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

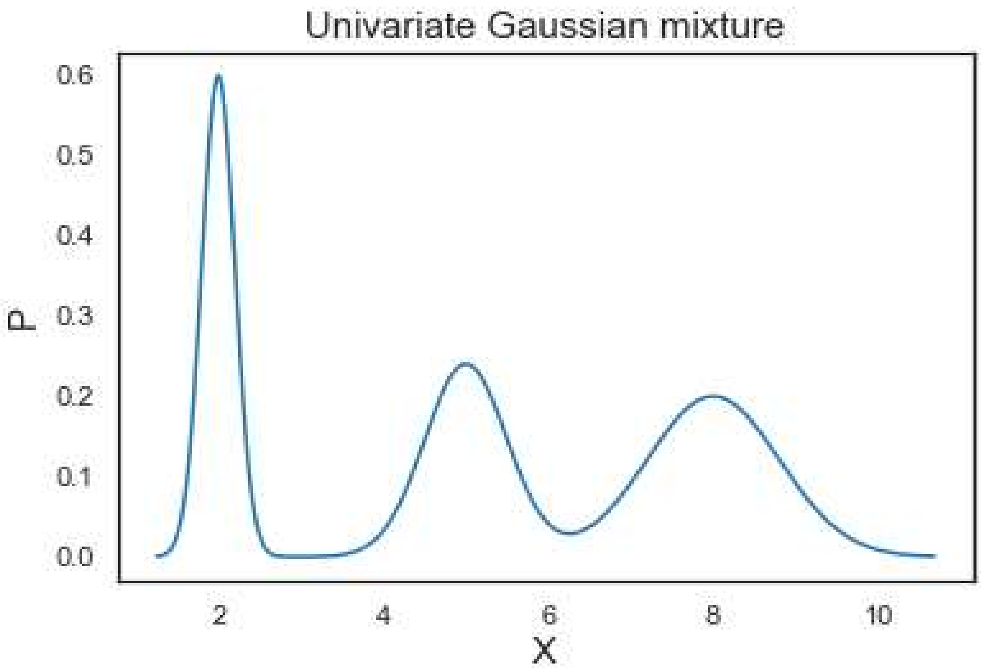
When put altogether, the pdf of the mixture model is formulated as:

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

Example 1: 1-Dimensional Gaussian Mixture:

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

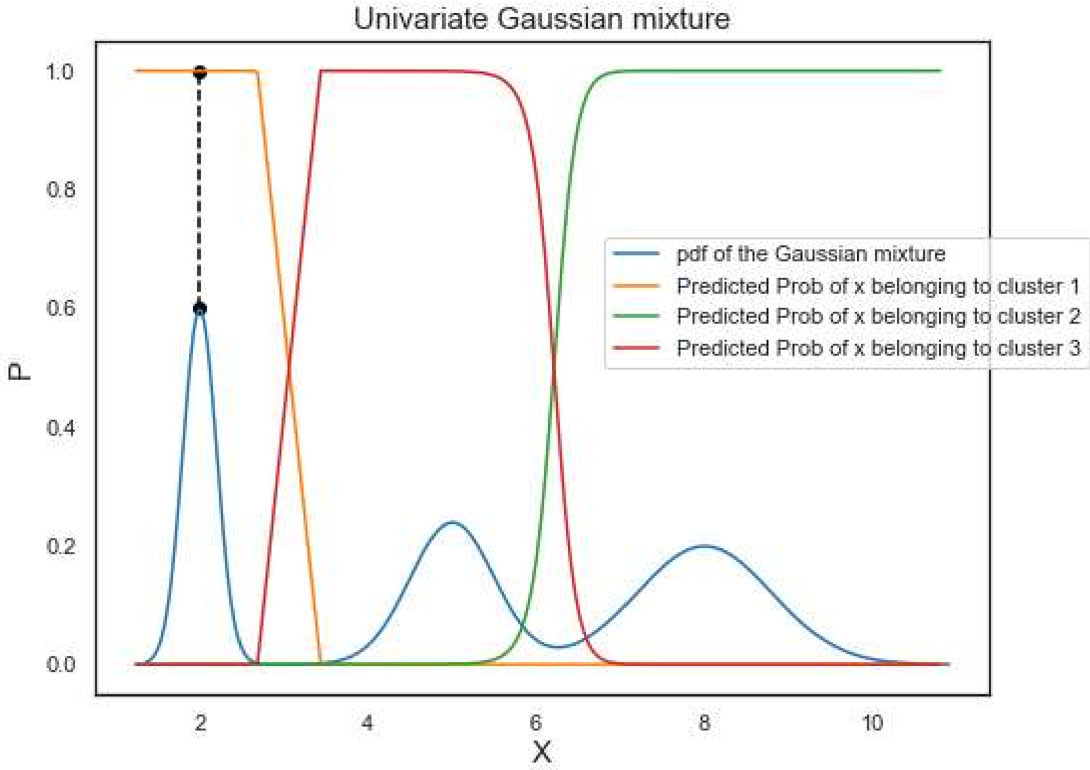
- means equal to **2, 5, 8** respectively
- std equal to **0.2, 0.5, 0.8** respectively
- component weight equal to **0.3, 0.3, 0.4** respectively



