

MCMC Methods: Gibbs Sampling and the Metropolis-Hastings Algorithm

Patrick Lam

Outline

Introduction to Markov Chain Monte Carlo

Gibbs Sampling

The Metropolis-Hastings Algorithm

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Basically a fancy way of saying we can take quantities of interest of a distribution from simulated draws from the distribution.

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We can approximate the integrals via Monte Carlo Integration by simulating M values from $p(\theta)$ and calculating

$$\hat{I}_M = \frac{1}{M} \sum_{i=1}^M g(\theta^{(i)})$$

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We know this to be true from the Strong Law of Large Numbers.

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Let X_1, X_2, \dots be a sequence of **independent** and identically distributed random variables, each having a finite mean $\mu = E(X_i)$.

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But what if we can't generate draws that are **independent**?

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If we can sample slightly dependent draws using a **Markov chain**, then we can still find quantities of interests from those draws.

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$$p(\theta^{(t+1)} | \theta^{(1)}, \theta^{(2)}, \dots, \theta^{(t)}) = p(\theta^{(t+1)} | \theta^{(t)})$$

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The jumping rules are governed by a **transition kernel**, which is a mechanism that describes the probability of moving to some other state based on the current state.

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For continuous state space (infinite possible states), the transition kernel is a bunch of conditional PDFs: $f(\theta_j^{(t+1)}|\theta_i^{(t)})$

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4. At iteration t , our distribution $\Pi^{(t)}$ (from which $\theta^{(t)}$ is drawn) is $\Pi^{(t)} = \Pi^{(t-1)} \times \mathbf{P} = \Pi^{(0)} \times \mathbf{P}^t$

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For all the MCMC algorithms we use in Bayesian statistics, the Markov chain will typically **converge** to π regardless of our starting points.

So if we can devise a Markov chain whose stationary distribution π is our desired posterior distribution $p(\theta|y)$, then we can run this chain to get draws that are approximately from $p(\theta|y)$ once the chain has converged.

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As a matter of practice, most people throw out a certain number of the first draws, known as the **burn-in**. This is to make our draws closer to the stationary distribution and less dependent on the starting point.

However, it is unclear how much we should **burn-in** since our draws are all slightly dependent and we don't know exactly when convergence occurs.

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Luckily, we have the **Ergodic Theorem**.

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But what does it mean for a chain to be *aperiodic*, *irreducible*, and *positive recurrent*, and therefore ergodic?

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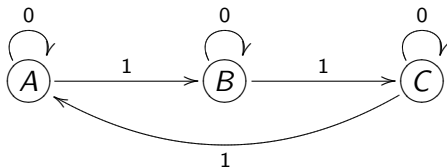
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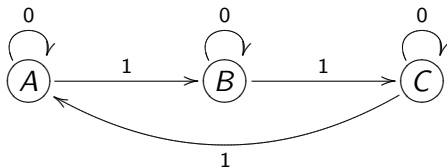
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As long as the chain is not repeating an identical cycle, then the chain is **aperiodic**.

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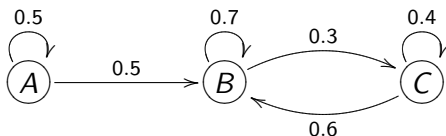
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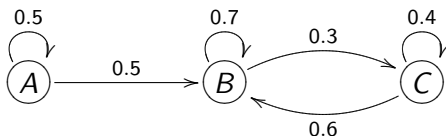
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The chain is not irreducible because we cannot get to A from B or C regardless of the number of steps we take.

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So if our Markov chain is **aperiodic**, **irreducible**, and **positive recurrent** (all the ones we use in Bayesian statistics usually are), then it is ergodic and the ergodic theorem allows us to do Monte Carlo Integration by calculating quantities of interest from our draws, ignoring the dependence between draws.

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- ▶ Shown to increase the variance of your Monte Carlo estimates.

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In Bayesian statistics, there are generally two MCMC algorithms that we use: the Gibbs Sampler and the Metropolis-Hastings algorithm.

Outline

Introduction to Markov Chain Monte Carlo

Gibbs Sampling

The Metropolis-Hastings Algorithm

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How can we know the joint distribution simply by knowing the full conditional distributions?

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But how do we figure out the full conditionals?

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4. Repeat steps 2 and 3 for all parameter blocks.

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Our result is a Markov chain with a bunch of draws of θ that are approximately from our posterior. We can do Monte Carlo Integration on those draws to get quantities of interest.

An Example (Robert and Casella, 10.17)¹

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Our likelihood is $\prod_{i=1}^{10} \text{Poisson}(\lambda_i t_i)$.

