Markov Chain Sampling Methods for Dirichlet Process Mixture Models

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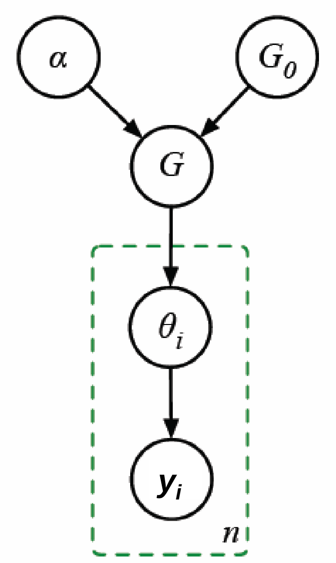
Introduction

- Some problems are more accurately represented with non-conjugate priors
  - Audio interpolation (Godsill & Rayner, 1995)
  - Climatology opinion quantification (Al-Awadhi & Garthwaite, 2001)
  - Financial risk assessment (Siu & Yang, 1999)
- Non-conjugate priors + Gibbs = headache.
  - Update integrals are nasty to compute
- Solution? Metropolis-Hastings + partial Gibbs.

Dirichlet process mixture models

- Basic idea
  - Given data $y_1,\ldots,y_n$ ind. drawn from an unknown distribution (y_i may be multivariate)
  - Model the unknown distribution as being drawn from of a mixture of distributions $F(\theta)$, w/ mixing distribution over θ being G.
  - Let prior for G be a Dirichlet process w/ concentration parameter α and base distribution G_0.
  - Then you have:

$$\begin{aligned} y_i \mid \theta_i &\sim F(\theta_i) \\ \theta_i \mid G &\sim G \\ G &\sim D(G_0, \alpha) \end{aligned}$$



Dirichlet process mixture models

- Integrate over G in previous model, giving a representation of the prior distribution of θ_i in terms of previous θ's:

$$\theta_i \mid \theta_1, \ldots, \theta_{i-1} \quad \sim \quad \frac{1}{i-1+\alpha} \sum_{j=1}^{i-1} \delta(\theta_j) \; + \; \frac{\alpha}{i-1+\alpha} G_0$$

- $\delta(\theta)$ is distribution concentrated at point θ.
- You might notice the "Chinese Restaurant Process" at work here

Dirichlet process mixture models

- You can also get here by letting K (# of components) go to ∞…

$$\begin{aligned} y_i \mid c, \phi &\sim F(\phi_{c_i}) \\ c_i \mid p &\sim \text{Discrete}(p_1, \ldots, p_K) \\ \phi_c &\sim G_0 \\ p_1, \ldots, p_K &\sim \text{Dirichlet}(\alpha/K, \ldots, \alpha/K) \end{aligned}$$

- c_i is the latent class associated with y_i
- The parameters φ_c determine the distribution of observations from c

Dirichlet process mixture models

- Integrate over mixing proportions p_c to write prior of c_i as follows:

$$P(c_i = c \mid c_1, \ldots, c_{i-1}) \quad = \quad \frac{n_{i,c} + \alpha/K}{i - 1 + \alpha}$$

- Where $n_{i,c}$ is the number of c_j for $j < i$ equal to c. Letting K go to ∞, we get c_i's prior as:

$$P(c_i = c \mid c_1, \ldots, c_{i-1}) \quad \to \quad \frac{n_{i,c}}{i - 1 + \alpha}$$

$$P(c_i \neq c_j \text{ for all } j < i \mid c_1, \ldots, c_{i-1}) \quad \to \quad \frac{\alpha}{i - 1 + \alpha}$$

Gibbs sampling w/ conjugate priors

- Exact computation of posterior for DP mixture models not feasible, so use Monte Carlo approaches
- Sample from posterior of $\theta_1,\ldots,\theta_n$ by simulating a Markov chain with this posterior as its equilibrium distribution
- Gibbs sampling is the natural approach here for conjugate priors
- 3 main ways of doing this

Algorithm 1 (Escobar, 1994)

Algorithm 1: Let the state of the Markov chain consist of $\theta_1, \ldots, \theta_n$. Repeatedly sample as follows:

- For $i = 1, \ldots, n$: Draw a new value from $\theta_i \mid \theta_{-i}, y_i$ as defined by equation (7).

