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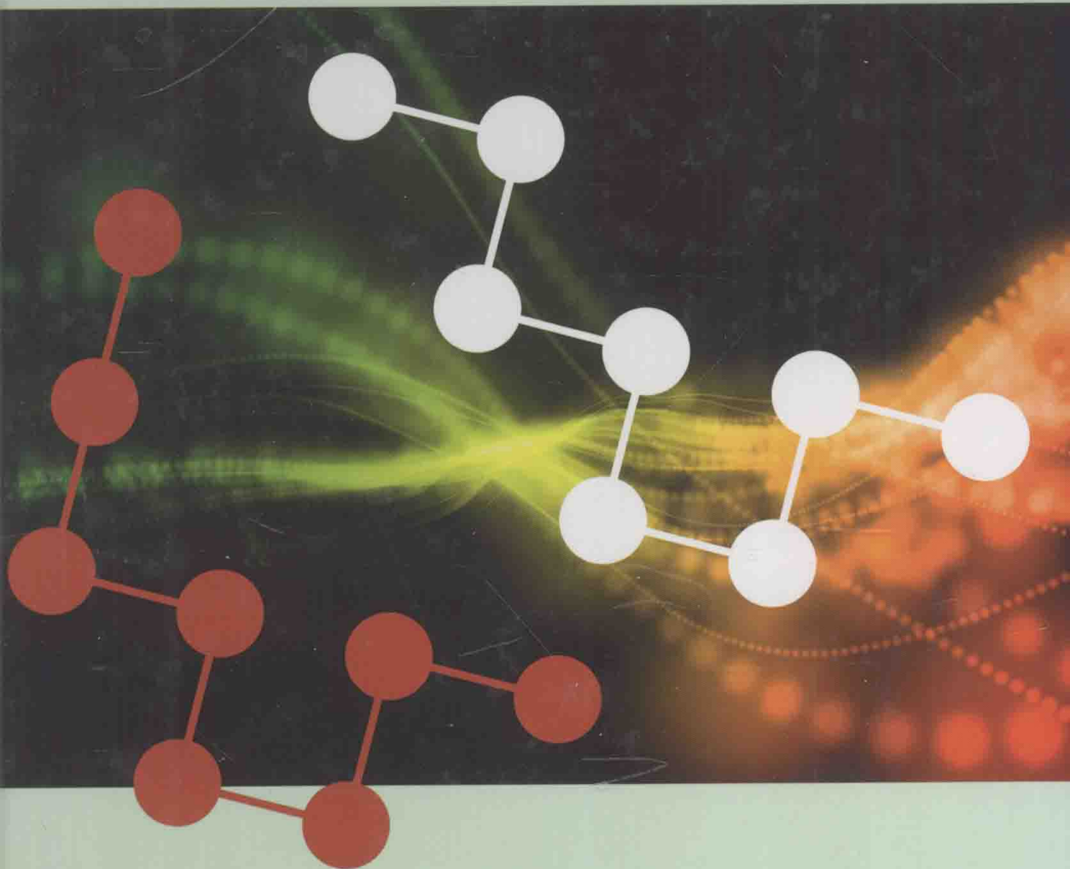

Faming Liang, Chuanhai Liu, Raymond J. Carroll

ADVANCED MARKOV CHAIN MONTE CARLO METHODS

LEARNING FROM PAST SAMPLES

WILEY

Advanced Markov Chain Monte Carlo Methods

Learning from Past Samples

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To our families

Preface

The Markov Chain Monte Carlo (MCMC) method is rooted in the work of physicists such as Metropolis and von Neumann during the period 1945–55 when they employed modern electronic computers for the simulation of some probabilistic problems in atomic bomb designs. After five decades of continual development, it has become the dominant methodology in the solution of many classes of computational problems of central importance to science and technology.

Suppose that one is interested in simulating from a distribution with the density/mass function given by $f(x) \propto \exp\{-H(x)/t\}$, $x \in \mathcal{X}$, where $H(x)$ is called the energy function, and t is called the temperature. The Metropolis algorithm (Metropolis *et al.*, 1953) is perhaps the first sampling algorithm for iterative simulations. It has an extremely simple form. Starting with any point $x_0 \in \mathcal{X}$, it proceeds by iterating between the following two steps, what we call the proposal-and-decision steps:

1. (*Proposal*) Propose a random 'unbiased perturbation' of the current state x_t generated from a symmetric proposal distribution $T(x_t, y)$, i.e., $T(x_t, y) = T(y, x_t)$.

