Dirichlet Process Mixture Models

General Principles

To discover group structures or clusters in data without pre-specifying the number of groups, we can use a **Dirichlet Process Mixture Model (DPMM)** Gershman and Blei (2012). This is a unsupervised clustering method . Essentially, the model assumes the data is generated from a collection of different Gaussian distributions, and it simultaneously tries to figure out:

1. **How many clusters (`K`) exist**: Unlike algorithms like K-Means, the DPMM infers the most probable number of clusters directly from the data.
2. **The properties of each cluster**: For each inferred cluster, it estimates its location and its spread.
3. **The assignment of each data point**: It determines the probability of each data point belonging to each cluster.

Considerations

Caution

- A DPMM is a Bayesian model that considers uncertainty in all its parameters. The core idea is to use the Dirichlet Process prior that allows for a potentially infinite number of clusters. In practice, we use a finite approximation where we cap the maximum number of clusters at K and use the Stick-Breaking Process .
- The key parameters and their priors are:
  - **Concentration** α: This single parameter controls the tendency to create new clusters. A low favors fewer, larger clusters, while a high allows for many smaller clusters. We typically place a `Gamma` prior on α to learn its value from the data.
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  - **Cluster Weights** `w`: Generated via the Stick-Breaking process from α. These are the probabilities of drawing a data point from any given cluster.

  - **Cluster Parameters** (μ, Σ): Each potential cluster has a mean μ and a covariance matrix Σ. If the data have multiple dimensions, we use a multivariate normal distribution (see chapter, 14). However, if the data is one-dimensional, we use a univariate normal distribution.

- 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.

Example

Below is an example of a DPMM implemented in BI. The goal is to cluster a synthetic dataset into its underlying groups. The code first generates data with 4 distinct centers and then applies the DPMM to recover these clusters.

Python

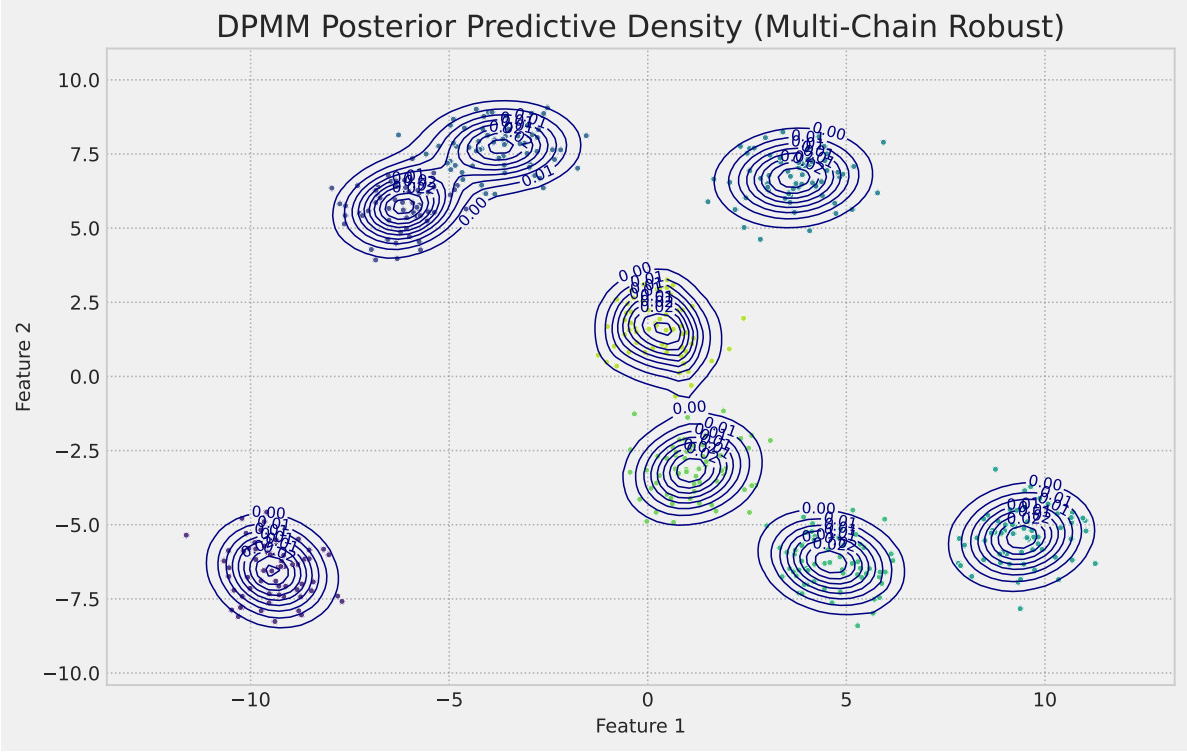
```
from BI import bi, jnp
from sklearn.datasets import make_blobs
import numpyro

m = bi(rand_seed = False)

# Generate synthetic data
data, true_labels = make_blobs(
    n_samples=500, centers=8, cluster_std=0.8,
    center_box=(-10,10), random_state=101
)
data_mean = jnp.mean(data, axis=0)
data_std = jnp.std(data, axis=0)*2

#  The model
def dpmm(data, K, data_mean, data_std):
    N, D = data.shape  # Number of features


    # 1) stick-breaking weights
    alpha = m.dist.gamma(1.0, 10.0,name='alpha')
```

```
    with m.dist.plate("beta_plate", K - 1):
        beta = m.dist.beta(1, alpha, name = "beta")

    w = numpyro.deterministic("w",m.models.dpmm.mix_weights(beta))

    # 2) component parameters
    with m.dist.plate("components", K):
        mu = m.dist.multivariate_normal(loc=data_mean, covariance_matrix=data_std*jnp.eye(D)
        sigma = m.dist.log_normal(0.0, 1.0,shape=(D,),event=1,name='sigma')# shape (T, D)
        Lcorr = m.dist.lkj_cholesky(dimension=D, concentration=1.0,name='Lcorr')# shape (T, D

        scale_tril = sigma[..., None] * Lcorr  # shape (T, D, D)

    # 3) Latent cluster assignments for each data point
    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
        ),
        obs=data
    )

m.data_on_model = dict(data=data,K = 10, data_mean=data_mean, data_std=data_std)
m.fit(dpmm)  # Optimize model parameters through MCMC sampling
m.plot(X=data,sampler=m.sampler) # Prebuild plot function for GMM
```

```
jax.local_device_count 32
```

```
  0%|          | 0/1000 [00:00<?, ?it/s]warmup:   0%|          | 1/1000 [00:01<17:29,  1.05s/
```

```
Model found 8 clusters.
```


