`bnplib`: A Nonparametric C++ Library

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Abstract

We present a C++ library that exploits a Bayesian nonparametric setting in order to conduct monodimensional 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.

1 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 form of 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

Let $M > 0$, and let G_0 be a probability measure defined on S. A Dirichlet process (DP) with parameters (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 $\{y_1, \ldots, y_n\}$, the basic DP model takes the following form:

$$\begin{aligned} y_i|G &\overset{\text{iid}}{\sim} G, \quad i = 1, \ldots, n \\ G &\sim DP(MG_0) \end{aligned} \tag{1}$$

A key property is that the DP is conjugate with respect to independent and identically distributed 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:

$$G|y_1, \ldots, y_n \sim DP\left(MG_0 + \sum_{i=1}^{n} \delta_{y_i}\right). \tag{2}$$

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

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

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

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

An important property of the DP is the discrete nature of G. Since it is a discrete random probability measure, 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 $m_k \overset{\text{iid}}{\sim} G_0$ for $k \in \mathbb{N}$ and the random weights constructed as $w_k = v_k \prod_{l<k}(1 - v_l)$ where $v_k \overset{\text{iid}}{\sim} Be(1, M)$.
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 Θ be a finite-dimensional parameter space and G_0 a probability measure on Θ. The Dirichlet process mixture (DPM) model convolves the densities $f(\cdot|\vartheta)$ from a parametric family $F = \{f(\cdot|\vartheta), \vartheta \in \Theta\}$ using the DP as mixture weights. The obtained model has the following form:

$$\begin{aligned} y_i|G \sim f_G(\cdot) &= \int_\Theta f(\cdot|\vartheta)\, G(\mathrm{d}\vartheta), \quad i = 1, \dots, n \\ G &\sim DP(MG_0) \end{aligned} \tag{3}$$

An equivalent hierarchical model is:

$$\begin{aligned} y_i|\vartheta_i &\overset{\perp\!\!\!\perp}{\sim} f(\cdot|\vartheta_i), \quad i = 1, \dots, n \\ \vartheta_i|G &\overset{\text{iid}}{\sim} G, \quad i = 1, \dots, n \\ G &\sim DP(MG_0) \end{aligned} \tag{4}$$

where the *latent variables* ϑ_i are introduced, one per unit. Since G is discrete, we know that two independent draws ϑ_i and ϑ_j from G can be equal with positive probability. In this way the DPM model induces a probability model on clusters and an object of interest that derives from this model is the partitioning induced by the clustering, as well as the density estimation.
Considering n data units, each ϑ_i will have one of the k unique values ϕ_j. An estimation of the number of the unique values is $M \log(n) \ll n$. Defining c_i the *allocation* parameters to the clusters such that $c_i = j$ if $\vartheta_i = \phi_j$, the model can be thought as the limit as K goes to infinity of finite mixture model with K components:

$$\begin{aligned} y_i|\phi, c_i &\sim f(\cdot|\phi_{c_i}) \\ c_i|\mathbf{p} &\sim \sum_{k=1}^{K} p_k \delta_k(\cdot) \\ \phi_c &\sim G_0 \\ \mathbf{p} &\sim \mathrm{Dir}(M/K, \dots, M/K) \end{aligned} \tag{5}$$

where $\mathbf{p} = (p_1, \ldots, p_K)$ represents the mixing proportions for the classes and each ϑ is characterized by the latent class c and the corresponding parameters ϕ_c.

1.2.1 Normal Normal-InverseGamma model

A very common choice for the DPM model is the gaussian mixture model, also known as 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:

$$\begin{aligned} f(y|\vartheta) &= N(y|\mu, \sigma^2) \\ G_0(\vartheta|\mu_0, \lambda_0, \alpha_0, \beta_0) &= N\left(\mu|\mu_0, \frac{\sigma^2}{\lambda_0}\right) \times \text{Inv-Gamma}(\sigma^2|\alpha_0, \beta_0) \end{aligned} \tag{6}$$

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

$$p(\widetilde{y}|\mu_0, \lambda_0, \alpha_0, \beta_0) = \int_\Theta f(\widetilde{y}|\vartheta)\, G_0(\mathrm{d}\vartheta) = \mathrm{t}_{\widetilde{\nu}}\left(\widetilde{y}|\widetilde{\mu}, \widetilde{\sigma}\right)$$

where the following parameters are set:

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

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

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

with:

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

2 Algorithms

For the task of density estimation, we investigated several Markov chain methods to sample from the posterior distribution of a Dirichlet process mixture model.
Starting from the hierarchical model (3), a first direct approach is simply drawing values for each ϑ_i from its conditional given the data and the other ϑ_j. However, as previously discussed, we have high probability for ties among them which can lead to slow convergence, since the ϑ values are not updated for more than one observation simultaneously.
For this reason, special attention was paid to the three of them we present in this section. 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

$\phi_{\mathbf{c}}$. 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, which eventually reaches convergence. Moreover, all methods can be extended with additional steps for hierarchical extensions. For example, we can place priors to hyperparamaters of the centering measure G_0 or to the total mass M.

