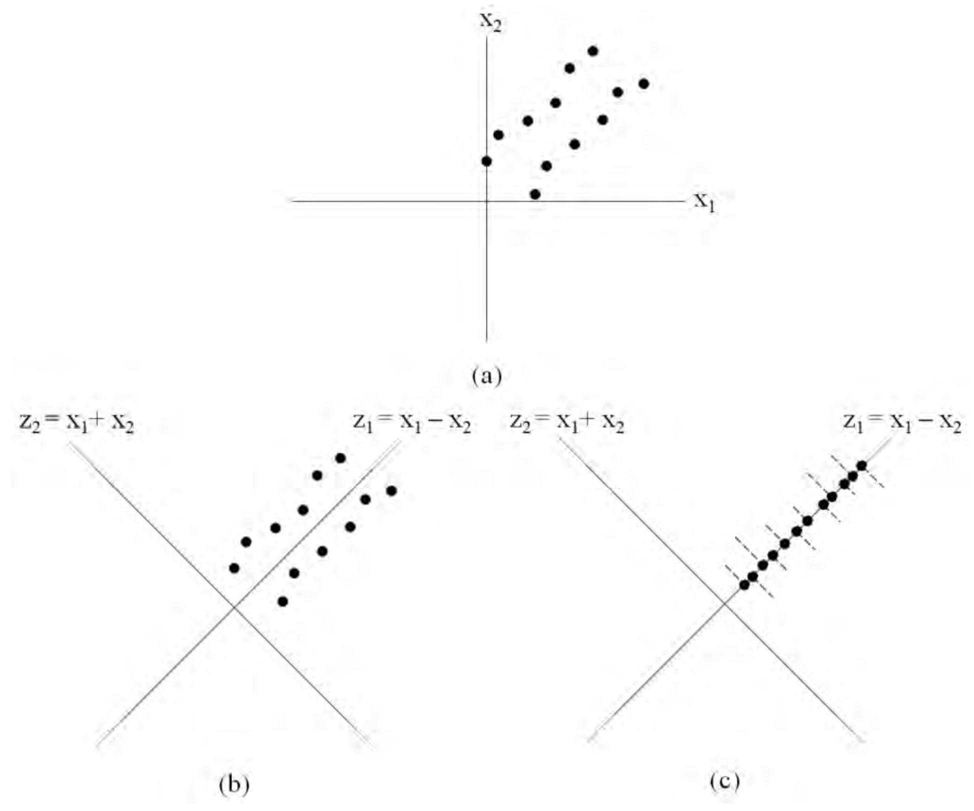


Figure 20: PC example

It is clear from Figure 20(a) that the x_1 and x_2 features are highly correlated, which implies redundancy. This suggests that the two dimensions of data can be reduced to one, with a limited amount of information loss.

[49] References for this subsection include Alpaydin (2014), Ham and Kostanic (2001), Lorraine (2019) and Timm (2002).

[50] Adapted from Abdullatif (2018).

To accommodate this, the axes is realigned so that the first principal axis, z_1, is in the direction that produces of the largest possible variance for the dataset and the second principal axis, z_2, is orthogonal to the first. As shown in Figure 20(b), for this example, this results from a 45 degrees rotation of the axes. Thus, $z_1 = x_1 - x_2$ (i.e., $x_1 = x_2$) and $z_2 = x_1 + x_2$ (i.e., $x_1 = - x_2$).

Now, since the variance of the data along the z_1 axis is much larger than the variance of the data along the z_2 axis, PCA suggests that only the principal axis, z_1, be maintained. To accommodate this, the data points are projected onto the z_1 axis, as shown by the dashed lines in Figure 20(c). This results in a 1D dataset in place of the original 2D dataset.

8.1.1 Insurance applications of PCA

Chen et al (2008) provides an example of a PCA application in insurance.

8.2 Singular value decomposition (SVD)[51]

Singular value decomposition (SVD) can be thought of as the decomposition of vectors onto orthogonal axes.

