Python Data Science Handbook

Essential Tools for Working with Data

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March 8, 2023

Contents

Chapter 1

In Depth: Gaussian Mixture Models

In particular, the nonprobabilistic nature of k-means and its use of simple distance from cluster center to assign cluster membership leads to poor performance for many real-world situations. Gaussian mixture models can be viewed as an extension of the ideas behind k-means, but can also be a powerful tool for estimation beyond simple clustering.

An important observation for k-means is that these cluster models must be circular: k-means has no built-in way of accounting for oblong or elliptical clusters.

These two disadvantages of k-means—its lack of flexibility in cluster shape and lack of probabilistic cluster assignment—mean that for many datasets (especially low-dimensional datasets) it may not perform as well as you might hope.

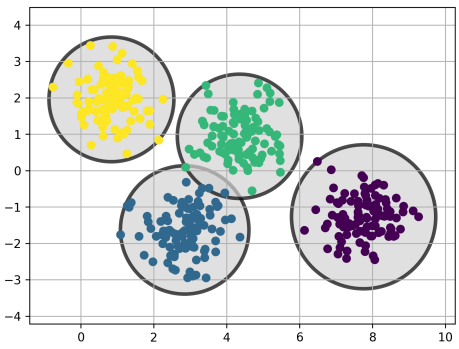
1.1 Generalizing E–M: Gaussian Mixture Models

A **Gaussian mixture model** (GMM) attempts to find a mixture of multidimensional Gaussian probability distributions that best model any input dataset.

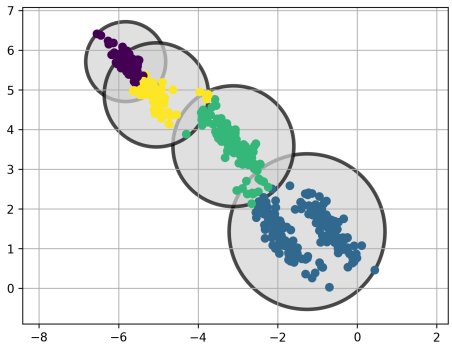
Under the hood, a Gaussian mixture model is very similar to k-means: it uses an expectation–maximization approach, which qualitatively does the following:

1. Choose starting guesses for the location and shape.
2. Repeat until converged:
   (a) E-step: For each point, find weights encoding the probability of membership in each cluster.
   (b) M-step: For each cluster, update its location, normalization, and shape based on all data points, making use of the weights.

The result of this is that each cluster is associated not with a hard-edged sphere, but with a smooth Gaussian model. Just as in the k-means expectation–maximization approach, this algorithm can sometimes miss the globally optimal solution, and thus in practice multiple random initializations are used.



(a) The circular clusters implied by the k-means model



(b) Poor performance of k-means for noncircular clusters

Figure 1.1: Motivating Gaussian Mixtures: Weaknesses of k-Means

1.2 Choosing the Covariance Type

If you look at the details of the preceding fits, you will see that the `covariance_type` option was set differently within each. This hyperparameter controls the degrees of freedom in the shape of each cluster; it's essential to set this carefully for any given problem. The default is `covariance_type="diag"`, which means that the size of the cluster along each dimension can be set independently, with the resulting ellipse constrained to align with the axes. `covariance_type="spherical"` is a slightly simpler and faster model, which constrains the shape of the cluster such that all dimensions are equal. The resulting clustering will have similar characteristics to that of k-means, though it's not entirely equivalent. A more complicated and computationally expensive model (especially as the number of dimensions grows) is to use `covariance_type="full"`, which allows each cluster to be modeled as an ellipse with arbitrary orientation.

1.3 Gaussian Mixture Models as Density Estimation

Though the GMM is often categorized as a clustering algorithm, fundamentally it is an algorithm for density estimation. That is to say, the result of a GMM fit to some data is technically not a clustering model, but a generative probabilistic model describing the distribution of the data.

A GMM is convenient as a flexible means of modeling an arbitrary multidimensional distribution of data. The fact that a GMM is a generative model gives us a natural means of determining the optimal number of components for a given dataset. A generative model is inherently a probability distribution for the dataset, and so we can simply evaluate the likelihood of the data under the model, using cross-validation to avoid overfitting. Another means of correcting for overfitting is to adjust the model likelihoods using some analytic criterion such as the Akaike information criterion (AIC) or the Bayesian information criterion (BIC).