Appendix 3

Markov Chain Monte Carlo and Gibbs Sampling

Far better an approximate answer to the right question, which is often vague, than an exact answer to the wrong question, which can always be made precise – Tukey (1962)

A constant theme in the development of statistics has been the search for justifications for what statisticians do — Blasco (2001)

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A historical impediment to the more widespread use of Bayesian approaches was computational — obtaining the posterior distribution usually requires the integration of high-dimensional functions. This can be very difficult, but several analytic approxmations short of direct integration have been proposed (reviewed by Smith 1991, Evans and Swartz 1995, Tanner 1996). Now, however, the widespread development of **Markov Chain Monte Carlo** (**MCMC**) methods, has made computation of very complex posteriors rather easy. Indeed, MCMC methods allow Bayesian approaches to often handle much higher dimensional problems than other approaches. MCMC methods offer a general approach for simulating direct draws from just about any complex distribution of interest. MCMC approaches are so-named because one uses the previous sample value to randomly generate the next sample value, generating a **Markov chain** (as the transition probabilities between sample values are only a function of the most recent value).

The realization in the early 1990's (Gelfand and Smith 1990) that one particular MCMC method, the **Gibbs sampler**, is very widely applicable to a broad class of Bayesian problems sparked the current exponential expansion in the use of Bayesian analysis. MCMC methods have their roots in the Metropolis algorithm (Metropolis and Ulam 1949, Metropolis et al. 1953), an attempt by physicists to compute complex integrals by expressing them as expectations for some distribution and then estimate this expectation by drawing samples from that distribution. The Gibbs sampler (Geman and Geman 1984) has its origins in image processing. It is thus somewhat ironic that the powerful machinery of MCMC methods had essentially no impact on the field of statistics until rather recently. MCMC methods are reviewed by Tanner (1996), Gammerman (1997), Chen et al. (2000), and Robert and Casella (2004).

MONTE CARLO INTEGRATION

The original **Monte Carlo** approach was a method developed by physicists to use random number generation to compute integrals. Suppose we wish to compute a complex integral

$$\int_a^b h(x)\, dx \qquad \text{(A3.1a)}$$

If we can decompose $h(x)$ into the product of a function $f(x)$ and a probability density function $p(x)$ defined over the interval (a, b), then note that

$$\int_a^b h(x)\,dx = \int_a^b f(x)\,p(x)\,dx = E_{p(x)}[\,f(x)\,], \qquad \text{(A3.1b)}$$

so that the integral can be expressed as an expectation of $f(x)$ over the density $p(x)$. Sampling a large number $x_1, \cdots, x_n$ of random variables from the density $p(x)$,

$$\int_a^b h(x)\,dx = E_{p(x)}[\,f(x)\,] \simeq \frac{1}{n}\sum_{i=1}^{n} f(x_i) \qquad \text{(A3.1c)}$$

This is referred to as **Monte Carlo integration**.

Monte Carlo integration can be used to approximate posterior (or marginal posterior) distributions required for a Bayesian analysis. Consider the integral $I(y) = \int f(y\,|\,x)\,p(x)\,dx$, which we approximate by

$$\widehat{I}(y) = \frac{1}{n}\sum_{i=1}^{n} f(y\,|\,x_i) \qquad \text{(A3.2a)}$$

where x_i are draws from the density $p(x)$. The estimated **Monte Carlo standard error** is given by

$$\text{SE}^2[\,\widehat{I}(y)\,] = \frac{1}{n}\left(\frac{1}{n-1}\sum_{i=1}^{n}\Big(f(y\,|\,x_i) - \widehat{I}(y)\Big)^2\right) \qquad \text{(A3.2b)}$$

where the inner term estimates the sampling variance.

Example A3.0. A very interesting quantitative-genetic application of Monte Carlo integration was suggested by Ovaskainen et al. (2008), who proposed a Bayesian method for comparing whether two $\mathbf{G}$ matrices are similar. As we detail in Volume 3, there are a large number of proposed methods for comparing matrices, but Ovaskainen suggest a (conceptully) simple approach. The $\mathbf{G}$ matrix for a given population is really a description of the distribution of breeding values, and as such we can think of comparing $\mathbf{G}$ matrices as being akin to comparing two multivariate population distributions, whose densities are denoted f and g. If $\mathbf{x}$ denotes a draw from one of these distributions, the probability it originates in distribution g is just $g(\mathbf{x})/[g(\mathbf{x}) + f(\mathbf{x})]$. Hence, the probability q that a random draw from f is incorrectly assigned to g is just

$$q(f, g) = \int \frac{g(\mathbf{x})}{g(\mathbf{x}) + f(\mathbf{x})}\,f(\mathbf{x})\,d\mathbf{x} \qquad \text{(A3.xxa)}$$

If the two probability distributions are essentially indistinquishable, then $q(f, g) = 0.5$, while if they are completely distinquishable then $q(f, g) = 0$. Hence $1 - 2q(f, g)$, which ranges from zero (indistinquishable) to one (fully distinquishable), provides a simple metric of the difference in between then, and hence the difference in the two $\mathbf{G}$ matrices that comprise the distributions f versus g. Ovaskainen et al. modify this futher, suggesting the metric

$$d(f, g) = \sqrt{1 - 2q(f, g)} \qquad \text{(A3.xxb)}$$

While Equation A3.xxb is an extremely complex integral, Equation A3.2a suggests

$$\widehat{q}(f, g) = \frac{1}{n}\sum_{i=1}^{n} \frac{g(\mathbf{x}_i)}{g(\mathbf{x}_i) + f(\mathbf{x}_i)} \rightarrow q(f, g) \qquad \text{(A3.xxc)}$$

where $\mathbf{x}_1, \cdots, \mathbf{x}_n$ are random draws from f. For example, if f is a multivariate normal with mean vector **0** and variance-covariance matrix $\mathbf{G}_1$, then

$$f(\mathbf{x}) = (2\pi)^{-n/2} |\, \mathbf{G}_1 \,| \exp\left(- \frac{\mathbf{x}^T \mathbf{G}_1^{-1} \mathbf{x}}{2} \right)$$

with g is similarly defined, but with $\mathbf{G}_2$ replacing $\mathbf{G}_1$, giving

$$\widehat{q}(f,g) = \frac{1}{n} \sum_{i=1}^{n} \frac{|\, \mathbf{G}_2 \,| \exp\left(-\mathbf{x}_i^T \mathbf{G}_2^{-1} \mathbf{x}_i/2\right)}{|\, \mathbf{G}_2 \,| \exp\left(-\mathbf{x}_i^T \mathbf{G}_2^{-1} \mathbf{x}_i/2\right) + |\, \mathbf{G}_1 \,| \exp\left(-\mathbf{x}_i^T \mathbf{G}_1^{-1} \mathbf{x}_i/2\right)} \qquad \text{(A3.xxb)}$$

Importance Sampling

Suppose the density $p(x)$ roughly approximates the density $q(x)$ of interest, then

$$\int f(x)\, q(x) dx = \int f(x) \left(\frac{q(x)}{p(x)} \right) p(x) dx = E_{p(x)} \left[f(x) \left(\frac{q(x)}{p(x)} \right) \right] \qquad \text{(A3.3a)}$$

This forms the basis for the method of **importance sampling**, with

$$\int f(x)\, q(x) dx \simeq \frac{1}{n} \sum_{i=1}^{n} f(x_i) \left(\frac{q(x_i)}{p(x_i)} \right) \qquad \text{(A3.3b)}$$

where again the x_i are drawn from the distribution given by $p(x)$. For example, if we are interested in a marginal density as a function of y, $J(y) = \int f(y \,|\, x)\, q(x) dx$, we approximate this by

$$J(y) \simeq \frac{1}{n} \sum_{i=1}^{n} f(y \,|\, x_i) \left(\frac{q(x_i)}{p(x_i)} \right) \qquad \text{(A3.4)}$$

where x_i are drawn from the approximating density p.

