Bayesian Modeling, Inference and Prediction

3a: Simulation-Based Computation

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3.1 Continuous Outcomes

Part 2 examined the modeling of **binary outcomes**, where the judgment of **exchangeability** and **de Finetti's Theorem for 1s and 0s** leads to a **Bernoulli/binomial likelihood** with a **single parameter** $\theta \in (0, 1)$; it was **convenient** (but not necessary) to employ a **conjugate** Beta prior distribution for θ.

For outcomes that live on the **entire real line** $\mathbb{R}$ there's an analogue of **de Finetti's Theorem** that's **equally central** to Bayesian model-building (e.g., Draper 2007):

Representation of exchangeable predictive distributions for continuous observables (de Finetti 1937): If I'm willing to regard $(y_1, \dots, y_n)$ as the first n terms in an infinitely exchangeable sequence $(y_1, y_2, \dots)$ of continuous values on $\mathbb{R}$, then

- $F(t) = \lim_{n \to \infty} F_n(t)$ must exist for all t and must be a valid CDF, where F_n is the **empirical CDF** based on $(y_1, \dots, y_n)$ (i.e., $F_n(t) = \frac{1}{n} \sum_{i=1}^{n} I(y_i \le t)$, in which $I(A)$ is the indicator function (1 if A is true, otherwise 0)), and the marginal distribution (given F) for each of the y_i must be $(y_i | F) \sim F$;

de Finetti's Theorem For Continuous Outcomes

- $G(F) = \lim_{n \to \infty} P(F_n)$ must also exist, where P is my **joint probability distribution** on $(y_1, y_2, \ldots)$; and $p(y_1, \ldots, y_n)$ can be expressed as

$$p(y_1, \ldots, y_n) = \int_{\mathcal{F}} \prod_{i=1}^{n} F(y_i) \, dG(F), \tag{1}$$

  where $\mathcal{F}$ is the space of **all possible CDFs** on $\mathbb{R}$.

Equation (1) says informally that **exchangeability** of my uncertainty about an observable process unfolding on the real line is **functionally equivalent** to assuming the **Bayesian hierarchical model**

$$\begin{array}{ccc} F & \sim & p(F) \\ (y_i|F) & \stackrel{\text{IID}}{\sim} & F, \end{array} \tag{2}$$

where $p(F)$ is a **prior distribution** on $\mathcal{F}$.

This prior makes the continuous form of de Finetti's Theorem **considerably harder to apply**: to take the elicitation task seriously is to try to specify a probability distribution on a **function space** (F is in effect an **infinite-dimensional** parameter).

Data-Analytic Model-Building

(**NB** This task is not unique to Bayesians — it's equivalent to asking **"Where does the likelihood come from?"** in frequentist analyses of observational data.)

What people often do in practice is to appeal to considerations that narrow down the field, such as an **a priori** judgment that the Y_i ought to be **symmetrically** distributed about a measure of center μ, and then try to use a fairly **rich parametric family** satisfying (e.g.) the symmetry restriction as a substitute for all of $\mathcal{F}$.

A **standard approach** to **model-building**, in fact, is to **choose** this **parametric family** by **looking at the data** to make the **most plausible choice** — let's call this the data-analytic approach.

From the **Bayesian** point of view this is **incoherent**: it amounts to **using the data** to **specify** the prior on $\mathcal{F}$ and then **using the same data** to **update** that prior.

Failing to acknowledge the **data-driven search** through the space $\mathcal{M}$ of **all possible models** will typically result in an **under-assessment** of

Model Uncertainty

model uncertainty (e.g., Draper 1995), and this will manifest itself in **poor calibration**: **inferential** and **predictive** intervals that are **narrower** than they should be.

This is a **modeling dilemma** for both **frequentists** and **Bayesians**; from the **Bayesian** viewpoint, not looking at the data to specify the prior on $\mathcal{F}$ can permit the data to **surprise** me in ways that would make me want to go back and **revise** my prior (this is an example of **Cromwell's Rule** in action: if A is a **proposition** of unknown truth value to me and D is a data set I'll collect in the future that's relevant to A, if I set $P(A) = 0$ (or 1) then $P(A|D) = 0$ (or 1) **no matter how the data set D comes out**).

I'm aware of **two potential ways out of this dilemma**:

- a **Bayesian** form of **cross-validation** (3CV: Draper and Krnjajić 2007), in which I **look at the data** to specify $p(F)$ but I do so in a way that **pays the appropriate price** for this "cheating"; and

- **Bayesian non-parametric** (BNP) modeling, which involves constructing **prior distributions on CDFs** in a way that **avoids the Cromwell's**

3CV

Rule dilemma by (in a particular technical sense) **not placing prior probability 0 on anything**.

$\boxed{\textbf{3CV in detail:}}$ Taking the usual **cross-validation** idea **one step further**,

(1) Partition data at random into *three* (non-overlapping and exhaustive) subsets S_i.

(2) Fit tentative {likelihood + prior} to S_1; **expand** initial model in all feasible ways suggested by data exploration using S_1; **iterate** until you're happy.