2. (*Decision*) Calculate the energy difference $\Delta H = H(y) - H(x_t)$. Set $x_{t+1} = y$ with probability $\min\{1, \exp(-\Delta H/t)\}$, and set $x_{t+1} = x_t$ with the remaining probability.

This algorithm was later generalized by Hastings (1970) to allow asymmetric proposal distributions to be used in generating the new state y. The generalized algorithm is usually called the Metropolis-Hastings algorithm. A fundamental feature of the Metropolis-Hastings update is its localness, the new state being generated in a neighborhood of the current state. This feature allows one to break a complex task into a series of manageable pieces. On the other hand, however, it tends to suffer from the local-trap problem when the energy function has multiple local minima separated by high energy barriers. In this situation, the Markov chain will be indefinitely trapped in local energy minima. Consequently, the simulation process may fail to sample from the relevant parts of the sample space, and the quantities of interest cannot be estimated with satisfactory accuracies. Many applications of the MCMC method, such as protein folding, combinatorial optimization, and spin-glasses, can be dramatically enhanced by sampling algorithms which allow the process to avoid being trapped in local energy minima.

Developing MCMC sampling algorithms that are immune to the local-trap problem has long been considered as one of the most important topics in MCMC research. During the past two decades, various advanced MCMC algorithms which address this problem have been developed. These include: the Swendsen-Wang algorithm (1987); parallel tempering (Geyer, 1991; Hukushima and Nemoto, 1996), multicanonical Monte Carlo (Berg and Neuhaus, 1991, 1992); simulated tempering (Marinari and Parisi, 1992; Geyer and Thompson, 1995); dynamic weighting (Wong and Liang, 1997; Liu *et al.*, 2001; Liang, 2002b); slice sampler (Higdon, 1998; Edwards and Sokal, 1988); evolutionary Monte Carlo (Liang and Wong, 2000, 2001b), adaptive Metropolis algorithm (Haario *et al.*, 2001); the Wang-Landau algorithm (Wang and Landau, 2001; Liang, 2005b); equi-energy sampler (Kou *et al.*, 2006); sample Metropolis-Hastings algorithm (Lewandowski and Liu, 2008); and stochastic approximation Monte Carlo (Liang *et al.*, 2007; Liang, 2009b), among others.

In addition to the local-trap problem, the Metropolis-Hastings algorithm also suffers from the inability in sampling from distributions with the mass/density function involving intractable integrals. Let $f(x) \propto c(x)\psi(x)$, where $c(x)$ denotes an intractable integral. Clearly, the Metropolis-Hastings algorithm cannot be applied to simulate from $f(x)$, as the acceptance probability would involve the intractable ratio $c(y)/c(x)$, where y denotes the candidate sample. To overcome this difficulty, advanced MCMC algorithms have also been proposed in recent literature. These include the Møller algorithm (Møller *et al.*, 2006), the exchange algorithm (Murray *et al.*, 2006), the double Metropolis-Hastings algorithm (Liang, 2009c; Jin and Liang, 2009), the Monte Carlo dynamically weighted importance sampling algorithm (Liang and Cheon, 2009), and the Monte Carlo Metropolis-Hastings sampler (Liang and Jin, 2010), among others.

One common key idea behind these advanced MCMC algorithms is *learning from past samples*. For example, stochastic approximation Monte Carlo (Liang *et al.*, 2007) modifies its invariant distribution from iteration to iteration based on its past samples in such a way that each region of the sample space can be drawn from with a desired frequency, and thus the local-trap problem can be avoided essentially. The adaptive Metropolis algorithm modifies its proposal distribution from iteration to iteration based on its past samples such that an "optimal" proposal distribution can be achieved dynamically. In the dynamic weighting algorithm, the importance weight carries the information of past samples, which helps the system move across steep energy barriers even in the presence of multiple local energy minima. In parallel tempering and evolutionary Monte Carlo, the state of the Markov chain is extended to a population of independent samples, for which, at each iteration, each sample can be updated based on entire samples of the current population. Hence, parallel tempering and evolutionary Monte Carlo can also be viewed as algorithms for learning from past samples, although they can only learn within a fixed horizon.

