## bnplib: A Nonparametric C++ Library

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https://github.com/poliprojects/BNPlib

#### Abstract

We present a C++ library that exploits a Bayesian nonparametric setting in order to conduct unidimensional and multidimensional data analysis. In such a setting, our main goals are density estimation and clustering analysis. Several algorithms are available that make use of Gibbs sampling, building a Markov chain that reaches convergence at a reasonably fast pace. In particular, we focused on implementing some algorithms introduced by Neal in 2000. After running one of these algorithms, density and cluster estimation can then be conducted by using the provided auxiliary tools. In this report, after an overview of the underlying Bayesian model and a roundup of the algorithms' state of the art, we delve into the details of our implementation and then present an example of data analysis, whilst providing the theoretical background for our estimates. We also include a description for the implemented Python interface of this C++ library.

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## Introduction

This report presents the development of a C++ library containing Markov chain sampling algorithms for two major goals: estimation of the density and clustering analysis of a given set of data points. In a Bayesian nonparametric setting, we focused on the Dirichlet process, one of the most widely used priors due to its flexibility and computational ease, and its extensions. Hereafter, we will assume that the underlying model for the given data points is a Dirichlet process mixture model, which is an enhancement of the simpler Dirichlet model. We shall now briefly describe these models and their relevant properties. (For a more detailed discussion of the nonparametric models, as well as references for all theoretical details included in this section, see [1] chapter 1 and 2.)

## 1.1 Dirichlet process model

Let M > 0, and let  $G_0$  be a probability measure defined on the state space S. A Dirichlet process with parameters M and  $G_0$ , noted as  $DP(M, G_0)$ , is a random probability measure G defined on S which assigns probability G(B) to every set B such that for each finite partition  $B_1, \ldots, B_k$  of S, the joint distribution of the vector  $(G(B_1), \ldots, G(B_k))$  is the Dirichlet distribution with parameters

$$(MG_0(B_1), \ldots, MG_0(B_k)).$$

The parameter M is called the precision or total mass parameter,  $G_0$  is the centering measure, and the product  $MG_0$  is the base measure of the DP. Having observed the independent and identically distributed sample  $\{y_1, \ldots, y_n\}$   $\subseteq \mathbb{R}$ , the basic DP model takes the following form:

$$y_i|G \stackrel{\text{iid}}{\sim} G, \quad i = 1, \dots, n$$
  
 $G \sim DP(MG_0)$  (1.1)

A key property is that the DP is conjugate with respect to iid sampling, so that the posterior base distribution is a weighted average of the prior base distribution  $G_0$  and the empirical distribution of the data, with the weights controlled by M:

$$G|y_1, \dots, y_n \sim DP\left(MG_0 + \sum_{i=1}^n \delta_{y_i}\right).$$
 (1.2)

Moreover, the marginal distribution for the data will be the product of the sequence of increasing conditionals:

$$p(y_1, \dots, y_n) = p(y_1) \prod_{i=2}^n p(y_i|y_1, \dots, y_{i-1}),$$

with  $y_1 \sim G_0$  and the conditional for  $i = 2, 3, \ldots$  being the following:

$$p(y_i|y_1,\ldots,y_{i-1}) = \frac{1}{M+i-1} \sum_{h=1}^{n-1} \delta_{y_h}(y_i) + \frac{M}{M+i-1} G_0(y_i).$$

Another important property is the discrete nature of the random probability measure G. Because of this, we can always write G as a weighted sum of point masses. A useful consequence of this property is its stick-breaking representation, i.e. G can be written as:

$$G(\cdot) = \sum_{k=1}^{+\infty} w_k \delta_{m_k}(\cdot),$$

with  $m_k \stackrel{\text{iid}}{\sim} G_0$  for  $k \in \mathbb{N}$  and the random weights constructed as  $w_k = v_k \prod_{l < k} (1 - v_l)$  where  $v_k \stackrel{\text{iid}}{\sim} Be(1, M)$ .

In many applications in which we are interested in a continuous density estimation, this discreteness can represent a limitation. Oftentimes a Dirichlet process mixture (DPM) model is used, where the DP random measure is the mixing measure for the parameters of a parametric continuous kernel function.

#### 1.2 Dirichlet process mixture model

Let  $\Theta$  be a finite-dimensional parameter space and  $G_0$  a probability measure on  $\Theta$ . The Dirichlet process mixture (DPM) model convolves the densities  $f(\cdot|\boldsymbol{\vartheta})$  from a parametric family  $\mathcal{F} = \{f(\cdot|\boldsymbol{\vartheta}), \boldsymbol{\vartheta} \in \Theta\}$  using the DP as mixture weights. The obtained model has the following form:

$$y_i|G \stackrel{\text{iid}}{\sim} f_G(\cdot) = \int_{\Theta} f(\cdot|\boldsymbol{\vartheta}) G(d\boldsymbol{\vartheta}), \quad i = 1, \dots, n$$

$$G \sim DP(MG_0)$$
(1.3)

An equivalent hierarchical model is:

$$y_i | \boldsymbol{\vartheta}_i \stackrel{\text{ind}}{\sim} f(\cdot | \boldsymbol{\vartheta}_i), \quad i = 1, \dots, n$$
  
 $\boldsymbol{\vartheta}_i | G \stackrel{\text{iid}}{\sim} G, \quad i = 1, \dots, n$   
 $G \sim DP(MG_0)$  (1.4)

where the *latent variables*  $\vartheta_i$  are introduced, one per unit. Since G is discrete, we know that two independent draws  $\vartheta_i$  and  $\vartheta_j$  from G can be equal with positive probability. In this way the DPM model induces a probability model on clusters of  $\vartheta_i$ . An object of interest that derives from this model is the partitioning induced by the clustering.

Considering n data points, each  $\vartheta_i$  will have one of the k unique values  $\phi_j$ . An estimation of the number of the unique values is  $M \log(n) \ll n$ . Defining  $\mathbf{c} = (c_1, \ldots, c_n)$  the allocation parameters to the clusters such that  $c_i = j$  if  $\vartheta_i = \phi_j$ , model (1.4) can be thought of as the limit as  $K \to +\infty$  of a finite mixture model with K components (recall instead that k is the number of unique values):

$$y_{i}|\phi_{1},\ldots,\phi_{k},c_{i} \stackrel{\text{ind}}{\sim} f(\cdot|\phi_{c_{i}}), \quad i=1,\ldots,n$$

$$c_{i}|\mathbf{p} \stackrel{\text{iid}}{\sim} \sum_{j=1}^{K} p_{j}\delta_{j}(\cdot), \quad i=1,\ldots,n$$

$$\phi_{c} \stackrel{\text{iid}}{\sim} G_{0}, \quad c=1,\ldots,k$$

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

$$(1.5)$$

where  $\mathbf{p} = (p_1, \dots, p_K)$  represents the mixing proportions for the clusters and each  $\vartheta_i$  is characterized by the latent cluster  $c_i$  and the corresponding parameters  $\phi_{c_i}$ .

