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

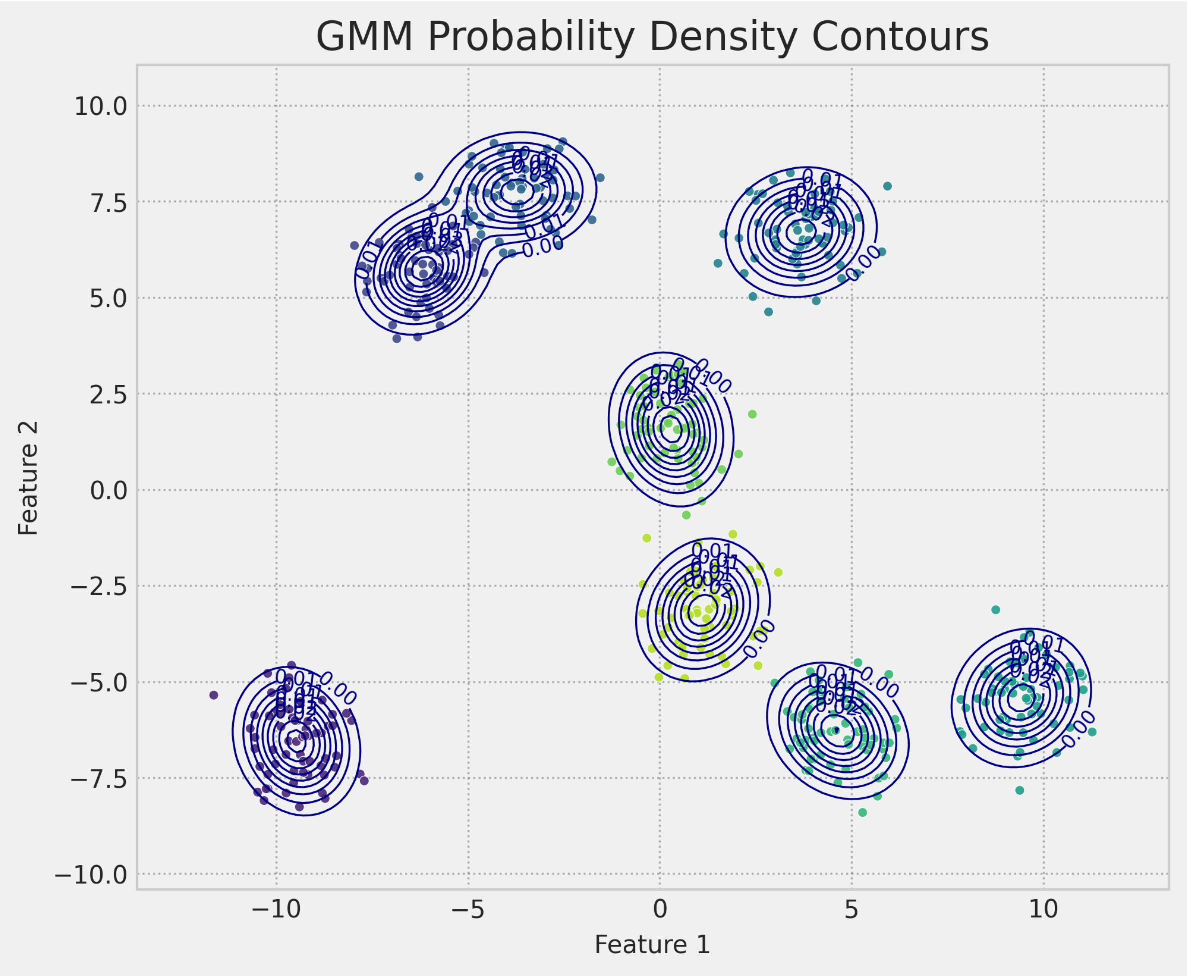
```python
from BI import bi, jnp
from sklearn.datasets import make_blobs

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, crea
        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) # Optimize model parameters through MCMC sampling
m.plot(X=data,sampler=m.sampler) # Prebuild plot function for GMM
```

```
jax.local_device_count 16
```

```
  0%|          | 0/1000 [00:00<?, ?it/s]warmup:   0%|          | 1/1000 [00:04<1:22:50,  4.98
```

```
 This function is still in development. Use it with caution.
 This function is still in development. Use it with caution.
```


GMM Probability Density Contours
Feature 1
Feature 2
−10
−5
0
5
10
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
0.00
0.01

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, crea
        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 DxD covariance matrix of the *k*-th cluster (it is composed from σ_k and Ω_k).
- Diag(σ_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.

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 DxD covariance matrix of the k-th cluster (it is composed from σ_k and Ω_k).
- σ_k is a diagonal matrix of standard deviations for the k-th cluster.
- 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.

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)