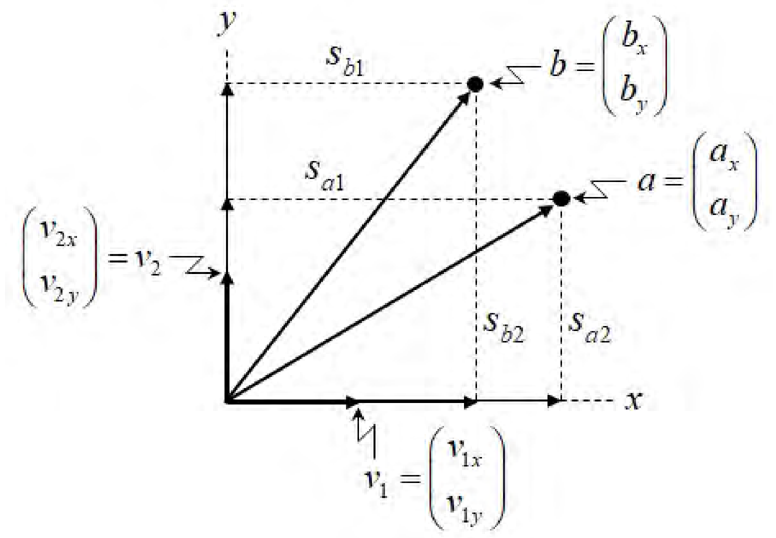
Every matrix A can be factored as $A = U\Sigma V^T$, which is known as the singular value decomposition of A. In this formulation, Σ is a diagonal matrix, whose entries, the number of which are equal to the rank[52] of A, are nonnegative numbers called singular values. Similarly, the columns of U and V, the number of which are also equal to the rank of A, are called left and right singular vectors, respectively.

Figure 21[53] depicts a representation of SVD in the 2-D case,

[51] References for this subsection include Abdullatif (2019) and Math3ma (2020).

[52] The rank of a matrix is the maximum number of linearly independent column or row vectors in the matrix.

[53] This figure and related discussion is adapted from Abdullatif (2019).



y
s_{b1}
$b = \begin{pmatrix} b_x \\ b_y \end{pmatrix}$
s_{a1}
$a = \begin{pmatrix} a_x \\ a_y \end{pmatrix}$
$\begin{pmatrix} v_{2x} \\ v_{2y} \end{pmatrix} = v_2$
s_{b2}
s_{a2}
x
$v_1 = \begin{pmatrix} v_{1x} \\ v_{1y} \end{pmatrix}$

Figure 21: a representation of SVD in the 2-D case

where:

a, b ≡ vectors

S_{ai}, S_{bi}, i = 1, 2 ≡ line segments

v_i, i = 1, 2 ≡ unit vectors

In what follows we validate that Figure 21 is a representation of SVD.

From the figure, the length of the projection of s_{a1} is the dot product of the transpose of a, a^T, and the unit vector v_1, that is,

$$a^T v_1 = (a_x \; a_y)\begin{pmatrix} v_{1x} \\ v_{1y} \end{pmatrix} = s_{a1}.$$

Thus, more generally, if

$$A = \begin{pmatrix} a_x & a_y \\ b_x & b_y \end{pmatrix},\; V = \begin{pmatrix} v_{1x} & v_{2x} \\ v_{1y} & v_{2y} \end{pmatrix}, \text{ and } S = \begin{pmatrix} s_{a1} & s_{a2} \\ s_{b1} & s_{b2} \end{pmatrix}$$

then

$A \cdot V = S$ or $A = S\,V^{-1} = S\,V^T$. [54]