2.1 Neal's Algorithm 2

In order to speed up the 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 (5), 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. Assuming that the current state of Markov chain is composed of $(c_1, \ldots, c_n)$ and the component parameters ϕ_c for all c, the Gibbs sampler first draws values for each c_i given the following conditional probabilities:

$$\mathbb{P}(c_i = c|\mathbf{c}_{-i}, y_i, \boldsymbol{\phi}) \propto \frac{n_{-i,c} + M/K}{n - 1 + M} f(y_i|\phi_c) \tag{7}$$

where $n_{-i,c}$ is the number of c_j equal to c excluding c_i. Consequently, the sampler draws a new value for each ϕ_c given the data belonging to that class. The passage to the infinite case is done taking the limit as K goes to infinity in the conditional distribution of c_i which becomes as follows:

$$\begin{aligned} \mathbb{P}(c_i = c|\mathbf{c}_{-i}, y_i, \boldsymbol{\phi}) &\propto \frac{n_{-i,c}}{n - 1 + M} f(y_i|\phi_c) \\ \mathbb{P}(c_i \neq c_j \text{ for all } j|\mathbf{c}_{-i}, y_i, \boldsymbol{\phi}) &\propto \frac{M}{n - 1 + M} \int_{\Theta} f(y_i|\phi)\, G_0(\mathrm{d}\phi) \end{aligned} \tag{8}$$

and considering only the ϕ_c associated with some observation, keeping the sampling finite and thus computationally feasible. At this point the algorithm works iteratively by sampling c and ϕ. For each observation i, c_i is updated according to its conditional distribution. 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 ϕ_{c_i} is drawn from the posterior distribution H_i, based on the prior G_0 and the single observation y_i. Then for all the classes the sample for ϕ_c is done considering the posterior distribution based on the prior and all the observations belonging to the specific class. The probability of setting c_i to a new component involves the integral $\int_{\Theta} f(y_i|\phi)\, G_0(\mathrm{d}\phi)$, which is difficult to compute in the non-conjugate case, as well as the sample from the posterior H_i. For this reason the algorithm is applied when there is conjugacy and it is possible to compute exactly 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 where the state is extended by the addition of auxiliary parameters: the `Neal8` algorithm. This technique allows to update the c_i while avoiding the integration with respect to G_0.

In this case the prior for c_i is:

$$\begin{aligned} \text{If } c = c_j \text{ for some } j\text{: } \mathbb{P}(c_i = c|\mathbf{c}_{-i}) &= \frac{n_{-i,c}}{n-1+M} \\ \mathbb{P}(c_i \neq c_j \text{ for all } j) &= \frac{M}{n-1+M} \end{aligned} \tag{9}$$

where the probability of selecting a new component is evenly split among the m auxiliary components, which will also be referred to as *auxiliary blocks*. Whilst maintaining the same structure as the `Neal2`, the `Neal8` is composed of two steps, where the components of the Markov chain state (c, ϕ) are repeatedly sampled. The first step scans all the observations and evaluates each c_i. If it is equal to another c_j, then all the auxiliary variables are drawn from G_0. If the corresponding cluster is a singleton, then it is linked to one of the auxiliary variable with the corresponding value of ϕ_c, while the others are drawn as before from G_0. Then, c_i is updated according to the following conditional probabilities:

$$\mathbb{P}(c_i = c|\mathbf{c}_{-i}, y_i, \phi_1, \ldots, \phi_h) \propto \begin{cases} \dfrac{n_{-i,c}}{n-1+M} f(y_i|\phi_c), & \text{for } 1 \leq c \leq k^- \\ \\ \dfrac{M/m}{n-1+M} f(y_i|\phi_c), & \text{for } k^- + 1 < c \leq h, \end{cases} \tag{10}$$

indicating with k^- the number of distinct c_j excluding the current c_i and setting $h = k^- + m$.
Once all the ϕ_c that are no longer associated with any observation are discarded, the algorithm proceeds with the sampling for ϕ_c for all the classes.