(3) Use final model (fit to S_1) from (2) to create predictive distributions for all data points in S_2; compare actual outcomes with these distributions, checking for **predictive calibration**; go back to (2), change likelihood as necessary, **retune prior** as necessary, to get good calibration; **iterate** until you're happy.

(4) Announce **final model** (fit to $S_1 \cup S_2$) from (3), and report **predictive calibration** of this model on data points in S_3 as indication of how well it would perform with new data.

3CV (continued)

With **large** n probably only need to do this **once**; with **small** and **moderate** n probably best to **repeat** (1–4) several times and **combine** results in some appropriate way (e.g., **model averaging** (e.g., Draper 1995)).

How large should the S_i be? **Preliminary answer:** With moderate sample sizes a good choice for the proportion of data in the three subsets is roughly $(0.5, 0.25, 0.25)$.

In other words, with $n =$ **1,000** I should be prepared to **pay about 250 observations worth of information** in **quoting my final uncertainty assessments** (i.e., making these uncertainty bands **about** $\sqrt{\frac{n}{0.75n}} \doteq 15\%$ **wider** than those based on the full data set), to **account in a well-calibrated manner** for my **search for a good model**.

To **focus** on **other points** I'll often use the **data-analytic approach** in this short course.

Case Study: Measurement of physical constants. What used to be called the National Bureau of Standards (NBS) in Washington, DC, conducts

Continuous Outcome Modeling

extremely high precision measurement of physical constants, such as the actual weight of so-called **check-weights** that are supposed to serve as reference standards (e.g., the official kg).

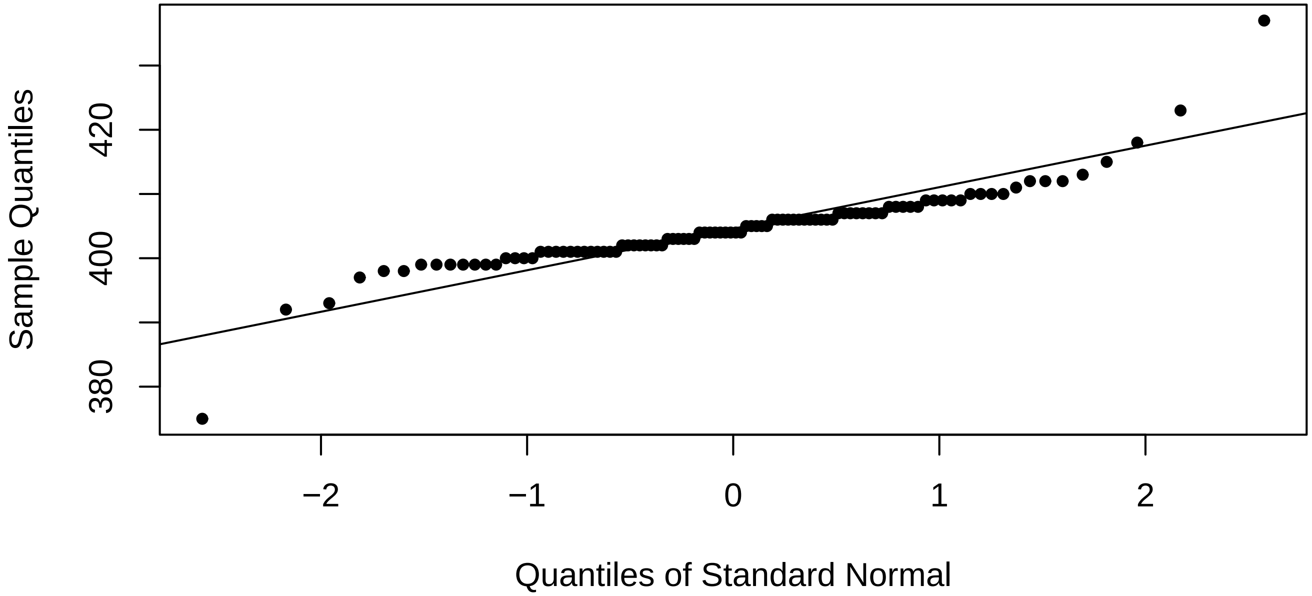
In 1962–63, for example, $n = 100$ weighings (listed below) of a block of metal called **NB10**, which was supposed to weigh exactly 10g, were made under conditions **as close to IID as possible** (Freedman et al., 1998); the measurements are expressed in **micrograms below 10g**.

Value	375	392	393	397	398	399	400	401
Frequency	1	1	1	1	2	7	4	12
Value	402	403	404	405	406	407	408	409
Frequency	8	6	9	5	12	8	5	5
Value	410	411	412	413	415	418	423	437
Frequency	4	1	3	1	1	1	1	1

Q: (a) How much does NB10 **really weigh**? (b) How certain am I given the data that the true weight of NB10 is **less than** (say) 405.25? And (c) How accurately can I **predict** the 101st measurement?

t Likelihood

The graph below is a **normal qqplot** of the 100 measurements $y = (y_1, \ldots, y_n)$, which have a mean of $\bar{y} = 404.6$ and an SD of $s = 6.5$.



Evidently it's plausible in answering Q1–Q3 to assume **symmetry** of the underlying CDF F in de Finetti's Theorem, but the **tails** are **substantially heavier** than those of the **Gaussian** distribution.

