

# BNPlib: A Nonparametric C++ Library

(part 3)

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<https://github.com/poliprojects/BNPlib>

# Model

# DP and DPM models

Having observed the iid sample  $\{y_i\}_i$ ,  $i = 1, \dots, n$ :

- Dirichlet process model (discrete):

$$y_i | G \stackrel{\text{iid}}{\sim} G$$
$$G \sim DP(MG_0)$$

- Dirichlet process mixture (**DPM**) model (continuous):

$$y_i | G \stackrel{\text{iid}}{\sim} f_G(\cdot) = \int_{\Theta} f(\cdot | \boldsymbol{\vartheta}) G(d\boldsymbol{\vartheta})$$
$$G \sim DP(MG_0)$$

# Equivalent formulations (1)

- (DPM) is equivalent to:

$$y_i | \boldsymbol{\vartheta}_i \stackrel{\text{iid}}{\sim} f(\cdot | \boldsymbol{\vartheta}_i), \quad i = 1, \dots, n$$

$$\boldsymbol{\vartheta}_i | G \stackrel{\text{iid}}{\sim} G, \quad i = 1, \dots, n$$

$$G \sim DP(MG_0)$$

- State  $\forall i$ :  $\boldsymbol{\vartheta}_i$  latent variables (discrete)

## Equivalent formulations (2)

- (DPM) is also equivalent to:

$$y_i | c_i, \phi_1, \dots, \phi_k \stackrel{\text{iid}}{\sim} f(\cdot | \phi_{c_i}), \quad i = 1, \dots, n$$

$$c_i | \mathbf{p} \stackrel{\text{iid}}{\sim} \sum_{j=1}^K p_j \delta_j(\cdot), \quad i = 1, \dots, n$$

$$\phi_c \stackrel{\text{iid}}{\sim} G_0, \quad c = 1, \dots, k$$

$$\mathbf{p} \sim \text{Dir}(M/K, \dots, M/K)$$

$$K \rightarrow +\infty$$

- State  $\forall i$ :  $c_i$  **allocations** to clusters
- State  $\forall i$ :  $\phi_{c_i}$  **unique values** for each cluster
- Only the finitely many  $\phi_c$  used are kept track of

# Case study

- (DPM) with a Normal Normal-InverseGamma (**NNIG**) hierarchy:

$$y_i | \boldsymbol{\vartheta}_i \stackrel{\text{ind}}{\sim} f(\cdot | \boldsymbol{\vartheta}_i), \quad i = 1, \dots, n$$

$$\boldsymbol{\vartheta}_i | G \stackrel{\text{iid}}{\sim} G, \quad i = 1, \dots, n$$

$$G \sim DP(MG_0)$$

$$f(y | \boldsymbol{\vartheta}) = N(y | \mu, \sigma^2)$$

$$G_0(\boldsymbol{\vartheta} | \mu_0, \lambda_0, \alpha_0, \beta_0) = N\left(\mu | \mu_0, \frac{\sigma^2}{\lambda_0}\right) \times \text{Inv-Gamma}(\sigma^2 | \alpha_0, \beta_0)$$

- Latent variables:  $\boldsymbol{\vartheta} = (\mu, \sigma)$
- State  $\forall i$ :  $c_i, \phi_{c_i}$

# Algorithms

# General structure

```
template<template <class> class Hierarchy,  
        class Hypers, class Mixture> class Algorithm  
  
    void step(){  
        sample_allocations();  
        sample_unique_values();  
    }  
  
    void run(){  
        initialize();  
        unsigned int iter = 0;  
        while(iter < maxiter){  
            step();  
            if(iter >= burnin){  
                save_iteration(iter);  
            }  
            iter++;  
        }  
    }
```



# Auxiliary classes

- Specific common interface
- `Mixture`  $\rightarrow$  `SimpleMixture`
- `Hypers`  $\rightarrow$  `HypersFixedNNIG`
- `Hierarchy<Hypers>`  $\rightarrow$  `HierarchyNNIG<Hypers>`