#### 1.2.1 Normal Normal-InverseGamma model

A very common choice for the DPM model (1.3) is the Normal-Normal-InverseGamma (Normal-NIG) model, opting for a Normal kernel and the conjugate Normal-InverseGamma as base measure  $G_0$ . That is, letting  $\vartheta = (\mu, \sigma)$ , we have:

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

$$G_0(\boldsymbol{\vartheta}|\mu_0, \lambda_0, \alpha_0, \beta_0) = N\left(\mu|\mu_0, \frac{\sigma^2}{\lambda_0}\right) \times \text{Inv-Gamma}(\sigma^2|\alpha_0, \beta_0).$$
(1.6)

Note that in this model we have a full prior for  $\sigma^2$  and instead a prior for  $\mu$  that is conditioned on the value of  $\sigma^2$ . Thanks to conjugacy, the predictive distribution for a new observation  $\tilde{y}$  can be computed analytically, finding a Student's t (see [4] section 3.5):

$$p(\widetilde{y}|\mu_0, \lambda_0, \alpha_0, \beta_0) = \int_{\Theta} f(\widetilde{y}|\boldsymbol{\vartheta}) G_0(d\boldsymbol{\vartheta}) = t_{\widetilde{\nu}}(\widetilde{y}|\widetilde{\mu}, \widetilde{\sigma})$$

where the following parameters are set:

$$\widetilde{\nu} = 2\alpha_0, \quad \widetilde{\mu} = \mu_0, \quad \widetilde{\sigma}^2 = \frac{\beta_0(\lambda_0 + 1)}{\alpha_0 \lambda_0}$$

Moreover, the marginal distribution for a given observation has the same expression.

The posterior distribution is again a Normal-InverseGamma (see [4] section 3.3):

$$p(\boldsymbol{\vartheta}|y_1,\ldots,y_n,\mu_0,\lambda_0,\alpha_0,\beta_0) = N\left(\mu|\mu_n,\frac{\sigma^2}{\lambda_0+n}\right) \times \text{Inv-Gamma}(\sigma^2|\alpha_n,\beta_n)$$

with:

$$\mu_n = \frac{\lambda_0 \mu_0 \bar{y} + n}{\lambda_0 + n}, \quad \alpha_n = \alpha_0 + \frac{n}{2}, \quad \beta_n = \beta_0 + \frac{1}{2} \sum_{i=1}^n (y_i - \bar{y})^2 + \frac{\lambda_0 n(\bar{y} - \mu_0)^2}{2(\lambda_0 + n)}.$$

# Algorithms

For the task of density estimation, we investigated several Markov chain methods to sample from the posterior distribution of a DPM model.

Starting from the hierarchical model (1.3), a first direct approach is simply drawing values for each  $\vartheta_i$  from its conditional distribution, given the data and the other  $\vartheta_j$ . However, as previously discussed, we have high probability for ties among them which can lead to slow convergence, since the  $\vartheta_i$  are not updated for more than one observation simultaneously.

For this reason, special attention was paid to the three methods we present in this chapter. They are Gibbs samplers with a similar base structure, sharing the two steps for the sampling of the allocations  $\mathbf{c}$  and of the unique values  $\phi_c$ . The set of allocations and unique values at a given iteration constitutes the *state* of that iteration. As the state is being updated at each iteration, a *chain* is formed and the mean of the state values eventually reaches convergence, as well as the estimate for the data distribution, as we will see in section 4.2. Moreover, all methods can be extended with additional steps for hierarchical extensions. For example, we can place priors to hyperparameters of the centering measure  $G_0$  or to the total mass M.

## 2.1 Neal's Algorithm 2

In order to speed up convergence in case of ties, Neal first proposed (see [2] section 3 as well as [1] chapter 2) a more efficient Gibbs sampling method based on the discrete model (1.5), but where the mixing proportions  $\mathbf{p}$  have been integrated out. We will refer to this method as Neal's Algorithm 2, or Neal2 for short. Before getting to the algorithm, let us start from the discrete model (1.5). Assuming that the current state of Markov chain is composed of  $(c_1, \ldots, c_n)$  and the unique values  $\phi_c$  for all  $c = 1, \ldots, k$ , the Gibbs sampler should first draw a new value c for each  $c_i$  according to the following probabilities:

If 
$$c = c_j$$
 for some  $j$ :  $\mathbb{P}(c_i = c | c_{-i}, y_i, \phi_1, \dots, \phi_k) \propto \frac{n_{-i,c} + M/K}{n - 1 + M} f(y_i | \phi_c)$  (2.1)

where  $c_{-i}$  is c minus the i-th component, and  $n_{-i,c}$  is the number of  $c_j$  equal to c excluding  $c_i$ . The transition to the infinite case, that is, to the reference DPM model (1.4), is handled by taking the limit as K goes to infinity in the

conditional distribution of  $c_i$ , which becomes as follows:

If 
$$c = c_j$$
 for some  $j$ :  $\mathbb{P}(c_i = c | \mathbf{c}_{-i}, y_i, \boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_k) \propto \frac{n_{-i,c}}{n-1+M} f(y_i | \boldsymbol{\phi}_c)$   
 $\mathbb{P}(c_i \neq c_j \text{ for all } j | \mathbf{c}_{-i}, y_i, \boldsymbol{\phi}_1, \dots, \boldsymbol{\phi}_k) \propto \frac{M}{n-1+M} \int_{\Theta} f(y_i | \boldsymbol{\vartheta}) G_0(\mathrm{d}\boldsymbol{\vartheta})$ 

$$(2.2)$$

and considering only the  $\phi_c$  associated with some observation, keeping the sampling finite and thus computationally feasible. The former expression is proportional to the cardinality of that cluster (excluding the *i*-th observation), while the latter is instead proportional to the total mass M and represents the probability of creating a new cluster. Moreover, the integral  $m(y_i) = \int_{\Theta} f(y_i|\boldsymbol{\vartheta}) G_0(\mathrm{d}\boldsymbol{\vartheta})$  represents the marginal distribution of the data points evaluated in  $y_i$ .

