Markov Chain Monte Carlo

26.1 Introduction

The Markov chain Monte Carlo (MCMC) revolution sweeping statistics is drastically changing how statisticians perform integration and summation. In particular, the Metropolis algorithm and Gibbs sampling make it straightforward to construct a Markov chain that samples from a complicated conditional distribution. Once a sample is available, then any conditional expectation can be approximated by forming its corresponding sample average. The implications of this insight are profound for both classical and Bayesian statistics. As a bonus, trivial changes to the Metropolis algorithm yield simulated annealing, a general-purpose algorithm for solving difficult combinatorial optimization problems.

Our limited goal in this chapter is to introduce a few of the major MCMC themes, particularly Gibbs sampling. In describing the various methods we will use the notation of discrete-time Markov chains. Readers should bear in mind that most of the methods carry over to chains with continuous state spaces; our examples exploit this fact. One issue of paramount importance is how rapidly the underlying chains reach equilibrium. This is the Achilles heel of the whole business and not just a mathematical nicety. Our two numerical examples illustrate some strategies for accelerating convergence. We undertake a formal theoretical study of convergence in the next chapter.

Readers interested in pursuing MCMC methods and simulated annealing further will enjoy the pioneering articles [9, 12, 16, 19, 24]. The elementary surveys [3, 6] of Gibbs sampling and the Metropolis algorithm are quite readable, as are the books [8, 10, 15, 22, 28, 32]. The well-tested program WinBugs [29] is one of the best vehicles for Gibbs sampling. *Numerical Recipes* [27] provides a compact implementation of simulated annealing.

26.2 The Hastings-Metropolis Algorithm

The Hastings-Metropolis algorithm is a device for constructing a Markov chain with a prescribed equilibrium distribution $\pi$ on a given state space [16, 24]. Each step of the chain is broken into two stages, a proposal stage and an acceptance stage. If the chain is currently in state $i$, then in the proposal stage a new destination state $j$ is proposed according to a probability density $q_{ij} = q(j \mid i)$. In the subsequent acceptance stage, a random number is drawn uniformly from $[0, 1]$ to determine whether the proposed
step is actually taken. If this number is less than the Hastings-Metropolis acceptance probability

$$a_{ij} = \min \left\{ \frac{\pi_j q_{ji}}{\pi_i q_{ij}}, 1 \right\}, \quad (26.1)$$

then the proposed step is taken. Otherwise, the proposed step is declined, and the chain remains in place.

A few comments about this strange procedure are in order. First, the resemblance of the Hastings-Metropolis algorithm to acceptance-rejection sampling should make the reader more comfortable. Second, like most good ideas, the algorithm has gone through successive stages of abstraction and generalization. For instance, Metropolis et al. [24] considered only symmetric proposal densities with \( q_{ij} = q_{ji} \). In this case the acceptance probability reduces to

$$a_{ij} = \min \left\{ \frac{\pi_j}{\pi_i}, 1 \right\}. \quad (26.2)$$

In this simpler setting it is clear that any proposed destination \( j \) with \( \pi_j > \pi_i \) is automatically accepted. Finally, in applying either formula (26.1) or formula (26.2), it is noteworthy that the \( \pi_i \) need only be known up to a multiplicative constant.

To prove that \( \pi \) is the equilibrium distribution of the chain constructed from the Hastings-Metropolis scheme (26.1), it suffices to check that detailed balance holds. If \( \pi \) puts positive weight on all points of the state space, it is clear that we must impose the requirement that the inequalities \( q_{ij} > 0 \) and \( q_{ji} > 0 \) are simultaneously true or simultaneously false. This requirement is also implicit in definition (26.1). Now suppose without loss of generality that the fraction

$$\frac{\pi_j q_{ji}}{\pi_i q_{ij}} \leq 1$$

for some \( j \neq i \). Then detailed balance follows immediately from

$$\pi_i q_{ij} a_{ij} = \pi_i q_{ij} \frac{\pi_j q_{ji}}{\pi_i q_{ij}} = \pi_j q_{ji} = \pi_j q_{ji} a_{ji}.$$

Besides checking that \( \pi \) is the equilibrium distribution, we should also be concerned about whether the Hastings-Metropolis chain is irreducible and aperiodic. Aperiodicity is the rule because the acceptance-rejection step allows the chain to remain in place. Problem 4 states a precise result and a counterexample. Irreducibility holds provided the entries of \( \pi \) are positive and the proposal matrix \( Q = (q_{ij}) \) is irreducible.