$$\theta_i \mid \theta_{-i}, y_i \sim \sum_{j \neq i} q_{i,j}\, \delta(\theta_j) + r_i\, H_i$$

- Where H_i is the posterior for θ based on the prior G_0 and y_i, having likelihood $F(y_i, \theta)$ and:

$$\begin{aligned} q_{i,j} &= b\, F(y_i, \theta_j) \\ r_i &= b\, \alpha \int F(y_i, \theta)\, dG_0(\theta) \end{aligned}$$

- Convergence may be slow due to groups of observations that are highly probably to be associated with the same θ

Algorithm 2 (West, Muller, & Escobar, 1994)

Algorithm 2: Let the state of the Markov chain consist of $c_1, \ldots, c_n$ and $\phi = (\phi_c \;:\; c \in \{c_1, \ldots, c_n\})$. Repeatedly sample as follows:

- For $i = 1, \ldots, n$: If the present value of c_i is associated with no other observation (ie, $n_{-i,c_i} = 0$), remove ϕ_{c_i} from the state. Draw a new value for c_i from $c_i \mid c_{-i}, y_i, \phi$ as defined by equation (11). If the new c_i is not associated with any other observation, draw a value for ϕ_{c_i} from H_i and add it to the state.
- For all $c \in \{c_1, \ldots, c_n\}$: Draw a new value from $\phi_c \mid y_i$ s.t. $c_i = c$.

$$\begin{aligned}
\text{If } c = c_j \text{ for some } j \neq i\text{:} \quad P(c_i = c \mid c_{-i}, y_i, \phi) &= b\, \frac{n_{-i,c}}{n-1+\alpha}\, F(y_i, \phi_c) \\
P(c_i \neq c_j \text{ for all } j \neq i \mid c_{-i}, y_i, \phi) &= b\, \frac{\alpha}{n-1+\alpha} \int F(y_i, \phi)\, dG_0(\phi)
\end{aligned} \tag{11}$$

Algorithm 3 (Neal, 1992)

Algorithm 3: Let the state of the Markov chain consist of $c_1, \ldots, c_n$. Repeatedly sample as follows:

- For $i = 1, \ldots, n$: Draw a new value from $c_i \mid c_{-i}, y_i$ as defined by equation (12).

$$\begin{aligned} \text{If } c = c_j \text{ for some } j \neq i\text{:} \quad P(c_i = c \mid c_{-i}, y_i) &= b \frac{n_{-i,c}}{n-1+\alpha} \int F(y_i, \phi)\, dH_{-i,c}(\phi) \\ P(c_i \neq c_j \text{ for all } j \neq i \mid c_{-i}, y_i) &= b \frac{\alpha}{n-1+\alpha} \int F(y_i, \phi)\, dG_0(\phi) \end{aligned} \tag{12}$$

Methods for handling non-conjugate priors

- If G_0 is not the conjugate prior for F, the integrals for sampling from the posterior might not be feasible to compute.
- West, Muller, and Escobar suggested a Monte Carlo approximation to compute the integral (1994).
  - Slower convergence
  - New values of c_i are likely to be discarded during following Gibbs iteration, leading to wrong distribution.

Algorithm 4 (MacEachern & Muller, 1998)

Algorithm 4: Let the state of the Markov chain consist of $c_1, \ldots, c_n$ and $\phi = (\phi_c \ : \ c \in \{c_1, \ldots, c_n\})$. Repeatedly sample as follows:

- For $i = 1, \ldots, n$: Let k^- be the number of distinct c_j for $j \neq i$, and let these c_j have values in $\{1, \ldots, k^-\}$. If $c_i \neq c_j$ for all $j \neq i$, then with probability $k^- / (k^- + 1)$ do nothing, leaving c_i unchanged. Otherwise, label c_i as $k^- + 1$ if $c_i \neq c_j$ for all $j \neq i$, or draw a value for ϕ_{k^-+1} from G_0 if $c_i = c_j$ for some $j \neq i$. Then draw a new value for c_i from $\{1, \ldots, k^- + 1\}$ using the following probabilities:

$$P(c_i = c \mid c_{-i}, y_i, \phi_1, \ldots, \phi_{k^-+1}) \ = \begin{cases} b\, n_{-i,c} F(y_i, \phi_c) & \text{if } 1 \leq c \leq k^- \\ b\,[\alpha/(k^- + 1)]\, F(y_i, \phi_c) & \text{if } c = k^- + 1 \end{cases}$$

  where b is the appropriate normalizing constant. Change the state to contain only those ϕ_c that are now associated with an observation.