An alternative formulation of importance sampling is to use

$$\int f(x)\, q(x) dx \simeq \widehat{I} = \sum_{i=1}^{n} w_i f(x_i) \Big/ \sum_{i=1}^{n} w_i, \quad \text{where} \quad w_i = \frac{g(x_i)}{p(x_i)} \qquad \text{(A3.5a)}$$

withthe x_i drawn from $p(x)$. This has an associated Monte Carlo variance of

$$\text{Var}\left(\widehat{I}\right) = \sum_{i=1}^{n} w_i \left(f(x_i) - \widehat{I} \right)^2 \Big/ \sum_{i=1}^{n} w_i \qquad \text{(A3.5b)}$$

INTRODUCTION TO MARKOV CHAINS

Before introducing two of the most common MCMC methods, the Metropolis-Hastings algorithm and the Gibbs sampler, a few introductory comments on Markov chains are in order. Let X_t denote the value of a random variable at time t, and let the **state space** refer to the range of possible X values. The random variable is a **Markov process** if the transition probabilities between different values in the state space depend only on the random variable's current state, i.e.,

$$\Pr(X_{t+1} = s_j \mid X_0 = s_k, \cdots, X_t = s_i) = \Pr(X_{t+1} = s_j \mid X_t = s_i) \tag{A3.6}$$

For a Markov random variable, the only information about the past needed to predict the future is the current state of the random variable, as knowledge of the values of earlier states does not change the transition probability. A **Markov chain** refers to a sequence of random variables $(X_0, \cdots, X_n)$ generated by a Markov process. A particular chain is defined by its **transition probabilities** (or the **transition kernel**), $P(i,j) = P(i \to j)$, which is the probability that a process at state space s_i moves to state s_j in a single step,

$$P(i,j) = P(i \to j) = \Pr(X_{t+1} = s_j \mid X_t = s_i) \tag{A3.7a}$$

We use the notation $P(i \to j)$ to imply a move from i to j, as some texts define $P(i,j) = P(j \to i)$, so we will use the arrow notation in an attempt to avoid confusion. Let

$$\pi_j(t) = \Pr(X_t = s_j) \tag{A3.7b}$$

denote the probability that the chain is in state j at time t, and let $\boldsymbol{\pi}(t)$ denote the row vector of the state space probabilities at step/time t. We start the chain by specifying a starting vector $\boldsymbol{\pi}(0)$. Often all the elements of $\boldsymbol{\pi}(0)$ are zero except for a single element of 1, corresponding to the process starting in that particular state. As the chain progresses, the probability values become more dispersed over the possible state space. The probability that the chain has state value s_i at time/step $t+1$ is given by the **Chapman-Kolomogrov (CK) equation**, which sums over the probability of being in a particular state at the current step t and the transition probability from that state into state s_i,

$$\begin{aligned}\pi_i(t+1) &= \Pr(X_{t+1} = s_i)\\ &= \sum_k \Pr(X_{t+1} = s_i \mid X_t = s_k) \cdot \Pr(X_t = s_k)\\ &= \sum_k P(k \to i)\, \pi_k(t) = \sum_k P(k,i)\, \pi_k(t)\end{aligned} \tag*{(A3.7c)}$$

Successive iteration of the CK equation describes the evolution of the chain.

We can more compactly write the CK equations in matrix form as follows. Define the **probability transition matrix P** as the matrix whose ij-th element is $P(i,j)$, the probability of moving from state i to state j, $P(i \to j)$. This implies that the rows of $\mathbf{P}$ sum to one. Considering the ith row, $\sum_j P(i,j) = \sum_j P(i \to j) = 1$. In matrix form, the Chapman-Kolomogrov equation becomes

$$\boldsymbol{\pi}(t+1) = \boldsymbol{\pi}(t)\mathbf{P} \tag{A3.8a}$$

Hence,

$$\boldsymbol{\pi}(t) = \boldsymbol{\pi}(t-1)\mathbf{P} = (\boldsymbol{\pi}(t-2)\mathbf{P})\mathbf{P} = \boldsymbol{\pi}(t-2)\mathbf{P}^2 \tag{A3.8b}$$

Continuing in this fashion yields the probability distribution in generation t as

$$\boldsymbol{\pi}(t) = \boldsymbol{\pi}(0)\mathbf{P}^t \tag{A3.8c}$$

Defining the n-step transition probability $p_{ij}^{(n)}$ as the probability that the process is in state j given that it started in state i n steps ago, i..e.,

$$p_{ij}^{(n)} = \Pr(X_{t+n} = s_j \mid X_t = s_i) \tag{A3.8d}$$

it immediately follows that $p_{ij}^{(n)}$ is just the ij-th element of $\mathbf{P}^n$, the nth power of the single-step transition matrix.

Finally, a Markov chain is said to be **irreducibile** if there exists a positive integer n_{ij} such that $p_{ij}^{(n_{ij})} > 0$ for all ij. That is, all states **communicate** with each other, in that the process can always move from any state to any other state (although this may multiple steps). Likewise, a chain is said to be **aperiodic** when the number of steps required to move between two states (say x and y) is not required to be multiple of some integer. Put another way, the chain is not forced into some cycle of fixed length between certain states.

Example A3.1. Suppose the state space consists of three possible weather conditions (Rain, Sunny, Cloudy) and weather patterns follows a Markov process (of course, they do not!). Thus, the probability of tomorrow's weather simply depends on today's weather, and not on any other previous days. If this is the case, the observation that it has rained for three straight days does not alter the probability of tomorrow's weather compared to the situation where (say) it rained today but was sunny for the last week. Suppose the probability transitions given today is rainy are

P(Rain tomorrow | Rain today) = 0.5,
P(Sunny tomorrow | Rain today) = 0.25,
P(Cloudy tomorrow | Rain today) = 0.25,

The first row of the transition probability matrix thus becomes $(0.5, 0.25, 0.25)$. Suppose the rest of the transition matrix is given by

$$\mathbf{P} = \begin{pmatrix} 0.5 & 0.25 & 0.25 \\ 0.5 & 0 & 0.5 \\ 0.25 & 0.25 & 0.5 \end{pmatrix}$$

Note that this Markov chain is irreducible, as all states communicate with each other.

