

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
import jax.numpy as jnp
from sklearn.datasets import make_blobs

m = bi()
# 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 = m.dist.dirichlet(concentration=alpha_prior, name='weights')

    with m.dist.plate("components", K): # Use fixed K
        mu = m.dist.multivariate_normal(loc=initial_means, covariance_matrix=0.1*jnp.eye(D),
        sigma = m.dist.half_cauchy(1, shape=(D,), event=1, name='sigma')

```

```

Lcorr = m.dist.lkj_cholesky(dimension=D, concentration=1.0, name='Lcorr')

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

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

# Kmeans clustering do initiate the means
m.ml.KMEANS(data, n_clusters=8)
m.data_on_model = {"data": data, "K": 8 }
m.data_on_model['initial_means'] = m.ml.results['centroids']

m.fit(gmm, progress_bar=False) # Optimize model parameters through MCMC sampling
m.plot(X=data, sampler=m.sampler) # Prebuild plot function for GMM

```

/home/sosa/work/3.12venv/lib/python3.10/site-packages/tqdm/auto.py:21: TqdmWarning:

IProgress not found. Please update jupyter and ipywidgets. See <https://ipywidgets.readthedocs.io/en/latest/README.html>

BI v 0.0.46 package loaded
jax.local_device_count 32

R



Julia

```
@BI function gmm(data, K, initial_means)
    D = data.shape[1]
    alpha_prior = 0.5 * jnp.ones(K)
    w = m.dist.dirichlet(concentration=alpha_prior, name="weights")

    # We capture the output of the pywith block
    # The block returns a tuple (mu, scale_tril)
    mu, scale_tril = pywith(m.dist.plate("components", K)) do _
```

```

mu_inner = m.dist.multivariate_normal(
    loc=initial_means,
    covariance_matrix=0.1*jnp.eye(D),
    name="mu"
)

sigma = m.dist.half_cauchy(1, shape=(D,), event=1, name="sigma")
Lcorr = m.dist.lkj_cholesky(dimension=D, concentration=1.0, name="Lcorr")

# FIX: Use expand_dims instead of slicing
scale_tril_inner = jnp.expand_dims(sigma, -1) * Lcorr

# Return them so they are available outside
(mu_inner, scale_tril_inner)
end

m.dist.mixture_same_family(
    mixing_distribution=m.dist.categorical(probs=w, create_obj=true),
    component_distribution=m.dist.multivariate_normal(loc=mu, scale_tril=scale_tril, create_obj=true),
    name="obs",
    obs=data
)
end

# Run
m.fit(gmm)
m.summary()

```

Mathematical Details

This section describes the generative process for a GMM.

$$\begin{pmatrix} Y_{i,1} \\ \vdots \\ Y_{i,D} \end{pmatrix} \sim \text{MVN} \left(\begin{pmatrix} \mu_{z_i,1} \\ \vdots \\ \mu_{z_i,D} \end{pmatrix}, \Sigma_{z_i} \right)$$

$$\begin{pmatrix} \mu_{k,1} \\ \vdots \\ \mu_{k,D} \end{pmatrix} \sim \text{MVN} \left(\begin{pmatrix} A_{k,1} \\ \vdots \\ A_{k,D} \end{pmatrix}, B \right)$$

$$\Sigma_k = \text{Diag}(\sigma_k) \Omega_k \text{Diag}(\sigma_k)$$

$$\sigma_{[k,d]} \sim \text{HalfCauchy}(1)$$

$$\Omega_k \sim \text{LKJ}(2)$$

$$z_i \sim \text{Categorical}(\pi)$$

$$\pi \sim \text{Dirichlet}(0.5, \dots, 0.5)$$

Where :

- $\begin{pmatrix} Y_{[i,1]} \\ \vdots \\ Y_{[i,D]} \end{pmatrix}$ is the i -th observation of a D -dimensional data array.
- $\begin{pmatrix} \mu_{[k,1]} \\ \vdots \\ \mu_{[k,D]} \end{pmatrix}$ is the k -th parameter vector of dimension D .
- $\begin{pmatrix} A_{[k,1]} \\ \vdots \\ A_{[k,D]} \end{pmatrix}$ is a prior for the k -th mean vector as derived by a *KMEANS* clustering algorithm.
- B is the prior covariance of the cluster means, and is setup as a diagonal matrix with 0.1 along the diagonal.
- Σ_k is the $D \times D$ covariance matrix of the k -th cluster (it is composed from σ_k and Ω_k).
- $\text{Diag}(\sigma_k)$ is a diagonal matrix whose diagonal entries are the standard deviations:

$$\text{Diag}(\sigma_k) = \begin{pmatrix} \sigma_{[k,1]} & 0 & \cdots & 0 \\ 0 & \sigma_{[k,2]} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \sigma_{[k,D]} \end{pmatrix}.$$

- σ_k is a D -vector of standard deviations for the k -th cluster where each element, d , has a half-cauchy prior.
- Ω_k is a correlation matrix for the k -th cluster.
- z_i is a latent variable that maps observation i to cluster k .
- π is a vector of K cluster weights.

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- σ_k is a diagonal matrix of standard deviations for the k -th cluster.
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Notes

i 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)