Normalizing the columns of S by dividing them by their magnitudes,

$$\sigma_i = \sqrt{(s_{ai})^2 + (s_{bi})^2}\text{ , i = 1, 2,}$$

[54] If a square matrix is orthogonal, its transpose is equal to its inverse. [Ayres (1962: 103)]

gives

$$S = \begin{pmatrix} \frac{s_{a1}}{\sigma_1} & \frac{s_{a2}}{\sigma_2} \\ \frac{s_{b1}}{\sigma_1} & \frac{s_{b2}}{\sigma_2} \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} = \begin{pmatrix} u_{a1} & u_{a2} \\ u_{b1} & u_{b2} \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix} = U\ \Sigma.$$

That is, normalizing the columns of S results in the conventional SVD formula

$$A = U\ \Sigma\ V^T.$$

8.2.1 Insurance applications of SVD

Kossi et al (2006) provides an example of a SVD application in insurance.

9 Reinforcement learning[55]

Sutton and Barto (2018), in the introduction to their popular book, observed that "Reinforcement learning ... is a computational approach to learning whereby an agent tries to maximize the total amount of reward it receives while interacting with a complex, uncertain environment." One vivid example of this was AlphaGo, the first computer program to defeat a world-class champion at the game of Go.[56]

Operationally, reinforcement learning may be thought of as involving a two-tier process: exploration and exploitation. At the beginning of the learning process, prior to any knowledge having been acquired, the system is in its exploration mode, and actions taken by it are random in nature. In this mode, the results of trying potential actions are documented as to whether they produce positive, negative, or neutral rewards. Once sufficient feedback is acquired, the system enters its exploitation mode, where it uses its learned knowledge to produce deterministic, rather than random, actions.

In this section, two reinforcement learning algorithms are presented that exemplify these characteristics: Markov decision processes and genetic algorithms.

[55] References for this section include Broekens (2007), Joshi (2020), Mnih et al (2016), and Sutton and Barto (2018).

[56] Silver et al (2017) gives an interesting overview of the recent status of reinforcement learning as applied to board games.

9.1 Markov decision process[57]

A Markov decision process (MDP) is a discrete-time stochastic control process that models decision making in situations where outcomes are partly random and partly under the control of a decision maker. It involves a standard reinforcement learning setting, where an agent interacts with the environment over a number of discrete-time steps. During this progression, the agent encounters various states and chooses various actions, subject to given policy. As with Markov chains, the only information available for this decision making is associated with the current state of the agent. At each new state, the agent receives a reward. The process continues until the agent reaches a terminal state.

Key parameters of the model, for t = 0,1,2, ..., T, are

$S = \{s_t\} \equiv$ a finite set of all the possible decision states,

$A = \{a_t\} \equiv$ a finite set of all the valid actions,

$P = \{p_t\} \equiv$ a matrix of state transition probabilities,

$R = \{r_t\} \equiv$ set of all the possible rewards,

$\Pi = \{\pi(a_t \,|\, s_t)\} \equiv$ set of policy functions that specify the action, a_t, given s_t

$= \{\pi_t\}$, for short

Figure 22 shows a representation of the role of these parameters in a MDP flowchart over the time interval t-1 to t+2.