- Has a vector of  $m$  `aux_unique_values`
- `initialize()`
- `sample_allocations()`: for all observations  $i = 1, \dots, n$ 
  - ▶ compute  $\text{card}[c] = n_{-i,c}$  for all clusters  $c = 1, \dots, k$
  - ▶ if  $c_i$  is a singleton, move  $\phi_{c_i}$  to `aux_unique_values[0]`
  - ▶ draw all (other) `aux_unique_values` iid from  $G_0$
  - ▶ draw a new value  $c$  for  $c_i$  according to:

$$\mathbb{P}(c_i = c | \mathbf{c}_{-i}, y_i, \phi_1, \dots, \phi_h) \propto \begin{cases} \frac{n_{-i,c}}{n-1+M} f(y_i | \phi_c), & \text{for } 1 \leq c \leq k^- \\ \frac{M/m}{n-1+M} f(y_i | \phi_c), & \text{for } k^- + 1 < c \leq h \end{cases}$$

with  $k^-$  unique values excluding  $c_i$  and  $h = k^- + m$

- ▶ update `card` and `allocations` (4 cases)
- `sample_unique_values()`: for all clusters  $c = 1, \dots, k$ 
  - ▶ build `curr_data` that contains all observations in cluster  $c$
  - ▶ draw  $\phi_c$  from its posterior distribution given `curr_data`

- For conjugate models only, e.g. (DPM)+(NNIG)
- `initialize()`
- `sample_allocations()`: for all observations  $i = 1, \dots, n$ 
  - ▶ compute  $\text{card}[c] = n_{-i,c}$  for all clusters  $c = 1, \dots, k$
  - ▶ draw a new value  $c$  for  $c_i$  according to:

$$\text{If } c = c_j \text{ for some } j: \mathbb{P}(c_i = c | \mathbf{c}_{-i}, y_i, \phi) \propto \frac{n_{-i,c}}{n-1+M} f(y_i | \phi_c)$$

$$\mathbb{P}(c_i \neq c_j \text{ for all } j | \mathbf{c}_{-i}, y_i, \phi) \propto \frac{M}{n-1+M} \int_{\Theta} f(y_i | \boldsymbol{\vartheta}) G_0(d\boldsymbol{\vartheta})$$

- ▶ if the latter, draw a new  $\phi_c$  from its posterior given  $y_i$
  - ▶ update card and allocations (4 cases)
- `sample_unique_values()`: for all clusters  $c = 1, \dots, k$ 
  - ▶ build `curr_data` that contains all observations in cluster  $c$
  - ▶ draw  $\phi_c$  from its posterior distribution given `curr_data`

# Applications

# Set-up

- $n = 100$  observations:
  - ▶  $y_1, \dots, y_{50} \stackrel{\text{iid}}{\sim} \mathcal{N}(4, 1)$
  - ▶  $y_{51}, \dots, y_{100} \stackrel{\text{iid}}{\sim} \mathcal{N}(7, 1)$
- Prior parameters for the Normal-NIG model:
  - ▶  $\mu_0 = 5$
  - ▶  $\lambda_0 = 1$
  - ▶  $\alpha_0 = 2$
  - ▶  $\beta_0 = 2$
- Neal8
  - ▶  $m = 3$
  - ▶ `maxiter` = 20000
  - ▶ `burnin` = 5000
  - ▶  $K = 15000$  valid iterations

# Cluster estimation

```
unsigned int cluster_estimate();
```

$$\hat{k} = \arg \min_k \left\| D^{(k)} - \bar{D} \right\|_F^2 = \arg \min_k \sum_{i,j} \left( D_{ij}^{(k)} - \bar{D}_{ij} \right)^2$$

- $D^{(k)}$ : dissimilarity matrix at iteration  $k$
- $\bar{D} = \frac{1}{K} \sum_k D^{(k)}$ : mean over  $K$  iterations