Suppose today is sunny. What is the expected weather two days from now? Seven days? Here $\boldsymbol{\pi}(0) = (\, 0 \quad 1 \quad 0 \,)$, giving

$$\boldsymbol{\pi}(2) = \boldsymbol{\pi}(0)\mathbf{P}^2 = (\, 0.375 \quad 0.25 \quad 0.375 \,)$$

and

$$\boldsymbol{\pi}(7) = \boldsymbol{\pi}(0)\mathbf{P}^7 = (\, 0.4 \quad 0.2 \quad 0.4 \,)$$

Conversely, suppose today is rainy, so that $\boldsymbol{\pi}(0) = (\, 1 \quad 0 \quad 0 \,)$. The expected weather becomes

$$\boldsymbol{\pi}(2) = (\, 0.4375 \quad 0.1875 \quad 0.375 \,) \quad \text{and} \quad \boldsymbol{\pi}(7) = (\, 0.4 \quad 0.2 \quad 0.4 \,)$$

Note that after a sufficient amount of time, the expected weather is *independent of the starting value*. In other words, the chain has reached a stationary distribution, where the probability values are independent of the actual starting value.

As the above example illustrates, a Markov chain may reach a **stationary distribution** $\boldsymbol{\pi}^*$, where the vector of probabilities of being in any particular given state is independent of the initial starting distribution. The stationary distribution satisfies

$$\boldsymbol{\pi}^* = \boldsymbol{\pi}^* \mathbf{P} \tag{A3.9}$$

In other words, $\boldsymbol{\pi}^*$ is the left eigenvalue associated with the eigenvalue $\lambda = 1$ of $\mathbf{P}$. One condition for the existance of a stationary distribution is that the chain is irreducible and aperiodic. When a chain is periodic, it can cycle in a deterministic fashion between states and hence never settles down to a stationary distribution (in effect, this cycling *is* the stationary distribution for this chain). A little thought will show that if $\mathbf{P}$ has no eigenvalues equal to -1 that it is aperiodic.

A sufficient condition for a unique stationary distribution is that the **detailed balance equation** holds (for all i and j),

$$P(j \to i)\, \pi_j^* = P(i \to j)\, \pi_i^* \tag{A3.10}$$

That is, at equilibrium, the amount of probability flux from state j to stage i is exactly balanced by the probability flux on the opposite direction (for i to j), so that a balance is reached, with no *net* flow of probability over the states. If Equation A3.10 holds for all ik, the Markov chain is said to be **reversible**, and hence Equation A3.10 is also called the **reversibility condition**. Note that this condition implies $\boldsymbol{\pi}^* = \boldsymbol{\pi}^*\mathbf{P}$, as the jth element of $\boldsymbol{\pi}^*\mathbf{P}$ is

$$(\boldsymbol{\pi}^*\mathbf{P})_j = \sum_i \pi_i^*\, P(i \to j) = \sum_i \pi_j^*\, P(j \to i) = \pi_j^* \sum_i\, P(j \to i) = \pi_j^*$$

where the key middle step following from Equation A3.10, while the last step follows since rows of $\mathbf{P}$ sum to one.

The basic idea of discrete-state Markov chain can be generalized to a continuous state Markov process by having a probability kernel $P(x, y)$ that satisfies

$$\int P(x, y)\, dy = 1$$

and the continuous extension of the Chapman-Kologronvo equation becomes

$$\pi_t(y) = \int \pi_{t-1}(x) P(x, y)\, dx \tag{A3.11a}$$

At equilibrium, that stationary distribution satisfies

$$\pi^*(y) = \int \pi^*(x) P(x, y)\, dx \tag{A3.11b}$$

THE METROPOLIS-HASTING ALGORITHM

One problem with applying Monte Carlo integration is in obtaining samples from some complex probability distribution $p(x)$. Attempts to solve this problem are the roots of MCMC methods. In particular, they trace to attempts by mathematical physicists to integrate very complex functions by random sampling (Metropolis and Ulam 1949, Metropolis et al. 1953, Hastings 1970), and the resulting Metropolis-Hastings algorithm. A detailed review of this method is given by Chib and Greenberg (1995).

Suppose our goal is to draw samples from some distribution $p(\theta)$ where $p(\theta) = f(\theta)/K$, where the normalizing constant K may not be known, and very difficult to compute. The **Metropolis algorithm** (Metropolis and Ulam 1949, Metropolis et al. 1953), which generates a sequence of draws from this distribution, is as follows:

1. Start with any initial value θ_0 satisfying $f\,(\theta_0) > 0$.

2. Using current θ value, sample a **candidate point** θ^* from some **jumping distribution** $q(\theta_1, \theta_2)$, which is the probability of returning a value of θ_2 given a previous value of θ_1. This distribution is also referred to as the **proposal** or **candidate-generating distribution**. The only restriction on the jump density in the Metropolis algorithm is that it is symmetric, i.e., $q(\theta_1, \theta_2) = q(\theta_2, \theta_1)$.

3. Given the candidate point θ^*, calculate the ratio of the density at the candidate (θ^*) and current (θ_{t-1}) points,
$$\alpha = \frac{p(\theta^*)}{p(\theta_{t-1})} = \frac{f(\theta^*)}{f(\theta_{t-1})}$$
Notice that because we are considering the ratio of $p(x)$ under two different values, the normalizing constant K cancels out.

4. If the jump increases the density ($\alpha > 1$), accept the candidate point (set $\theta_t = \theta^*$) and return to step 2. If the jump decreases the density ($\alpha < 1$), then with probability α accept the candidate point, else reject it and return to step 2.

We can summarize the Metropolis sampling as first computing
$$\alpha = \min\left(\frac{f(\theta^*)}{f(\theta_{t-1})}, 1\right) \tag{A3.12}$$
and then accepting a candidate point with probability α (the **probability of a move**). This generates a Markov chain $(\theta_0, \theta_1, \cdots, \theta_k, \cdots)$, as the transition probabilities from θ_t to θ_{t+1} depends only on θ_t and not $(\theta_0, \ \cdots, \theta_{t-1})$. Following a sufficient **burn-in period** (of, say, k steps), the chain approaches its stationary distribution and (as we will demonstrate shortly), samples from the vector $(\theta_{k+1}, \cdots, \theta_{k+n})$ are samples from $p(x)$.

Hastings (1970) generalized the Metropolis algorithm by using an arbitrary (as opposed to strictly symmetric) transition probability function $q(\theta_1, \theta_2) = \Pr(\theta_1 \rightarrow \theta_2)$, and setting the acceptance probability for a candidate point as
$$\alpha = \min\left(\frac{f(\theta^*)\, q(\theta^*, \theta_{t-1})}{f(\theta_{t-1})\, q(\theta_{t-1}, \theta^*)}, 1\right) \tag{A3.13}$$
This is the **Metropolis-Hastings algorithm**. Assuming that the proposal distribution is symmetric, i.e., $q(x, y) = q(y, x)$, recovers the original Metropolis algorithm

