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 $X_1, X_2, \ldots$ 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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$$p(\boldsymbol{\theta}^{(t+1)}|\boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)}, \ldots, \boldsymbol{\theta}^{(t)}) = p(\boldsymbol{\theta}^{(t+1)}|\boldsymbol{\theta}^{(t)})$$

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What are the rules governing how the chain jumps from one state to another at each period?

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: $f(\boldsymbol{\theta}_{\mathbf{j}}^{(t+1)} \mid \boldsymbol{\theta}_{\mathbf{i}}^{(t)})$

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

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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 $p(\boldsymbol{\theta}|y)$, then we can run this chain to get draws that are approximately from $p(\boldsymbol{\theta}|y)$ once the chain has converged.

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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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Let $\boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)}, \ldots, \boldsymbol{\theta}^{(M)}$ be M values from a Markov chain that is *aperiodic*, *irreducible*, and *positive recurrent* (then the chain is ergodic), and $E[g(\boldsymbol{\theta})] < \infty$.

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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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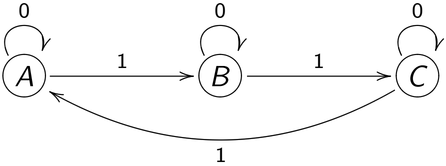

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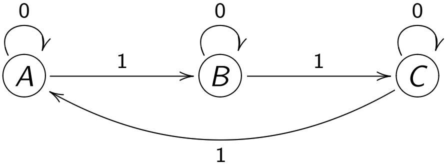

As long as the chain is not repeating an identical cycle, then the chain is **aperiodic**.

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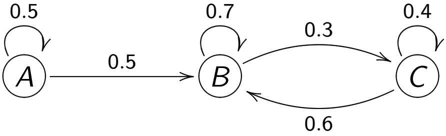

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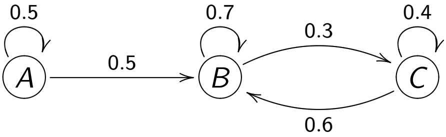

The chain is not irreducible because we cannot get to A from B or C regardless of the number of steps we take.

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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 $\boldsymbol{\theta}$ that are approximately from our posterior. We can do Monte Carlo Integration on those draws to get quantities of interest.

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

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Finding the full conditionals:

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> beta.update <- function(alpha, gamma, delta, lambda, y) {
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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

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

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5. Repeat steps 2-4 M times to get M draws from $p(\boldsymbol{\theta}|\mathbf{y})$, 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 $p(\boldsymbol{\theta}|\mathbf{y})$ *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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$$r = \frac{p(\boldsymbol{\theta}^*|\mathbf{y})/J_t(\boldsymbol{\theta}^*)}{p(\boldsymbol{\theta}^{(t-1)}|\mathbf{y})/J_t(\boldsymbol{\theta}^{(t-1)})}$$

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

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If your acceptance rate is too high, the chain is probably not mixing well (not moving around the parameter space quickly enough).

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What is too high and too low depends on your specific algorithm, but generally

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

A Simple Example

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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)
```