UNIT IV

UNSUPERVISED LEARNING

EM Algorithm- Mixtures of Gaussians

The EM algorithm is considered a latent variable model to find the local maximum likelihood parameters of a statistical model, proposed by Arthur Dempster, Nan Laird, and Donald Rubin in 1977. The EM (Expectation-Maximization) algorithm is one of the most commonly used terms in machine learning to obtain maximum likelihood estimates of variables that are sometimes observable and sometimes not. However, it is also applicable to unobserved data or sometimes called latent. It has various real-world applications in statistics, including obtaining the mode of the posterior marginal distribution of parameters in machine learning and data mining applications.

In most real-life applications of machine learning, it is found that several relevant learning features are available, but very few of them are observable, and the rest are unobservable. If the variables are observable, then it can predict the value using instances. On the other hand, the variables which are latent or directly not observable, for such variables Expectation-Maximization (EM) algorithm plays a vital role to predict the value with the condition that the general form of probability distribution governing those latent variables is known to us. In this topic, we will discuss a basic introduction to the EM algorithm, a flow chart of the EM algorithm, its applications, advantages, and disadvantages of EM algorithm, etc.

What is an EM algorithm?

The Expectation-Maximization (EM) algorithm is defined as the combination of various unsupervised machine learning algorithms, which is used to determine the local maximum likelihood estimates (MLE) or maximum a posteriori estimates (MAP) for unobservable variables in statistical models. Further, it is a technique to find maximum likelihood estimation when the latent variables are present. It is also referred to as the latent variable model.

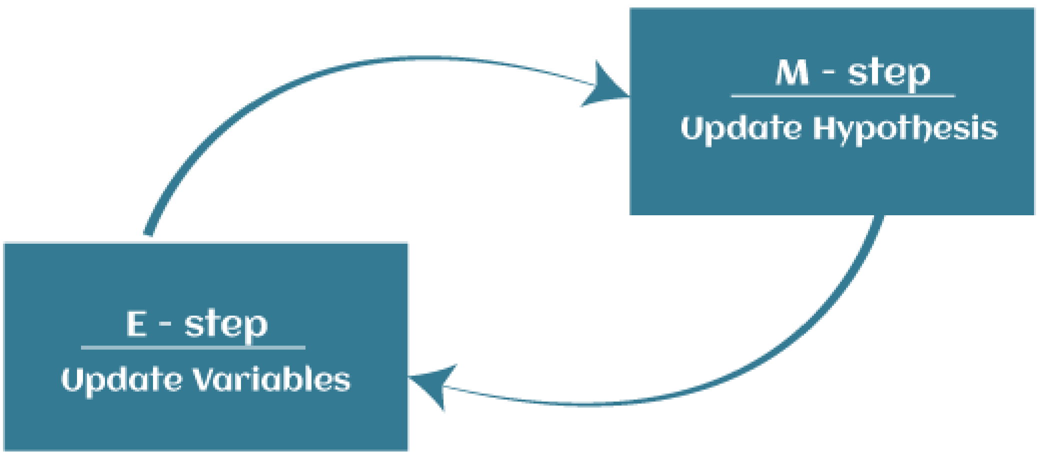
A latent variable model consists of both observable and unobservable variables where observable can be predicted while unobserved are inferred from the observed variable. These unobservable variables are known as latent variables.

Key Points:

1. It is known as the latent variable model to determine MLE and MAP parameters for latent variables.
2. It is used to predict values of parameters in instances where data is missing or unobservable for learning, and this is done until convergence of the values occurs.

EM Algorithm

The EM algorithm is the combination of various unsupervised ML algorithms, such as the **k-means clustering algorithm**. Being an iterative approach, it consists of two modes. In the first mode, we estimate the missing or latent variables. Hence it is referred to as the **Expectation/estimation step (E-step)**. Further, the other mode is used to optimize the parameters of the models so that it can explain the data more clearly. The second mode is known as the **maximization-step or M-step.**



Expectation step (E - step): It involves the estimation (guess) of all missing values in the dataset so that after completing this step, there should not be any missing value.

Maximization step (M - step): This step involves the use of estimated data in the E-step and updating the parameters.

Repeat E-step and M-step until the convergence of the values occurs.