DPMM Posterior Predictive Density (Multi-Chain Robust)
Feature 1
Feature 2
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−10
−5
0
5
10

R

Julia

```
using BayesianInference
using PythonCall
numpyro = pyimport("numpyro")

m = importBI(rand_seed = false)

# 1. Generate Data
sk_datasets = pyimport("sklearn.datasets")
output = sk_datasets.make_blobs(n_samples=500, centers=8, cluster_std=0.8, center_box=(-10,
data = output[0]
```

```
data_mean = jnp.mean(data, axis=0)
data_std = jnp.std(data, axis=0) * 2
m.data_on_model = pydict(data=data, K=10, data_mean = data_mean, data_std = data_std)


@BI function dpmm(data, K, data_mean , data_std)
    N, D = data.shape

    alpha = m.dist.gamma(1.0, 10.0, name="alpha")

    beta = pywith(m.dist.plate("beta_plate", K - 1)) do _
        m.dist.beta(1, alpha, name = "beta")
    end

    w = numpyro.deterministic("w", m.models.dpmm.mix_weights(beta))

    mu, scale_tril = pywith(m.dist.plate("components", K)) do _
        mu_val = m.dist.multivariate_normal(
            loc=data_mean,
            covariance_matrix=data_std * jnp.eye(D),
            name="mu"
        )

        sigma = m.dist.log_normal(0.0, 1.0, shape=(D,), event=1, name="sigma")
        Lcorr = m.dist.lkj_cholesky(dimension=D, concentration=1.0, name="Lcorr")
        scale_tril_inner = jnp.expand_dims(sigma, -1) * Lcorr
        (mu_val, 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
        ),
        obs=data
    )
end

# 4. Run
```

```
m.fit(dpmm)

@pyplot m.models.dpmm.plot_dpmm(m.data_on_model["data"], m.sampler)
```

Mathematical Details

The process involves two keys submodels. The first, aims to identify the location and scale of K potential clusters. The second, aims to identify which cluster is most likely to have generated a given data point.

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

$$\begin{pmatrix} \mu_{k,1} \\ \vdots \\ \mu_{k,D} \end{pmatrix} \sim \text{MVN}\left(\begin{pmatrix} A_1 \\ \vdots \\ A_D \end{pmatrix}, B \right)$$

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

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

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

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

$$\pi_i(\beta_{1:K}) = \beta_i \prod_{j<K} (1 - \beta_j)$$

$$\beta_k \sim \text{Beta}(1, \alpha)$$

$$\alpha \sim \text{Gamma}(1, 10)$$

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.
- $\begin{pmatrix} A_1 \\ \vdots \\ A_D \end{pmatrix}$ is a prior for the mean vector as derived from mean of the raw data.
- 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).
- $\text{Diag}(\sigma_k)$ 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, some of which may be close to zero if the predicted number of clusters is less than the maximum number of clusters.
- β_k: The set of K Beta-distributed random variables used in the stick-breaking process to construct the mixture weights.
- α: The concentration parameter, controlling the effective number of clusters.

Notes

> **Note**
>
> - The primary advantage of the DPMM is the **automatic inference of the number of clusters**. The posterior distribution of the weights `w` reveals which components are "active", giving a probabilistic estimate of `K`.
> - Prior α strongly influence the predicted number of clusters. Below are examples of this relationship:

Table 1: Impact of Gamma Prior Hyperparameters on Cluster Counts

Shape	Rate	Behavior
1	15	Forces very few clusters
5	1	Encourages many small clusters
10	2	Same mean, less variance
2	0.5	Moderately many clusters
15	1	Explosive prior cluster count

Reference(s)

https://en.wikipedia.org/wiki/Dirichlet_process https://pyro.ai/examples/dirichlet_process_mixture.html

Gershman, Samuel J, and David M Blei. 2012. "A Tutorial on Bayesian Nonparametric Models." *Journal of Mathematical Psychology* 56 (1): 1–12.