Let us now introduce the actual Neal2 algorithm, which works iteratively in two steps, in which we sample  $(c_1, \ldots, c_n)$  and  $(\phi_1, \ldots, \phi_k)$ , respectively. First, for each observation i,  $c_i$  is updated according to the conditional probabilities (2.2). It can be set either to one of the other components currently associated with some observation, or to a new mixture component. If the new value of  $c_i$  is different from all the other  $c_j$ , a value for  $\phi_{c_i}$  is created by drawing it from the posterior distribution  $H_i$ , given the prior  $G_0$  and the single observation  $y_i$ ; this means that in this case, a new cluster has been created.

Then, for all clusters, the sampling of their unique value  $\phi_c$  is conducted by considering their posterior distribution given the prior  $G_0$  and all observations belonging to that cluster. The probability of setting  $c_i$  to a new component involves the computation of the marginal, which is difficult to compute in the non-conjugate case, as well as the sampling from the posterior  $H_i$ . For this reason, the algorithm is only used under conjugacy and hence it is possible to exactly compute the integral.

## 2.2 Neal's Algorithm 8

To handle non-conjugate priors, Neal proposed (see [2] section 6 and [1] chapter 2) a second Markov chain sampling procedure, the Neal8 algorithm, where the state is extended by the addition of m auxiliary parameters. This technique allows to update the  $c_i$  while avoiding the integration with respect to  $G_0$  for the computation of the marginal.

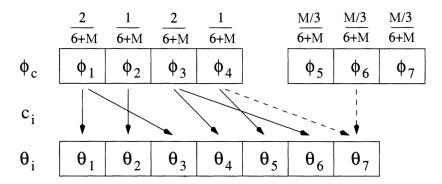
In this case the sampling probabilities for the  $c_i$  given all other  $c_j$  are:

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

$$\mathbb{P}(c_i \neq c_j \text{ for all } j) = \frac{M}{n - 1 + M}$$
(2.3)

where the latter probability of creating a new cluster is evenly split among the m auxiliary components, which will also be referred to as the *auxiliary blocks*. Maintaining the same structure as the Neal2 algorithm, Neal8 is composed of two steps, where the components of the Markov chain state  $(c_1, \ldots, c_n)$  and  $(\phi_1, \ldots, \phi_k)$  are repeatedly sampled.

The first step scans all the observations and evaluates each  $c_i$ . If it is equal to some other  $c_j$ , i.e. if the current cluster of observation i is not a singleton, then



Graphical representation of the variables: the allocations are visualized as arrows linking each  $\vartheta_i$  with either one of the four old clusters or one of the new components (image taken from [2])

all auxiliary variables are iid drawn from  $G_0$ . If instead the cluster corresponding to  $c_i$  is a singleton, then it is linked to one of the auxiliary blocks (i.e. the first one, without loss of generality) while keeping its old unique value  $\phi_{c_i}$  (as shown in the above figure), whereas the other blocks are drawn normally from  $G_0$  as before. Then,  $c_i$  is updated according to the following conditional probabilities:

$$\mathbb{P}(c_{i} = c | \boldsymbol{c}_{-i}, y_{i}, \boldsymbol{\phi}_{1}, \dots, \boldsymbol{\phi}_{h}) \propto \begin{cases} \frac{n_{-i,c}}{n - 1 + M} f(y_{i} | \boldsymbol{\phi}_{c}), & \text{for } 1 \leq c \leq k^{-} \\ \frac{M/m}{n - 1 + M} f(y_{i} | \boldsymbol{\phi}_{c}), & \text{for } k^{-} + 1 < c \leq h, \end{cases}$$
(2.4)

indicating with  $k^-$  the number of distinct  $c_j$  excluding the current  $c_i$  and setting  $h = k^- + m$ . Again, the probabilities of being placed in an already existing cluster or in a newly created cluster are proportional to the cluster's cardinality (sans observation i) and to the total mass, respectively.

Once all the  $\phi_c$  that are no longer associated with any observation are discarded, the algorithm proceeds, for each cluster, with the sampling of  $\phi_c$  from the posterior computed with the observations of the specific cluster, similarly to the Neal2 algorithm.

#### 2.3 Blocked Gibbs

Another Gibbs sampling method that is applicable in the considered DPM model is the one proposed by Ishwaran and James (see [3] section 5), where the prior P is assumed to be a finite dimensional stick-breaking measure, allowing the update of whole blocks of parameters. A key point of the method is that it does not marginalize over the prior; instead, by grouping more variables together, it samples from their joint distribution conditioned on all other variables. This sampler needs to draw from the following conditionals:

$$egin{aligned} oldsymbol{\phi}_1, \dots, oldsymbol{\phi}_k &\sim \mathcal{L}(\cdot|c_1, \dots, c_n, oldsymbol{y}) \ c_1, \dots, c_n &\sim \mathcal{L}(\cdot|oldsymbol{\phi}_1, \dots, oldsymbol{\phi}_k, oldsymbol{p}, oldsymbol{y}) \ oldsymbol{p} &\sim \mathcal{L}(\cdot|c_1, \dots, c_n) \end{aligned}$$

The drawing of the unique values can also be handled in the non-conjugate case by applying standard Markov chain Monte Carlo methods.

This algorithm is not explored in detail as it has not implemented yet in our library. For a full explanation, see [3].

# Implementation

As far as code implementation goes, the aforementioned algorithms all share the following structure:

```
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++;
    }
}
```

In particular, the blocked Gibbs algorithm has an additional phase in step(),  $sample_weights()$ . Moreover, as discussed in chapter 2, all the algorithms can be generalized including further Gibbs sampling steps to update the hyperparameters of  $G_0$  or the total mass parameter M. Each implemented algorithm will be discussed in detail in its own section. As for the general structure of an algorithm class, a template approach was chosen, to allow the use of several layers of complexity based on the needs of the user:

That is, Hierarchy<>, Hypers, and Mixture are not actual implemented classes, but rather proxy names for classes which will be received as *parameters* by the algorithm class. These classes must have a *common interface* in order for them to be passed as parameters, as explained in the following section. An example with actual class names, as found in the main.cpp file, is:

Neal8<NNIGHierarchy, HypersFixed, SimpleMixture> sampler8;

As a final introductory note, probability distributions and random sampling were handled through the Stan library, whilst the popular Eigen library was exploited for the creation of the necessary matrix-like objects and the use of matrix-algebraic operations throughout the code.