A natural choice for the **likelihood** here would be a version of the t distribution:

Multi-Parameter Inferential Problems

$$\begin{aligned} (\mu, \sigma^2, \nu) & \sim & p(\mu, \sigma^2, \nu) \\ (y_i | \mu, \sigma^2, \nu) & \stackrel{\text{IID}}{\sim} & t_\nu(\mu, \sigma^2) \ , \end{aligned} \qquad (3)$$

where $t_\nu(\mu, \sigma^2)$ denotes the **scaled t distribution** with mean μ, scale parameter σ^2, and shape parameter ν ($W \sim t_\nu(\mu, \sigma^2) \iff \frac{W-\mu}{\sigma}$ follows the standard t distribution with ν **degrees of freedom**).

$\boxed{\textbf{3.2 Bayesian inference with multivariate } \theta\textbf{.}}$ This is **more complicated** than the Bernoulli modeling in Part 2; here the parameter θ is a **vector** (μ, σ^2, ν) of length $k = 3$.

When $k > 1$ I can still use Bayes' Theorem directly to obtain the **joint posterior distribution**,

$$\begin{aligned} p(\theta | y) & = & p(\mu, \sigma^2, \nu | y) = c \, p(\theta) \, l(\theta | y) \\ & = & c \, p(\mu, \sigma^2, \nu) \, l(\mu, \sigma^2, \nu | y), \end{aligned} \qquad (4)$$

where $y = (y_1, \ldots, y_n)$, although making this calculation directly requires a k-dimensional **integration** to evaluate the normalizing constant c; for example, in this case

Integration Is the Challenge

$$\begin{aligned} c &= [p(y)]^{-1} = \left(\iiint p(\mu, \sigma^2, \nu, y) \, d\mu \, d\sigma^2 \, d\nu \right)^{-1} \\ &= \left(\iiint p(\mu, \sigma^2, \nu) \, l(\mu, \sigma^2, \nu | y) \, d\mu \, d\sigma^2 \, d\nu \right)^{-1} . \qquad (5) \end{aligned}$$

Usually, however, I'll be more interested in the **marginal posterior distributions**, in this case $p(\mu|y)$, $p(\sigma^2|y)$ and $p(\nu|y)$.

Obtaining these requires k integrations, each of dimension $(k-1)$, a process that people refer to as marginalization or **integrating out the nuisance parameters** — for example,

$$p(\mu|y) = \int_0^\infty \int_0^\infty p(\mu, \sigma^2, \nu | y) \, d\sigma^2 \, d\nu \, . \qquad (6)$$

Predictive distributions also involve a k-dimensional integration: for example, with $y = (y_1, \ldots, y_n)$,

$$\begin{aligned} p(y_{n+1}|y) &= \iiint p(y_{n+1}, \mu, \sigma^2, \nu | y) \, d\mu \, d\sigma^2 \, d\nu \qquad (7) \\ &= \iiint p(y_{n+1} | \mu, \sigma^2, \nu) \, p(\mu, \sigma^2, \nu | y) \, d\mu \, d\sigma^2 \, d\nu. \end{aligned}$$

Multivariate Unknown θ

And, finally, if I'm interested in a **function of the parameters**, I have some more hard integrations ahead of me.

For instance, suppose I wanted the posterior distribution for the **coefficient of variation** $\lambda = g_1(\mu, \sigma^2, \nu) = \frac{\sqrt{\sigma^2}}{\mu}$ in model (3).

Then one **fairly direct way** to get this posterior (e.g., Bernardo and Smith, 1994) is to

(a) introduce **two additional functions** of the parameters, say $\eta = g_2(\mu, \sigma^2, \nu)$ and $\psi = g_3(\mu, \sigma^2, \nu)$, such that the mapping $f = (g_1, g_2, g_3)$ from (μ, σ^2, ν) to (λ, η, ψ) is **invertible**;

(b) compute the joint posterior for (λ, η, ψ) through the usual **change-of-variables formula**

$$p(\lambda, \eta, \psi|y) = p_{\mu,\sigma^2,\nu}[f^{-1}(\lambda, \eta, \psi)|y] \left| J_{f^{-1}}(\lambda, \eta, \psi) \right|, \qquad (8)$$

where $p_{\mu,\sigma^2,\nu}(\cdot, \cdot, \cdot|y)$ is the joint posterior for (μ, σ^2, ν) and $\left| J_{f^{-1}} \right|$ is the **determinant** of the **Jacobian** of the inverse transformation; and

(c) **marginalize** in λ by integrating out η and ψ in $p(\lambda, \eta, \psi|y)$, in a manner

Simulation-Based Computation

analogous to (6).

This process involves **two integrations**, one (of dimension k) to get the normalizing constant that defines (8) and one (of dimension $(k-1)$) to get rid of η and ψ.

It's clear that when k is a lot bigger than 2 all these integrals may create **severe computational problems** — this was the **big stumbling block** for applied Bayesian work for a long time.

More than 200 years ago **Laplace** (1774) — the second Bayesian in history (after Bayes himself) — developed, as one avenue of solution to this problem, what people now call **Laplace approximations** to high-dimensional integrals of the type arising in Bayesian calculations (see, e.g., Tierney and Kadane, 1986).