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%.

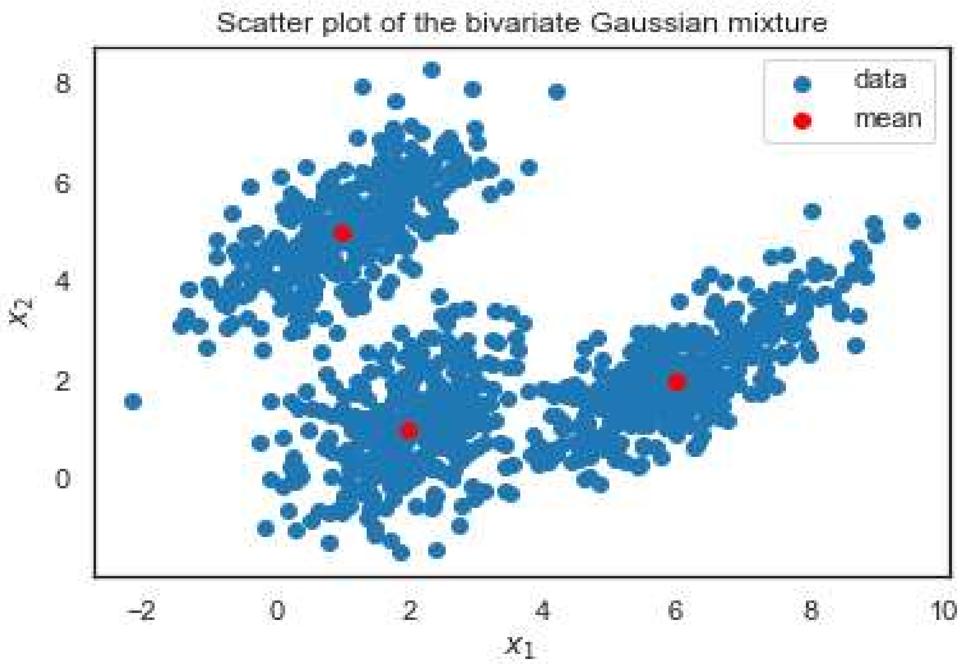
▼ Click here for the code used for this example!

```
import numpy as np
import scipy.stats as ss
import matplotlib.pyplot as plt
from sklearn.mixture import GaussianMixture

means=[2,5,8]
stds=[0.2, 0.5, 0.8]
weights=[0.3, 0.3, 0.4]

mixture_idx = np.random.choice(3, size=10000, replace=True, p=weights)
# generate 10000 possible values of the mixture
X = np.fromiter((ss.norm.rvs(loc=means[i], scale=stds[i]) for i in
        mixture_idx), dtype=np.float64)

# create x axis of the plot
xs = np.linspace(X.min(), X.max(), 300)
ps = np.zeros_like(xs)
```

```
for mu, s, w in zip(means, stds, weights):
    ps += ss.norm.pdf(xs, loc=mu, scale=s) * w

# sort X in ascending order for plotting purpose
X_sorted = np.sort(X.reshape(-1)).reshape(-1,1)

# fit the GMM
GMM = GaussianMixture(n_components=3, random_state=10)
GMM.fit(X_sorted)

# store the predicted probabilities in y1_prob
probs = GMM.predict_proba(X_sorted)

# plot the Gaussian mixture pdf
plt.figure(figsize=(8,6))
plt.plot(xs, ps, label='pdf of the Gaussian mixture')
plt.xlabel("X", fontsize=15)
plt.ylabel("P", fontsize=15)
plt.title("Univariate Gaussian mixture", fontsize=15)

# plot the predicted prior probabilities
plt.plot(X_sorted, probs[:,0], label='Predicted Prob of x belonging to
        cluster 1')
plt.plot(X_sorted, probs[:,1], label='Predicted Prob of x belonging to
        cluster 2')
plt.plot(X_sorted, probs[:,2], label='Predicted Prob of x belonging to
        cluster 3')
plt.scatter(2, 0.6, color='black')
plt.scatter(2, 1.0, color='black')
plt.plot([2, 2], [0.6, 1.0],'--', color='black')
plt.legend(bbox_to_anchor=(0.6,0.7), borderaxespad=0)
```