#### 3.1 Auxiliary classes

First of all, we must briefly describe the auxiliary classes that are used as parameters for the algorithms:

- The Mixture classes contain all information about the mixing part of the DPM model, namely the total mass parameter and its prior distribution, if any. We implemented the SimpleMixture class, which represents a fixed total mass parameter without any prior on it, and contains the totalmass member as well as a getter and a setter (get\_totalmass(), set\_totalmass()).
- The Hypers classes contain all information about the hyperparameters of the hierarchy, including their values (if fixed) or their prior distributions (if not). We implemented the HypersFixedNNIG class, which contains the four fixed parameters mu0, lambda, alpha0, and beta0 of the Normal-NIG hierarchical model, and their respective getters and setters.
- The Hierarchy<Hypers> classes are template classes themselves and accept any Hypers class as template parameter. A Hierarchy<> class contains a vector state which stores the current values of the likelihood parameters, as well as a pointer to a Hypers object this is why Hypers is required as a parameter for Hierarchy<>. A pointer is chosen instead of an actual object, since multiple Hierarchy<> objects will be created and stored by the algorithms; the states of these objects will of course share the same prior, and with a pointer to Hypers the updating of the prior will only happen once rather than one time per object. A Hierarchy<> class also contains functions to:
  - evaluate the marginal distribution (provided it is known in closed form) and the log-likelihood in a given set of points, given the current state:
  - compute the posterior parameters with respect to a given set of observations;
  - generate new values for the state both according to its prior and to its posterior distribution;
  - get and set class members, as with the other classes.

In particular, we implemented the HierarchyNNIG class, which represents the Normal-NIG model described in section 1.2.1. The state holds the values for  $\phi = (\mu, \sigma)$ .

Any class representing any type of hierarchy or parameters can be built as long as it possesses the above interface, which is required for their use in the implemented algorithms.

We will be now first examining the Neal8 class as an example.

## 3.2 Neal8 algorithm

Relying on the algorithm described in section 2.2, we proceed to describe our implementation of it. Aside from the usual getters and setters, as well as constructors, the Neal8 class contains the following members:

```
unsigned int n_aux;
unsigned int maxiter;
unsigned int burnin;
unsigned int num_clusters;
std::mt19937 rng; // random number generating engine
```

These are the parameters of the method, and are rather self-explanatory. Their values are initialized either via the constructors or the setters. If num\_clusters is not provided, it will be automatically set equal to the number of data points, thus starting the algorithm with one datum per cluster.

The data and values containers were implemented as follows:

```
std::vector<double> data;
std::vector<unsigned int> allocations;
std::vector<Hierarchy<Hypers>> unique_values;
std::vector<Hierarchy<Hypers>> aux_unique_values;
Mixture mixture;
```

The algorithm will keep track of the labels representing assignments to clusters via the allocations vector. For instance, if one has allocations [5] = 2, it means that datum number 5 is associated to cluster number 2. Note that indexing for both data and clusters starts at zero, so this actually means that we have the sixth datum being assigned to the third cluster.

The containers for the unique values  $\phi$  hold objects of type Hierarchy<br/>> because each  $\phi$  is associated to a cluster, which is in fact a small hierarchy that can have its own hyperprior in the general case. The same reasoning goes for aux\_unique\_values, the m auxiliary blocks, from which the algorithm may draw in order to generate new clusters.

As for the members used for running the algorithm:

```
void initialize();
void sample_allocations();
void sample_unique_values();
void step(){
    sample_allocations();
    sample_unique_values();
}
void save_iteration(unsigned int iter);
void run();
```

Aside from run(), whose code was shown at the beginning of this section, we shall briefly describe the implementation of these functions:

- initialize() creates num\_clusters clusters and randomly assigns each datum to one of them, while making sure that each cluster contains at least one. This assignment is done through changing allocations components, as explained earlier.
- In sample\_allocations(), a loop is performed over all observations i =1: n. A vector card is first filled, with card[j] being the cardinality of cluster j. The algorithm mandates that  $\mathtt{data[i]}$  be moved to another cluster; thus, if the current cluster is a singleton, its  $\phi$  values are transferred to the first auxiliary block. Then, each auxiliary block (except the first one if the above case occurred) generates new  $\phi$  values via the hierarchy's draw() function. Now a new cluster, that is, new  $\phi$  values, for data[i] needs to be drawn. A vector probas with n\_unique+n\_aux components is filled with the probabilities of each  $\phi$  being extracted, in line with (2.4). Computations involve, among other things, the card vector, the likelihood like() evaluated in data[i], and the total mass parameter. Then, the new value for allocations[i] is randomly drawn according to the computed probas. Finally, four different cases of updating unique\_values and card are handled separately, depending on whether the old cluster was a singleton or not, and whether an auxiliary block or an already existing cluster was chosen as the new cluster for data[i]. This is done because depending on the case, clusters are either unchanged, increased by one, decreased by one, or moved around.
- In sample\_unique\_values(), for each cluster j, their φ values are updated through the sample\_given\_data() function, which takes as argument the vector curr\_data of data points which belong to cluster j. Since we only keep track of clusters via their labels in allocations, we do not have a vector of actual data points stored for each cluster. Thus we must fill, before the loop on j, a matrix clust\_idxs whose column k contains the index of data points belonging to cluster k. clust\_idxs is then used in the j loop to fill curr\_data with the actual data points of cluster j.
- save\_iteration will be examined in the next section.

## 3.3 Neal2 algorithm

The structure of the Neal2 class is similar to the one of Neal8 described above. The only relevant differences are the obvious lack of aux\_unique\_values and most of the sample\_allocations() phase. As discussed in section 2.1, this algorithm exploits conjugacy, thus this function requires specifically implemented hierarchies, in which the marginal distribution of the data with respect to  $\vartheta$  is provided in closed form. In our case, a Normal-NIG specialization for the Neal2 template class was implemented. In sample\_allocations(), a loop is performed over observations i and the card vector is built, just as before. The probas vector of weights for the new allocation value is computed, according to the probabilities (2.2), by also using the marginal density in data[i], which is known to be a Student's t as mentioned in section 1.2.1. After the new allocations[i] is drawn according to probas, four cases are handled separately as before, depending on whether the old cluster was a singleton and

whether data[i] is assigned to a new cluster. Indeed, in such a case, a new  $\phi$  value for it must be generated, and this must be handled differently by the code if an old singleton cluster was just destroyed (as the new cluster must take its former place).

# Part II Applications

# **Applications**

These algorithms can also be used for two useful practical purposes: *cluster estimation* and *density estimation*. Both processes, however, require the whole chain to be saved, that is, at each iteration the current values of states and allocations must be stored in some data structure. For this purpose, we used the Protocol Buffers library, which needs a short introduction.