Here I'll describe another, more general, **simulation-based** approach: **Markov chain Monte Carlo** (MCMC), which dates from the **1940s** and whose **history** is tied up in the development of the **atom bomb** and **digital computers**.

3.3 Markov Chain Monte Carlo (MCMC) Methods

Computation via conjugate analysis (Part 2) produces **closed-form results** (good) but is **limited in scope** to a fairly small set of models for which straightforward conjugate results are possible (bad); for example, there is **no conjugate prior** for (μ, σ^2, ν) in the t model above.

This was a **severe limitation** for Bayesians for almost 250 years (from the 1750s to the 1980s).

Over the past 25 years or so the Bayesian community has "discovered" and developed an entirely new computing method, **Markov chain Monte Carlo (MCMC)** ("discovered" because the physicists first figured it out about 60 years ago: Metropolis and Ulam, 1949; Metropolis et al., 1953).

It became clear above that the **central Bayesian practical challenge** is the **computation of high-dimensional integrals**.

People working on the first atom bomb in World War II faced a **similar challenge**, and noticed that **digital computers** (which were then passing from theory (Turing 1943) to reality) offered an **entirely new approach** to solving the problem.

Simulation-Based Computation

The idea (Metropolis and Ulam, 1949) was based on the observation that **anything I want to know about a probability distribution can be learned to arbitrary accuracy by sampling from it**.

Suppose, for example, that I'm interested in a posterior distribution $p(\theta|y)$ which **cannot be worked with (easily) in closed form**, and initially (to keep things simple) think of θ as a **scalar** (real number) rather than a vector.

Three things of direct interest to me about $p(\theta|y)$ would be

- its low-order moments, including the **mean** $\mu = E(\theta|y)$ and **standard deviation** $\sigma = \sqrt{V(\theta|y)}$,
- its **shape** (basically I'd like to be able to trace out (an estimate of) the entire **density curve**), and
- one or more of its **quantiles** (e.g., to construct a 95% central posterior interval for θ I need to know the **2.5% and 97.5% quantiles**, and sometimes the **posterior median** (the **50th percentile**) is of interest too).

Simulation-Based Computation (continued)

Suppose I could take an **arbitrarily large random sample** from $p(\theta|y)$, say $\theta_1^*, \ldots, \theta_m^*$.

Then each of the above three aspects of $p(\theta|y)$ can be **estimated** from the θ^* sample:

- $\hat{E}(\theta|y) = \bar{\theta}^* = \frac{1}{m}\sum_{j=1}^m \theta_j^*$, and $\sqrt{\hat{V}(\theta|y)} = \sqrt{\frac{1}{m-1}\sum_{j=1}^m \left(\theta_j^* - \bar{\theta}^*\right)^2}$;
- the density curve can be estimated by a **histogram** or **kernel density estimate**; and
- percentiles can be estimated by **counting** how many of the θ^* values fall below a series of specified points — e.g., to find an estimate of the 2.5% quantile I solve the equation

$$\hat{F}_\theta(t) = \frac{1}{m}\sum_{j=1}^m I(\theta_j^* \leq t) = 0.025 \tag{9}$$

  for t, where $I(A)$ is the **indicator function** (1 if A is true, otherwise 0).

These are called Monte Carlo estimates of the true summaries of $p(\theta|y)$ (in

IID Sampling

honor of the casinos) because they're based on the **controlled use of chance**.

Theory shows that with large enough m, each of the Monte Carlo (or **simulation-based**) estimates can be made arbitrarily close to the truth with arbitrarily high probability, under some reasonable assumptions about the **nature of the random sampling**.

One way to achieve this, of course, is to make the sampling **IID** (interestingly, this is **sufficient** but **not necessary** — see below).

If, for example, $\bar{\theta}^* = \frac{1}{m} \sum_{j=1}^{m} \theta_j^*$ is based on an IID sample of size m from $p(\theta|y)$, I can use the **frequentist fact** that in repeated sampling $V\left(\bar{\theta}^*\right) = \frac{\sigma^2}{m}$, where (as above) σ^2 is the variance of $p(\theta|y)$, to construct a **Monte Carlo standard error** (MCSE) for $\bar{\theta}^*$:

$$\widehat{SE}\left(\bar{\theta}^*\right) = \frac{\hat{\sigma}}{\sqrt{m}}, \qquad (10)$$

where $\hat{\sigma}$ is the **sample SD** of the θ^* values.

This can be used, possibly after some **preliminary experimentation**, to decide on m, the Monte Carlo **sample size**, which later will be called the

An IID Example

length of the **monitoring run**.

An IID example. Consider the posterior distribution $p(\theta|y) = \text{Beta}(76.5, 353.5)$ in the **AMI mortality example** in Part 2.

Theory says that the **posterior mean** of θ in this example is $\frac{76.5}{76.5+353.5} \doteq 0.1779$; let's see how well the Monte Carlo method does in estimating this **known truth**.

