Rejection Sampling

Example. In the spring of 1993 a survey was taken of **bicycle** and other **traffic** in the vicinity of the University of California, Berkeley, campus (Gelman et al. 1995).

As part of this survey 10 city blocks on **residential** streets with **bike routes** were chosen at random from all such blocks at Berkeley; on one of those blocks n vehicles were observed on a randomly chosen **Tuesday afternoon from 3 to 4pm**, and s of them were bicycles.

To draw inferences about the underlying **proportion θ of bicycle traffic** (PBT) on blocks similar to this one at times similar to Tuesday afternoons from 3 to 4pm, it's natural (as in the AMI mortality case study) to employ the **model**

$$\left\{ \begin{array}{c} \theta \sim \text{Beta}(\alpha_0, \beta_0) \\ (S|\theta) \sim \text{Binomial}(n, \theta) \end{array} \right\} \rightarrow (\theta|s) \sim \text{Beta}(\alpha_0 + s, \beta_0 + n - s), \tag{6}$$

provided that whatever **prior information** I have about θ can be meaningfully captured in the **Beta** family.

After **reflection** I realize that I'd be quite surprised if the PBT in residential city blocks with bike routes in Berkeley on Tuesday afternoons from 3 to 4pm was **less than 5%** or **greater than 50%**.

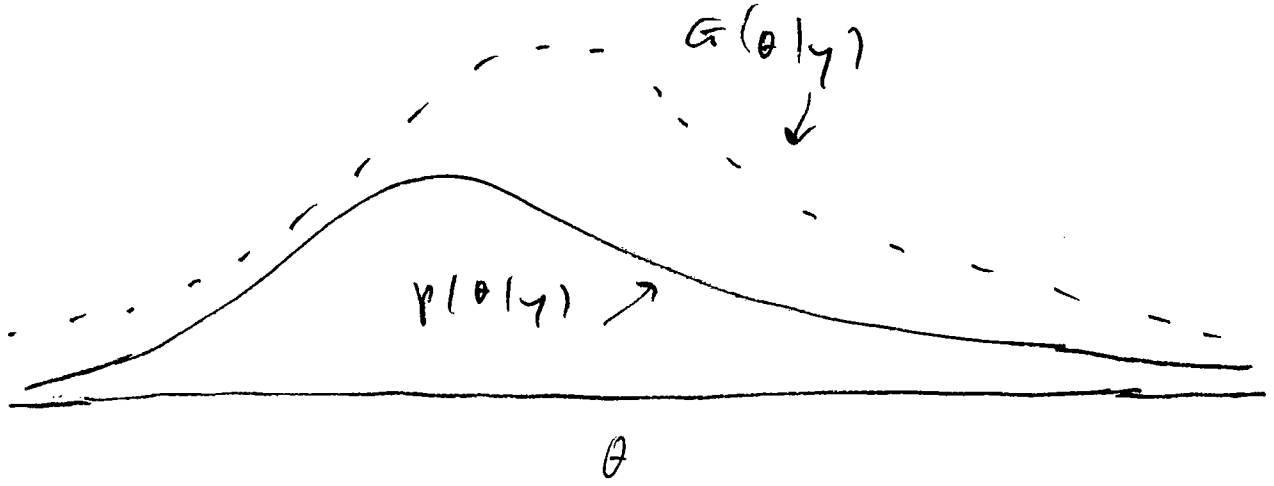
Making this operational by assuming that in the prior $p(0.05 \leq \theta \leq 0.5) = \mathbf{0.9}$, and putting **half** of the remaining prior probability in each of the **left** and **right tails** of the Beta distributions, yields (via numerical methods similar to those in the AMI case study) $(\alpha_0, \beta_0) =$ **(2.0, 6.4)** (this Beta distribution has prior mean and SD **0.24** and **0.14**, respectively).

In the city block in question the **data** came out $(n, s) =$ **(74, 16)**, so that the data mean was **0.216**, and the posterior is then $\text{Beta}(\alpha_0 + s, \beta_0 + n - s) =$ **Beta(18.0, 64.4)**.

Rejection Sampling (continued)

Pretend for the sake of illustration of **rejection sampling** that you didn't know the formulas for the mean and SD of a Beta distribution, and suppose that you wanted to use **IID Monte Carlo sampling** from the Beta$(\alpha_0 + s, \beta_0 + n - s) =$ posterior to estimate the **posterior mean**.