Protocol Buffers, or protobuf for short, was developed by Google and allows automatic generation of data-storing C++ classes by defining a class skeleton in a .proto file. This also allows easy interfacing with other programming languages such as R and Python.

We built our template as follows:

```
message UniqueValues {
    repeated double params = 1;
}
message IterationOutput {
    repeated int32 allocations = 1;
    repeated UniqueValues phi = 2;
}
message ChainOutput {
    repeated IterationOutput state = 1;
}
```

Here message and repeated are the protobuf equivalent of classes and vectors respectively, while the numbers 1 and 2 just act as identifiers for the fields in the messages. After generating the corresponding C++ classes via the protoc compiler, we were able to add the following members to the Neal8 and Neal2 classes:

```
ChainOutput chain;
IterationOutput best_clust;
std::pair< std::vector<double>, Eigen::VectorXd > density;
```

For each iteration after the burn-in phase, the <code>save\_iteration()</code> function saves all state values of the current iteration into the <code>chain</code> pseudo-vector in the appropriate structure. On the other hand, <code>best\_clust</code> represents the state of a single iteration, and it is the object where the result of the clustering analysis will be saved. The <code>density</code> object shares a similar purpose for the density

estimation part, albeit not actually generated via protobuf. It will be filled with a grid of points in which the density will be evaluated, and the evaluations of the density themselves.

We will be explaining in thorough detail these two useful applications in the next lines.

#### 4.1 Cluster estimation

Suppose we wish to estimate the real clustering of the data, assuming the DPM model holds true. A first rough estimate is the *final clustering*, that is, the state values corresponding to the last iteration of the algorithm. This estimate does not require an appropriate function to be implemented, since the state values are already available in allocations and unique\_values after the algorithm is run(). However, due to the oscillating behavior of the clusters (as we shall see later on), the last clustering may not be the optimal one. Instead, we chose to implement a *least square* estimate in the following function:

#### unsigned int cluster\_estimate();

This function exploits the chain pseudo-vector, in which states of all iterations of the algorithm were saved via save\_iteration() (of course, only after the burn-in phase) and the protobuf library. This function loops over all IterationOutput objects in chain, finds the iteration at which the best clustering occurred, saves the whole object into the best\_clust class member, and returns the iteration number of this best clustering. As briefly touched upon earlier, the best clustering is found via the minimization of the squared posterior Binder's loss function. An equivalent approach (see [9] lecture on BNP clustering) is computing the so-called dissimilarity matrix for each iteration, computing its sample mean over all iterations, and finding the iteration that is the closest to the mean with respect to the Frobenius norm. More specifically, for each iteration k, the dissimilarity matrix  $D^{(k)}$  is a symmetric, binary n-by-n matrix (where n is the number of available observations) whose entries  $D_{ij}^{(k)}$  are 1 if datum i and j are placed in the same cluster at iteration k and 0 otherwise. After each  $D^{(k)}$  and the sample mean  $\bar{D} = \frac{1}{K} \sum_k D^{(k)}$  are computed, where Kis the number of iterations (not counting the ones in the burn-in phase), the best clustering  $\hat{k}$  is found by minimizing the Frobenius norm of the difference with  $\bar{D}$ :

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

By virtue of the involved matrices being symmetric, the latter summation can be computed over all i < j instead of all i, j for efficiency.

The convergence in mean of the algorithm grants the correctness of this least square estimate, at it is the closest available approximation to the mean dissimilarity matrix.

## 4.2 Density estimation

One other important application of clustering algorithms is the estimation of the density according to which the data points are distributed. This is done differently in both the Neal2 and Neal8 algorithms, as the former can exploit the conjugacy of the hierarchical model. In either case, the following function was implemented:

void eval\_density(const std::vector<double> grid);

It accepts a grid of points in which the density will be evaluated. This grid is stored in the density member object, as well as the computed evaluations themselves in form of a vector from the Eigen library. Just like for the cluster estimate, the computation will access all iterations stored in the chain pseudovector. In both Neal8 and Neal2, a loop is performed over the iterations k. Suppose this iterations has J clusters, that is, j=0:J-1. The card vector is once again computed, where  ${\tt card[j]}=n_j^{(k)}$  is the cardinality of cluster j. Then, for each point x in  ${\tt grid}$ , we compute the local estimate of the density, that is, only taking iteration k into account:

$$\hat{f}^{(k)}(x) = \sum_{j} \frac{n_j^{(k)}}{M+n} f\left(x|\phi_j^{(k)}\right) + \frac{M}{M+n} m(x)$$
 (4.1)

That is, the local estimate is a weighted mean of the likelihood given the unique values  $\phi_j^{(k)}$  of cluster j and the marginal distribution m(x), taken from the appropriate function in the Hierarchy<> class. The weights of the clusters are proportional to their size  $n_j^{(k)}$ , while the "virtual" cluster of the marginal counts as having size M, the total mass parameter (n is the total number of observations, as per usual). The marginal distribution is only known under the conjugacy assumption in the Neal2 algorithm. In particular, for a Normal-NIG model m(x) is a Student's t as explained in section 1.2.1. In the Neal8 algorithm, m(x) is not available in closed form, and thus it is replaced in the above formula by the following approximation:

$$\hat{m}(x) = \frac{1}{m} \sum_{h=0}^{m-1} f(x|\phi_h)$$
 (4.2)

where we use m unique values, that is, one for each of the  $m = n_aux$  auxiliary blocks of the algorithm, drawn from the base measure:  $\phi_h \stackrel{\text{iid}}{\sim} G_0$ , h = 0 : m - 1. Finally, the *empirical density* is computed as the mean over all K iterations:

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

and saved into the density object. Again, this estimate approaches the true posterior density of the data thanks to the convergence in mean of the chain.

## 4.3 Saving estimates to files

We also implemented the following functions in each Algorithm class, which save data from the class into text files in order to ease exportation to other programs or computers:

They can be called as need be from the main.cpp file. If a file name is not provided, the above default names will be used. The former two create a .csv file with the columns being, in order, data index, data value, allocation, unique values (one per column). write\_chain\_to\_file() has the same columns as the previous functions, but adds one more column containing the iteration number (starting from 0) as the first one. Finally, write\_density\_to\_file() has values of x in the first column and the corresponding  $\hat{f}(x)$  in the second one.

## Collectors

Once a BNP algorithm is run, one may be interested, as mentioned above, in an estimate of the density given a grid of points or in an identification of a partition through the clustering obtained in the algorithm, which we call best clustering, i.e. the one that optimizes the binder loss function. In any case we need to be able to retrieve the information of each iteration of the algorithm, such as allocations and unique values, which characterize the state of the chain. In order to do it without saving the entire chain of states as a member of the Algorithm class we have implemented the collectors classes. A collector is therefore a class outside the algorithm class meant to store the state of a Markov chain at all iterations, in order to be able to use the states chain after the algorithm run, for density and clustering estimates.

