BNPlib for density estimation A nonparametric C++ library

Bruno Guindani Elena Zazzetti



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https://github.com/poliprojects/BNPlib

Non-Parametric statistics

- Goal: density estimation
- Infinite-dimensional parameters, e.g. functions

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$$\mathcal{P}:\Omega \to M(S)$$
 fixed $\left[\ \omega \mapsto G(\cdot) \ \right]$

Model name: BNP model

Dirichlet Process prior

$$y_i|G \stackrel{\text{iid}}{\sim} G$$

$$G \sim \mathcal{P} = DP(MG_0)$$

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

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- Discreteness (stick-breaking): $G(\cdot) = \sum_{k=1}^{+\infty} w_h \delta_{m_h}(\cdot)$
- Conjugacy: $G|\mathbf{y} \sim DP(MG_0 + \sum_i \delta_{y_i}) \implies \text{density estimation}$

Continuous density estimation

• **Mixtures** (kernel f + mixing distribution <math>G):

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- Model name: **DPM model**
- Equivalent to:

$$\begin{aligned} y_i | \vartheta_i &\overset{\perp}{\sim} f_{\vartheta_i} \\ \vartheta_i | G &\overset{\text{iid}}{\sim} G \\ G \sim DP(MG_0) \end{aligned}$$

• ϑ_i "latent variables" $\forall i = 1, \dots, n$

Clustering in the DPM

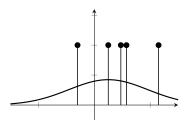
- Discreteness: the ϑ_i have one of the k unique values ϕ_j $(j=1,\ldots,k)$
- $k \simeq M \log(n) \ll n$
- ullet All i s.t. $artheta_i=\phi_j$ belong to cluster S_j $_{(j=1,\ldots,k)}$, and $n_j=|S_j|$

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- Conditional prior for ϑ_i :

$$\mathcal{L}(\vartheta_i|\boldsymbol{\vartheta}_{-i}) \propto \sum_{j=1}^{k^-} n_j^- \delta_{\phi_j^-}(\vartheta_i) + MG_0(\vartheta_i)$$

$$\uparrow \qquad \uparrow$$

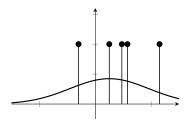


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• Conditional posterior for ϑ_i :

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

Discrete model

Equivalent models as $K \to +\infty$:

$$\begin{aligned} (Y_i|\vartheta_i) &\sim F(\vartheta_i) \\ (\vartheta_i|G) &\sim G \\ G &\sim DP(M,G_0) \end{aligned} & \begin{aligned} (Y_i|\phi,c_i) &\sim F(\phi_{c_i}) \\ (c_i|\mathbf{p}) &\sim \mathsf{Discrete}(p_1,\ldots,p_K) \\ \phi_c &\sim G_0 \\ \mathbf{p} &\sim \mathsf{Dirichlet}(M/K,\ldots,M/K) \end{aligned}$$
 (discrete model)

with
$$c_i=j\iff \vartheta_i\in S_j$$
 allocation parameters and $m{artheta}\iff (m{\phi}, \mathbf{c})$

Neal's Algorithm 2

Gibbs sampling algorithm:

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

If
$$c=c_j$$
 for some $j\neq i$: $\mathbb{P}(c_i=c|c_{-i},y_i,\pmb{\phi})\propto \frac{n_{-i,c}}{n-1-M}F(y_i,\phi_c)$
$$\mathbb{P}(c_i\neq c_j \text{ for all } j|c_{-i},y_i,\pmb{\phi})\propto \frac{M}{n-1-M}\int F(y_i,\phi)\mathrm{d}G_0(\phi)$$

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

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

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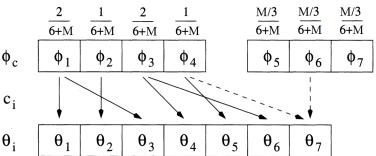
Advantages

- Feasible if we can compute $\int F(y_i, \phi) dG_0(\phi)$ and sample from H_i (generally conjugate case)
- ullet Change the artheta for more than one observation simultaneously

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Neal's Algorithm 8

ullet Gibbs sampling to the state extended by the addition of m auxiliary parameters



• Prior for c_i :

If
$$c=c_j$$
 for some j : $\mathbb{P}(c_i=c|c_{-i})=\frac{n_{-i,c}}{n-1-M}$
$$\mathbb{P}(c_i\neq c_j \text{ for all } j)=\frac{M}{n-1-M}\Rightarrow \begin{array}{c} \text{split among the } m \\ \text{auxiliary parameters} \end{array}$$

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Neal's Algorithm 8

Algorithm:

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

The other ϕ values drawn from G_0

▶ Draw c_i as follows:

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

- lacktriangle Discard ϕ values not associated to any cluster
- For $c \in \{c_1, ..., c_n\}$: update ϕ_c given y_i such that $c_i = c$

Advantages

- Models with non-conjugate priors
- As $m \to +\infty$ it approaches Algorithm 2 but equilibrium distribution is exact
- More efficient than similar algorithms (e.g. no-gaps)
- Hierarchical extensions

Stick-Breaking Priors

$$\begin{split} \mathscr{P}(\cdot) &= \sum_{k=1}^N p_k \delta_{Z_k}(\cdot) \\ p_k &= V_1 \text{ and } p_k = (1-V_1)(1-V_2) \cdot \cdot \cdot (1-V_{k-1})V_k \\ &\qquad \qquad \mathbf{Z_k} \overset{\text{iid}}{\sim} H \\ V_k \overset{\text{iid}}{\sim} Beta(a_k,b_k) \\ \mathbf{a} &= (a_1,a_2,\ldots) \text{ and } \mathbf{b} = (b_1,b_2,\ldots) \\ 0 &\leq p_k \leq 1 \text{ and } \sum_{k=1}^N p_k = 1 \end{split}$$

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

Blocked Gibbs Algorithm

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

$$(Y_i|\phi, \mathbf{c}) \stackrel{\text{iid}}{\sim} F(\phi_{c_i}), \ i = 1, ..., n$$
$$(c_i|\mathbf{p}) \stackrel{\text{iid}}{\sim} \sum_{k=1}^N p_k \delta_k(\cdot)$$
$$\mathbf{p} \sim \mathscr{GD}(\mathbf{a}, \mathbf{b})$$
$$\phi_c \sim G_0$$

Blocked Gibbs Algorithm

Algorithm:

Repeatedly drawing values from conditional distributions of the blocked variables:

- \bullet $(\phi | \mathbf{c}, \mathbf{Y})$
- $(\mathbf{c}|\phi,\mathbf{p},\mathbf{Y})$
- (p|c)

Direct sampling of the posterior $\mathscr{P}(\cdot|\mathbf{Y})$:

- ullet The Algorithm produces draws from $(\phi, \mathbf{c}, \mathbf{p} | \mathbf{Y})$
- \bullet Each draw $(\phi, \mathbf{c}, \mathbf{p})$ defines a measure $P(\cdot) = \sum\limits_{k=1}^N p_k \delta_{\phi_k}(\cdot)$
- ullet Each P is a drawn from $\mathscr{P}(\cdot|\mathbf{Y})$

Advantages

- Handles the issue of conjugacy
- Good mixing
- Hierarchical extensions

Bibliography

- 陯 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