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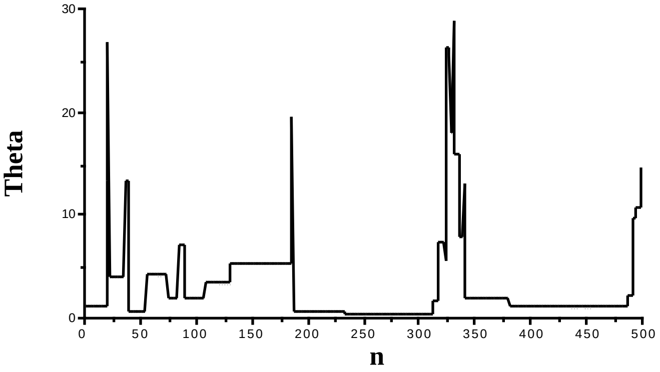
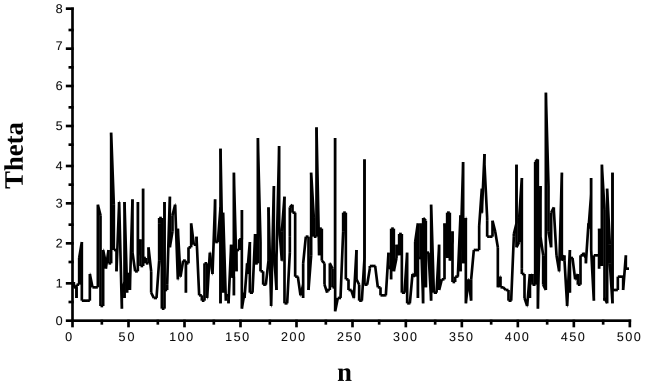
Example A3.2. Consider the scaled inverse-χ^2 distribution,
$$p(\theta) = C \cdot \theta^{-n/2} \cdot \exp\left(\frac{-a}{2\theta}\right)$$
We wish to simulate draws from this distribution with $n = 5$ degrees of freedom and scaling factor $a = 4$, using the Metropolis algorithm. Thus, $f(x) = x^{-5/2} \exp[-4/(2x)\,]$.

Suppose we take as our candidate-generating distribution a uniform distribution on (say) $(0, 100)$. Clearly, there is probability mass above 100 for the scaled inverse-χ^2, but we assume this is sufficiently small that we can ignore it. Now let's run the algorithm. Take $\theta_0 = 1$ as our starting value, and suppose the uniform returns a candidate value of $\theta^* = 39.82$. Computing α,
$$\alpha = \min\left(\frac{f(\theta^*)}{f(\theta_{t-1})}, 1\right) = \min\left(\frac{(39.82)^{-2.5} \cdot \exp(-2/39.82)}{(1)^{-2.5} \cdot \exp(-2/2 \cdot 1)}, 1\right) = 0.0007$$
Since (this case) $\alpha < 1$, θ^* is accepted with probability 0.007. Thus, we randomly draw U from a uniform $(0, 1)$ and accept θ^* if $U \leq \alpha$. In this case, the candidate is rejected, and we draw another candidate value from the proposal distribution (which turns out to be 71.36) and continue as above. The resulting first 500 values of θ are plotted below.



Notice that there are long flat periods (corresponding to all θ^* values being rejected). Such a chain is called **poorly mixing**.

In contrast, suppose we use as our proposal distribution a χ_1^2. Here, the candidate distribution is no longer symmetric, and we must employ Metropolis-Hastings (see Example A3.3 for the details). In this case, a resulting Metropolis-Hastings sampling run is shown below. Note that the time series looks like **white noise**, and the chain is said to be **well mixing**.



Metropolis-Hasting Sampling as a Markov Chain

To demonstrate that the Metropolis-Hasting sampling generates a Markov chain whose equilibrium density is that candidate density $p(x)$, it is sufficient to show that the Metropolis-Hasting transition kernel satisfy the detailed balance equation (Equation A3.10) with $p(x)$, as we show below.

Under Metropolis-Hasting, we sample from $q(x, y) = \Pr(x \rightarrow y \mid q)$ and then accept the move with probability $\alpha(x, y)$, so that the transition probability kernel is given by

$$\Pr(x \rightarrow y) = q(x, y)\,\alpha(x, y) = q(x, y) \cdot \min\left[\frac{p(y)\,q(y, x)}{p(x)\,q(x, y)}, 1\right] \tag{A3.14}$$

Thus if the Metropolis-Hasting kernel satisfies $P(x \rightarrow y)\,p(x) = P(y \rightarrow x)\,p(y)$, or

$$q(x, y)\,\alpha(x, y)\,p(x) = q(y, x)\,\alpha(y, x)\,p(y) \quad \text{for all } x, y$$

then that stationary distribution from this kernel corresponds to draws from the target distribution $p(x)$. We show that the balance equation is indeed satisfied with this kernel by considering the three possible cases for any particular x, y pair.

1. $q(x,y)\,p(x) = q(y,x)\,p(y)$. Here $\alpha(x,y) = \alpha(y,x) = 1$ implying

$$P(x,y)\,p(x) = q(x,y)\,p(x) \quad \text{and} \quad P(y,x)p(y) = q(y,x)\,p(y)$$

and hence $P(x,y)\,p(x) = P(y,x)\,p(y)$, showing that (for this case), the detailed balance equation holds.

2. $q(x,y)\,p(x) > q(y,x)\,p(y)$, in which case

$$\alpha(x,y) = \frac{p(y)\,q(y,x)}{p(x)\,q(x,y)} \quad \text{and} \quad \alpha(y,x) = 1$$

Hence

$$\begin{aligned} P(x,y)\,p(x) &= q(x,y)\,\alpha(x,y)\,p(x) \\ &= q(x,y)\,\frac{p(y)\,q(y,x)}{p(x)\,q(x,y)}\,p(x) \\ &= q(y,x)\,p(y) = q(y,x)\,\alpha(y,x)\,p(y) \\ &= P(y,x)\,p(y) \end{aligned}$$

3. $q(x,y)\,p(x) < q(y,x)\,p(y)$. Here

$$\alpha(x,y) = 1 \quad \text{and} \quad \alpha(y,x) = \frac{q(x,y)\,p(x)}{q(y,x)\,p(y)}$$

Hence

$$\begin{aligned} P(y,x)\,p(y) &= q(y,x)\,\alpha(y,x)\,p(y) \\ &= q(y,x)\left(\frac{q(x,y)\,p(x)}{q(y,x)\,p(y)}\right)p(y) \\ &= q(x,y)\,p(x) = q(x,y)\,\alpha(x,y)\,p(x) \\ &= P(x,y)\,p(x) \end{aligned}$$

Burning-in the Sampler

A key issue in the successful implementation of Metropolis-Hastings, or any other MCMC sampler, is the number of runs (steps) until the chain approaches stationarity (the length of the **burn-in period**). Typically the first 1000 to 5000 values of the chain are thrown out, and then various convergence tests (see below) are used to assess whether stationarity has indeed been reached.

A poor choice of starting values and/or proposal distribution can greatly increase the required burn-in time, and an area of much current research is whether an optimal starting point and proposal distribution can be found. For now, we simply offer some basic rules. One suggestion for a starting value is to start the chain as close to the center of the distribution as possible, for example taking a value close to the distribution's mode (such as using an approximate MLE as the starting value).

A chain is said to be **poorly mixing** if it says in small regions of the parameter space for long periods of time, as opposed to a **well mixing** chain that seems to happily explore the entire space. A poorly mixing chain can arise because the target distribution is multimodal and our choice of starting values traps us near one of the modes (such multimodal posteriors can arise if we have a strong prior in conflict with the observed data). Two approaches have been suggested for situations where the target distribution may have multiple peaks. The most straightforward is to use widely dispersed initial values to start several different chains (Gelman and Rubin 1992). A less obvious approach is to use **simulated annealing** on a single-chain.

