# February 11, 2020

## Abstract

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## 2 Introduction

This report presents the development of a Bayesian Non parametric library containing methods for density estimation and clustering. In a Bayesian Non-parametric setting we focused on the Dirichlet process (DP) and its extensions, one of the most widely used priors due to its flexibility and computational ease.

### 3 Dirichlet Process

**Formal definition**: Let M > 0 and  $G_0$  be a probability measure defined on S. A DP with parameters  $(M, G_0)$  is a random probability measure G defined on S which assigns probability G(B) to every (measurable) set B such that for each (measurable) finite partition  $B_1, ..., B_k$  of S, the joint distribution of the vector  $(G(B_1), ..., G(B_k))$  is the Dirichlet distribution with parameters

$$(MG_0(B_1), ..., MG_0(B_k)).$$
 (1)

The parameter M is called the precision or total mass parameter,  $G_0$  is the centering measure, and the product  $MG_0$  is referred to as the base measure of the DP.

The basic DP model has the form:

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

A key property is that the DP is conjugate with respect to i.i.d 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 weighting controlled by M:

$$G|\mathbf{y} \sim DP(MG_0 + \sum_{i=1}^n \delta_{y_i}).$$
 (2)

And the marginal distribution will be the result of the product of the conditionals:

$$p(y_i|y_1, ..., y_{i-1}) = \frac{1}{M+i-1} \sum_{h=1}^{n-1} \delta_{y_h}(y_i) + \frac{M}{M+i-1} G_0(y_i).$$
 (3)

An important property of the DP is the discrete nature of G. As a discrete random probability measure we can always write G as a weighted sum of point masses. A useful property based on the discrete nature of the process is his stick-breaking representation, i.e. G can be written as:

$$G(\cdot) = \sum_{k=1}^{+\infty} w_k \delta_{m_k}(\cdot) \tag{4}$$

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

In many applications in which we are interested in a continuous density estimation this discreteness can represents a limit. It's common choice to use a Dirichlet Process Mixture (DPM) model where the DP random measure is the mixing measure for the parameters of a parametric continuous kernel function.

## 4 Dirichlet Process Mixture Model

Extending the DP by convolving G with a kernel F, the model will have the form:

$$y_i|G \sim F_G(y) = \int F(y, \vartheta) G(d\vartheta), \quad i = 1, \dots, n$$
  
 $G \sim DP(MG_0)$ 

An equivalent hierarchical model is:

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

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 and an object of interest starting from this model is the partitioning induced by the clustering as well as the density estimation.

Considering n data units, each  $\vartheta_i$  will have one of the k unique values  $phi_j$ . An estimation of the number of the unique values is  $M\log(n) \ll n$ . Calling  $c_i$  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:

$$(Y_i|\phi, c_i) \sim F(\cdot, \phi_{c_i})$$
  
 $(c_i|\mathbf{p}) \sim \sum_{k=1}^K p_k \delta_k(\cdot)$   
 $\phi_c \sim G_0$   
 $\mathbf{p} \sim \text{Dir}(M/K, \dots, M/K)$ 

where  $(p_1, ..., p_K)$  represent the mixing proportions for the classes and each theta is defined by the latent class c and the corresponding parameters  $\phi_c$ .

## 4.1 Normal Normal-InverseGamma Model

A very common choice is the Gaussian Mixture Model, opting for a Normal kernel and as base measure  $G_0$  the conjugate Normal-InverseGamma:

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

Thanks to the conjugacy the predictive distribution for a new observation  $\tilde{y}$ can be found analytically:

$$p(\widetilde{y}|\mu_0, \lambda_0, \alpha_0, \beta_0) = \int k(\widetilde{y}|\vartheta) p(\vartheta, G_0) d\vartheta = \frac{1}{\widetilde{\sigma}} \text{t-Student}\left(\frac{\widetilde{y} - \widetilde{\mu}}{\widetilde{\sigma}}, |\widetilde{v}\right)$$
(5)

where 
$$\widetilde{v}=2\alpha_0$$
,  $\widetilde{\mu}=\mu_0$  and  $\widetilde{\sigma}=\sqrt{\frac{\beta_0(\lambda_0+1)}{\alpha_0\lambda_0}}$   
The posterior distribution is again a Normal-InvGamma:

$$p(\vartheta|y, \mu_0, \lambda_0, \alpha_0, \beta_0) = N\left(\mu|\mu_n, \frac{\sigma^2}{\lambda_0 + n}\right) \text{Inv-Gamma}(\sigma^2|\alpha_n, \beta_n)$$
 (6)

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

#### Methods 5

Starting from the hierarchical model (n) a direct approach is simply drawing values for each  $\vartheta_i$  from its conditional given the data and the other  $\vartheta_i$ , but as we discussed before there is an high probability for ties among them and this can result in a slow convergence.

#### 5.1 Neal2

To solve and make it more efficient Neal proposed, starting from the discrete model (n), a Gibbs sampling method, integrating out the mixing proportion **p.** Assuming the current state of Markov chain consists of  $(c_1,...,c_n)$  and the component parameters  $\phi_c$  for all c, the Gibbs sampler consists of drawing values for each  $c_i$  given the conditional probabilities:

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

and consequently a new value for each  $\phi_c$  given the data belonging to that class. The passage to the infinite case is done taking the limit of K to infinity in the conditional distribution of  $c_i$  that becomes:

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

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

e considering only the  $\phi_c$  associated with some observation, keeping feasible the sampling.

- **5.2** Neal8
- 5.3 Blocked Gibbs

## 6 Implementation

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

```
void step(){
    sample_allocations();
    sample_unique_values();
    sample_weights();
}
void run(){
    initalize();
    unsigned int iter = 0;
    while(iter < maxiter){</pre>
        step();
        if(iter >= burnin){
             save_iteration(iter);
        }
        iter++;
    }
}
```

In particular, the Neal2 and Neal8 algorithms do not have a sample\_weights() phase. 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 it would be called from the main.cpp) is:

Neal8<NNIGHierarchy, HypersFixed, SimpleMixture> sampler8;

#### 6.1 Auxiliary classes

- 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 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 earlier.

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.

#### 6.2 Neal8 algorithm

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-explainatory. 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 are 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, which will be referred to as the vector of auxiliary blocks, from which the algorithm may draw in order to generate new clusters.

As for the members used for running the algorithm:

```
void initalize();
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  $\phi$  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 a new  $\phi$  value, 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. Computations involve, among other things, the card vector, the log\_like() evaluated in data[i], and the total mass parameter, as shown in the previous sections. 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  $\phi$  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.

#### 6.3 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. Since this algorithm exploits conjugacy, this function must be specifically implemented for each different hierarchy. In our case, a Normal-NIG specialization for the Neal2 template class was implemented. In sample\_allocations(), a loop is performed over data points is card vector is built, just as before. The probas vector of weights for the new allocation value is computed by also using the marginal density in data[i], which is known to be a Student's t as mentioned in the appropriate section. 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).

# 7 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.

#### 7.1 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.

#### 7.2 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 oscillating behaviour, 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  $\bar{D}$ :

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

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.

#### 7.3 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 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 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:

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

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 ?. 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:

$$\tilde{m}(x) = \sum_{h=0}^{m-1} \frac{M}{m} F(x|\phi_h)$$

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 iterations:

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

and saved into the density object.

#### 7.4 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:

They can be called as need be from the main.cpp. If a file name is not provided, the above default names will be used.

#### 8 Results

TBD

## 9 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 Neal(2000) section 7.
- Hierarchies other than the Normal-NIG can be created. This is enough to run Neal8 by passing the class name as parameter, but other algorithms such as the conjugacy-dependent Neal2 may need an hoc implementation of some segments of code.
- 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 readapted 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

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