Here is von Neumann's basic idea: suppose the target density $p(\theta|y)$ is **difficult** to sample from, but you can find an integrable **envelope function** $G(\theta|y)$ such that (a) G **dominates** p in the sense that $G(\theta|y) \geq p(\theta|y) \geq 0$ for all θ and (b) the density g obtained by normalizing G—later to be called the **proposal distribution**—is easy and fast to sample from.



Then to get a **random draw** from p, make a draw θ^* from g instead and **accept** or **reject** it according to an **acceptance probability** $\alpha_R(\theta^*|y)$; if you **reject** the draw, **repeat** this process until you accept.

von Neumann showed that the **choice**

$$\alpha_R(\theta^*|y) = \frac{p(\theta^*|y)}{G(\theta^*|y)} \tag{7}$$

correctly produces IID draws from p, and you can **intuitively** see that he's right by the following argument.

Rejection Sampling (continued)

Making a **draw** from the posterior distribution of interest is like choosing a point **at random** (in two dimensions) under the density curve $p(\theta|y)$ in such a way that **all possible points are equally likely**, and then writing down its θ value.

If you instead draw from G so that all points under G are equally likely, to get **correct** draws from p you'll need to throw away any point that falls between p and G, and this can be accomplished by **accepting** each sampled point θ^* with probability $\frac{p(\theta^*|y)}{G(\theta^*|y)}$, as von Neumann said.

A **summary** of this method is as follows.

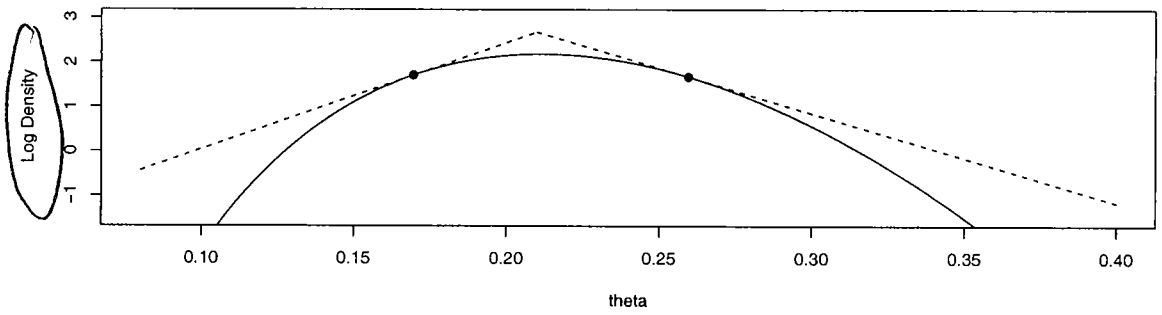
Algorithm (rejection sampling). To make m draws at random from the density $p(\theta|y)$ for real-valued θ, select an integrable **envelope function** G—which when normalized to integrate to 1 is the **proposal distribution** g—such that $G(\theta|y) \geq p(\theta|y) \geq 0$ for all θ; define the acceptance probability $\alpha_R(\theta^*|y) = \frac{p(\theta^*|y)}{G(\theta^*|y)}$; and

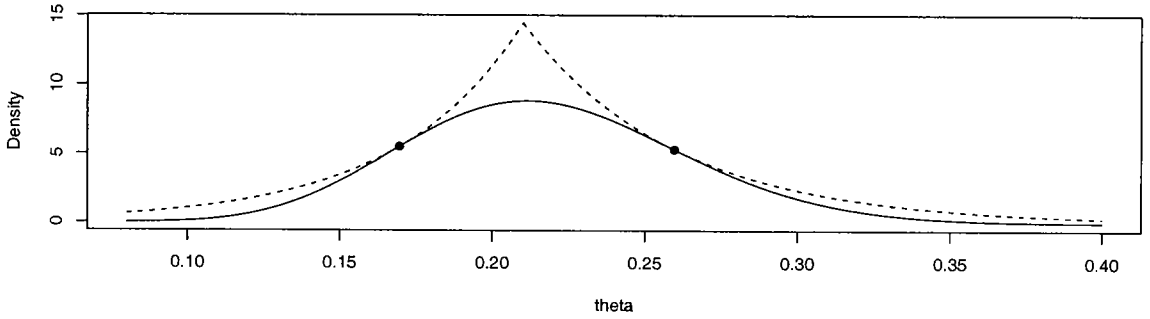
```
Initialize t ← 0
Repeat {
  Sample θ* ~ g(θ|y)
  Sample u ~ Uniform(0, 1)
  If u ≤ α_R(θ*|y) then
    { θ_{t+1} ← θ*; t ← (t + 1) }
}
until t = m.
```

(8)

The **figure** below demonstrates this method on the Beta(18.0, 64.4) density arising in the **Beta-Bernoulli example** above.