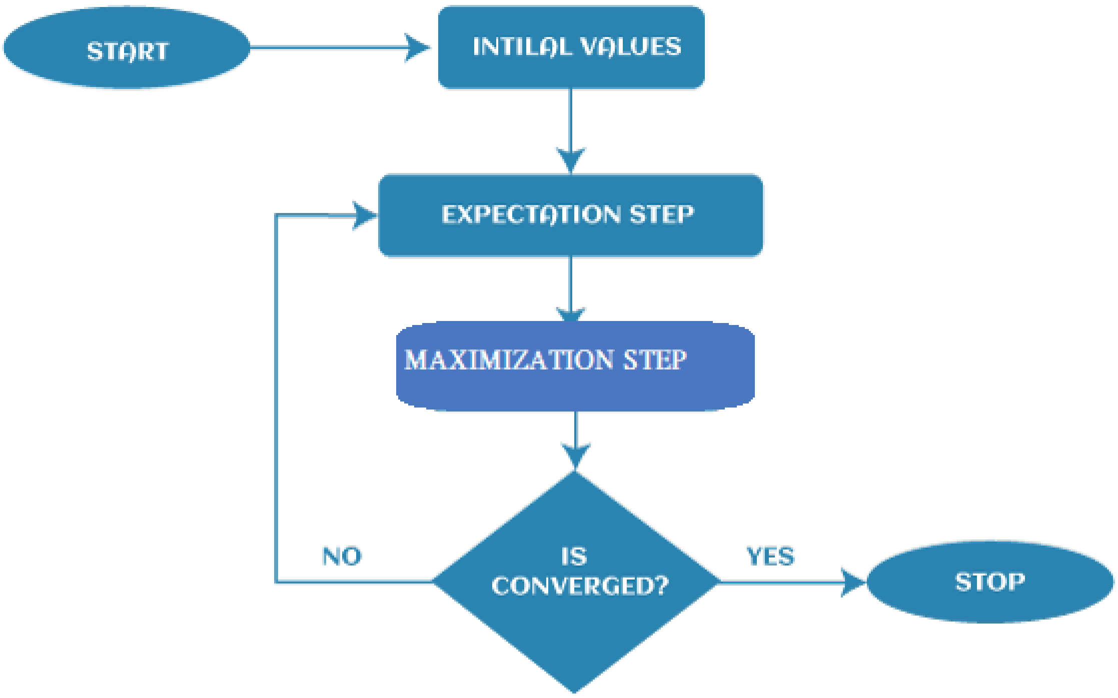
The primary goal of the EM algorithm is to use the available observed data of the dataset to estimate the missing data of the latent variables and then use that data to update the values of the parameters in the M-step.

What is Convergence in the EM algorithm?

Convergence is defined as the specific situation in probability based on intuition, e.g., if there are two random variables that have very less difference in their probability, then they are known as converged. In other words, whenever the values of given variables are matched with each other, it is called convergence.

Steps in EM Algorithm

The EM algorithm is completed mainly in 4 steps, which include Initialization Step, Expectation Step, Maximization Step, and convergence Step. These steps are explained as follows:



EM Algorithm in Machine Learning

1st Step: The very first step is to initialize the parameter values. Further, the system is provided with incomplete observed data with the assumption that data is obtained from a specific model.

2nd Step: This step is known as Expectation or E-Step, which is used to estimate or guess the values of the missing or incomplete data using the observed data. Further, E-step primarily updates the variables.

3rd Step: This step is known as Maximization or M-step, where we use complete data obtained from the 2nd step to update the parameter values. Further, M-step primarily updates the hypothesis.

4th step: The last step is to check if the values of latent variables are converging or not. If it gets "yes", then stop the process; else, repeat the process from step 2 until the convergence occurs.

Gaussian Mixture Model (GMM)

The Gaussian Mixture Model or GMM is defined as a mixture model that has a combination of the unspecified probability distribution function. Further, GMM also requires estimated statistics values such as mean and standard deviation or parameters. It is used to estimate the parameters of the probability distributions to best fit the density of a given training dataset. Although there are plenty of techniques available to estimate the parameter of the Gaussian Mixture Model (GMM), the Maximum Likelihood Estimation is one of the most popular techniques among them.

Let's understand a case where we have a dataset with multiple data points generated by two different processes. However, both processes contain a similar Gaussian probability distribution and combined data. Hence it is very difficult to discriminate which distribution a given point may belong to.