Here's a function written in the statistical computing environment `R` to construct **Monte Carlo estimates** of the **posterior mean** and **MCSE values** for these estimates.

```
beta.sim <- function( m, alpha, beta, n.sim, seed ) {
  set.seed( seed )
  theta.out <- matrix( 0, n.sim, 2 )
  for ( i in 1:n.sim ) {
    theta.sample <- rbeta( m, alpha, beta )
    theta.out[ i, 1 ] <- mean( theta.sample )
    theta.out[ i, 2 ] <- sqrt( var( theta.sample ) / m )
  }
```

IID Example (continued)

```
  return( theta.out )
}
```

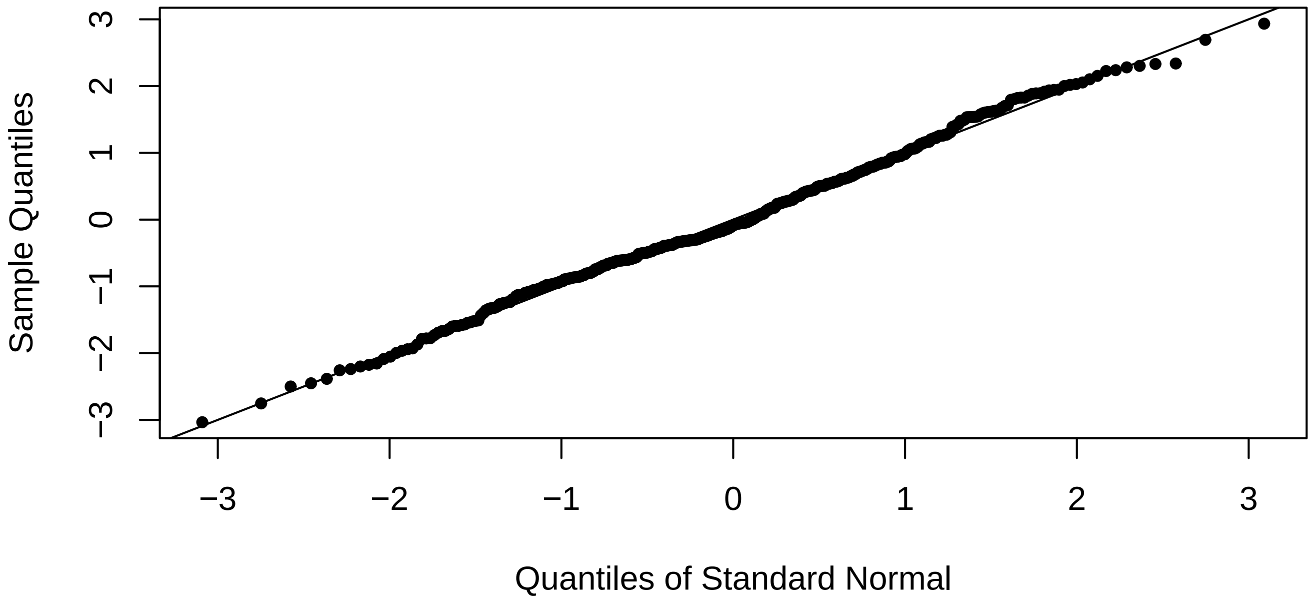
This function simulates, `n.sim` times, the process of taking an **IID sample** of size m from the Beta(α, β) distribution and **calculating** $\bar{\theta}^*$ and $\widehat{SE}\left(\bar{\theta}^*\right)$.

```
> m <- 100
> alpha <- 76.5
> beta <- 353.5
> n.sim <- 500
> seed <- c( 6425451, 9626954 )
> theta.out <- beta.sim( m, alpha, beta, n.sim, seed )
# This took about 0.2 second at 1.6 Unix GHz.
> theta.out[ 1:5, ]
           [,1]        [,2]
 [1,] 0.1756400 0.001854220
 [2,] 0.1764806 0.001703780
 [3,] 0.1781742 0.001979863
 [4,] 0.1793588 0.002038532
 [5,] 0.1781556 0.001596011
```

IID Example (continued)

The $\bar{\theta}^*$ values fluctuate around the truth with a **give-or-take** of about 0.0018, which agrees well with the **theoretical SE** $\frac{\sigma}{\sqrt{m}} = \frac{0.0184}{\sqrt{100}} \doteq 0.00184$ (the SD value 0.0184 comes from page 47 in Part 2).

```
> theta.bar <- theta.out[ , 1 ]
> qqnorm( ( theta.bar - mean( theta.bar ) ) / sd( theta.bar ),
    xlab = "Quantiles of Standard Normal", main = "", pch = 20 )
> abline( 0, 1 )
```



IID Example (continued)

Each of the $\bar{\theta}^*$ values is the mean of $m = 100$ IID draws, so (by the CLT) the **distribution** of the random variable $\bar{\theta}^*$ should be **closely approximated by a Gaussian**, and you can see from the qqplot above that this is true.

```
> truth <- alpha / ( alpha + beta )
> theta.bar.SE <- theta.out[ , 2 ]
> qnorm( 0.025 )
> sum( ( theta.bar - 1.96 * theta.bar.SE < truth ) *
>   ( truth < theta.bar + 1.96 * theta.bar.SE ) ) / n.sim
> [1] 0.94
```

With this set of **pseudo-random numbers**, **94%** of the nominal **95% Monte Carlo confidence intervals** for the posterior mean **included the truth**.