Simulated Annealing

Simulated annealing was developed as an approach for finding the maximum of complex functions with multiple peaks where standard hill-climbing approaches may trap the algorithm at a less that optimal peak. The idea is that when we initially start sampling the space, we will accept a reasonable probability of a down-hill move in order to explore the entire space. As the process proceeds, we decrease the probability of such down-hill moves. The analogy (and hence the term) is the annealing of a crystal as temperate decreases — initially there is a lot of movement, which gets smaller and smaller as the temperature cools. Simulated annealing is very closely related to Metropolis sampling, differing only in that the probability α of a move is given by

$$\alpha_{SA} = \min\left[1, \left(\frac{p(\theta^*)}{p(\theta_{t-1})}\right)^{1/T(t)}\right] \tag{A3.15a}$$

where the function $T(t)$ is called the **cooling schedule** (setting $T = 1$ recovers Metropolis sampling), and the particular value of T at any point in the chain is called the **temperature**. For example, suppose that $p(\theta^*)/p(\theta_{t-1}) = 0.5$. With $T = 100$, $\alpha = 0.93$, while for $T = 1$, $\alpha = 0.5$, and for $T = 1/10$, $\alpha = 0.0098$. Hence, we start off with a high probability of a jump and then cool down to a very low jump probability.

Typically, a function with geometric decline for the temperature is used. For example, to start out at T_0 and "cool" down to a final "temperature" of T_f over n steps, we can set

$$T(t) = T_0\left(\frac{T_f}{T_0}\right)^{t/n} \tag{A3.15b}$$

More generally if we wish to cool off to T_f by time n, and then keep the temperature constant at T_f for the rest of the run, we can take

$$T(t) = \max\left(T_0\left(\frac{T_f}{T_0}\right)^{t/n}, T_f\right) \tag{A3.15c}$$

Thus, to cool down to Metropolis sampling, we set $T_f = 1$ and the cooling schedule becomes

$$T(t) = \max\left(T_0^{1-t/n}, 1\right) \tag{A3.15c}$$

Choosing a Jumping (Proposal) Distribution

The Metropolis sampler works with any symmetric distribution, while Metropolis-Hastings works with even more general distribution. How do we determine our best option for a proposal distribution? There are two general approaches — random walks and independent chain sampling. Under a sampler using a proposal distribution based on a **random walk chain**, the new value y equals the current value x plus a random variable z,

$$y = x + z$$

In this case, $q(x, y) = g(y - x) = g(z)$, the density associated with the random variable z. If $g(z) = g(-z)$, i.e., the density for the random variable z is symmetric (as occurs with a normal or multivariate normal with mean zero, or a uniform centered around zero), then we can use Metropolis sampling as $q(x, y)/q(y, x) = g(z)/g(-z) = 1$. The variance of the proposal distribution can be thought of as a **tuning parameter** that we can adjust to get better mixing.

Under a proposal distribution using an **independent chain**, the probability of jumping to point y is independent of the current position (x) of the chain, i.e., $q(x, y) = g(y)$. Thus the candidate value is simply drawn from a distribution of interest, independent of the current value. Again, any number of standard distributions can be used for $g(y)$. Note that in this case, the proposal distribution is generally not symmetric, as $g(x)$ is generally not equal to $g(y)$, and Metropolis-Hasting sampling must be used.

As mentioned, we can tune the proposal distribution to adjust the mixing, and in particular the acceptance probability, of the chain. This is generally done by adjusting the standard deviation (SD), of the proposal distribution. For example, by adjusting the variance (or the eigenvalues of the covariance matrix) for a normal (or multivariate normal), increasing or decreasing the range $(-a, a)$ if a uniform is used, or changing the degrees of freedom if a χ^2 is used (variance increasing with the df). To increase the acceptance probability, one *decreases* the proposal distribution SD (Draper 2000). Draper notes a tradeoff in that if the SD is too large, moves are large (which is good), but are not accepted often (bad). This leads to high autocorrelation (see below) and very poor mixing, requiring much longer chains. If the proposal SD is too small, moves are generally accepted (high acceptance probability), but they are also small, again generating high autocorrelations and poor mixing.

Example A3.3. Suppose we wish to use a χ^2 distribution as our candidate density, by simply drawing from a χ^2 distribution independent of the current position. Recall for $x \sim \chi^2_n$, that

$$g(x) \propto x^{n/2-1} e^{-x/2}$$

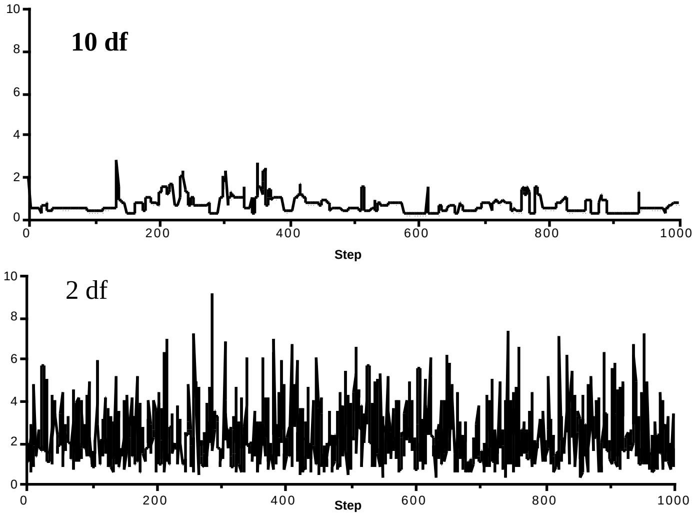
Thus, $q(x, y) = g(y) = C \cdot y^{n/2-1} e^{-y/2}$. Note that $q(x, y)$ is not symmetric, as $q(y, x) = g(x) \neq g(y) = q(x, y)$. Hence, we must use Metropolis-Hastings sampling, with acceptance probability

$$\alpha(x, y) = \min\left[\frac{p(y)\, q(y, x)}{p(x)\, q(x, y)}, 1\right] = \min\left[\frac{p(y)\, x^{n/2-1} e^{-x/2}}{p(x)\, y^{n/2-1} e^{-y/2}}, 1\right]$$

Using the same target distribution as in Example A3.2 (a scaled inverse χ^2), $p(x) = C \cdot x^{-2.5}\, e^{-2/x}$, the rejection probability becomes

$$\alpha(x, y) = \min\left[\frac{(\, y^{-2.5}\, e^{-2/y}\,)\,(\, x^{n/2-1} e^{-x/2}\,)}{(\, x^{-2.5}\, e^{-2/x}\,)\,(\, y^{n/2-1} e^{-y/2}\,)}, 1\right]$$

Results for a run of the sampler under two different proposal distributions (a χ^2_2 and a χ^2_{10}) are plotted below. The χ^2_2 has the smaller variance, and thus a higher acceptance probability.



