

# Gaussian Mixture Models

## General Principles

To discover group structures or clusters in data, we can use a **Gaussian Mixture Model (GMM)**. This is a parametric clustering method. A GMM assumes that the data is generated from a mixture of a **pre-specified number (K)** of different Gaussian distributions. The model's goal is to figure out:

1. **The properties of each of the K clusters:** For each of the K clusters, it estimates its center (mean  $\mu$ ) and its shape/spread (covariance  $\Sigma$ ).
2. **The mixture weights:** It estimates the proportion of the data that belongs to each cluster.
3. **The assignment of each data point:** It determines the probability of each data point belonging to each of the K clusters.

## Considerations

### Caution

- A GMM is a Bayesian model that considers uncertainty in all its parameters, *except for the number of clusters, K*, which must be fixed in advance.
- The key parameters and their priors are:
  - **Number of Clusters K:** This is a **fixed hyperparameter** that you must choose before running the model. Choosing the right K often involves running the model multiple times and using model comparison criteria (like cross-validation, AIC, or BIC).
  - **Cluster Weights  $w$ :** These are the probabilities of drawing a data point from any given cluster. Since there are a fixed number K of them and they must sum to 1, they are typically given a **Dirichlet** prior. A symmetric **Dirichlet** prior (e.g., `Dirichlet(1, 1, ..., 1)`) represents an initial belief that all clusters are equally likely.

- **Cluster Parameters** ( $\mu$ ,  $\Sigma$ ): Each of the  $K$  clusters has a mean  $\mu$  and a covariance matrix  $\Sigma$ . We place priors on these to define our beliefs about their plausible values.
- Like the DPMM, the model is often implemented in its marginalized form . Instead of explicitly assigning each data point to a cluster, we integrate out this choice. This creates a smoother probability surface for the inference algorithm to explore, leading to much more efficient computation.
- To increase accuracy we run a k-means algorithm to initialize the cluster mean priors.

## Example

Below is an example of a GMM implemented in BI. The goal is to cluster a synthetic dataset into a **pre-specified K=4 groups**.

## Python

```
from BI import bi
from sklearn.datasets import make_blobs

# Generate synthetic data
data, true_labels = make_blobs(
    n_samples=500, centers=8, cluster_std=0.8,
    center_box=(-10,10), random_state=101
)

# The model
def gmm(data, K, initial_means): # Here K is the *exact* number of clusters
    D = data.shape[1] # Number of features
    alpha_prior = 0.5 * jnp.ones(K)
    w = dist.dirichlet(concentration=alpha_prior, name='weights')

    with dist.plate("components", K): # Use fixed K
        mu = dist.multivariatenormal(loc=initial_means, covariance_matrix=0.1*jnp.eye(D), name='mu')
        sigma = dist.halfcauchy(1, shape=(D,), event=1, name='sigma')
        Lcorr = dist.lkjcholesky(dimension=D, concentration=1.0, name='Lcorr')
```

```

        scale_tril = sigma[..., None] * Lcorr

    dist.mixturestamefamily(
        mixing_distribution=dist.categorical(probs=w, create_obj=True),
        component_distribution=dist.multivariateNormal(loc=mu, scale_tril=scale_tril, create_obj=True),
        name="obs",
        obs=data
    )

m.data_on_model = {"data": data, "K": 4 }
m.fit(gmm) # Optimize model parameters through MCMC sampling
m.plot(X=data, sampler=m.sampler) # Prebuild plot function for GMM

```

## R

### Mathematical Details

This section describes the generative process for a GMM.

$$\begin{aligned}
 Z_i | \pi &\sim \text{Categorical}(\pi) \\
 X_i | Z_i = k, \mu_k, \Sigma_k &\sim \text{MultivariateNormal}(\mu_k, \Sigma_k) \\
 \pi &\sim \text{Dirichlet}([0.5, \dots, 0.5]) \\
 \text{for } k \text{ in } 1, \dots, K : \\
 \mu_k &\sim \text{MultivariateNormal}(\mu_{0,k}, 0.1 \cdot I_D) \\
 \Sigma_k &= \text{diag}(\sigma_k) \cdot \Omega_k \cdot \text{diag}(\sigma_k) \\
 \sigma_{k,d} &\sim \text{HalfCauchy}(1) \quad \text{for } d \text{ in } 1, \dots, D \\
 \Omega_k &\sim \text{LKJ}(1)
 \end{aligned}$$

**Parameter Definitions:** \* **Observed Data:** \*  $x_i$ : The  $i$ -th observed  $D$ -dimensional data point.

- **Latent Variables (Inferred):**

- $z_i$ : The integer cluster assignment for the  $i$ -th data point.

- $w$ : The  $K$ -dimensional vector of mixture weights.
- $\mu_k$ : The  $D$ -dimensional mean vector of the  $k$ -th cluster.
- $\Sigma_k$ : The  $D \times D$  covariance matrix of the  $k$ -th cluster (composed of  $\sigma_k$  and  $L_{\text{corr},k}$ ).

- **Hyperparameters (Fixed):**

- $K$ : The total number of clusters.
- $\alpha_0$ : The concentration parameter vector for the Dirichlet prior on weights (e.g.,  $[1, 1, \dots, 1]$ ).
- $\mu_0$ : The prior mean for the cluster centers.
- $\Sigma_0$ : The prior covariance for the cluster centers.

## Notes

### Note

The primary challenge of the GMM compared to the DPMM is the need to **manually specify the number of clusters  $K$** . If the chosen  $K$  is too small, the model may merge distinct clusters. If  $K$  is too large, it may split natural clusters into meaningless subgroups. Therefore, applying a GMM often involves an outer loop of model selection where one fits the model for a range of  $K$  values and uses a scoring metric to select the best one.

## Reference(s)

C. M. Bishop (2006). *Pattern Recognition and Machine Learning*. Springer. (Chapter 9)