Example 2: 2-Dimensional Gaussian Mixture:

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

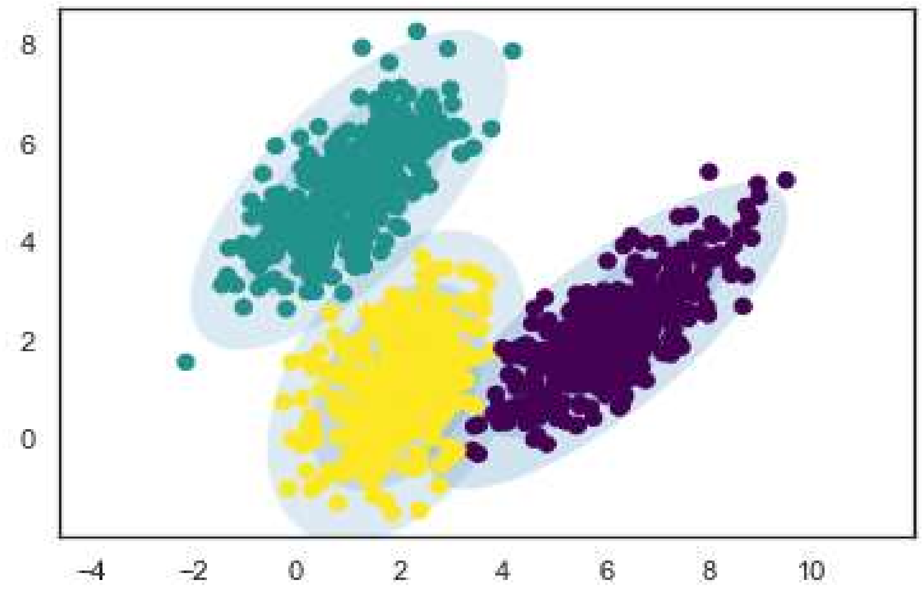


▼ Click here for the code used for simulating the 2d dataset!

```
means = [(1,5), (2,1), (6,2)]
cov1 = np.array([[0.5, 1.0],[1.0, 0.8]])
cov2 = np.array([[0.8, 0.4],[0.4, 1.2]])
cov3 = np.array([[1.2, 1.3],[1.3, 0.9]])
covs = [cov1, cov2, cov3]
weights = [0.3, 0.3, 0.4]

mixture_idx = np.random.choice(3, size=10000, replace=True, p=weights)

# generate 10000 possible values of the mixture
X = np.fromiter(chain.from_iterable(multivariate_normal.rvs(mean=means[i],
        cov=covs[i]) for i in mixture_idx),
            dtype=float)
X.shape = 10000, 2

xs1 = y[:,0]
xs2 = y[:,1]

plt.scatter(xs1, xs2, label="data")

L = len(means)
for l, pair in enumerate(means):
    plt.scatter(pair[0], pair[1], color='red')
    if l == L-1:
        break
plt.scatter(pair[0], pair[1], color='red', label="mean")
```

```
plt.xlabel("$x_1$")
plt.ylabel("$x_2$")
plt.title("Scatter plot of the bivariate Gaussian mixture")
plt.legend()
```

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!

```
import numpy as np
import cv2
from sklearn.mixture import GaussianMixture as GMM

img = cv2.imread('cat.jpeg')
# If img is greyscale, then change to .reshape(-1, 1):
```

```
x = img.reshape(-1, 3)
# The number of components; you can change this to a positive integer
        of your choice!:
n = 8
gmm = GMM(n_components=n, covariance_type='tied')
gmm.fit(x)
labels = gmm.predict(x)
seg = np.zeros(x.shape)
for label in range(n):
    seg[labels == label] = gmm.means_[label]
seg = seg.reshape(img.shape).astype(np.uint8)
cv2.imwrite(f'gauss-cat-{n}.jpeg', seg)
```