2.3 Blocked Gibbs

Another Gibbs Sampling method applicable in the considered Bayesian hierarchical models 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 in this way to update blocks of parameters. A key point of the method is that it does not marginalize over the prior, instead, grouping more variables together, it samples from their joint distribution conditioned on all other variables.
It needs to draw from the conditionals:

$$\begin{aligned} \boldsymbol{\phi} &\sim \mathcal{L}(\boldsymbol{\phi}|\mathbf{c}, \mathbf{y}) \\ \mathbf{c} &\sim \mathcal{L}(\mathbf{c}|\boldsymbol{\phi}, \mathbf{p}, \mathbf{y}) \\ \mathbf{p} &\sim \mathcal{L}(\mathbf{p}|\mathbf{c}) \end{aligned}$$

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

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()`. 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:

```
template<template <class> class Hierarchy, class Hypers,
         class Mixture> class Algorithm
```

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 `state`s 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 data points;
  - 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 proceeded with our implementation. 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 ϕ hold objects of type `Hierarchy<>` because each ϕ 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 data points $i = 1 : n$. A vector `card` is first filled, with `card[j]` being the cardinality of cluster j. The algorithm mandates that `data[i]` be moved to another cluster; thus, if the current cluster is a singleton, its ϕ values are transferred to the first auxiliary block. Then, each auxiliary block (except the first one if the above case occurred) generates new ϕ values via the hierarchy's `draw()` function. Now, a new cluster, that is a new ϕ value, for `data[i]` needs to be drawn. A vector `probas` with `n_unique+n_aux` components is filled with the probabilities of each ϕ being extracted, in line with 10. Computations involve, among other things, the `card` vector, the `log_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 a later 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 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 data points i `card` vector is built, just as before. The `probas` vector of weights for the new allocation value is computed, according to probabilities in 8, 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 ϕ 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).

4 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.

4.1 Storing values with `protobuf`

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 `save_iteration()` function saves all state values of the current iteration into the `chain` pseudo-vector in the appropriate structure. On the other hand, `best_clust` represents the state of a single iteration, and it is the object where the result of the clustering analysis will be saved. The `density` 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.

4.2 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 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 data points) 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 K is 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.

4.3 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` pseudo-vector. 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 `card[j]` $= n_j^{(k)}$ is the cardinality of cluster j. Then, for each point x in `grid`, we compute the local estimate of the density, that is, only taking iteration k into account:

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

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 instead the number of data points, 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:

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

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: $\phi_h \overset{\text{iid}}{\sim} G_0,\ h = 0 : m-1$. Finally, the *empirical density* is computed as the mean over all iterations:

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

and saved into the `density` object.

4.4 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:

```
const void write_final_clustering_to_file(
           std::string filename = "final_clust.csv");
const void write_best_clustering_to_file(
           std::string filename = "best_clust.csv");
const void write_chain_to_file(
           std::string filename = "chain.csv");
const void write_density_to_file(
           std::string filename = "density.csv");
```

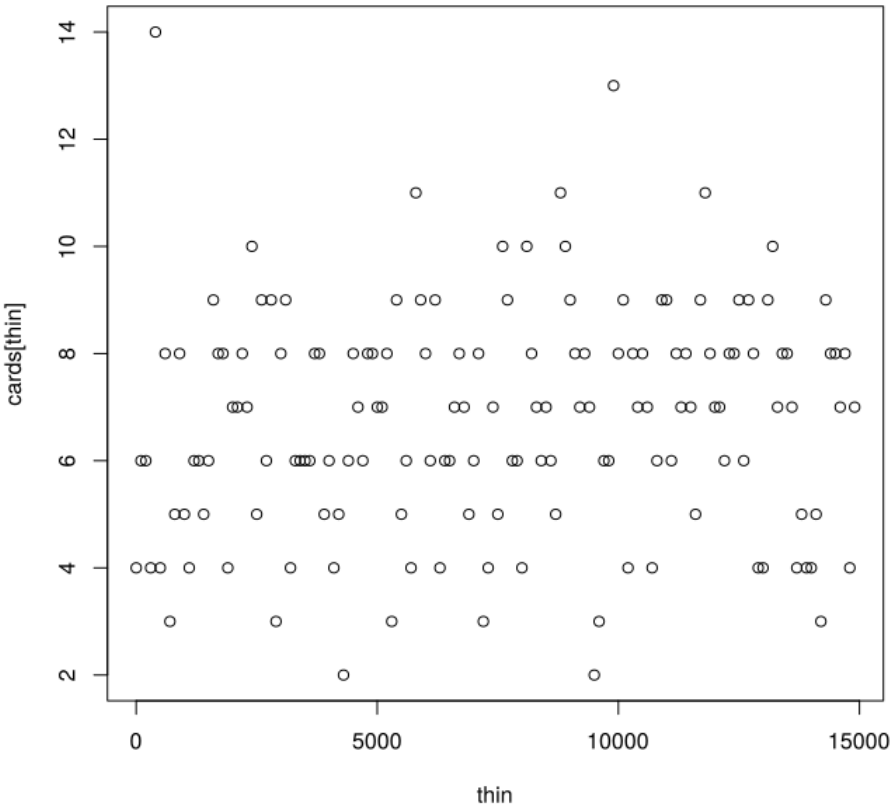
They can be called as need be from the `main.cpp` file. If a file name is not provided, the above default names will be used. The former two create a `.csv` file with the columns being, in order, data index, data value, allocation, unique values (one per column). `write_chain_to_file()` has the same 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.