# Density estimation

```
void eval_density(const std::vector<double> grid);
```

$$\hat{f}^{(k)}(x) = \sum_j \frac{n_j^{(k)}}{M+n} f(x|\phi_j^{(k)}) + \frac{M}{M+n} m(x)$$

$$\hat{m}(x) = \frac{1}{m} \sum_{h=0}^{m-1} f(x|\phi_h)$$

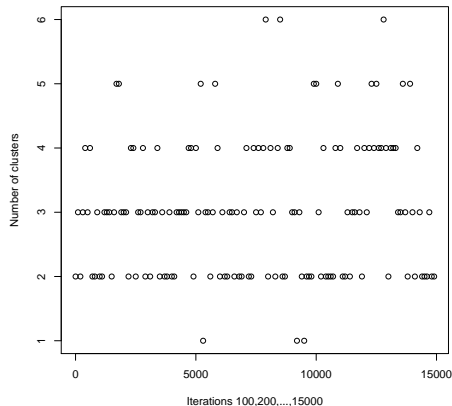
$$\implies \hat{f}(x) = \frac{1}{K} \sum_k \hat{f}^{(k)}(x)$$

# Results

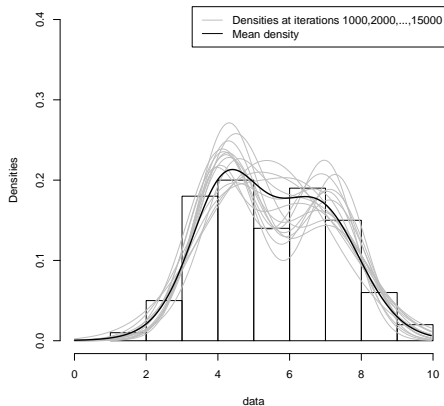


# Oscillations

Number of clusters at single iterations

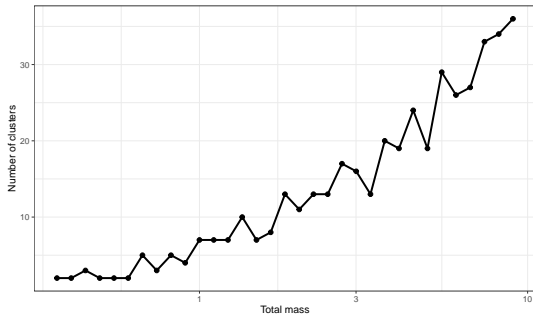


Local density estimates at single iterations

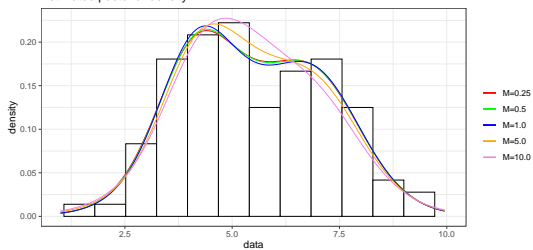


# Total mass

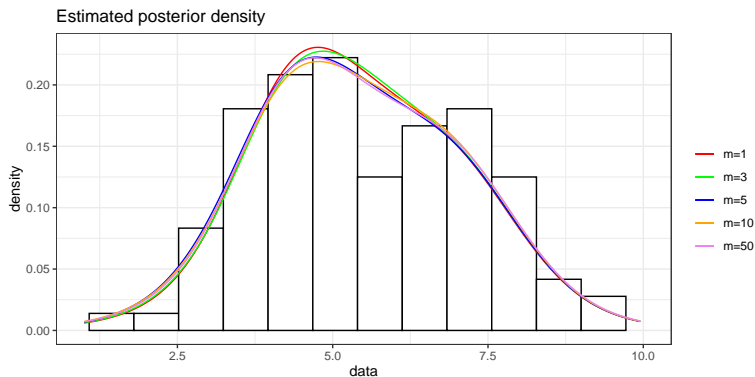
Number of clusters as a function of the total mass



