Springer Series in Statistics

Jun S. Liu

Monte Carlo Strategies in Scientific Computing

科学计算中的蒙特卡罗策略

Springer

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With 56 Figures

Springer
世界图书出版公司

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Library of Congress Cataloging-in-Publication Data
Liu, Jun S.
Monte Carlo strategies in scientific computing / Jun S. Liu
p. cm. — (Springer series in statistics)
Includes bibliographical references and index.
ISBN 0-387-95230-6 (hc. : alk. paper)
1. Science—Statistical methods. 2. Monte Carlo method. I. Title. II. Series
Q180.55.S7 L58 2001
501'519282—dc21 00-069243

ISBN 0-387-95230-6

www.springer-ny.com

Springer-Verlag New York Berlin Heidelberg
A member of BertelsmannSpringer Science+Business Media GmbH

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To my wife Wei

Preface

An early experiment that conceives the basic idea of Monte Carlo computation is known as "Buffon's needle" (Dörrie 1965), first stated by Georges Louis Leclerc Comte de Buffon in 1777. In this well-known experiment, one throws a needle of length l onto a flat surface with a grid of parallel lines with spacing D ($D > l$). It is easy to compute that, under ideal conditions, the chance that the needle will intersect one of the lines is $2l/\pi D$. Thus, if we let p_N be the proportion of "intersects" in N throws, we can have an estimate of π as

$$\hat{\pi} = \lim_{N \to \infty} \frac{2l}{p_N D},$$

which will "converge" to π as N increases to infinity. Numerous investigators actually used this setting to estimate π. The idea of simulating random processes so as to help evaluate certain quantities of interest is now an essential part of scientific computing.

A systematic use of the Monte Carlo method for real scientific problems appeared in the early days of electronic computing (1945-55) and accompanied the development of the world's first programmable "super" computer, MANIAC (Mathematical Analyzer, Numerical Integrator and Computer), at Los Alamos during World War II. In order to make a good use of these fast computing machines, scientists (Stanislaw Ulam, John von Neumann, Nicholas Metropolis, Enrico Fermi, etc.) invented a statistical sampling-based method for solving numerical problems concerning random neutron diffusion in fissile material in atomic bomb designs and for estimating eigenvalues of the Schrödinger equation. The basic idea underlying

the method was first brought up by Ulam and deliberated between him and von Neumann in a car when they drove together from Los Alamos to Lamy. Allegedly, Nick Metropolis coined the name "Monte Carlo," which played an essential role in popularizing the method.

In the early 1950s, statistical physicists (N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller, and E. Teller) introduced a Markov-chain-based dynamic Monte Carlo method for the simulation of simple fluids. This method was later extended to cover more and more complex physical systems, including spin glass models, harmonic crystal, polymer models, etc. In the 1980s, statisticians and computer scientists developed Monte-Carlo-based methods for a wide variety of tasks such as combinatorial optimizations, nonparametric statistical inference (e.g., jackknife and bootstrap), likelihood computation with missing observations, statistical genetics analysis, Bayesian modeling and computations, and others. In the 1990s, the method began to play an important role in computational biology and was used to solve problems in sequence motif identification and the analysis of complex pedigree. Now, the list of application areas of Monte Carlo methods includes biology (Leach 1996, Karplus and Petsko 1990, Lawrence, Altschul, Boguski, Liu, Neuwald and Wootton 1993), chemistry (Alder and Wainwright 1959), computer science (Kirkpatrick, Gelatt and Vecchi 1983), economics and finance (Gouriérourx and Monfort 1997); engineering (Geman and Geman 1984), material science (Frenkel and Smit 1996), physics (Metropolis, Rosenbluth, Rosenbluth, Teller and Teller 1953, Goodman and Sokal 1989, Marinari and Parisi 1992), statistics (Efron 1979, Gelfand and Smith 1990, Rubin 1987, Tanner and Wong 1987), and many others. Among all Monte Carlo methods, *Markov chain Monte Carlo* (MCMC) provides an enormous scope for dealing with very complicated stochastic systems and has been the central pillar in the study of macromolecules and other physical systems. Recently, the MCMC methodology has drawn much attention from statisticians because the method enables them to entertain more sophisticated and realistic statistical models.

Being attracted by the extreme flexibility and power of the Monte Carlo method, many researchers in different scientific areas have contributed to its development. However, because a substantial amount of domain-specific knowledge is required in order to understand problems in any of these fields, communications among researchers in these fields are very limited. Many efforts have been devoted to the reinvention of techniques that have been developed in other fields. It is therefore desirable to develop a relatively general framework in which scientists in every field — e.g., theoretical chemists, statistical physicists, structural biologists, statisticians, econometricians, and computer scientists — can compare their Monte Carlo techniques and learn from each other. For a large number of scientists and engineers who employ Monte Carlo simulation and related global optimization techniques (such as simulated annealing) as an essential tool in their work, there is also a need to keep up to date with recent advances in Monte Carlo method-

ologies and to understand the nature and connection of various proposed methods. The aim of this book is to provide a self-contained, unified, and up-to-date treatment of the Monte Carlo method.

This book is intended to serve three audiences: researchers specializing in the study of Monte Carlo algorithms; scientists who are interested in using advanced Monte Carlo techniques; and graduate students in statistics, computational biology, and computer sciences who want to learn about Monte Carlo computations. The prerequisites for understanding most of the methods described in this book are rather minimal: a one-semester course on probability theory (Pitman 1993) and a one-semester course on theoretical statistics (Rice 1994), both at the undergraduate level. However, it would be more desirable if the reader has some background in a specific scientific field such as artificial intelligence, computational biology, computer vision, engineering, or Bayesian statistics in which heavy computations are involved. This book is most suitable for a second-year graduate-level course on Monte Carlo methods, with an emphasis on their relevance to scientific and statistical research.