Rejection Sampling (continued)





Rejection sampling permits considerable **flexibility** in the choice of **envelope function**; here, borrowing an idea from Gilks and Wild (1992), I've noted that the relevant Beta density is **log concave** (a real-valued function is log concave if its **second derivative** on the log scale is **everywhere non-positive**), meaning that it's easy to construct an envelope on that scale in a **piecewise linear** fashion, by choosing points on the log density and constructing **tangents** to the curve at those points.

The **simplest** possible such envelope involves **two line segments**, one on either side of the **mode**.

The **optimal** choice of the tangent points would maximize the marginal **probability of acceptance** of a draw in the rejection algorithm, which can be shown to be

$$\left[\int G(\theta)\, d\theta\right]^{-1}; \tag{9}$$

Rejection Sampling (continued)

in other words, you should **minimize** the area under the (un-normalized) envelope function subject to the constraint that it **dominates** the target density $p(\theta|y)$.

Here this optimum turns out to be attained by locating the two tangent points at about **0.17** and **0.26**, as in the figure above; the resulting acceptance probability of about **0.75** could clearly be **improved** by adding more tangents.

Piecewise linear envelope functions on the log scale are a **good choice** because the resulting envelope density on the raw scale is a piecewise set of **scaled exponential distributions** (see the bottom panel in the figure above), from which random samples can be taken **quickly**.

A **preliminary** sample of $m_0 = 500$ IID draws from the Beta(18.0, 64.4) distribution using the above rejection sampling method yields $\bar{\theta}^* = \mathbf{0.2197}$ and $\hat{\sigma} = \mathbf{0.04505}$, meaning that the posterior mean has already been estimated with an **MCSE** of only $\frac{\hat{\sigma}}{\sqrt{m_0}} = 0.002$ even with just **500** draws.

Suppose, however, that—as in equation (4) above—I want $\bar{\theta}^*$ to **differ** from the true posterior mean μ by no more than some (perhaps even smaller) **tolerance** ϵ_1 with Monte Carlo probability at least $(1 - \epsilon_2)$; then equation (5) tells me how long to **monitor** the simulation output.

For instance, to pin down **three significant figures** (sigfigs) in the posterior mean in this example with high Monte Carlo accuracy I might take $\epsilon_1 = 0.0005$ and $\epsilon_2 = 0.05$, which yields a **recommended IID sample size** of $\frac{(0.04505^2)(1.96)^2}{0.0005^2} \doteq 31,200$.

Rejection Sampling (continued)

So I take another sample of **30,700** (which is virtually instantaneous at 550 Unix MHz) and **merge** it with the 500 draws I already have; this yields $\bar{\theta}^* = 0.21827$ and $\hat{\sigma} = 0.04528$, meaning that the **MCSE** of this estimate of μ is $\frac{0.04528}{\sqrt{31200}} \doteq 0.00026$.

I might **announce** that I think $E(\theta|y)$ is about **0.2183**, give or take about **0.0003**, which accords well with the true value **0.2184**.

Of course, **other aspects** of $p(\theta|y)$ are equally easy to monitor; for example, if I want a Monte Carlo estimate of $p(\theta \leq q|y)$ for some q, as noted above I just work out the **proportion** of the sampled θ^* values that are no larger than q.

Or, even better, I recall that $P(A) = E[I(A)]$ for any event or proposition A, so to the MC data set consisting of 31,200 rows and one column (the θ_t^*) I add a column monitoring the values of the **derived variable** which is 1 whenever $\theta_t^* \leq q$ and 0 otherwise; the **mean** of this derived variable is the Monte Carlo estimate of $p(\theta \leq q|y)$, and I can attach an **MCSE** to it in the same way I did with $\bar{\theta}^*$.