CONVERGENCE DIAGONISTICS

The careful reader will note that we have still not answered the vexing question of how to determine whether the sampler has reached its stationary distribution. Further, given that adjacent members in a Metropolis-Hasting sampling chain are very likely correlated, how does this affect use of the sequence for estimating parameters of interest from the distribution? We (partly) address these issues here.

Autocorrelation and Sample Size Inflation

We expect adjacent members from a Metropolis-Hastings sequence to be positively correlated, and we can quantify the nature of this correlation by using an **autocorrelation function**. Consider a sequence $(\theta_1, \cdots, \theta_n)$ of length n. Correlations can occur between adjacent members $(\rho(\theta_i, \theta_{i+1}) \neq 0)$, and (more generally) between more distant members $(\rho(\theta_i, \theta_{i+k}) \neq 0)$. The kth order autocorrelation ρ_k can be estimated by

$$\widehat{\rho}_k = \frac{\text{Cov}(\theta_t, \theta_{t+k})}{\text{Var}(\theta_t)} = \frac{\sum\limits_{t=1}^{n-k} \left(\theta_t - \overline{\theta}\right)\left(\theta_{t+k} - \overline{\theta}\right)}{\sum\limits_{t=1}^{n-k} \left(\theta_t - \overline{\theta}\right)^2}, \quad \text{with} \quad \overline{\theta} = \frac{1}{n}\sum_{t=1}^{n} \theta_t \tag{A3.16}$$

An important result from the theory of time series analysis is that if the θ_t are from a stationary (and correlated) process, correlated draws still provide an unbiased picture of the distribution ***provided the sample size is sufficiently large***.

Some indication of the required sample size comes from the theory of a **first-order autoregressive process** (or AR_1), where

$$\theta_t = \mu + \alpha(\,\theta_{t-1} - \mu\,) + \epsilon \tag{A3.17a}$$

where ϵ is **white noise**, $\epsilon \sim N(0, \sigma^2)$. Here $\rho_1 = \alpha$ and the kth order autocorrelation is given by $\rho_k = \rho_1^k = \alpha^k$. Under this process, $E(\,\overline{\theta}\,) = \mu$ with standard error

$$\text{SE}\left(\,\overline{\theta}\,\right) = \frac{\sigma}{\sqrt{n}}\sqrt{\frac{1+\rho}{1-\rho}} \tag{A3.17b}$$

The first ratio is the standard error for white noise, while the second ratio, $\sqrt{(1+\rho)/(1-\rho)}$, is the **sample size inflation factor**, or **SSIF**, which shows how the autocorrelation inflates the sampling variance. For example, for $\rho = 0.5$, 0.75, 0.9, 0.95, and 0.99, the associated SSIF are 3, 7, 19, 39, and 199 (respectively). Thus with an autocorrelation of 0.95 (which is not uncommon in a Metropolis-Hastings sequence), roughly forty times as many points are required for the same precision as with an uncorrelated sequence.

One strategy for reducing autocorrelation is **thinning** the output, storing only every m-th point after the burn-in period. Suppose a Metropolis-Hastings sequence follows an AR_1 model with $\rho_1 = 0.99$. In this case, sampling every 50, 100, and 500 points gives the correlation between the thinned samples as $0.605\ (= 0.99^{50})$, 0.366, and 0.007 (respectively). In addition to reducing autocorrelation, thinning the sequence also saves computer memory.

Tests for Convergence

As shown in Examples A3.2 and A3.3, one should always look at the **time series trace**, the plot of the random variable(s) being generated versus the number of iterations. In addition to showing evidence for poor mixing, such traces can also suggest a ***minimum*** burn-in period for some starting value. For example, suppose the trace moves very slowly away from the initial value to a rather different value (say after 5000 iterations) after which it appears to settle down. Clearly, the burn-in period is ***at least*** 5000 in this case. It must be cautioned that the actual time may be far longer than suggested by the trace. Nevertheless, the trace often indicates that the burn-in is still not complete.

Two other graphs that are very useful in accessing a run from an MCMC sampler plot serial autocorrelations as a function of the time lag. A plot of α_k vs. k (the kth order autocorrelation vs. the lag) should show geometric decay is the sampler series closely follows an AR_1 model. A plot of the **partial autocorrelations** as a function of lag is also useful. The kth partial autocorrelation is the excess correlation not accounted for by a $k-1$ order autogressive model (AR_{k-1}). Hence, if the first order model fits, the second order partial autocorrelation is zero, as the lagged autocorrelations are completed accounted for the AR_1 model (i.e., $\rho_k = \rho_1^k$). Both of these autocorrelation plots may indicate underlying correlation structure in the series not obvious from the time series trace.

What formal tests are available to test for stationarity of the sampler after a given point? We consider two here (additional diagnostic checks for stationary are discussed by Geyer 1992; Gelman and Rubin 1992; Raftery and Lewis 1992b; and Robert 1995). The **Geweke test** (Geweke 1992) splits the sample (after removing a burn-in period) into two parts: say the first 10% and last 50%. If the chain is at stationarity, the means of the two samples should be equal. A modified z-test can be used to compare the two subsamples, and the resulting test statistic is often referred to as a **Geweke z-score**. A value larger than 2 indicates that the mean of the series is still drifting, and a longer burn-in is required before monitoring the chain (to extract a sampler) can begin.

A more informative approach is the **Raftery-Lewis test** (Raftery and Lewis 1992a). Here, one specifies a particular quantile q of the distribution of interest (typically 2.5% and 97.5%, to give a 95% confidence interval), an accuracy ϵ of the quantile, and a power $1-\beta$ for achieving this accuracy on the specified quantile. With these three parameters set, the Raftery-Lewis test breaks the chain into a (1,0) sequence — 1 if $\theta_t \leq q$, zero otherwise. This generates a two-state Markov chain, and the Raftery-Lewis test uses the sequence to estimate the transition probabilities between states. With these probabilities in hand, one can then estimate the number of addition burn-ins (if any) required to approach stationarity, the thinning ratio (how many points should be discarded for each sampled point), and the total chain length required to achieve the preset level of accuracy.

One Long Chain or Many Smaller Chains?

One can either use a single long chain (Geyer 1992, Raftery and Lewis 1992b) or multiple chains each starting from different initial values (Gelman and Rubin 1992). Note that with parallel processing machines, using multiple chains may be computationally more efficient than a single long chain. Geyer, however, argues that using a single longer chain is the best approach. If long burn-in periods are required, or if the chains have very high autocorrelations, using a number of smaller chains may result in each not being long enough to be of any value. Applying the diagnostic tests discussed above can resolve some of these issues for any particular sampler.

THE GIBBS SAMPLER

The **Gibbs sampler** (introduced in the context of image processing by Geman and Geman 1984), is a special case of Metropolis-Hastings sampling wherein the random value is always accepted (i.e., $\alpha = 1$). The task remains to specify how to construct a Markov Chain whose values converge to the target distribution. The key to the Gibbs sampler is that one only considers ***univariate*** conditional distributions — the distribution when all of the random variables but one are assigned fixed values. Such conditional distributions are far easier to simulate than complex joint distributions and usually have simple forms (often being normals, inverse χ^2, or other common prior distributions). Thus, one simulates n random variables sequentially from the n univariate conditionals rather than generating a single n-dimensional vector in a single pass using the full joint distribution.