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$$p(\lambda, \beta | \mathbf{y}, \mathbf{t}) \propto \left(\prod_{i=1}^{10} \text{Poisson}(\lambda_i t_i) \times \text{Gamma}(\alpha, \beta) \right) \times \text{Gamma}(\gamma, \delta)$$

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 p(\lambda_i | \lambda_{-i}, \beta, \mathbf{y}, \mathbf{t}) &\propto \lambda_i^{y_i + \alpha - 1} e^{-(t_i + \beta) \lambda_i} \\
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```
> beta.update <- function(alpha, gamma, delta, lambda, y) {  
+   rgamma(1, length(y) * alpha + gamma, delta + sum(lambda))  
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6. Make it into a function.

```

> gibbs <- function(n.sims, beta.start, alpha, gamma, delta,
+   y, t, burnin = 0, thin = 1) {
+   beta.draws <- c()
+   lambda.draws <- matrix(NA, nrow = n.sims, ncol = length(y))
+   beta.cur <- beta.start
+   lambda.update <- function(alpha, beta, y, t) {
+     rgamma(length(y), y + alpha, t + beta)
+   }
+   beta.update <- function(alpha, gamma, delta, lambda,
+     y) {
+     rgamma(1, length(y) * alpha + gamma, delta + sum(lambda))
+   }
+   for (i in 1:n.sims) {
+     lambda.cur <- lambda.update(alpha = alpha, beta = beta.cur,
+       y = y, t = t)
+     beta.cur <- beta.update(alpha = alpha, gamma = gamma,
+       delta = delta, lambda = lambda.cur, y = y)
+     if (i > burnin & (i - burnin)%%thin == 0) {
+       lambda.draws[(i - burnin)/thin, ] <- lambda.cur
+       beta.draws[(i - burnin)/thin] <- beta.cur
+     }
+   }
+   return(list(lambda.draws = lambda.draws, beta.draws = beta.draws))
+ }

```

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```
> posterior <- gibbs(n.sims = 10000, beta.start = 1, alpha = 1.8,  
+   gamma = 0.01, delta = 1, y = y, t = t)  
> colMeans(posterior$lambda.draws)  
  
[1] 0.07113 0.15098 0.10447 0.12321 0.65680 0.62212 0.86522 0.85465  
[9] 1.35524 1.92694  
  
> mean(posterior$beta.draws)  
  
[1] 2.389  
  
> apply(posterior$lambda.draws, 2, sd)  
  
[1] 0.02759 0.08974 0.04012 0.03071 0.30899 0.13676 0.55689 0.54814  
[9] 0.60854 0.40812  
  
> sd(posterior$beta.draws)  
  
[1] 0.6986
```

Outline

Introduction to Markov Chain Monte Carlo

Gibbs Sampling

The Metropolis-Hastings Algorithm

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If all else fails, we can use the **Metropolis-Hastings** algorithm, which will always work.

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3. Compute an acceptance ratio (probability):

$$r = \frac{p(\theta^*|\mathbf{y})/J_t(\theta^*|\theta^{(t-1)})}{p(\theta^{(t-1)}|\mathbf{y})/J_t(\theta^{(t-1)}|\theta^*)}$$

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5. Repeat steps 2-4 M times to get M draws from $p(\theta|\mathbf{y})$, with optional burn-in and/or thinning.

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Otherwise, we are starting with a value that cannot be drawn.

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Generally speaking, chain will behave well only if the jumping distribution has heavier tails than the posterior.

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Note that since r is a ratio, we only need $p(\theta|\mathbf{y})$ *up to a constant of proportionality* since $p(\mathbf{y})$ cancels out in both the numerator and denominator.

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For example, if we are very likely to jump to some $\boldsymbol{\theta}^*$, then $J_t(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(t-1)})$ is likely to be high, so we should accept less of them than some other $\boldsymbol{\theta}^*$ that we are less likely to jump to.

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In the case of independent Metropolis-Hastings sampling,

$$r = \frac{p(\boldsymbol{\theta}^*|\mathbf{y})/J_t(\boldsymbol{\theta}^*)}{p(\boldsymbol{\theta}^{(t-1)}|\mathbf{y})/J_t(\boldsymbol{\theta}^{(t-1)})}$$

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Unlike in rejection sampling, each iteration always produces a draw, either θ^* or $\theta^{(t-1)}$.

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- ▶ random walk: somewhere between 0.25 and 0.50 is recommended
- ▶ independent: something close to 1 is preferred

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```
> mh.gamma <- function(n.sims, start, burnin, cand.sd, shape, rate) {  
+   theta.cur <- start  
+   draws <- c()  
+   theta.update <- function(theta.cur, shape, rate) {  
+     theta.can <- rnorm(1, mean = theta.cur, sd = cand.sd)  
+     accept.prob <- dgamma(theta.can, shape = shape, rate = rate)/dgamma(theta.cur,  
+       shape = shape, rate = rate)  
+     if (runif(1) <= accept.prob)  
+       theta.can  
+     else theta.cur  
+   }  
+   for (i in 1:n.sims) {  
+     draws[i] <- theta.cur <- theta.update(theta.cur, shape = shape,  
+       rate = rate)  
+   }  
+   return(draws[(burnin + 1):n.sims])  
+ }  
> mh.draws <- mh.gamma(10000, start = 1, burnin = 1000, cand.sd = 2,  
+   shape = 1.7, rate = 4.4)
```