By this approach, for instance, the **Monte Carlo estimate** of $p(\theta \leq 0.15|y)$ based on the 31,200 draws examined above comes out $\hat{p} =$ **0.0556** with an MCSE of **0.0013**.

Percentiles are typically harder to pin down with equal Monte Carlo accuracy (in terms of sigfigs) than means or SDs, because the 0/1 scale on which they're based is **less information-rich** than the θ^* scale itself; if I wanted an MCSE for $\hat{p}$ of 0.0001 I would need an IID sample of more than **5 million draws** (which would still only take a **few seconds** at contemporary workstation speeds).

Beyond Rejection Sampling

IID sampling is not necessary. Nothing in the Metropolis-Ulam idea of Monte Carlo estimates of posterior summaries requires that these estimates be based on **IID samples from the posterior**.

This is lucky, because in practice it's often difficult, particularly when θ is a **vector of high dimension** (say k), to figure out how to make such an IID sample, via rejection sampling or other methods (e.g., imagine trying to find an **envelope function** for $p(\theta|y)$ when k is 10 or 100 or **1,000**).

Thus it's necessary to **relax** the assumption that $\theta_j^* \overset{\text{IID}}{\sim} p(\theta|y)$, and to consider samples $\theta_1^*, \ldots, \theta_m^*$ that form a **time series**: a series of draws from $p(\theta|y)$ in which θ_j^* may **depend on** $\theta_{j'}^*$ for $j' < j$.

In their pioneering paper Metropolis et al. (1953) allowed for **serial dependence** of the θ_j^* by combining von Neumann's idea of rejection sampling (which had itself only been published a few years earlier in 1951) with concepts from a subject in the theory of **stochastic processes** called **Markov chains**.

Combining **Monte Carlo sampling** with **Markov chains** gives rise to the name now used for this technique for solving the Bayesian high-dimensional integration problem: **Markov chain Monte Carlo** (MCMC).

Markov Chains

Markov chains. A **stochastic process** is just a collection of random variables $\{\theta_t^*, t \in T\}$ for some **index set** T, usually meant to stand for **time**.

In practice T can be either **discrete**, e.g., $\{0, 1, \ldots\}$, or **continuous**, e.g., $[0, \infty)$.

Markov chains are a special kind of stochastic process that can either unfold in discrete or continuous time—we'll talk here about **discrete-time Markov chains**, which is all you need for MCMC.

The **possible values** that a stochastic process can take on are collectively called the **state space** S of the process—in the simplest case S is **real-valued** and can also either be discrete or continuous.

Intuitively speaking, a Markov chain (e.g., Feller, 1968; Roberts, 1996; Gamerman, 1997) is a stochastic process unfolding in time in such a way that the **past and future states of the process are independent given the present state**—in other words, to figure out where the chain is likely to go next you don't need to pay attention to where it's been, you just need to consider **where it is now**.

More formally, a stochastic process $\{\theta_t^*, t \in T\}$, $T = \{0, 1, \ldots\}$, with state space S is a **Markov chain** if, for any set $A \in S$,

$$P(\theta_{t+1}^* \in A | \theta_0^*, \ldots, \theta_t^*) = P(\theta_{t+1}^* \in A | \theta_t^*). \qquad (10)$$

The theory of Markov chains is **harder mathematically** if S is continuous (e.g., Tierney, 1996), which is what we need for MCMC with real-valued parameters, but **most of the main ideas emerge with discrete state spaces**, and I'll assume discrete S in the intuitive discussion here.

Markov Chains (continued)

Example. For a simple example of a **discrete-time Markov chain** with a **discrete state space**, imagine a **particle** that moves around on the integers $\{\ldots, -2, -1, 0, 1, 2, \ldots\}$, starting at 0 (say).

Wherever it is at time t—say at i—it **tosses a (3-sided) coin** and moves to $(i-1)$ with probability p_1, stays at i with probability p_2, and moves to $(i+1)$ with probability p_3, for some $0 < p_1, p_2, p_3 < 1$ with $p_1 + p_2 + p_3 = 1$—these are the **transition probabilities** for the process.

This is called a **random walk** (on the integers), and it's **clearly a Markov chain**.

Nice behavior. The most **nicely-behaved** Markov chains satisfy **three properties**:

- They're **irreducible**, which basically means that no matter where it starts the chain has to be able to reach any other state in a finite number of iterations with positive probability;

- They're **aperiodic**, meaning that for all states i the set of possible **sojourn times**, to get back to i having just left it, can have no divisor bigger than 1 (this is a **technical** condition; periodic chains still have some nice properties, but the nicest chains are aperiodic).