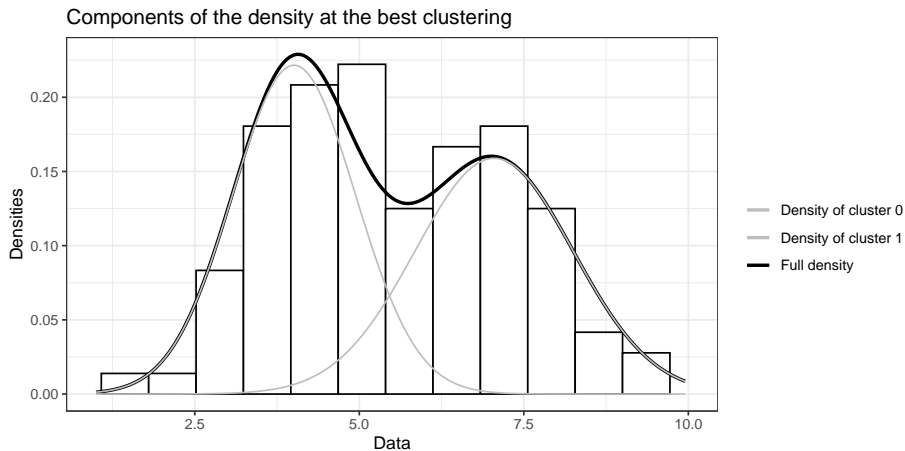
Estimated posterior density



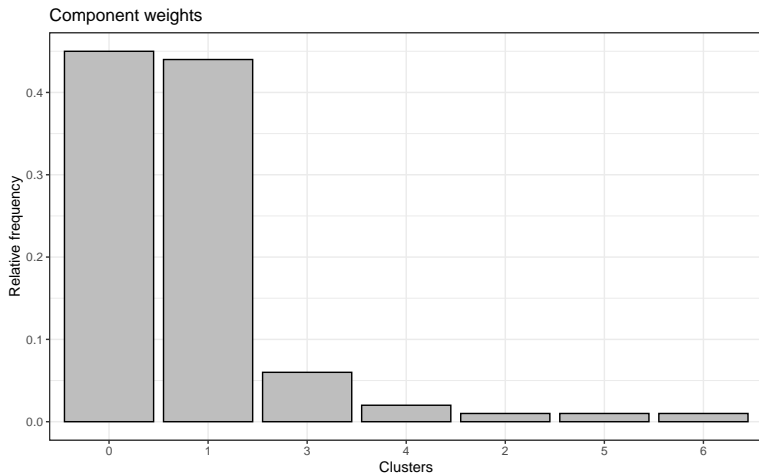
# Auxiliary parameters



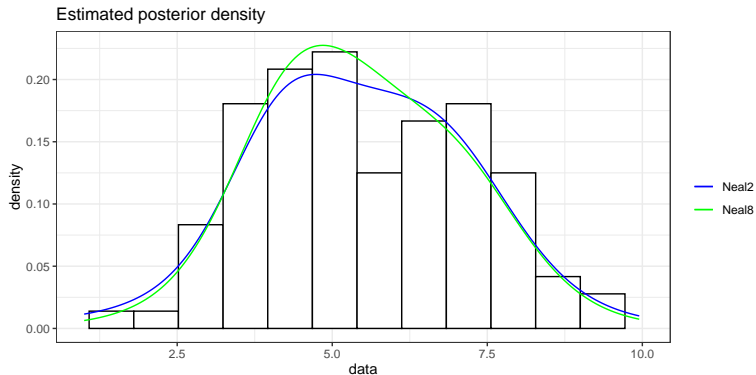
# Density components



# Clustering












# Neal2 vs Neal8



# Extensions

- Adaptation to Hypers containing hyper-priors
- Implementation of other Hierarchy classes
- Adaptation to other Mixture classes
- Interface with R and Python
- Integration of conjugacy-dependent algorithms to handle non-conjugacy
- Full generalization

# Bibliography

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-  GitHub codes of Mario Beraha and Riccardo Corradin for similar projects
-  Course material for Bayesian Statistics: <https://beep.metid.polimi.it/web/2019-20-bayesian-statistics-alessandra-guglielmi-/>