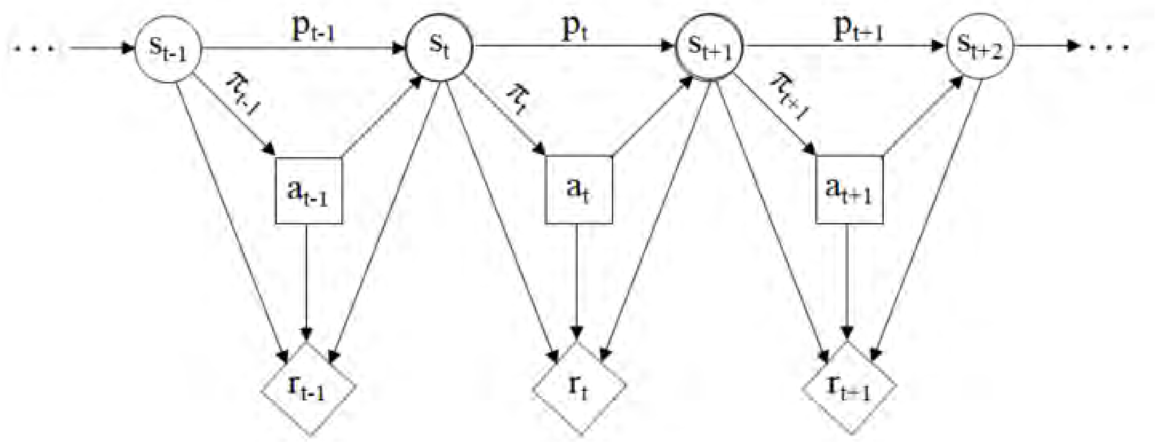


Figure 22: MDP flowchart

[57] References for this subsection include Chhabra (2018), Clayton (2011), Marbach (1998), Mnih et al (2016) and Sloan (2014).

Focusing on time t, the system is in state s_t , the agent takes the action a_t in response to the policy function π_t, the environment transitions to a new state s_{t+1} with a probability p_t, and the agent acquires reward r_t .

9.1.1 Insurance applications of MDP

Dellaert et al (1993) provides an example of a MDP application in insurance.

9.2 Genetic algorithms[58]

GAs are automated heuristics that perform optimization by emulating biological evolution. They are particularly well suited for solving problems that involve loose constraints, such as discontinuity, noise, high dimensionality, and multimodal objective functions.

GAs can be thought of as an automated, intelligent approach to trial and error, based on principles of natural selection. In this sense, they are modern successors to Monte Carlo search methods. The flow chart in Figure 23[59] gives a representation of the process.

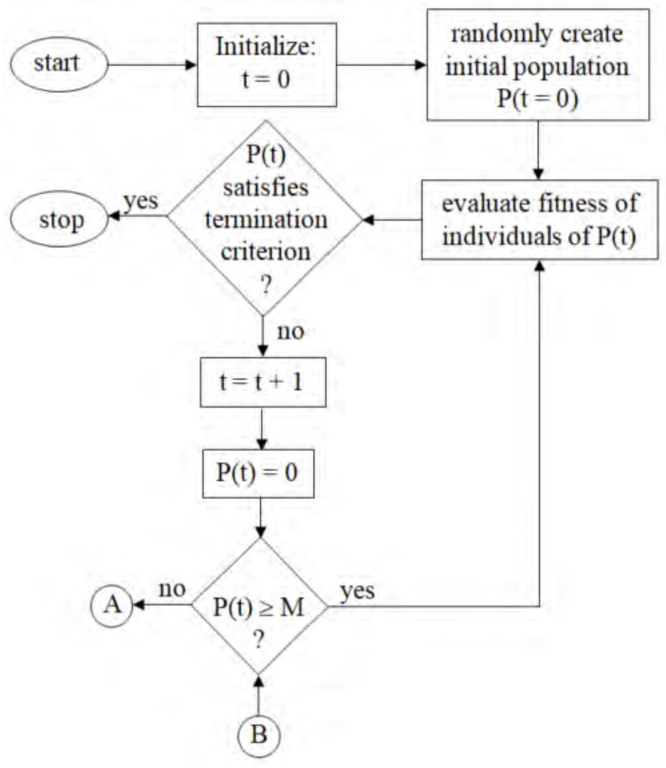

start
Initialize: t = 0
randomly create initial population P(t = 0)
evaluate fitness of individuals of P(t)
P(t) satisfies termination criterion ?
yes
stop
no
t = t + 1
P(t) = 0
P(t) ≥ M ?
no
A
yes
B

Figure 23: Flowchart of a GA

[58] References for this subsection include Shapiro (2000a).

[59] Figure 23 and Figure 24 were adapted from Shapiro (2000a), Figures 8 and 9.

As indicated, GAs are iterative procedures, where each iteration (t) represents a generation. The process starts with an initial population of solutions, P(0), which are randomly generated. From this initial population, the best solutions are "bred" with each other and the worse are discarded. The process ends when the termination criterion is satisfied.

