

BNPlib for density estimation:

A nonparametric C++ library

Bruno Guindani
Elena Zazzetti

November 22nd, 2019



POLITECNICO
MILANO 1863

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

Non-Parametric Statistics

- Goal: density estimation
- **Infinite-dimensional** parameters
- For example: functions
- Bayesian Non-Parametric (**BNP**) model:

$$y_i | G \stackrel{\text{iid}}{\sim} G, \quad i = 1, \dots, n$$
$$G \sim \mathcal{P} \quad (G \text{ random pr. measure})$$

Dirichlet Process Prior

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

- Parameters: $M > 0$, $G_0 \in M(S)$
- Defining property: $\forall \{B_{1:k}\}$ partition of S ,

$$[G(B_1), \dots, G(B_k)] \sim \text{Dir}(MG_0(B_1), \dots, MG_0(B_k))$$

- **Discreteness** (stick-breaking): $G(\cdot) = \sum_{k=1}^{+\infty} w_k \delta_{m_k}(\cdot)$
- **Conjugacy**: $G | \mathbf{y} \sim \mathcal{DP}(MG_0 + \sum_{i=1}^n \delta_{y_i}) \implies$ density estimation

Continuous Density Estimation

- **Mixtures** (kernel F + mixing distribution G):

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

- Model name: Dirichlet-Process Mixture (**DPM**) model
- Equivalent to a hierarchical model:

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

- ϑ_i *latent variables*, one per unit

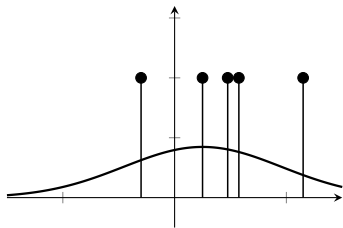
Clustering In The DPM

- Discreteness: the ϑ_i have one of k **unique values** ϕ_j
- Data units: $i = 1, \dots, n$
- Unique values: $j = 1, \dots, k \simeq M \log n \ll n$
- c_i **allocation** parameters to the clusters: $c_i = j$ if $\vartheta_i = \phi_j$

Clustering In The DPM

- Discreteness: the ϑ_i have one of k **unique values** ϕ_j
- Data units: $i = 1, \dots, n$
- Unique values: $j = 1, \dots, k \simeq M \log n \ll n$
- c_i **allocation** parameters to the clusters: $c_i = j$ if $\vartheta_i = \phi_j$
- Conditional prior for ϑ_i , $i = 1, \dots, n$:

$$\mathcal{L}(\vartheta_i | \boldsymbol{\vartheta}_{-i}) \propto \sum_{j=1}^{k^-} \underset{\uparrow}{n_j^-} \underset{\uparrow}{\delta_{\phi_j^-}(\vartheta_i)} + M G_0(\vartheta_i)$$



- Conditional posterior for ϑ_i :

$$\mathcal{L}(\vartheta_i | \boldsymbol{\vartheta}_{-i}, y_i) \propto \sum_{j=1}^{k^-} F(y_i, \vartheta) \delta_{\phi_j^-}(\vartheta_i) + M r_i G_0(\vartheta_i | y_i)$$

Discrete Model

$$\begin{array}{ll} (Y_i|\vartheta_i) \sim F(\cdot, \vartheta_i) & (Y_i|\phi, c_i) \sim F(\cdot, \phi_{c_i}) \\ (\vartheta_i|G) \sim G & (c_i|\mathbf{p}) \sim \sum_{k=1}^K p_k \delta_k(\cdot) \\ G \sim \mathcal{DP}(M, G_0) & \xleftrightarrow{K \rightarrow \infty} \\ & \phi_c \sim G_0 \\ & \mathbf{p} \sim \text{Dir}(M/K, \dots, M/K) \\ \text{(hierarchical model)} & \text{(K-discrete model)} \end{array}$$

with $\vartheta \longleftrightarrow (\phi, \mathbf{c})$

Neal's Algorithm 2

Gibbs sampling algorithm:

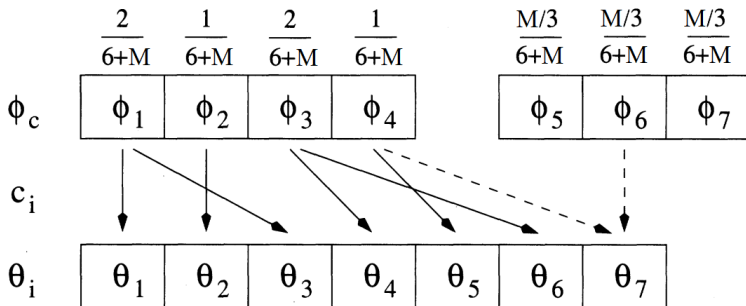
- (ϕ, \mathbf{c}) is the **state** of a Markov chain
- For $i = 1, \dots, n$: update c_i
 - ▶ If c_i allocates ϕ_{c_i} to a singleton, remove ϕ_{c_i} from the state
 - ▶ Sample c_i as follows:

$$\begin{aligned} \text{If } c = c_j \text{ for some } j \neq i: \mathbb{P}(c_i = c | \mathbf{c}_{-i}, y_i, \phi) &\propto \frac{n_{-i,c}}{n-1+M} F(y_i, \phi_c) \\ \text{total } \mathbb{P}(c_i \neq c_j \text{ for all } j | \mathbf{c}_{-i}, y_i, \phi) &\propto \frac{M}{n-1+M} \int F(y_i, \phi) G_0(d\phi) \end{aligned}$$

- ▶ If the new c_i allocates ϕ_{c_i} to a singleton, draw $\phi_{c_i} \sim G_0(\cdot | y_i)$ and add it to the state
- For $c \in \{c_1, \dots, c_n\}$: update ϕ_c , given all the y_i with $c_i = c$

Neal's Algorithm 8

- **Gibbs sampling** on the state, which is extended by the addition of m **auxiliary parameters**

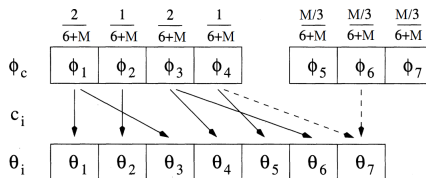


- Prior for c_i :

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

$$\text{total } \mathbb{P}(c_i \neq c_j \text{ for all } j) = \frac{M}{n - 1 + M} \Rightarrow \text{split among the } m \text{ auxiliary parameters}$$

Neal's Algorithm 8



Algorithm (with $h = k^- + m$):

- For $i = 1, \dots, n$: update c_i
 - ▶ Sample auxiliary parameters:
 - $c_i = c_j$ for some $j \Rightarrow$ no connection
 - $c_i \neq c_j \Rightarrow$ association to one of m

The other ϕ values drawn from G_0

- ▶ Draw c_i as follows:

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

- ▶ Discard values in ϕ not associated to any ϑ_j

- For $c \in \{c_1, \dots, c_n\}$: update ϕ_c given y_i such that $c_i = c$

Advantages

- Models with non-conjugate priors
- More efficient than similar algorithms (e.g. no-gaps)
- Hierarchical extensions

Stick-Breaking Priors

$$\mathcal{P}(\cdot) = \sum_{k=1}^N p_k \delta_{Z_k}(\cdot)$$

with $k = 1, \dots, N$ and:

- $Z_k \stackrel{\text{iid}}{\sim} H$ (locations)
- $V_k \stackrel{\text{iid}}{\sim} \text{Beta}(a_k, b_k)$ with $\mathbf{a} = (a_1, a_2, \dots)$ and $\mathbf{b} = (b_1, b_2, \dots)$
- $p_k = (1 - V_1)(1 - V_2) \cdots (1 - V_{k-1})V_k$ (weights),

with $0 \leq p_k \leq 1$, $\sum_{k=1}^N p_k = 1$

Dimension:

- $N < +\infty$: $\mathcal{P}_N(\mathbf{a}, \mathbf{b})$
 - ▶ $\mathbf{p} \sim \mathcal{GD}(\mathbf{a}, \mathbf{b})$ (Generalized Dirichlet)
 - ▶ e.g. all finite dimensional Dirichlet priors
- $N = +\infty$: $\mathcal{P}_\infty(\mathbf{a}, \mathbf{b})$
 - ▶ e.g. Dirichlet process, the two-parameter Poisson-Dirichlet process

Blocked Gibbs Algorithm

- Assumption: **finite-dimensional** prior $P \sim \mathcal{P}_N(\mathbf{a}, \mathbf{b})$
- Finite number of random variables \Rightarrow *blocks of parameters*
- Model:

$$(y_i | \phi, \mathbf{c}) \stackrel{\text{iid}}{\sim} F(\cdot, \phi_{c_i}), \quad i = 1, \dots, n$$

$$(c_i | \mathbf{p}) \stackrel{\text{iid}}{\sim} \sum_{k=1}^N p_k \delta_k(\cdot), \quad i = 1, \dots, n$$

$$\mathbf{p} \sim \mathcal{GD}(\mathbf{a}, \mathbf{b})$$

$$\phi_c \sim G_0, \quad c \in \{c_1, \dots, c_n\}$$

Blocked Gibbs Algorithm

Algorithm:

- Repeatedly draw values from the conditional distributions of the blocked variables:

$$\phi \sim \mathcal{L}(\phi | \mathbf{c}, \mathbf{y})$$

$$\mathbf{c} \sim \mathcal{L}(\mathbf{c} | \phi, \mathbf{p}, \mathbf{y})$$

$$\mathbf{p} \sim \mathcal{L}(\mathbf{p} | \mathbf{c})$$

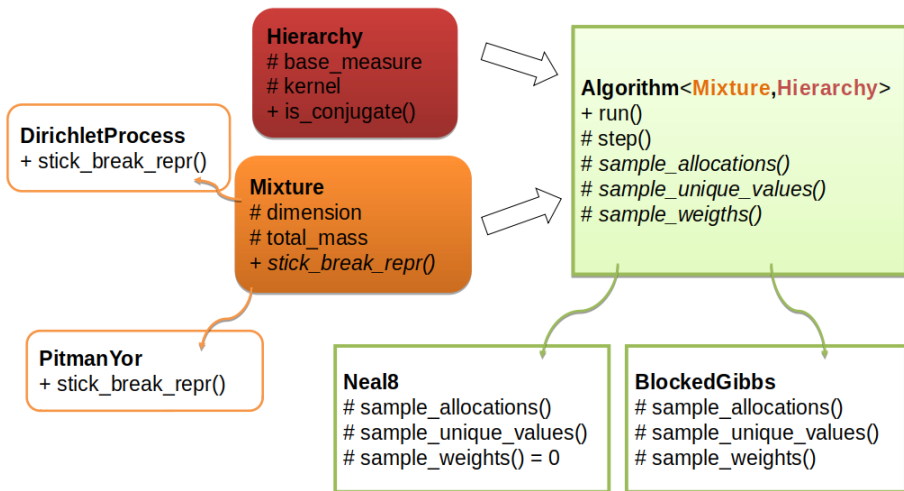
Direct sampling of the **posterior** $\mathcal{P}(\cdot | \mathbf{y})$:

- The algorithm produces draws from $(\phi, \mathbf{c}, \mathbf{p} | \mathbf{y})$
- Each draw $(\phi, \mathbf{c}, \mathbf{p})$ defines a measure $P(\cdot) = \sum_{k=1}^N p_k \delta_{\phi_k}(\cdot)$
- Each P is drawn from $\mathcal{P}(\cdot | \mathbf{y})$


Advantages

- Handling non-conjugate priors
- Approximation of DPM models
- Hierarchical extensions

Code Structure



Bibliography

-  Muller, Quintana, *Bayesian Nonparametric Data Analysis*
-  Neal (2000), *Markov Chain Sampling Methods for Dirichlet Process Mixture Models*
-  Ishwaran, James (2001), *Gibbs Sampling Methods for Stick-Breaking Priors*