The author is most grateful to his mentor and friend Wing Hung Wong for his many important suggestions, his overwhelming passion for Monte Carlo and scientific problems, and his continuous encouragement. The author is also grateful to Persi Diaconis for teaching him many things including Markov chain theory, group theory, and nonparametric Bayes methods, to both Susan Holmes and Persi for numerous enlightening conversations on Markov chain Monte Carlo and other related problems, to Donald B. Rubin for insights on the missing data formulation and the Bayesian thinking, to Jonathan Goodman for helpful comments on multigrid Monte Carlo, to Yingnian Wu and Songchun Zhu for their materials on pattern simulations and thoughts on conditional sampling, to Faming Liang for his supply of many examples and figures, and to Minghui Chen and David van Dyk for helpful comments. Several former graduate students in the statistics departments of Stanford and Harvard universities — Yuguo Chen, Lingyu Chen, Chiara Sabatti, Tanya Logvinenko, Zhaohui Qin and Juni Zhang — have contributed in many ways to the development of this book. Ms. Helen Tombropoulos has provided editorial assistance to the author both for this book and for many articles published earlier. Finally, the author is greatly indebted to his wife Wei for her love and her continuous support of his research activities these years. Part of the book was written when the author was on the faculty of the Statistics Department of Stanford University. This work was also partially supported by the National Science Foundation Grants DMS-9803649 and DMS-0094613.

Cambridge, Massachusetts
March 2001

Jun Liu

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Introduction and Examples

1.1 The Need of Monte Carlo Techniques

An essential part of many scientific problems is the computation of integral

$$I = \int_D g(\mathbf{x})d\mathbf{x},$$

where D is often a region in a high-dimensional space and $g(\mathbf{x})$ is the target function of interest. If we can draw independent and identically distributed (i.i.d.) random samples $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}$ uniformly from D (by a computer), an approximation to I can be obtained as

$$\hat{I}_m = \frac{1}{m}\{g(\mathbf{x}^{(1)}) + \cdots + g(\mathbf{x}^{(m)})\}.$$

The *law of large numbers* states that the average of many independent random variables with common mean and finite variances tends to stabilize at their common mean (see the Appendix); that is,

$$\lim_{m\to\infty} \hat{I}_m = I, \quad \text{with probability 1.}$$

Its convergence rate can be assessed by the *central limit theorem* (CLT):

$$\sqrt{m}(\hat{I}_m - I) \to N(0, \sigma^2), \quad \text{in distribution,}$$

where $\sigma^2 = \text{var}\{g(\mathbf{x})\}$. Hence, the "error term" of this Monte Carlo approximation is $O(m^{-1/2})$, regardless of the dimensionality of $\mathbf{x}$. This basic

setting underlies the potential role of the Monte Carlo methodology in science and statistics.

In the simplest case when $D = [0,1]$ and $I = \int_0^1 g(x)dx$, one can approximate I by

$$\tilde{I}_m = \frac{1}{m}\{g(b_1) + \cdots + g(b_m)\},$$

where $b_j = j/m$. This method can be called the *Riemann approximation.* When g is reasonably smooth, the Riemann approximation gives us an error rate of $O(m^{-1})$, better than that of the Monte Carlo method. More sophisticated methods such as Simpson's rule and the Newton-Cotes rules give better numerical approximations (Thisted 1988). However, a fatal defect of these deterministic methods is that they do not scale well as the dimensionality of D increases. For example, in a 10-dimensional space with $D = [0,1]^{10}$, we will have to evaluate $O(m^{10})$ grid points in order to achieve an accuracy of $O(m^{-1})$ in the Riemann approximation of I. In contrast, the naive Monte Carlo approach, which draws $x^{(1)}, \ldots, x^{(m)}$ uniformly from D, has an error rate $O(m^{-1/2})$ regardless of the dimensionality of D, at least theoretically.

Although the "error rate" of a Monte Carlo integration scheme remains the same in high-dimensional problems, two intrinsic difficulties arise: (a) when the region D is large in high-dimensional space, the variance σ^2, which measures how "uniform" the function g is in region D, can be formidably large; (b) one may not be able to produce uniform random samples in an arbitrary region D. To overcome these difficulties, researchers often employ the idea of *importance sampling* in which one generates random samples $\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}$ from a nonuniform distribution $\pi(\mathbf{x})$ that puts more probability mass on "important" parts of the state space D. One can estimate integral I as

$$\hat{\tilde{I}} = \frac{1}{m}\sum_{j=1}^{m} \frac{g(\mathbf{x}^{(j)})}{\pi(\mathbf{x}^{(j)})},$$

which has a variance $\sigma_\pi^2 = \mathrm{var}_\pi\{g(\mathbf{x})/\pi(\mathbf{x})\}$. In the most fortunate case, we may choose $\pi(\mathbf{x}) \propto g(\mathbf{x})$ when g is non-negative and I is finite, which results in an exact estimate of I. But in no known application of the Monte Carlo method has this "luckiest situation" ever occurred. More realistically, we may hope to find a good "candidate" π which will explore more in regions where the value of g is high. In such a situation, generating random draws from π can be a challenging problem.

Demands for sampling from a nonuniform distribution π are also seen from another set of problems in bioinformatics, computational chemistry, physics, structural biology, statistics, etc. In these problems, the desired probability distribution $\pi(\mathbf{x})$ of a complex system, where $\mathbf{x}$ is often called a *configuration* of the system, arises from basic laws in physics and statistical