- For all $c \in \{c_1, \ldots, c_n\}$: Draw a new value from $\phi_c \mid y_i$ s.t. $c_i = c$, or perform some other update to ϕ_c that leaves this distribution invariant.

Problem with Algorithm 4

- Algorithm 4 has a problem in that assigning c_i to a new component is reduced by a factor of $k^- + 1$.
- However, something similar without this problem is possible.

Metropolis-Hastings and partial Gibbs

- Use Metropolis-Hastings approach to update the c_i using the conditional prior as the proposal distribution.
- Draw a candidate state, compute its acceptance probability. If it's accepted, use the candidate state, else leave as is.
- We can apply this to the finite model from slide 6, again integrating out p_c

Algorithm 5 (Neal, 1998)

Algorithm 5: Let the state of the Markov chain consist of $c_1, \ldots, c_n$ and $\phi = (\phi_c \ : \ c \in \{c_1, \ldots, c_n\})$. Repeatedly sample as follows:

- For $i = 1, \ldots, n$, repeat the following update of c_i R times: Draw a candidate, c_i^*, from the conditional prior for c_i given by equation (16). If a c_i^* not in $\{c_1, \ldots, c_n\}$ is proposed, chose a value for $\phi_{c_i^*}$ from G_0. Compute the acceptance probability, $a(c_i^*, c_i)$, as in equation (15), and set the new value of c_i to c_i^* with this probability. Otherwise let the new value of c_i be the same as the old value.
- For all $c \in \{c_1, \ldots, c_n\}$: Draw a new value from $\phi_c \mid y_i$ s.t. $c_i = c$, or perform some other update to ϕ_c that leaves this distribution invariant.

$$a(c_i^*, c_i) \;=\; \min\left[1, \ \frac{F(y_i, \phi_{c_i^*})}{F(y_i, \phi_{c_i})}\right]$$

$$\text{If } c = c_j \text{ for some } j \neq i\text{:} \quad P(c_i = c \mid c_{-i}) \;=\; \frac{n_{-i,c}}{n - 1 + \alpha}$$

$$P(c_i \neq c_j \text{ for all } j \neq i \mid c_{-i}) \;=\; \frac{\alpha}{n - 1 + \alpha}$$

Algorithm 6 (Neal, 1998)

Algorithm 6: Let the state of the Markov chain consist of $\theta_1, \ldots, \theta_n$. Repeatedly sample as follows:

- For $i = 1, \ldots, n$, repeat the following update of θ_i R times: Draw a candidate, θ_i^*, from the following distribution:

$$\frac{1}{n-1+\alpha} \sum_{j \neq i} \delta(\theta_j) \; + \; \frac{\alpha}{n-1+\alpha} G_0$$

  Compute the acceptance probability

$$a(\theta_i^*, \theta_i) \;\; = \;\; \min[1,\, F(y_i, \theta_i^*) \,/\, F(y_i, \theta_i)]$$

  Set the new value of θ_i to θ_i^* with this probability; otherwise let the new value of θ_i be the same as the old value.

Algorithm 7 (Neal, 1998)

Algorithm 7: Let the state of the Markov chain consist of $c_1, \ldots, c_n$ and $\phi = (\phi_c \; : \; c \in \{c_1, \ldots, c_n\})$. Repeatedly sample as follows:

- For $i = 1, \ldots, n$, update c_i as follows: If c_i is a not a singleton (ie, $c_i = c_j$ for some $j \neq i$), let c_i^* be a newly-created component, with $\phi_{c_i^*}$ drawn from G_0. Set the new c_i to this c_i^* with probability

$$a(c_i^*, c_i) \;=\; \min\left[1, \; \frac{\alpha}{n-1} \frac{F(y_i, \phi_{c_i^*})}{F(y_i, \phi_{c_i})}\right]$$

  Otherwise, when c_i is a singleton, draw c_i^* from c_{-i}, choosing $c_i^* = c$ with probability $n_{-i,c} \,/\, (n-1)$. Set the new c_i to this c_i^* with probability

$$a(c_i^*, c_i) \;=\; \min\left[1, \; \frac{n-1}{\alpha} \frac{F(y_i, \phi_{c_i^*})}{F(y_i, \phi_{c_i})}\right]$$

  If the new c_i is not set to c_i^*, it is the same as the old c_i.

