Gaussian Mixture Models

Use cases of GMM:1

- **Recommender systems** that make recommendations to users based on preferences (such as Netflix viewing patterns) of similar users (such as neighbors).
- **Anomaly detection** that identifies rare items, events or observations which deviate significantly from the majority of the data and do not conform to a well defined notion of normal behavior.
- **Customer segmentation** that aims at separating customers into multiple clusters, and devise targeted marketing strategy based on each cluster's characteristics.

When is GMM better than K-Means?

Imagine you are a Data Scientist who builds a recommender for selling cars using K-Means clustering and you have two clusters. Everybody in cluster A is recommended to buy car A which costs **100k** with a **25k** profit margin and everyone in cluster B is recommended to buy car B which costs **50k** with a **10k** profit margin.

Let's say you want to get as many people in cluster A as possible, why not use an algorithm that informs you of exactly how likely somebody would be interested in purchasing car A, instead of one that only tells you a hard yes or no (This is what K-Means does!).

With GMM, not only will you be getting the predicted cluster labels, the algorithm will also give you the probability of a data point belonging to a cluster. How amazing is that!

Whoever is selling those cars should definitely work on a better plan for a customer with a 90% chance of purchasing than for someone with a 75% chance of purchasing, even though they might show up in the same cluster.

What are Gaussian Mixture Models (GMM)?

Put simply, Gaussian Mixture Models (GMM) is a clustering algorithm that:

- Fits Gaussian distributions to your data
- The data scientist (you) needs to determine the number of gaussian distributions (k)

Hard vs Soft Clustering:

- **Hard clustering** algorithms cluster each data point in exactly one cluster.
- **Soft clustering** algorithms can cluster data in partially one cluster and partially others.

GMM is a soft clustering algorithm.

Background:

A Gaussian mixture is a weighted combination of (k) Gaussians, where each is identified by the following parameters:

1. a mean vector $\boldsymbol{\mu}_i$
2. a covariance matrix $\boldsymbol{\Sigma}_i$
3. a component weight π_i that indicates the contribution of the ith Gaussian

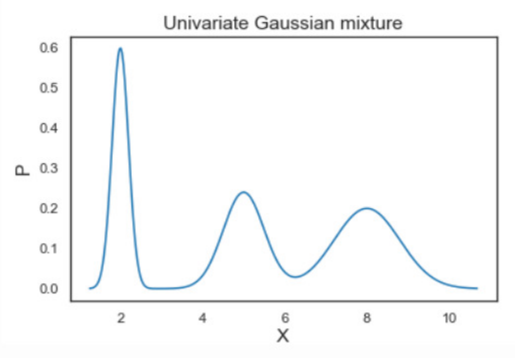
When put altogether, the pdf of the mixture model is formulated as:

$$p(\boldsymbol{x}) = \sum_{i=1}^{K} \pi_i \mathcal{N}(x|\boldsymbol{\mu_i}, \boldsymbol{\Sigma_i}), \sum_{i=1}^{K} \pi_i = 1$$

Example 1: 1-Dimensional Gaussian Mixture:

Let's look at a mixture of 3 univariate Gaussians with

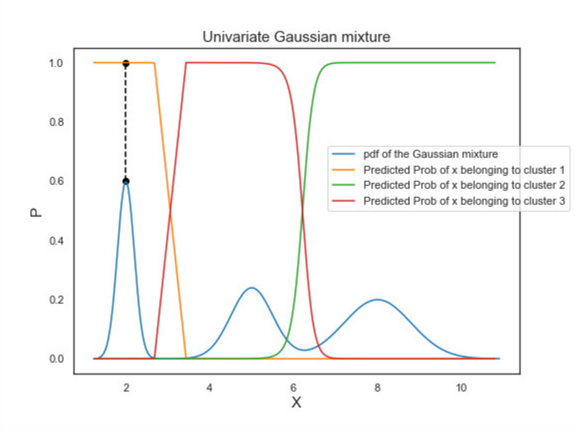
- means equal to **2, 5, 8** respectively
- std equal to **0.2, 0.5, 0.8** respectively
- component weight equal to **0.3, 0.3, 0.4** respectively



Thus, the means determine the centers of the mixed Gaussians; the standard deviations determine the width and shape of the mixed Gaussians; the weights determine the contributions of the Gaussians to the mixture.