There are three ways to develop a new generation of solutions: reproduction, crossover and mutation. Reproduction adds a copy of a fit individual to the next generation. Crossover emulates the process of creating children, and involves the creation of new individuals (children) from the two fit parents by a recombination of their genes (parameters). Under mutation, there is a small probability that some of the gene values in the population will be replaced with randomly generated values. This has the potential effect of introducing good gene values that may not have occurred in the initial population or which were eliminated during the iterations. The process is repeated until the new generation has the same number of individuals (M) as the current one.

A flowchart of the process for generating new populations of solutions is depicted in Figure 24.

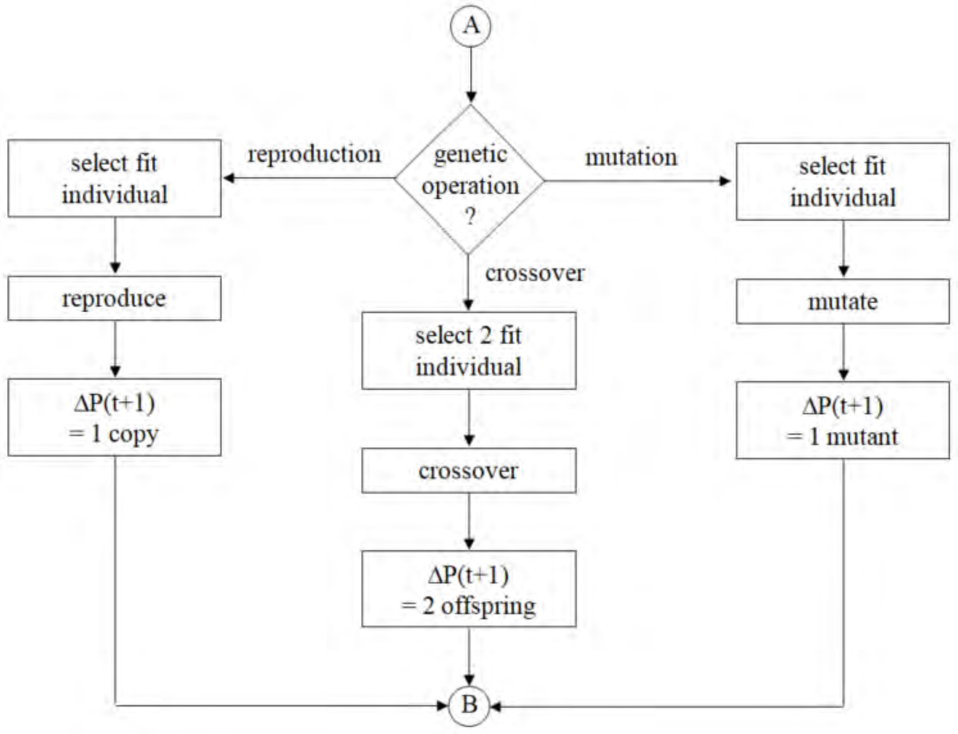


Figure 24: Reproduction, crossover, and mutation

9.2.1 Insurance applications involving GAs

Yan et al (2020) provides an example of a GA application in insurance.

10 Commentary

In this article, we explored the characteristics of some ML algorithms of each type of ML: supervised learning based on regression and classification, unsupervised learning based on clustering and dimensionality reduction, and reinforcement learning. In each instance, the focus was on conceptualization.

As mentioned previously, this version of this article should be viewed as preliminary, in the sense that subsequent versions will extend the discussion to include:

(1) more details with respect to the underlying mathematics of ML, to complement the current text,

(2) a broader discussion of the types of ML algorithms, and

(3) an overview of insurance applications related to ML algorithms.

This being a preliminary version notwithstanding, it is hoped that this article stimulates discussion and provides direction and insight for further research in this area. To the extent it does so, it will have served its purpose.

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