5 Results

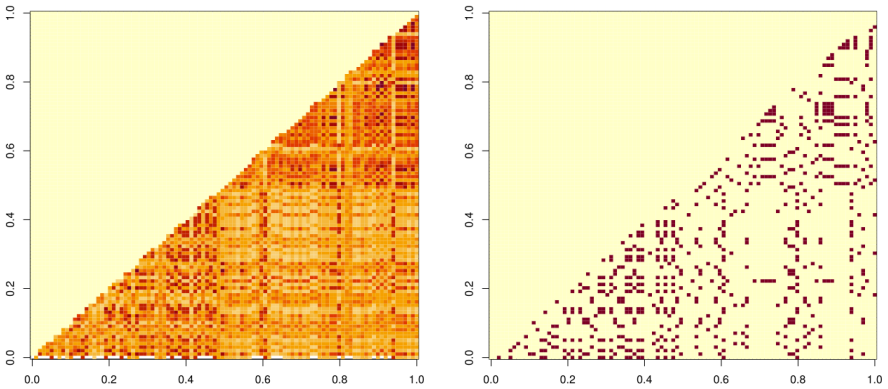
5.1 Clustering analysis

Our clustering analysis was conducted on 100 data points, the former 50 of which were iid sampled from a $\mathcal{N}(4, 1)$ and the latter from a $\mathcal{N}(6, 1)$. The `Neal8` algorithm with $m = 3$ auxiliary blocks was run for 20000 iterations, and the first

5000 were discarded as burn-in. Then, `cluster_estimate()` was called. The resulting best clustering is found at iteration 2975 and has 9 clusters in it.
The obtained clusterings are highly fluctuating in terms of the number of clusters, as shown by the below plot:



A thinning of one iteration every 100 was performed for better readability of the plot. Here, one can clearly see that the number of clusters at all iterations varies significantly bewteen 2 and 14, even in the last thousands of iterations, with most of the iterations hovering between 6 and 9 clusters. This shows that the best clustering in a *least sqaure* sense (via Binder's loss function, as previously discussed) does not necessarily have a small number of clusters.
Let us now take a closer look at the structure produced by `cluster_estimate()` by looking at the heat map for the mean dissimilarity matrix $\bar{D}$ (below, on the left) and for the best clustering (on the right). Darker, reddish colors indicate values closer to 1 (both data are in the same cluster), while light, yellowish colors indicate values closer to 0 (both data are in different clusters). We only show the lower triangular parts, as the matrices are symmetric and the diagonal entries are obviously all equal to 1. In the mean dissimilarity matrix, entries are numbers from 0 to 1, and they can be interpreted as probabilities of data



points belonging to the same cluster. More specifically, the more iterations keep datum i and j in the same cluster, the closer to 1 the corresponding entry $\bar{D}_{ij}$.

6 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. Of course this is a daunting task that is far beyond the scope of this library, although we do think it is possible to achieve with reasonable effort.

References

[1] P. Muller, F. A. Quintana, *Bayesian Nonparametric Data Analysis*

[2] R. M. Neal (2000), *Markov Chain Sampling Methods for Dirichlet Process Mixture Models*

[3] H. Ishwaran, L. F. James (2001), *Gibbs Sampling Methods for Stick-Breaking Priors*

[4] K. P. Murphy (2007), *Conjugate Bayesian analysis of the Gaussian distribution*

[5] Stan documentation: `http://mc-stan.org/math`. Code found at `https://github.com/stan-dev/math` (version 3.0.0 was used) and it also includes other needed libraries: Boost, Eigen, SUNDIALS, Intel TBB

[6] Eigen documentation: `https://eigen.tuxfamily.org/dox`.
Code is included in the Stan package (version 3.3.3 is used there)

[7] Protocol Buffers Tutorial for C++: `https://developers.google.com/protocol-buffers/docs/cpptutorial`.
Code found at `https://github.com/protocolbuffers/protobuf` (version 3.11.0 was used)

[8] Codes of Mario Beraha and Riccardo Corradin for similar projects, found at `https://github.com/mberaha/partial_exchangeability` and `https://github.com/rcorradin/BNPmix` respectively