At the end of each iteration of the algorithm allocations and unique values of the current state are stored in classes built via the Google Protocol Buffers library, also known as Protobuf. The protobuf-object of the state is then stored in a collector.

We have implemented two types of collector that we called FileCollector and MemoryCollector. The first saves the protobuf-objects related to the chain states on binary files while the second saves them on a deque.

The MemoryCollector, unlike the FileCollector, does not write chain states anywhere and all information contained in it is destroyed when the main that created it is terminated. It is therefore useful in situation in which writing to a file is not needed, for instance in a main program that both runs the algorithm and computes the estimates. Instead, the contents of a Filecollector are permanent, because every state collected by it remains ever after the termination of the main that created it, in Protobuf form, in the corresponding file. This approach is mandatory, for instance, if different main programs are used to run the algorithm and the estimates. Sharing the two a common interface we implemented an abstract base class, BaseCollector and two derived classes: FileCollector and MemoryCollector. Below are shown the structures of the classes:

The base class has as protected members the current size of the chain, which is updated during the run by increasing by one for each performed iteration, and the curr\_iter, a cursor useful for reading the chain, when this is done state by state.

Among the public methods useful functions for writing the chain are: the start() function, to initialize the collector, the collect() function to write the single state of the chain in the collector and finish() to close the collector for writing.

Two alternatives are possible for reading: using the get\_chain() method that returns the entire chain of states in protobuf-objects deque format or the get\_next\_state method that returns one state at a time, increasing the curr\_iter cursor by 1 to keep track of the current position. In case the second method is used, since the whole chain is not available, the get\_state method is implemented, which returns the state of a specific iteration, useful for instance in the cluster\_estimate function once it's identified the state of the chain corresponding to the best\_clustering.

## 5.1 Use in run function: writing-mode

In the main program, a DerivedCollector, chosen runtime, is instantiated before running the algorithm and a BaseCollector pointer points to the Derived Collector object. Then the Collector pointer is passed to the run() method and before the first step(), through the pointer, the Collector method start() is called, a function useful in case of FileCollector that initializes the collector for writing. Then, at the end of each iteration, the public function collect() is called which takes in input a Protobuf object related to the current state and writes it to the collector. At the end of all iterations, the Collector public method finish() is called, a function useful in the case of FileCollector to end the collector writing.

#### 5.1.1 FileCollector

In the specific case of FileCollector we pass the filename string to the constructor indicating the file name where the chain will be saved, while the other protected members are initialized by default. In the run() is then initially called the public method of the FileCollector start(), where through the function open() an open file description that refers to the file is created and a file descriptor that refers to that open file description is returned, which we save in the protected member outfd. Then we pass the unix file descriptor to FileOutputStream() which creates a stream that writes to the given Unix file descriptor and initialize the protected member fout as pointer to the created stream. After each iteration is then called the public function of the FileCollector collect() that takes in input the current state in Protobul object format and through SerializeDelimitedToZeroCopyStream () is written on file and the size member is increased by one.

At the end of all iterations the public FileCollector finish() method is called, in witch the close() function closes the file descriptor, e FileOutputStream::Close() flushes any buffers and closes the underlying file.

#### 5.1.2 MemoryCollector

In the case a Memorycollector is used, as before the collector-object is constructed in the main program that is pointed by a pointer to BaseCollector. In this case the default constructor is called. The start and finish methods of a

MemoryCollector do nothing while the collect method, called at the end of each iteration, inserts in the deque the protobul object related to the current state and increases the size by one.

#### 5.2 Use in estimates functions: reading-mode

Once the BNP algorithm run is completed, we proceed with density and clustering estimates. For both estimates it is necessary, as said before, to know the whole chain of states, so the BaseCollector pointer is passed as input in both the functions. Within the estimates functions we decided to call get\_chain , the collectors public methos that returns the whole chain in deque form. In the case of MemoryCollector is simply returned the protected member chain, while in the case of FileCollector the chain is read from file state by state with google::protobuf::util::ParseDelimitedFromZeroCopyStream(): each state is converted back into protobuf format and saved in the deque.

#### 5.2.1 Alternative of reading

A possible alternative to reading the chain could be to read status by status directly in the estimates functions when necessary, without saving the whole chain inside the function. With such an implementation, in the for loop of the estimates functions that runs the iterations, the get\_next\_state() Collectors method mentioned above, could be called for each iteration, in which the cursor curr\_iter, initialized to -1, is increased by one and the get\_next protected method, specific for each Derived Collector, returns the state relative to the current iteration. In the case of Memory collector get\_next simply returns the element of the deque relative to the current position up to size -1, when the curr\_iter is re-initialized for a possible recall by one of the estimates functions.

In the case of FileCollector, at the first iteration the file is opened for reading, the chain status is read and converted back to Protobuf-object form, while for the other iterations the reading of the file continues from the position of the previous iteration. When the curr\_iter is equal to size—1the curr\_iter is reset to -1 and the file is closed for reading.

When the estimates functions are executed in the same main program where the algorithm is run, the collectors contain the size information, corresponding to the number of iterations saved on the chain. If the estimates are made in a different main program, situation where the FileCollector is needed, the size information is lost with the destruction of the object created in the main program where the run() is executed. Therefore, it might be a plausible option to also save the size to file to easily recover it when needed.

In addition, in cluster\_estimate(), once the dissimilarity matrices have been calculated by reading the whole chain state by state, and the iteration related to the best\_clustering, i.e. the one that optimizes the binder loss function, is identified, the corresponding state must be retrieved and in the case of FileCollectors it is therefore necessary to re-read the file up to this iteration with get\_state(). get\_state() can be improved by saving the number of bytes corresponding to the individual protobuf-object and thus be able to recover a specific state without reading previous iterations. For sake of simplicity we have opted for a reading

of the whole chain, leaving in the collectors classes the functions get\_next\_state, get\_next and get\_state for a possible extension.