Evidently **frequentist ideas** can be used to work out how big m needs to be to have **any desired** **Monte Carlo accuracy** for $\bar{\theta}^*$ as an estimate of the posterior mean $E(\theta|y)$.

In practice, with $p(\theta|y)$ unknown, I would probably take an **initial sample** (in this case, of size $m = 100$) and look at the MCSE to decide **how big** m **really needs to be**.

IID Example (continued)

Let's say I ran the program with `n.sim` $= 1$ and $m = 100$ and got the following **results**:

```
> theta.bar <- beta.sim( m, alpha, beta, 1, seed )
> theta.bar
           [,1]        [,2]
[1,] 0.1756400 0.001854220
```

(1) Suppose I wanted the MCSE of $\bar{\theta}^*$ to be (say) $\epsilon = 0.00005$; then I could **solve the equation**

$$\frac{\hat{\sigma}}{\sqrt{m}} = \epsilon \quad \leftrightarrow \quad m = \frac{\sigma^2}{\epsilon^2}, \tag{11}$$

which says (unhappily) that the required m goes up as the **square** of the posterior SD and as the **inverse square** of ϵ.

The program results above show that $\frac{\hat{\sigma}}{\sqrt{100}} \doteq 0.001854220$, from which $\hat{\sigma} \doteq 0.01854220$, meaning that **to get** $\epsilon = 0.00005$ **I need a sample of size** $\frac{0.01854220^2}{0.00005^2} \doteq 137,525 \doteq 138\text{k}$.

IID Sample Size Determination

(2) Suppose instead that I wanted $\bar{\theta}^*$ to **differ** from the true posterior mean μ by **no more than** ϵ_1 with Monte Carlo probability **at least** $(1 - \epsilon_2)$:

$$P\left(\left| \bar{\theta}^* - \mu \right| \le \epsilon_1 \right) \ge 1 - \epsilon_2, \tag{12}$$

where $P(\cdot)$ here is based on the (frequentist) **Monte Carlo randomness** inherent in $\bar{\theta}^*$.

I know from the CLT and the calculations above that **in repeated sampling** $\bar{\theta}^*$ is approximately **Gaussian** with mean μ and variance $\frac{\sigma^2}{m}$; this leads to the inequality

$$m \ge \frac{\sigma^2 \left[\Phi^{-1} \left(1 - \frac{\epsilon_2}{2} \right) \right]^2}{\epsilon_1^2}, \tag{13}$$

where $\Phi^{-1}(q)$ is the place on the standard normal curve where $100q\%$ of the area is to the left of that place (the qth **quantile** of the standard Gaussian distribution).

(13) is like (11) except that the value of m from (11) has to be multiplied by $\left[\Phi^{-1} \left(1 - \frac{\epsilon_2}{2} \right) \right]^2$, which typically makes the required sample sizes **even bigger**.

A Closer Look at IID Sampling

For example, with $\epsilon_1 = 0.00005$ and $\epsilon_2 = 0.05$ — i.e., to have at least 95% Monte Carlo confidence that reporting the posterior mean as 0.1756 will be correct to about **four significant figures** — (13) says that I would need a monitoring run of at least $137,525(1.959964)^2 \doteq 528,296 \doteq 528\text{k}$.

This sounds like a long monitoring run but only takes about **2 seconds** at 1.6 Unix GHz, yielding $\left[\bar{\theta}^*, \widehat{SE}\left(\bar{\theta}^* \right) \right] = (0.1779052, 0.00002)$, which **compares favorably** with the **true value** 0.1779070.

It's evident from calculations like these that people often **report simulation-based answers** with numbers of significant figures **far in excess of what's justified** by the actual accuracy of the Monte Carlo estimates.

A closer look at IID sampling. I was able to easily perform the above **simulation study** because `R` has a large variety of built-in functions like `rbeta` for **pseudo-random-number generation**.

How would I go about **writing** such functions **myself**?

There are a number of **general-purpose** methods for generating random numbers (I won't attempt a survey here); the one we need to look closely at, to

Rejection Sampling

understand the algorithms that arise later in this part of the short course, is **rejection sampling** (von Neumann 1951), which is often one of the most **computationally efficient** ways to make IID draws from a distribution.

Example. Continuing the **AMI mortality case study** from Part 2, consider an **alternative prior specification** in which I'd like to put most (**90%**, say) of the prior mass in the interval **(0.05, 0.50)**; calculations like those in Part 2 within the **conjugate Beta family** yield **prior hyperparameter values** of $(\alpha_0, \beta_0) = \mathbf{(2.0,\ 6.4)}$ (this Beta distribution has prior mean and SD **0.24** and **0.14**, respectively).

Suppose that the sample size n was smaller at 74, and $s = 16$ AMI deaths were observed, so that the data mean was **0.216**; the posterior is then $\text{Beta}(\alpha_0 + s, \beta_0 + n - s) = \mathbf{Beta(18.0,\ 64.4)}$.

I'll pretend for the sake of illustration of **rejection sampling** that I don't know the formulas for the mean and SD of a Beta distribution, and suppose that I wanted to use **IID Monte Carlo sampling** from the $\text{Beta}(\alpha_0 + s, \beta_0 + n - s)$ posterior to estimate the **posterior mean**.