The processes used to generate the data point represent a latent variable or unobservable data. In such cases, the Estimation-Maximization algorithm is one of the best techniques which helps us to estimate the parameters of the gaussian distributions. In the EM algorithm, E-step estimates the expected value for each latent variable, whereas M-step helps in optimizing them significantly using the Maximum Likelihood Estimation (MLE). Further, this process is repeated until a good set of latent values, and a maximum likelihood is achieved that fits the data.

Applications of EM algorithm

The primary aim of the EM algorithm is to estimate the missing data in the latent variables through observed data in datasets. The EM algorithm or latent variable model has a broad range of real-life applications in machine learning. These are as follows:

- The EM algorithm is applicable in data clustering in machine learning.
- It is often used in computer vision and NLP (Natural language processing).
- It is used to estimate the value of the parameter in mixed models such as the **Gaussian Mixture Model**and quantitative genetics.
- It is also used in psychometrics for estimating item parameters and latent abilities of item response theory models.

- It is also applicable in the medical and healthcare industry, such as in image reconstruction and structural engineering.
- It is used to determine the Gaussian density of a function.

Advantages of EM algorithm

- It is very easy to implement the first two basic steps of the EM algorithm in various machine learning problems, which are E-step and M- step.
- It is mostly guaranteed that likelihood will enhance after each iteration.
- It often generates a solution for the M-step in the closed form.

Disadvantages of EM algorithm

- The convergence of the EM algorithm is very slow.
- It can make convergence for the local optima only.
- It takes both forward and backward probability into consideration. It is opposite to that of numerical optimization, which takes only forward probabilities.

Gaussian Mixture Model

Suppose there are K clusters (For the sake of simplicity here it is assumed that the number of clusters is known and it is K). So and are also estimated for each k. Had it been only one distribution, they would have been estimated by the **maximum-likelihood method**. But since there are K such clusters and the probability density is defined as a linear function of densities of all these K distributions, i.e.

where is the mixing coefficient for k^{th} distribution. For estimating the parameters by the maximum log-likelihood method, compute p(X| , ,).

Now define a random variable such that =p(k|X).

From Bayes theorem,

Now for the log-likelihood function to be maximum, its derivative

of with respect to , , and should be zero. So equating the

derivative of with respect to to zero and rearranging the terms,

Similarly taking the derivative with respect to and pi respectively, one can obtain the following expressions.

And

Note: *denotes the total number of sample points in the k*th *cluster. Here it is assumed that there is a total N number of samples and each sample containing d features is denoted by .*

So it can be clearly seen that the parameters cannot be estimated in closed form. This is where the **Expectation-Maximization algorithm** is beneficial.

Expectation-Maximization (EM) Algorithm

The Expectation-Maximization (EM) algorithm is an iterative way to find maximum-likelihood estimates for model parameters when the data is incomplete or has some missing data points or has some hidden variables. EM chooses some random values for the missing data points and estimates a new set of data. These new values are then recursively used to estimate a better first date, by filling up missing points, until the values get fixed.

In the Expectation-Maximization (EM) algorithm, the estimation step (E-step) and maximization step (M-step) are the two most important steps that are iteratively performed to update the model parameters until the model convergence.

Estimation Step (E-step):

- In the estimation step, we first initialize our model parameters like the mean (μk), covariance matrix (Σk), and mixing coefficients (πk).
- For each data point, We calculate the posterior probabilities of data points belonging to each centroid using the current parameter values. These probabilities are often represented by the latent variables γk.
- At the end Estimate the values of the latent variables γ k based on the current parameter values

Maximization Step

- In the maximization step, we update parameter values (i.e. , and) using the estimated latent variable γk.
- We will update the mean of the cluster point (μk) by taking the weighted average of data points using the corresponding latent variable probabilities
- We will update the covariance matrix (Σk) by taking the weighted average of the squared differences between the data points and the mean, using the corresponding latent variable probabilities.
- We will update the mixing coefficients (πk) by taking the average of the latent variable probabilities for each component.

Repeat the E-step and M-step until convergence

- We iterate between the estimation step and maximization step until the change in the log-likelihood or the parameters falls below a predefined threshold or until a maximum number of iterations is reached.
- Basically, in the estimation step, we update the latent variables based on the current parameter values.
- However, in the maximization step, we update the parameter values using the estimated latent variables
- This process is iteratively repeated until our model converges.

The Expectation-Maximization (EM) algorithm is a general framework and can be applied to various models, including Gaussian Mixture Models (GMMs). The steps described above are specifically for GMMs, but the overall concept of the Estimization-step and Maximization-step remains the same for other models that use the EM algorithm.