- For $i = 1, \ldots, n$: If c_i is a singleton (ie, $c_i \neq c_j$ for all $j \neq i$), do nothing. Otherwise, choose a new value for c_i from $\{c_1, \ldots, c_n\}$ using the following probabilities:

$$P(c_i = c \mid c_{-i}, \, y_i, \, \phi, \, c_i \in \{c_1, \ldots, c_n\}) \;=\; b \, \frac{n_{-i,c}}{n-1} \, F(y_i, \phi_c)$$

  where b is the appropriate normalizing constant.

- For all $c \in \{c_1, \ldots, c_n\}$: Draw a new value from $\phi_c \mid y_i$ s.t. $c_i = c$, or perform some other update to ϕ_c that leaves this distribution invariant.

Gibbs sampling w/ auxiliary parameters

- More flexible.
  - Basic idea is that we sample from a distribution π_x for x by sampling from distribution π_{xy} for (x, y).
  - Idea extendable to accommodate auxiliary variables which can be created/discarded during Markov chain simulation.
  - A variable y can be introduced temporarily:
    - Draw a value for y from its conditional given x
    - Perform an update of (x, y) leaving π_{xy} invariant
    - Discard y, leaving x.
  - This technique can be used to update c_i for the DPM without having to integrate w.r.t. G_0

Algorithm 8 (Neal, 1998)

Algorithm 8: Let the state of the Markov chain consist of $c_1, \ldots, c_n$ and $\phi = (\phi_c \,:\, c \in \{c_1, \ldots, c_n\})$. Repeatedly sample as follows:

- For $i = 1, \ldots, n$: Let k^- be the number of distinct c_j for $j \neq i$, and let $h = k^- + m$. Label these c_j with values in $\{1, \ldots, k^-\}$. If $c_i = c_j$ for some $j \neq i$, draw values independently from G_0 for those ϕ_c for which $k^- < c \leq h$. If $c_i \neq c_j$ for all $j \neq i$, let c_i have the label $k^- + 1$, and draw values independently from G_0 for those ϕ_c for which $k^- + 1 < c \leq h$. Draw a new value for c_i from $\{1, \ldots, h\}$ using the following probabilities:

$$P(c_i = c \mid c_{-i}, y_i, \phi_1, \ldots, \phi_h) = \begin{cases} b \, \dfrac{n_{-i,c}}{n-1+\alpha} F(y_i, \phi_c) & \text{for } 1 \leq c \leq k^- \\ b \, \dfrac{\alpha/m}{n-1+\alpha} F(y_i, \phi_c) & \text{for } k^- < c \leq h \end{cases}$$

  where $n_{-i,c}$ is the number of c_j for $j \neq i$ that are equal to c, and b is the appropriate normalizing constant. Change the state to contain only those ϕ_c that are now associated with one or more observations.

- For all $c \in \{c_1, \ldots, c_n\}$: Draw a new value from $\phi_c \mid y_i$ s.t. $c_i = c$, or perform some other update to ϕ_c that leaves this distribution invariant.

The Experiment

	Time per iteration in microseconds	*Autocorrelation time for k*	*Autocorrelation time for θ_1*
Alg. 4 ("no gaps")	7.6	13.7	8.5
Alg. 5 (Metropolis-Hastings, $R = 4$)	8.6	8.1	10.2
Alg. 6 (M-H, $R = 4$, no ϕ update)	8.3	19.4	64.1
Alg. 7 (mod M-H & partial Gibbs)	8.0	6.9	5.3
Alg. 8 (auxiliary Gibbs, $m = 1$)	7.9	5.2	5.6
Alg. 8 (auxiliary Gibbs, $m = 2$)	8.8	3.7	4.7
Alg. 8 ($m = 30$, approximates Alg. 2)	38.0	2.0	2.8

- k is the number of distinct c_i, θ_1 is the parameter associated with y_1
- Algorithm 8 with m=1 superior to algorithm 4 ("no gaps")
- Performance much worse for algorithm 6, where no updates for φ_c are included
- With m=30, algorithm 8 takes longer, but performance is great.