Rejection Sampling (continued)

Here's von Neumann's **basic idea**, which (as it turns out) works equally well for **scalar** or **vector** θ: 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**

$$\alpha_R(\theta^*|y) = \frac{p(\theta^*|y)}{G(\theta^*|y)} \tag{14}$$

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

Making a **draw** from the posterior distribution of interest is like choosing a

Rejection Sampling (continued)

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 on the next page.

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

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

Rejection Sampling (continued)

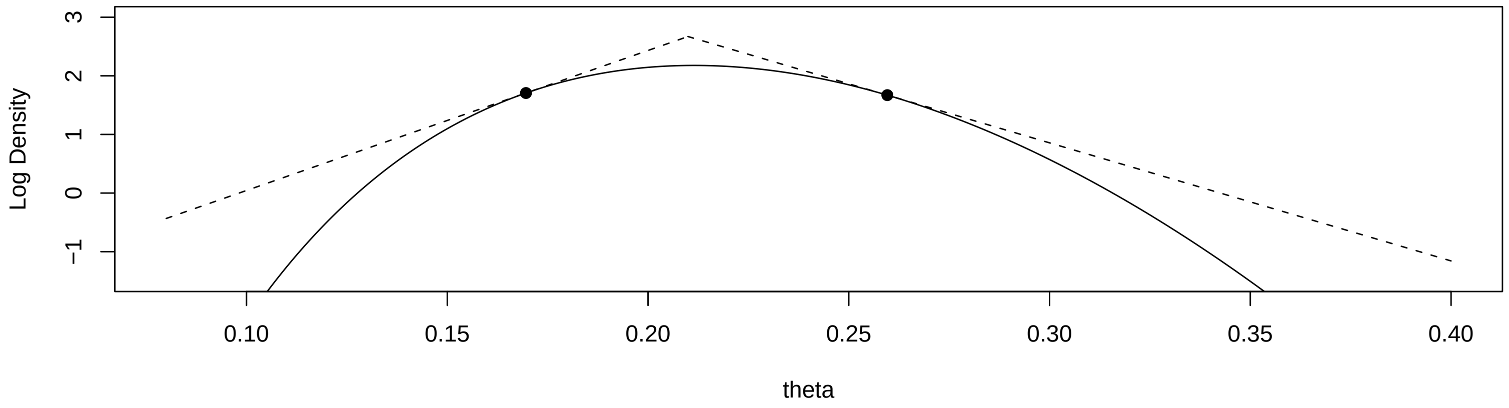
Algorithm (rejection sampling). To make m draws at random from the density $p(\theta|y)$ for scalar or vector θ, select an integrable **envelope function** G — which when normalized to integrate to 1 is the **proposal distribution** g — such that $G(\theta|y) \geq p(\theta|y) \geq 0$ for all θ; define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

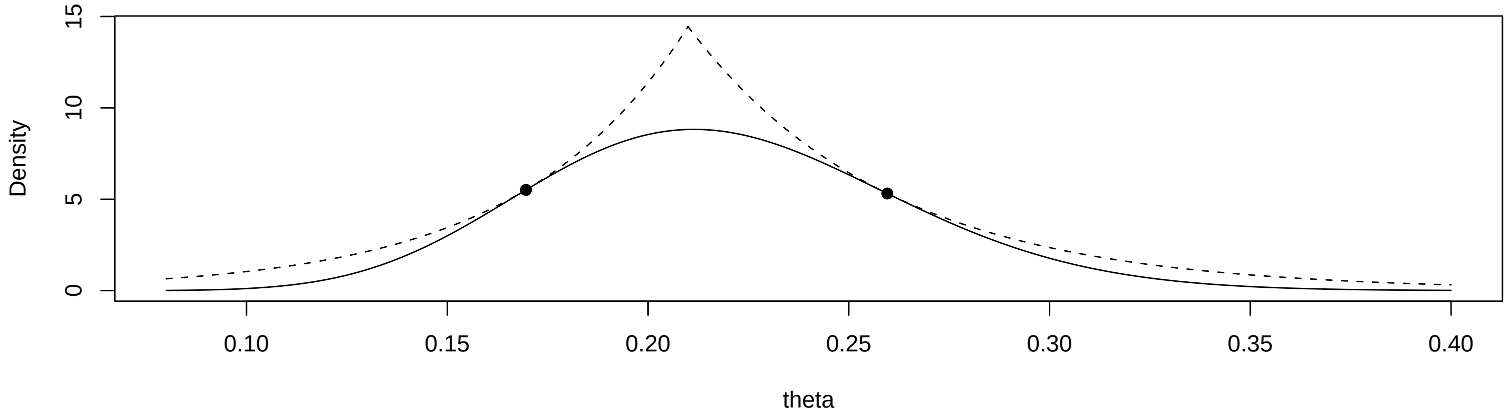
```
    Initialize $t \leftarrow 0$
    Repeat {
        Sample $\theta^* \sim g(\theta|y)$
        Sample $u \sim$ Uniform$(0, 1)$
        If $u \leq \alpha_R(\theta^*|y)$ then
            { $\theta_{t+1} \leftarrow \theta^*$;  $t \leftarrow (t + 1)$ }
    }
    until $t = m$.
```

tangents to the curve at those points.

