

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 μ) and its shape/spread (covariance Σ).
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** (μ, Σ): Each of the K clusters has a mean μ and a covariance matrix Σ . 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.multivariate_normal(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.mixturesamefamily(
    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. For each data point x_i , the model first selects one of the K clusters according to the weights w , and then draws the point from that cluster's Gaussian distribution.

$$z_i \sim \text{Categorical}(w) \text{ for } i = 1, \dots, N \\ x_i | z_i = k \sim \text{MultivariateNormal}(\mu_k, \Sigma_k) \text{ for } i = 1, \dots, N$$

$$w \sim \text{Dirichlet}(\alpha_0) \quad (\text{Mixture weights vector for } K \text{ clusters})$$

$$\mu_k \sim \text{MultivariateNormal}(\mu_0, \Sigma_0) \text{ for } k = 1, \dots, K \\ \sigma_k \sim \text{HalfCauchy}(1) \text{ for } k = 1, \dots, K \\ L_{\text{corr},k} \sim \text{LKJCholesky}(D, 1)$$

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.
- μ_k : The D-dimensional mean vector of the k -th cluster.
- Σ_k : The DxD covariance matrix of the k -th cluster (composed of σ_k and $L_{\text{corr},k}$).

- **Hyperparameters (Fixed):**
 - K : The total number of clusters.
 - α_0 : The concentration parameter vector for the Dirichlet prior on weights (e.g., $[1, 1, \dots, 1]$).
 - μ_0 : The prior mean for the cluster centers.
 - Σ_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)