# Factory

6.1

# Python interface

## 7.1 Creating the interface

A Python interface was implemented for easier usage and testing with respect to C++. The files are located in the src/python folder. This interface is made possible by two main pieces of software: the pybind11 Python package, and again the Protocol Buffers library. pybind11 allows transporting of C++ objects into a C++ library that can be read as if it were a Python library. In particular, the cpp\_exports subfolder contains several source files each containing a function that fulfills a specific role. This allows the user to be able to run the algorithm and execute the estimate at different points in time, since these two actions are completely independent – this is actually the main reason for why a FileCollector was implemented in the first place. Such independence is possible because after using the run unit, the Markov chain is automatically saved to a FileCollector, which can then be read and describlized thanks to the Python interface of the protobuf library. More specifically, the chain\_state.proto file that was used to generate the State class in C++ is also used to generate the same exact class in a Python file, again by running the Protobuf compiler protoc; the created file is called chain\_state\_pb2.py. All these units are included into the exports.cpp file, in which the macro PYBIND\_MODULE is invoked to create the Python version of the library by passing the created function objects by reference:

```
PYBIND11_MODULE(bnplibpy, m){
    m.doc() = "Nonparametric library for cluster and density
        estimation";
    m.def("run_NNIG_Dir", &run_NNIG_Dir);
    ...
}
```

(Note that the units included in the library must have a fixed hierarchy and mixture, since the choice at runtime for these objects is not available yet, as previously noted.) The library is then compiled into a shared .so C++ library by calling the Makefile rule, pybind\_generate. After the library is created, one can simply import bnplibpy in any Python script after adding its file path to the PYTHONPATH environment variable.

#### 7.2 Using the interface

In particular, a Python interface file, bnp\_interface.py was created to automatically import the library and implement several useful tools:

- get\_multidim\_grid() creates an hypercube grid of arbitrary side, dimension and step, which is useful for evaluating a higher-dimension density estimate;
- deserialize() exploits the aforementioned common interface provided by Protobuf to read a Markov chain from a FileCollector given its name and turn it into a list of State objects;
- chain\_barplot() loops over the Markov chain unpacked by deserialize() and produces a barplot which shows the distribution of the number of clusters over all saved iterations of the chain;
- plot\_density\_points() and plot\_density\_contour() both take a density evaluation file as input and plots them if possible, i.e. if the given density has the correct dimensions: 1D and 2D for the former, which is a regular function graph, and 2D for the latter, which is a map of the estimated contour lines of the function;
- plot\_clust\_cards() takes a clustering .csv file as input, most likely the best clustering computed and stored via the cluster\_estimate() method of the Algorithm class, and plots the cardinalities of clusters inside it;
- clust\_rand\_score() computes the so-called *adjusted Rand score* between a given predicted clustering and true clustering. This score is a value in [0, 1] that represents a measure of the proportion of correct decisions made by the clustering algorithm with respect to the true clustering.

The user can then call each of these tools and the ones in bnplibpy at will in their scripts. For instance, one may want to run the algorithm and get the Markov chain, visualize the distribution of clusters via chain\_barplot(), then compute the estimates; or maybe di all 3 at the same times. A typical Python script that uses this library looks as follows (extracted from console.py):

```
from bnp_interface import *

# Initialize parameters
mu0 = 5.0
lambda_ = 0.1
...

# Write file names
datafile = "csv/data_uni.csv"
collfile = "collector.recordio"
...

# Run algorithms, estimates, and plots
bnplibpy.run_NNIG_Dir(mu0, lambda_, alpha0, beta0, totalmass, datafile, algo, collfile, init, rng, maxit, burn, n_aux)
```

chain\_barplot(collfile, imgfilechain)
bnplibpy.estimates\_NNIG\_Dir(mu0, lambda\_, alpha0, beta0, totalmass, grid, algo,
collfile, densfile, clustfile, only)
plot\_clust\_cards(clustfile, imgfileclust)

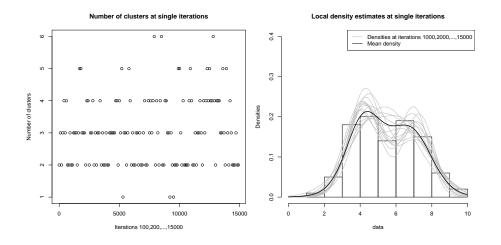
## Results

Our clustering analysis was conducted on n=100 observations, the former 50 of which were iid sampled from a  $\mathcal{N}(4,1)$  and the latter from a  $\mathcal{N}(7,1)$ , which were saved in the data.csv file. We chose the prior parameters for the Normal-NIG model (1.2.1) as follows:  $\mu_0=5, \lambda_0=1, \alpha_0=2, \beta_0=2$ . The Neal8 algorithm with m=3 auxiliary blocks was run for 20000 iterations, and the first 5000 were discarded as burn-in, for a total of K=15000 valid iterations. We will keep these parameters values fixed unless explicitly stated.

The following test data were all saved to .csv files and used for the realization of plots with the ggplot2 R package. All scripts and data sheets are available in the GitHub repository of our library.

#### 8.1 Oscillations

After running the algorithm as described above with total mass M = 0.25, we find that the obtained best clusterings (again, in the lest square sense) and local density estimates are highly fluctuating over the iterations of the algorithm:

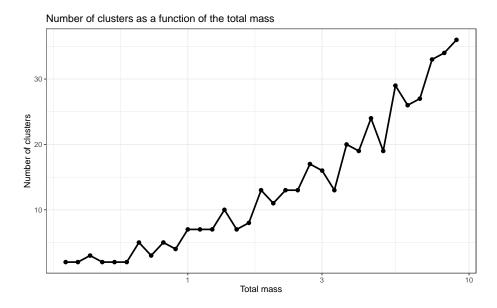


In both plots, a thinning of one iteration every 100 and every 2500, respectively, was performed for better readability of the plot. In the right side plot, the

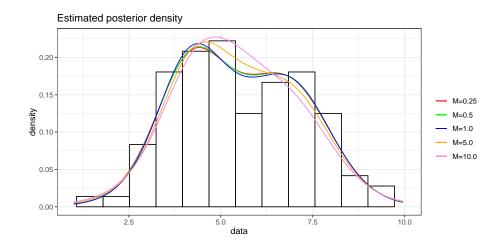
local densities are compared with the histogram of the data as well as the final estimate provided by the mean density. We can see that the number of clusters at all iterations varies significantly between 1 and 6, even in the last thousands of iterations, and the same behavior applies to the local density estimates. This is further confirmation of the fact that the single iterations themselves do not converge. Instead, as previously discussed, the convergence is in the *mean*, both for the density estimate and for the average dissimilarity matrix which we use to find the best clustering.