Let's fit a GMM with `n_components=3` to our simulated data and plot the prior probabilities. The **GaussianMixture** class from **Scikit-learn** allows us to estimate the parameters of a Gaussian mixture distribution.

GaussianMixture.predict_proba_ evaluates the components' density for each sample or for sample x_n the probability $p(i|x_n)$.

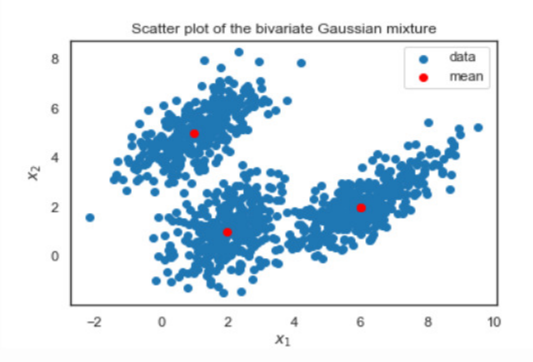


To interpret the predicted probabilities, let's take a look at the point colored in black as an example. On the Gaussian mixture pdf, the point is at the the peak of the first bell-shaped curve. Its corresponding probability of belonging to cluster 1 is equal to 1, which demonstrates that the probability of the center of a Gaussian distribution belonging to its own cluster is 100%.

▸ Click here for the code used for this example!

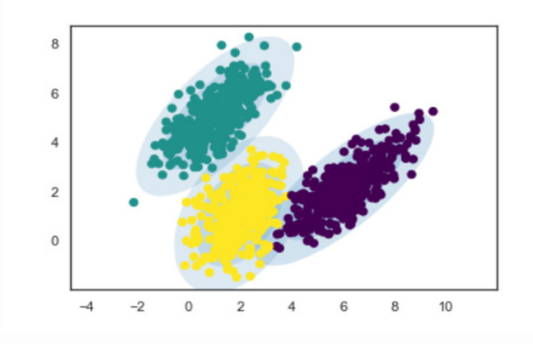
Example 2: 2-Dimensional Gaussian Mixture:

In this example, you have a simulated 2-dimensional data that looks like this:



▸ Click here for the code used for simulating the 2d dataset!

Like before, to work with GMM, we can use the **GaussianMixture** function from **sklearn.mixture**. We fit a GMM with **n_components** = **3** to the simulated dataset, and plot the clustering result as follows:



Awesome! The fitted clusters indeed match the individual Gaussians we simulated, and the ellipses drawn based on the estimated parameter values (means, covariances, weights) contain the clusters.

The default value of **covariance_type** in GMM is `full`, which allows each component (Gaussian) to have its own covariance matrix.

Since our dataset was simulated using three different covariance matrices, using the default covariance_type value would work the best.

However, note that sometimes you can't use **covariance_type** = **full**, because you won't be able to invert it and that will give you an error.

Example 3: Image Segmentation

Image segmentation is the process of segmenting an image into multiple important regions.

We can use a GMM to segment an image into **K** regions `(n_components = K)` according to significant colors.

Each pixel would be a data point with three features (r, g, b) (Or 1 feature if greyscale).

For instance, if we are working with a 256×256 image, you would have 65536 pixels in total and your data X would have a shape of 65536×3.

Let's look at an example using a picture of a house cat:

First let's segment our image using 2 gaussian distributions;

Then we replace each pixel with the "average color" or the mean RGB values of the gaussian distribution it belongs to:

Similarly, if we increase the number of components to 8:

Our segmented image looks remarkably similar to the original, even though it uses only 8 colors!

▸ Click here for the code used for this example!