- They're **positive recurrent**, meaning that (a) for all states i, if the process starts at i it will return to i with probability 1, and (b) the expected length of waiting time til the first return to i is finite.

Notice that this is a bit delicate: wherever the chain is now, we insist that it **must certainly come back here**, but we don't expect to have to **wait forever** for this to happen.

Markov Chains (continued)

The random walk defined above is clearly **irreducible** and **aperiodic**, but it may not be **positive recurrent** (depending on the p_i): it's true that it has positive probability of returning to wherever it started, but (because S is **unbounded**) this probability may not be 1, and on average you may have to wait forever for it to return.

We can fix this by **bounding** S: suppose instead that $S = \{-k, -(k-1), \ldots, -1, 0, 1, \ldots, k\}$, keeping the same transition probabilities except **rejecting** any moves **outside the boundaries** of S.

This bounded random walk now satisfies **all three of the nice properties**.

The value of nice behavior. Imagine running the bounded random walk for a long time, and look at the **distribution** of the **states** it visits—over time this distribution should **settle down** (converge) to a kind of limiting, **steady-state** behavior.

This can be demonstrated by **simulation**, for instance in R, and using the **bounded random walk** as an example:

```
rw.sim <- function( k, p, theta.start, n.sim, seed ) {

  set.seed( seed )

  theta <- rep( 0, n.sim + 1 )

  theta[ 1 ] <- theta.start

  for ( i in 1:n.sim ) {

    theta[ i + 1 ] <- move( k, p, theta[ i ] )

  }

  return( table( theta ) )

}
```

Markov Chain Simulation

```
move <- function( k, p, theta ) {

  repeat {

    increment <- sample( x = c( -1, 0, 1 ), size = 1, prob = p )

    theta.next <- theta + increment

    if ( abs( theta.next ) <= k ) {

      return( theta.next )

      break

    }

  }

}
```

```
rosalind 17> R

R : Copyright 2001, The R Development Core Team
Version 1.2.1  (2001-01-15)

> p <- c( 1, 1, 1 ) / 3

> k <- 5

> theta.start <- 0

> seed <- c( 6425451, 9626954 )

> rw.sim( k, p, theta.start, 10, seed )

theta
0 1 2
5 5 1

> rw.sim( k, p, theta.start, 100, seed )

-2 -1  0  1  2  3  4  5
 7  9 16 17 23 14  8  7
```

Simulation (continued)

```
> rw.sim( k, p, theta.start, 1000, seed )

 -5  -4  -3  -2  -1   0   1   2   3   4   5
 65 115 123 157 148 123 106  82  46  21  15

> rw.sim( k, p, theta.start, 10000, seed )

  -5   -4   -3   -2   -1    0    1    2    3    4    5
 581  877  941  976  959 1034 1009  982 1002  959  681

> rw.sim( k, p, theta.start, 100000, seed )

  -5   -4   -3   -2   -1    0    1    2    3    4    5
6515 9879 9876 9631 9376 9712 9965 9749 9672 9352 6274

> rw.sim( k, p, theta.start, 1000000, seed )

   -5    -4    -3    -2    -1     0     1     2     3     4     5
65273 98535 97715 96708 95777 96607 96719 96361 96836 95703 63767
```

You can see that the distribution of where the chain has visited is **converging** to something close to **uniform** on $\{-5,-4,\ldots,4,5\}$, except for the effects of the **boundaries**.

Letting q_1 denote the **limiting** probability of being in one of the 9 **non-boundary** states $(-4,-3,\ldots,3,4)$ and q_2 be the **long-run** probability of being in one of the 2 **boundary** states $(-5,5)$, on grounds of **symmetry** you can guess that q_1 and q_2 should satisfy

$$9q_1 + 2q_2 = 1 \quad \text{and} \quad q_1 = \frac{3}{2}q_2, \tag{11}$$

from which $(q_1, q_2) = \left(\frac{3}{31}, \frac{2}{31}\right) \doteq (0.096774, 0.064516)$.