#### 8.2 Total mass

Let us now examine the role of the total mass parameter, M. We ran the algorithm with several values for M whilst keeping the other parameters unchanged from the ones indicated at the beginning of the section. For each M, we saved the number of clusters of the best clustering produced by the algorithm, and plotted it against the corresponding M:



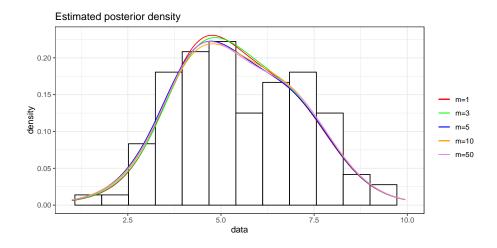
Note that the values for M were chosen so as to be evenly spaced in log-scale, thus the abscissa is in log-scale as well. We can note that the clusters are increasing with the total mass. This is consistent with the fact that the probability of creating a new cluster is proportional to M, as seen in (2.4). Moreover, the density estimates for some of the values of M (again, compared with the histogram of the data) are as follows:



In our case, lower values for the total mass account better for the distribution of the data points, with the modes being near the real expected values of the two normal distributions, 4 and 7. On the other hand, higher values tend to clump together all 100 observations as though they were extracted from a single distribution. As we can see, the total mass M acts as smoothing parameter and, given its strong influence on the number of mixture components, it is a prime candidate for a prior distribution being put onto it.

## 8.3 Auxiliary blocks

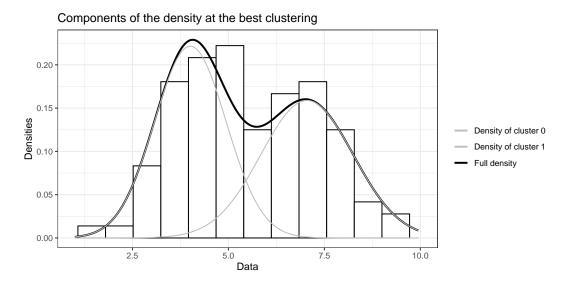
We shall now try and change the number of auxiliary blocks m, and check how this impacts the density estimation. For this test, a large total mass M=10 was chosen; the reason being that a small M would not allow significant differences as m changes. Indeed, m directly influences only the estimate (4.2) of the marginal distribution, that has a weight of  $\frac{M}{M+n}$  (as seen in (4.1)), which is negligible if M is small. Therefore, M=10 was picked, and the result was the following:



Note that a larger m gives a better estimate of the marginal, because the sample mean is computed over a larger number of terms and the algorithm approximates the behavior of the algorithm Neal2.

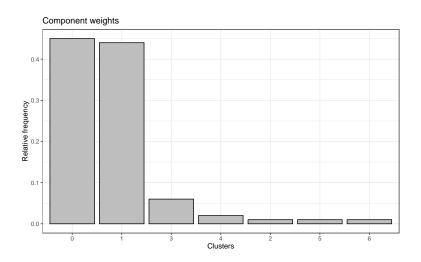
#### 8.4 Density components

We now wish to visualize how the local density is computed at a given sample iteration. Let us run again the Neal8 algorithm with both M=0.25 and m=3 fixed, and then use the cluster\_estimate() function to extract the best clustering for the data. We find that it is at iteration 2490, which gives 2 clusters. As shown in 4.1, each of these clusters has its own density estimate, which we refer to as *component*, and a weight attached to it proportional to its cardinality. The weighted sum of these components gives the "full" local estimate of the density for that iteration. This plot shows both the weighted components and their sum:



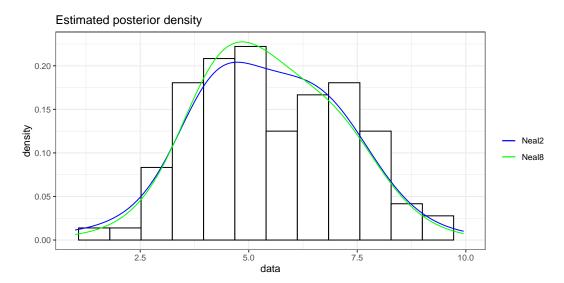
In this case the weights turn out to be approximately equal (0.52 and 0.48 respectively). Again, the two components are concentrated around the true means (4 and 7) of the likelihoods of the data points, as expected.

In other cases, the best clustering may produce more than 2 clusters. One such example is given by the best clustering of Neal8 run with M=1 (and m=3 as before), found at iteration 6611. Although there are 7 clusters, all weights bar the first two are insignificant, making the corresponding components have almost zero impact in the weighted sum of the local estimate:



#### 8.5 Neal2 vs Neal8

Finally, we ran the Neal2 algorithm with the same parameters as Neal8 (indicated at the beginning of the section) as well as M=10 for both. Again, a rather large total mass was chosen in order to better highlight the difference in the marginal estimate. In fact, in the Neal2 case, since the marginal distribution is known in closed form, the estimate is more accurate:



## Extensions

The bnplib library has several possible extensions:

- New types of Hypers classes can be implemented, for example ones containing hyper-priors for some of the parameters if the model. The algorithm must be modified accordingly, for instance by adding extra steps (which are skipped if the hyperparameters are fixed). Changes depend on the type of parameter for which a prior is used; for example, a prior on the total mass parameter involves different steps than a prior on the parameters of the base measure. For a general outline of the necessary changes, see [2] section 7.
- Hierarchies other than the Normal-NIG can be created. This is enough to run Neal8 and Neal2 by passing the class name as parameter, provided that the Hierarchy class has the appropriate interface.
- Interfaces with both R and Python can be easily implemented, thanks to the data structures provided by protobuf and the already-available libraries Rcpp and pybind respectively.
- Algorithms can be re-adapted for the use of other mixture models, such as the Pitman-Yor process.
- Conjugacy-dependent algorithms such as Neal2 can be re-adapted to account for non-conjugacy, for example by using an Hamiltonian Monte Carlo sampler.
- Finally, a full generalization of the library might be possible. That is, given the distributions of the likelihood, hyperparameters, etc, one might want an algorithm that works for the chosen specific model without needing and explicit implementation for it. This means, among other things, that one has to handle non-conjugacy for the general case. The main issue is that Stan distribution functions do not accept vectors of parameter values as arguments; thus, the updated values for distributions must be explicitly enumerated and given as arguments one by one to the Stan function. This requires to know in advance the number of parameters for all such distributions, which is impossible in the general case. Some advanced C++ techniques may be used to circumvent this hindrance,

such as argument unpackers that transform a vector into a list of function arguments, and variadic templates, which are templates that accept any number of arguments. Theoretically, the latter would also allow the use of priors on the parameters of the hyper-prior itself, and so on, adding layers of uncertainty ad libitum. Although it is a hard task, we do think it is possible to achieve with reasonable effort.

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