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

Rejection Sampling (continued)





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

Rejection Sampling (continued)

$$\left[\int G(\theta)\, d\theta \right]^{-1} ; \qquad (15)$$

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

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 easily and **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.

Rejection Sampling (continued)

Suppose, however, that — as in equation (12) 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 (13) 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 $\frac{(0.04505^2)(1.96)^2}{0.0005^2} \doteq 31,200$.

So I take another sample of **30,700** (which is virtually instantaneous at 1.6 Unix GHz) 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.

Beyond Rejection Sampling

Or, even better, I recall that $P(A) = E[I(A)]$ for any event or proposition A, so to the **Monte Carlo dataset** (see page 47 below) 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 $\hat{p} = \mathbf{0.0556}$ 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).

IID sampling is not necessary. Nothing in the Metropolis-Ulam idea of

MCMC

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 $\theta_j^* \stackrel{\text{IID}}{\sim} p(\theta|y)$, 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 **Markov chains**, a subject in the theory of **stochastic processes**.

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).

3.3 Brief Review of 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 — I'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 evolving 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**.

Markov Chains (continued)

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

$$P(\theta_{t+1}^* \in A | \theta_0^*, \dots, \theta_t^*) = P(\theta_{t+1}^* \in A | \theta_t^*). \tag{16}$$

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.

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 $\{\dots, -2, -1, 0, 1, 2, \dots\}$, starting at 0 (say).

Wherever it finds itself 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 a **random walk** (on the integers), and it's **clearly a Markov chain**.

Markov Chains (continued)

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:

Markov Chains (continued)

```
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 ) )
}
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
    }
  }
}
```

Markov Chains (continued)

```
greco 171> R
R version 2.5.1 (2007-06-27)
Copyright (C) 2007 The R Foundation for Statistical Computing
> 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
> 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
```

Markov Chains (continued)

```
> 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

$$9q_1 + 2q_2 = 1 \quad \text{and} \quad q_1 = \frac{3}{2} q_2, \tag{17}$$

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 you would estimate these

Markov Chains (continued)

probabilities **empirically** as

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

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
```

Markov Chains (continued)

```
> 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

$$\pi(j) = \sum_i \pi(i) P_{ij}(t) \tag{18}$$

for all states j and times $t \geq 0$, where $P_{ij}(t) = P(\theta_t^* = j | \theta_{t-1}^* = i)$ is the **transition matrix** of the chain.

The MCMC Payoff

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 four properties:

- It should have the **same state space** as θ,
- It should be **easy to simulate from**,
- It should work **equally well** with an **un-normalized** $p(\theta|y)$, so that it's **not necessary to evaluate the normalizing constant**, 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 as $m \rightarrow \infty$

$$\frac{1}{m}\sum_{t=1}^{m} f(\theta_t^*) \rightarrow E_\pi[f(\theta)] = \sum_i f(i)\,\pi(i), \tag{19}$$

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

The Monte Carlo and MCMC Datasets

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**?

The Monte Carlo and MCMC datasets. The basis of the Monte Carlo approach to obtaining **numerical approximations** to posterior summaries like means and SDs is the (weak) **Law of Large Numbers**: with IID sampling

The Monte Carlo and MCMC Datasets (continued)

the **Monte Carlo estimates** of the true summaries of $p(\theta|y)$ are **consistent**, meaning that they can be made arbitrarily close to the truth with arbitrarily high probability as the number of monitoring iterations $m \to \infty$.

Before we look at how Metropolis et al. attempted to achieve the same goal with a **non-IID Monte Carlo approach**, let's look at the **practical consequences** of switching from IID to Markovian sampling.

Running the **IID rejection sampler** on the AMI mortality example above for a total of m monitoring iterations would produce something that might be called the **Monte Carlo (MC) dataset**, with one **row** for each **iteration** and one **column** for each **monitored quantity**; in that example it might look like the table on the next page (MCSEs in parenthesis).

Running the **Metropolis sampler** on the same example would produce something that might be called the **MCMC dataset**.

It would have a **similar structure** as far as the **columns** are concerned, but the rows would be divided into **three phases**:

- Iteration 0 would be the value(s) used to **initialize** the Markov chain;

The MC and MCMC Data Sets

The MC Data Set:

Iteration	θ	$I(\theta \le 0.15)$
1	$\theta_1^* = 0.244$	$I_1^* = 0$
2	$\theta_2^* = 0.137$	$I_2^* = 1$
$\vdots$	$\vdots$	$\vdots$
$m = 31,200$	$\theta_m^* = 0.320$	$I_m^* = 0$
Mean	0.2183 (0.003)	0.0556 (0.0013)
SD	0.04528	—
Density	(like the bottom	
Trace	plot on page 29)	—

- Iterations 1 through b would be the **burn-in** period, during which the chain reaches its **equilibrium** or **stationary** distribution (as mentioned above, iterations 0 through b are generally **discarded**); and

- Iterations $(b + 1)$ through $(b + m)$ would be the **monitoring** run, on which **summaries** of the posterior (means, SDs, density traces, ...) will be based.