Meanwhile, many advanced techniques have been developed in the literature to accelerate the convergence of the Metropolis-Hastings algorithm and the Gibbs sampler; the latter can be viewed as a special form of the Metropolis-Hastings algorithm, with each component of the state vector being updated via a conditional sampling step. Such techniques include: blocking and collapsing (Liu *et al.*, 1994); reparameterization (Gelfand *et al.*, 1995); parameter expansion (Meng and van Dyk, 1999; Liu and Wu, 1999); multiple-try (Liu *et al.*, 2000); and alternating subspace-spanning resampling (Liu, 2003), among others.

The aim of this book is to provide a unified and up-to-date treatment of advanced MCMC algorithms and their variants. According to their main features, we group these advanced MCMC algorithms into several categories. The Gibbs sampler and acceleration methods, the Metropolis-Hastings algorithm and extensions, auxiliary variable-based MCMC algorithms, population-based MCMC algorithms, dynamic weighting, stochastic approximation Monte Carlo, and MCMC algorithms with adaptive proposals are described in Chapters 2–8. Chapter 1 is dedicated to brief descriptions of Bayesian inference, random number generation, and basic MCMC theory. Importance sampling, which represents another important area of Monte Carlo other than MCMC, is not fully addressed in this book. Those interested in this area should refer to Liu (2001) or Robert and Casella (2004).

This book is intended to serve three audiences: researchers specializing in Monte Carlo algorithms; scientists interested in using Monte Carlo methods; and graduate students in statistics, computational biology, engineering, and computer sciences who want to learn Monte Carlo methods. The prerequisites for understanding most of the material presented are minimal: a one-semester course on probability theory (Ross, 1998) and a one-semester course on statistical inference (Rice, 2007), both at undergraduate level. However, it would also be more desirable for readers to have a background in some specific scientific area such as Bayesian computation, artificial intelligence, or computational biology. This book is suitable as a textbook for one-semester courses on Monte Carlo methods, offered at the advanced Master's or Ph.D. level.

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Chuanhai Liu's interest in computational statistics is due largely to the support and encouragement from his M.S. advisor professor, Yaoting Zhang and PhD advisor professor, Donald B. Rubin. In the mid-1980s, Chuanhai Liu learned from Professor Yaoting Zhang the importance of statistical computing. Over a time period of more than ten years from late 1980s, Chuanhai Liu learned from Professor Donald B. Rubin statistical thinking in developing iterative methods, such as EM and Gibbs-type algorithms.

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Finally, we wish to thank our families for their constant love, understanding and support. It is to them that we dedicate this book.

F.L., C.L. and R.C.

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Contents

Chapter 1

Bayesian Inference and Markov Chain Monte Carlo

1.1 Bayes

Bayesian inference is a probabilistic inferential method. In the last two decades, it has become more popular than ever due to affordable computing power and recent advances in Markov chain Monte Carlo (MCMC) methods for approximating high dimensional integrals.

Bayesian inference can be traced back to Thomas Bayes (1764), who derived the inverse probability of the success probability θ in a sequence of independent Bernoulli trials, where θ was taken from the uniform distribution on the unit interval $(0, 1)$ but treated as unobserved. For later reference, we describe his experiment using familiar modern terminology as follows.

■ **Example 1.1 The Bernoulli (or Binomial) Model With Known Prior**

Suppose that $\theta \sim \text{Unif}(0, 1)$, the uniform distribution over the unit interval $(0, 1)$, and that $x_1, \ldots, x_n$ is a sample from Bernoulli(θ), which has the sample space $\mathcal{X} = \{0, 1\}$ and probability mass function (pmf)

$$\Pr(X = 1|\theta) = \theta \quad \text{and} \quad \Pr(X = 0|\theta) = 1 - \theta, \tag{1.1}$$

where X denotes the Bernoulli random variable (r.v.) with $X = 1$ for *success* and $X = 0$ for *failure*. Write $N = \sum_{i=1}^{n} x_i$, the observed number of successes in the n Bernoulli trials. Then $N|\theta \sim \text{Binomial}(n, \theta)$, the Binomial distribution with parameters size n and probability of success θ.

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