To introduce the Gibbs sampler, consider a bivariate random variable (x, y), and suppose we wish to compute one or both marginals, $p(x)$ and $p(y)$. The idea behind the sampler is that it is far easier to consider a sequence of conditional distributions, $p(x \,|\, y)$ and $p(y \,|\, x)$, than it is to obtain the marginal by integration of the joint density $p(x, y)$, e.g., $p(x) = \int p(x, y)dy$. The sampler starts with some initial value y_0 for y and obtains x_0 by generating a random variable from the conditional distribution $p(x \,|\, y = y_0)$. The sampler then uses x_0 to generate a new value of y_1, drawing from the conditional distribution based on the value x_0, $p(y \,|\, x = x_0)$. The sampler proceeds as follows

$$x_i \sim p(x \,|\, y = y_{i-1}) \tag{A3.18a}$$

$$y_i \sim p(y \,|\, x = x_i) \tag{A3.18b}$$

Repeating this process k times, generates a **Gibbs sequence** of length k, where a subset of points (x_j, y_j) for $1 \leq j \leq m < k$ are taken as our simulated draws from the full joint distribution. One iteration of all the univariate distributions is often called a **scan** of the sampler. To obtain the desired total of m sample points (here each element in the sampler is a vector of realizations of the two random variables), one samples the chain (i) after a sufficient burn-in to removal the effects of the initial starting values and (ii) at set time points (say every n samples) following the burn-in. The Gibbs sequence converges to a stationary (equilibrium) distribution that is independent of the starting values, and by construction this stationary distribution is the target distribution we are trying to simulate (Tierney 1994).

Example A3.4. Consider the following distribution from Casella and George (1992). Suppose the joint distribution of $x = 0, 1, \cdots n$ and $0 \leq y \leq 1$ is given by

$$p(x, y) = \frac{n!}{(n-x)!x!}\, y^{\,x+\alpha-1}\,(1-y)^{\,n-x+\beta-1}$$

Note that x is discrete and y continuous. While the joint density is complex, the conditional densities are simple distributions. To see this, first recall that a binomial random variable z has a density proportional to

$$p(z \mid q, n) \propto \frac{q^z (1-q)^{n-z}}{z!(n-z)!} \quad \text{for} \quad 0 \le z \le n$$

where $0 < q < 1$ is the success parameter and n the number of traits, and we denote $z \sim \mathrm{B}(n, p)$. Likewise recall the density for $z \sim \text{Beta}(a, b)$, a beta distribution with shape parameters a and b is given by

$$p(z \mid a, b) \propto z^{a-1}(1-z)^{b-1} \quad \text{for} \quad 0 \le z \le 1$$

Observe that the conditional distribution of x (treating y as a fixed constant) is $x \mid y \sim \mathrm{B}(n, y)$, while $y \mid x \sim \text{Beta}(x + \alpha, n - x + \beta)$.

The power of the Gibbs sampler is that by computing a sequence of these univariate conditional random variables (a binomial and then a beta) we can compute any feature of either marginal distribution. Suppose $n = 10$ and $\alpha = 1$, $\beta = 2$. Start the sampler with (say) $y_0 = 1/2$, and we will take the sampler through three full iterations.

(i) x_0 is obtained by generating a random $\mathrm{B}(n, y_0) = \mathrm{B}(10, 1/2)$ random variable, giving $x_0 = 5$ in our simulation.

(ii) y_1 is obtained from a $\text{Beta}(x_0 + \alpha, n - x_0 + \beta) = \text{Beta}(5+1, 10-5+2)$ random variable, giving $y_1 = 0.33$.

(iii) x_1 is a realization of a $\mathrm{B}(n, y_1) = \mathrm{B}(10, 0.33)$ random variable, giving $x_1 = 3$.

(iv) y_2 is obtained from a $\text{Beta}(x_1 + \alpha, n - x_1 + \beta) = \text{Beta}(3+1, 10-3+2)$ random variable, giving $y_2 = 0.56$.

(v) x_2 is obtained from a $\mathrm{B}(n, y_2) = \mathrm{B}(10, 0.56)$ random variable, giving $x_2 = 0.7$.

Our particular realization of the Gibbs sequence after three iterations is thus (5, 0.5), (3, 0.33), (7, 0.56). We can continue this process to generate a chain of the desired length. Obviously, the initial values in the chain are highly dependent upon the y_0 value chosen to start the chain. This dependence decays as the sequence length increases and so we typically start recording the sequence only after a sufficient number of burn-in iterations have occurred.

When more than two variables are involved, the sampler is extended in the obvious fashion. In particular, the value of the kth variable is drawn from the distribution $p(\theta^{(k)} \mid \boldsymbol{\Theta}^{(-k)})$ where $\boldsymbol{\Theta}^{(-k)}$ denotes a vector containing all of the variables but k. Thus, during the ith iteration of the sample, to obtain the value of $\theta_i^{(k)}$ we draw from the distribution

$$\theta_i^{(k)} \sim p(\theta^{(k)} \mid \theta^{(1)} = \theta_i^{(1)}, \cdots, \theta^{(k-1)} = \theta_i^{(k-1)}, \theta^{(k+1)} = \theta_{i-1}^{(k+1)}, \cdots, \theta^{(n)} = \theta_{i-1}^{(n)})$$

For example, if there are four variables, (w, x, y, z), the sampler becomes

$$\begin{aligned}
w_i &\sim p(w \mid x = x_{i-1}, y = y_{i-1}, z = z_{i-1}) \\
x_i &\sim p(x \mid w = w_i, y = y_{i-1}, z = z_{i-1}) \\
y_i &\sim p(y \mid w = w_i, x = x_i, z = z_{i-1}) \\
z_i &\sim p(z \mid w = w_i, x = x_i, y = y_i)
\end{aligned}$$

Gelfand and Smith (1990) illustrated the power of the Gibbs sampler to address a wide variety of statistical issues, while Smith and Roberts (1993) showed the natural marriage of the Gibbs sampler with Bayesian statistics for obtaining posterior distributions. A nice introduction to the sampler is given by Casella and George (1992), while further details can be found in Tanner (1996), Besag et al. (1995), and Lee (1997). Note that the Gibbs sampler can be thought of as a stochastic analog to the EM (Expectation-Maximization) approaches (LW Appendix 4) used to obtain likelihood functions when missing data are present. In the sampler, random sampling replaces the expectation and maximization steps.

