

More on Posterior Computation

PUBH 8442: Bayes Decision Theory and Data Analysis

Eric F. Lock
UMN Division of Biostatistics, SPH
elock@umn.edu

04/16/2024

Gibbs Sampling Techniques

- ▶ Several techniques exist to reduce autocorrelation and improve convergence in Gibbs sampling.
- ▶ *Augmented* sampling introduces auxiliary variables to condition on during sampling.
 - ▶ E.g: To compute posterior for variables A and B , introduce C and sample from $P(C | A, B)$, $P(A | B, C)$ and $P(B | A, C)$.
- ▶ *Collapsed* sampling marginalizes over some variables.
 - ▶ E.g: Rather than drawing from $P(A | B, C)$, marginalize over C and sample from $P(A | B)$.
- ▶ *Blocked* sampling draws from the joint distribution of variable sets rather than their separate full conditionals.
 - ▶ E.g.: Draw from $P(A, B | C)$ rather than $P(A | B, C)$ and $P(B | C, A)$.

Example: Normal-Inverse-Gamma mixture sampling

- ▶ Draw $z_i \in \{1, \dots, K\}$, to indicate the component that generated y_i , from $p(z_i = k \mid \mathbf{y}, \mathbf{q}, \theta)$
 - ▶ Augmenting with Z_i 's to facilitate sampling other parameters
- ▶ Draw weights q from $p(q \mid \mathbf{y}, \theta, \mathbf{z})$.
- ▶ Draw $\theta_k = (\mu_k, \sigma_k^2)$ from normal-inverse gamma posterior for $\mathbf{y}_k = \{y_i : z_i = k\}$:

Draw $\sigma_k^2 \mid \mathbf{z}, \mathbf{y}, q \sim IG(a + n_k/2 - 1/2, b + 1/2 \|\mathbf{y}_k - \bar{y}_k\|^2)$

Draw $\mu_k \mid \sigma_k^2, \mathbf{z}, \mathbf{y}, q \sim \text{Normal} \left(\frac{\sigma_k^2 \mu_0 + n_k \tau^2 \bar{y}_k}{n \tau^2 + \sigma_k^2}, \frac{\sigma_k^2 \tau^2}{n \tau^2 + \sigma_k^2} \right)$

- ▶ Blocking μ_k, σ_k^2
- ▶ Draw for σ_k^2 collapses over μ_k

Hamiltonian Monte Carlo

- ▶ *Hamiltonian* Monte Carlo is an enhanced variant of Metropolis-Hastings sampling
- ▶ Proposals are motivated by Hamiltonian dynamics
 - ▶ Borrowing ideas of “potential” and “kinetic” energy in physics
- ▶ Informed by first-order gradient of posterior at each step
 - ▶ Allows draws to move more quickly to regions of higher posterior probability
- ▶ Often improves on Gibbs or MH sampling for complex posteriors
- ▶ Default estimation approach for the [STAN software](#)
- ▶ For an overview see [this chapter](#) by RM Neal

Approximate Bayesian Computing (ABC)

- ▶ *Approximate Bayesian computing* simulates new data \mathbf{y}^* and assesses how well the simulated data fits the observed data \mathbf{y} .
- ▶ Let \mathbf{y} be discrete, with pmf specified by θ : $P(\mathbf{y} | \theta)$
- ▶ To draw from $p(\theta | \mathbf{y})$, consider the following algorithm:
 - ▶ Propose θ^* from prior $p(\theta)$
 - ▶ Draw \mathbf{y}^* from $P(\mathbf{y} | \theta^*)$
 - ▶ Accept θ^* if $\mathbf{y}^* = \mathbf{y}$
- ▶ The accepted θ^* represent direct draws from $p(\theta | \mathbf{y})$.

Approximate Bayesian Computing (ABC)

- ▶ If \mathbf{y} is continuous, accept θ^* if \mathbf{y}^* is “close” to \mathbf{y}
- ▶ E.g., if $\mathbf{y} \in \mathbb{R}^n$, accept if

$$\|\mathbf{y}^* - \mathbf{y}\|^2 < \epsilon$$

- ▶ Generally accepted θ^* yield draws from $p(\theta | \mathbf{y})$ as $\epsilon \rightarrow 0$
- ▶ Can be very inefficient – high rejection rates
 - ▶ Adaptive methods [like this approach](#) can help
- ▶ Only requires a way to generate samples \mathbf{y}^* given θ .
 - ▶ No need to fully specify the likelihood function $p(\mathbf{y} | \theta)$ or $P(\mathbf{y} | \theta)$
 - ▶ “likelihood-free”