Based on the run of **1,000,001 iterations** above we would estimate these probabilities **empirically** as

$$\left[\frac{98535+\ldots+95703}{(9)(1000001)}, \frac{65273+63767}{(2)(1000001)}\right] \doteq (0.096773, 0.064520).$$

Simulation (continued)

It should also be clear that the limiting distribution **does not depend** on the initial value of the chain:

```
> rw.sim( k, p, 5, 100000, seed )

  -5   -4   -3   -2   -1    0    1    2    3    4    5
6515 9879 9876 9624 9374 9705 9959 9738 9678 9365 6288
```

Of course, you get a **different limiting distribution** with a **different choice of** (p_1, p_2, p_3):

```
> p <- c( 0.2, 0.3, 0.5 )

> rw.sim( k, p, 0, 10, seed )

0 1 2 3
1 3 4 3

> rw.sim( k, p, 0, 100, seed )

 0  1  2  3  4  5
 1  3  6 13 30 48

> rw.sim( k, p, 0, 1000, seed )

  0   1   2   3   4   5
  1  18  71 157 336 418

> rw.sim( k, p, 0, 10000, seed )

  -5   -4   -3   -2   -1    0    1    2    3    4    5
   5   16   19   30   28   74  215  583 1344 3470 4217

> rw.sim( k, p, 0, 100000, seed )

   -5    -4    -3    -2    -1     0     1     2     3     4     5
    5    22    53   132   302   834  2204  5502 13489 34460 42998

> rw.sim( k, p, 0, 1000000, seed )
-5     -4     -3     -2     -1      0      1      2      3      4      5
61    198    511   1380   3398   8591  22117  54872 137209 343228 428436
```

Stationary Distributions

A positive recurrent and aperiodic chain is called **ergodic**, and it turns out that such chains possess a unique **stationary** (or **equilibrium**, or **invariant**) distribution π, characterized by the relation

$$\pi(j) = \sum_i \pi(i) P_{ij}(t) \tag{12}$$

for all states j and times $t \geq 0$, where $P_{ij}(t) = P(\theta_t^* = j | \theta_0^* = i)$ is the **transition matrix** of the chain.

Informally, the stationary distribution characterizes the **behavior that the chain will settle into** after it's been run for a long time, regardless of its initial state.

The point of all of this. Given a parameter vector θ and a data vector y, the Metropolis et al. (1953) idea is to **simulate** random draws from the posterior distribution $p(\theta|y)$, by constructing a **Markov chain** with the following three properties:

- It should have the **same state space** as θ,
- It should be **easy to simulate from**, and
- Its **equilibrium distribution** should be $p(\theta|y)$.

If you can do this, you can run the Markov chain for a long time, generating a huge sample from the posterior, and then use **simple descriptive summaries** (means, SDs, correlations, histograms or kernel density estimates) to extract any features of the posterior you want.

The Ergodic Theorem

The mathematical fact that underpins this strategy is the **ergodic theorem**: if the Markov chain $\{\theta_t^*\}$ is ergodic and f is any real-valued function for which $E_\pi|f(\theta)|$ is finite, then with probability 1

$$\frac{1}{M}\sum_{t=1}^{M} f(\theta_t^*) \to E_\pi[f(\theta)] = \sum_i f(i)\,\pi(i), \qquad (13)$$

in which the right side is just the **expectation** of $f(\theta)$ under the stationary distribution π.

In plain English this means that—as long as the stationary distribution **is** $p(\theta|y)$—you can learn (to arbitrary accuracy) about things like posterior means, SDs, and so on just by **waiting for stationarity to kick in** and **monitoring** thereafter **for a long enough period**.

Of course, as Roberts (1996) notes, the theorem is **silent** on the two key practical questions it raises: **how long you have to wait** for stationarity, and **how long to monitor** after that.

A third practical issue is what to use for the **initial value** θ_0^*: intuitively the **closer** θ_0^* is to the **center** of $p(\theta|y)$ the **less time** you should have to wait for stationarity.

The standard way to deal with **waiting for stationarity** is to (a) run the chain from a **good starting value** θ_0^* for B iterations, until **equilibrium** has been reached, and (b) **discard** this initial **burn-in** period.

All of this motivates the topic of **MCMC diagnostics**, which are intended to answer the following questions:

- What should I use for the **initial value** θ_0^*?
- How do I know when I've reached **equilibrium**? (This is equivalent to asking **how big** B should be.)
- Once I've reached equilibrium, how big should M be, i.e., how long should I **monitor the chain** to get posterior summaries with **decent accuracy**?