Using the Gibbs Sampler to Approximate Marginal Distributions

Any feature of interest for the marginals can be computed from the m realizations of the Gibbs sequence. If $\theta_1, \cdots \theta_m$ is an appropriately thinned and burned-in set of relatizations from a GIbbs sample, the expectation of any function f of the random variable θ is approximated by

$$E[f(\theta)]_m = \frac{1}{m} \sum_{i=1}^{m} f(\theta_i) \tag{A3.19a}$$

This is the **Monte-Carlo** (MC) **estimate** of $f(x)$, as $E[f(\theta)]_m \to E[f(\theta)]$ as $m \to \infty$. Likewise, the MC estimate for any function of n variables ($\theta^{(1)}, \cdots, \theta^{(n)}$) is given by

$$E[f(\theta^{(1)}, \cdots, \theta^{(n)})]_m = \frac{1}{m} \sum_{i=1}^{m} f(\theta_i^{(1)}, \cdots, \theta_i^{(n)}) \tag{A3.19b}$$

Example A3.5. Although the sequence of length 3 computed in Example A3.4 is too short (and too dependent on the starting value) to be a proper Gibbs sequence, for illustrative purposes we can use it to compute Monte-Carlo estimates. The MC estimate of the means of x and y are

$$\overline{x}_3 = \frac{5+3+7}{3} = 5, \quad \overline{y}_3 = \frac{0.5+0.33+0.56}{3} = 0.46$$

Similarly, $\left(\overline{x^2}\right)_3 = 27.67$ and $\left(\overline{y^2}\right)_3 = 0.22$, giving the MC estimates of the variances of x and y as

$$\text{Var}(x)_3 = \left(\overline{x^2}\right)_3 - \left(\overline{x}_3\right)^2 = 2.67$$

and

$$\text{Var}(y)_3 = \left(\overline{y^2}\right)_3 - \left(\overline{y}_3\right)^2 = 0.25$$

While computing the MC estimate of any moment using the sampler is straightforward, computing the actual *shape* of the marginal density is slightly more involved. While one might use the Gibbs sequence of (say) x_i values to give a rough approximation of the marginal distribution of x, this turns out to be inefficient, especially for obtaining the tails of the distribution. A better approach is to use the average of the conditional densities $p(x \mid y = y_i)$, as the function form of the conditional density contains more information about the shape of the entire distribution than the sequence of individual realizations x_i (Gelfand and Smith 1990, Liu et al. 1991). Since

$$p(x) = \int p(x \mid y)\, p(y)\, dy = E_y\left[\, p(x \mid y)\, \right] \tag{A3.20a}$$

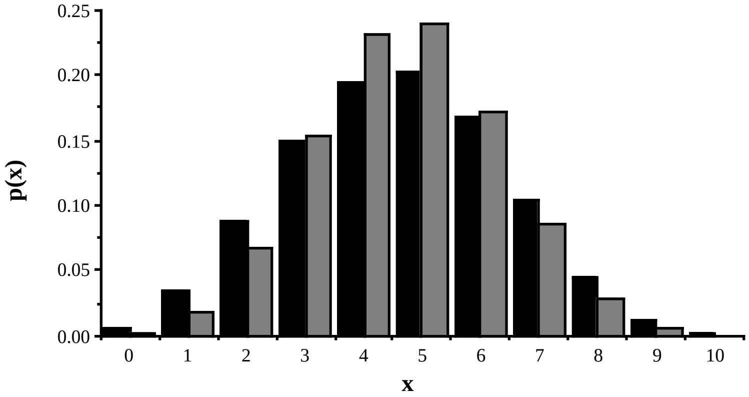
one can approximate the marginal density using

$$\widehat{p}_m(x) = \frac{1}{m} \sum_{i=1}^{m} p(x \,|\, y = y_i) \tag{A3.20b}$$

Example A3.6. Returning to the Gibbs sequence generated in Example A3.4, recall that the distribution of x given y is binomial, with $x \,|\, y \sim \mathrm{B}(n, y)$. Applying Equation A3.20b the estimate (based on this sequence) of the marginal distribution of x is the weighted sum of three binomials with success parameters 0.5, 0.33, and 0.56, giving

$$p_3(x) = 10! \left[\frac{0.5^x(1-0.5)^{10-x} + 0.33^x(1-0.33)^{10-x} + 0.56^x(1-0.56)^{10-x}}{3\,x!(10-x)!} \right]$$

As the figure below shows, the resulting distribution (solid bars), although a weighted sum of binomials, departs substantially from the binomial based on the average (here 0.46)of the success parameter (stripped bars).



The Monte Carlo Variance of a Gibbs-Sampler Based Estimate

Suppose we are interested in using an appropriately thinned and burned-in Gibbs sequence $\theta_1, \cdots, \theta_n$ to estimate some function $h(\theta)$ of the target distribution, such as a mean, variance, or specific quantile (cumulative probability value). Since we are drawing random variables, there is some sampling variance associated with the Monte Carlo estimate

$$\widehat{h} = \frac{1}{n} \sum_{i=1}^{n} h(\theta_i) \tag{A3.21}$$

By increasing the length of the chain (increasing n), we can decrease the sampling variance of $\widehat{h}$, but it would be nice to have some estimate of the size of this variance. One direct approach is to run several chains (or subsample a very long chain) and use the between-chain variance in $\widehat{h}$. Specifically, if $\widehat{h}_j$ denotes the estimate for chain j $(1 \le j \le m)$ where each of the m chains has the same length, then the estimated variance of the Monte Carlo estimate is

$$\mathrm{Var}\left(\widehat{h}\right) = \frac{1}{m-1} \sum_{j=1}^{m} \left(\widehat{h}_j - \widehat{h^*}\right)^2 \quad \text{where} \quad \widehat{h^*} = \frac{1}{m} \sum_{j=1}^{m} \widehat{h}_j \tag{A3.22}$$

Using only a single chain, an alternative approach is to use results from the theory of time series. Estimate the lag-k autocovariance associated with h by

$$\widehat{\gamma}(k) = \frac{1}{n} \sum_{i=1}^{n-k} \left[\left(h(\theta_i) - \widehat{h} \right) \left(h(\theta_{i+k}) - \widehat{h} \right) \right] \tag{A3.23}$$

This is natural generalization of the k-th order autocorrelation to the random variable generated by $h(\theta_i)$. The resulting estimate of the Monte Carlo variance is

$$\text{Var}\left(\widehat{h}\right) = \frac{1}{n} \left(\widehat{\gamma}(0) + 2 \sum_{i=1}^{2\delta+1} \widehat{\gamma}(i) \right) \tag{A3.24}$$

Here δ is the smallest positive integer satisfying $\widehat{\gamma}(2\delta) + \widehat{\gamma}(2\delta+1) > 0$, (i.e., the higher order (lag) autocovariances are zero).

One measure of the effects of autocorrelation between elements in the sampler is the **effective chain size**,

$$\widehat{n} = \frac{\widehat{\gamma}(0)}{\text{Var}\left(\widehat{h}\right)} \tag{A3.25}$$

In the absence of autocorrelation between members, $\widehat{n} = n$.

Convergence Diagonistics: The Gibbs Stopper

Our discussion of the various diagnostics for Metropolis-Hastings (MH) also applies to Gibbs sampler, as Gibbs is a special case of MH. As with MH sampling, we can reduce the autocorrelation between monitored points in the sampler sequence by increasing the thinning ratio (increasing the number of points discarded between each sampled point). Draper (2000) notes that the Gibbs sampler usually produces chains with smaller autocorrelations that other MCMC samplers.

Tanner (1996) discusses an approach for monitoring approach to convergence based on the **Gibbs stopper**, in which weights based on comparing the Gibbs sampler and the target distribution are computed and plotted as a function of the sampler iteration number. As the sampler approaches stationary, the distribution of the weights is expected to spike. See Tanner for more details.

ABC: APPROXIMATE BAYESIAN COMPUTATION

MCMC Without Computing Likelhioods

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