Example: socks

- Given m socks are picked from laundry, and y are unique, how many pairs of socks are in the load?¹



¹Example motivated by: <http://www.sumsar.net/blog/2014/10/tiny-data-and-the-socks-of-karl-broman/>

Example: socks

- ▶ Let n_{pairs} be the total number of pairs of socks
- ▶ Uniform prior on $n_{\text{pairs}} \in \{6, \dots, 50\}$
- ▶ Observe $y = 9$ unique socks in first $m = 12$ taken out
- ▶ Would like to find the posterior $p(n_{\text{pairs}} | y)$
- ▶ Avoid specifying the likelihood $P(y | n_{\text{pairs}})$ directly

Example: socks

- ▶ ABC approach:
 - ▶ Draw n_{pairs}^* uniformly from $\{6, \dots, 50\}$
 - ▶ Simulate a sample of $m = 12$ socks without replacement from n_{pairs}^* pairs ($2 \times n_{\text{pairs}}^*$ total)
 - ▶ Compute number of unique socks y^*
 - ▶ If $y^* = 9$, consider n_{pairs}^* a draw from $p(n_{\text{pairs}} \mid y)$
- ▶ Repeat above algorithm for 50,000 proposed draws

[http:](http://www.ericfrazerlock.com/More_on_Posterior_Computation_Rcode1.r)

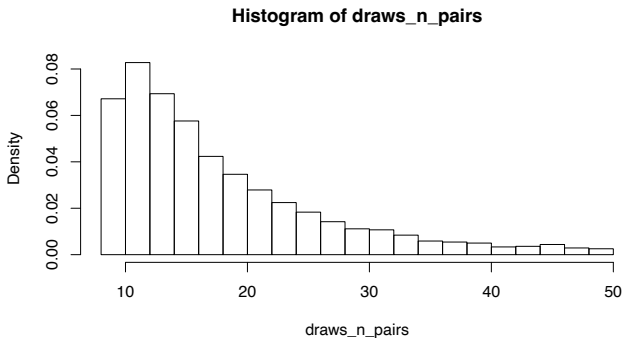
[//www.ericfrazerlock.com/More_on_Posterior_Computation_Rcode1.r](http://www.ericfrazerlock.com/More_on_Posterior_Computation_Rcode1.r)

```
m=12
y=9
T=50000
draws_n_pairs = c()
for(i in 1:T){
  n_pairs_star = sample(c(6:50),1)
  ## vector with two 1's, two 2's, etc.
  ##(each number represents a sock pair):
  sim_socks = rep(c(1:n_pairs_star),2)
  sock_sample = sample(sim_socks,m)
  y_star = length(unique(sock_sample))
  if(y_star==y) draws_n_pairs = c(draws_n_pairs,n_pairs_star)
}

hist(draws_n_pairs, freq=FALSE, breaks=20)

AcceptanceRate = length(draws_n_pairs)/T
```

Example: socks



- Acceptance rate: 0.11

Variational Bayes

- ▶ A *variational Bayes* algorithm approximates the posterior $p(\theta | \mathbf{y})$ by a *variational distribution* $q(\theta)$
- ▶ Where $q(\theta)$, or $q(\theta | \nu)$, represents a family of distributions, usually of simpler form than $p(\theta | \mathbf{y})$
- ▶ The approximation is determined by minimizing a distance $D(q, p)$
- ▶ In *mean-field variational Bayes* this distance is Kullback-Leibler divergence:

$$KL(q||p) = \int q(\theta) \log \frac{q(\theta)}{p(\theta | \mathbf{y})} d\theta$$

- ▶ For *expectation propagation*, the KL-divergence is reversed:
 $D = KL(p||q)$

Mean-field variational Bayes

- ▶ For mean-field variational Bayes we often assume the posterior can be factorized into M chunks:

$$q(\theta) = \prod_{i=1}^M q_i(\theta_i)$$

- ▶ Iteratively update q_i 's to maximize $KL(q||p)$
 - ▶ Uses the mean-field approximation and calculus of variations
 - ▶ Analogous to the EM-algorithm
- ▶ Converges to a local optimum
- ▶ For example, could optimize over

$$q(\theta_i) = N(\mu_i, \sigma_i^2)$$

Variational Bayes: Comments

- ▶ The accuracy of variational approximation q can depend on:
 - ▶ Appropriateness of simplifying assumptions on q
 - ▶ Convergence properties of the iterative algorithm - may converge to a local mode that is not close to optimal
- ▶ Variational techniques tend to underestimate posterior uncertainty.
- ▶ Could use variational techniques to initialize MCMC sampling
- ▶ For more information see [this tutorial](#) by C. Fox and S. Roberts