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The Fields Institute for Research in Mathematical Sciences

The Fields Institute is named in honour of the Canadian mathematician John Charles Fields (1863–1932). Fields was a visionary who received many honours for his scientific work, including election to the Royal Society of Canada in 1909 and to the Royal Society of London in 1913. Among other accomplishments in the service of the international mathematics community, Fields was responsible for establishing the world's most prestigious prize for mathematics research—the Fields Medal.

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Preface

This book is based on a graduate course that I gave at the Fields Institute for Research in Mathematical Sciences in Fall 1998, as part of the thematic year on Probability and Its Applications. The aim of the course was to introduce students to the theory and practice of Monte Carlo methods. I planned to cover a range of key topics to the depth necessary for the student to be able to design, implement and analyze a full Monte Carlo study of a mathematical or scientific problem. As in most courses, I had to compromise between breadth and depth. The lectures were designed to present material that could be comfortably handled in lecture format. For students who might later need more details on individual topics, I included frequent references to books and articles. This book is based closely upon the lectures and follows this approach.

The course was unique for me because it attracted a larger variety of students (and postdocs and others) than I am accustomed to: in attendance were people whose research was in mathematics, statistics, physics, chemistry, finance, computer science, and biology. The only formal prerequisite for the course was an undergraduate course in probability. The same is true for this book, although it is also helpful to know some basic statistics, and a knowledge of elementary Markov chain theory is assumed for Chapter 4. I have tried to keep the level of the book suitable for a beginning graduate student or an advanced undergraduate.

The first chapter contains an overview of what Monte Carlo is all about, as well as a brief summary of basic concepts from probability and statistics that the reader is assumed to have seen elsewhere. Chapter 2 describes various algorithms that produce "random variables" having desired distributions. Computer implementation of these algorithms are the fundamental building blocks of any Monte Carlo study. Chapter 3 describes techniques for improving the efficiency and accuracy of your Monte Carlo study, and illustrates the concepts with running examples from numerical integration, network reliability and queueing theory. Chapter 4 is devoted to Markov chain Monte Carlo, a powerful method for simulating complex random systems arising in statistics, physics, computer science, and other fields. Chapter 5 describes statistical methods for analyzing the output of a Monte Carlo study. Chapter 6 concludes the book with a discussion of the Ising model from statistical physics and Markov chain Monte Carlo methods that have been developed to study it.

I have tried to make this book broadly accessible to students with a variety of scientific backgrounds, although parts of it are designed more for students with a stronger mathematical inclination. I have also been rather selective in the choice of topics, with the result that I could have subtitled this work "A Personal View of Monte Carlo". With several fine and thorough texts on Monte Carlo available, I felt spared from the need to be complete, and I used the limitations imposed by the course timetable as a further excuse to abbreviate or omit various topics. I feel that the resulting lecture notes that comprise this book "cut to the chase" and allow the reader to survey quickly the main ideas and capabilities of Monte Carlo methods.

It is natural to reflect on the additional topics that I would have covered if the course had been much longer. High on the list would be the theory of convergence rates for Markov chain Monte Carlo (Sinclair (1993), Meyn and Tweedie (1993)), simulated tempering and other acceleration algorithms (Madras (1998)), and more detailed applications to various fields, such as statistics (Gilks, Richardson, and Spiegelhalter (1996)), communications networks (Rubinstein (1986)), physics (Frenkel and Smit (1996), Sokal (1997)), and the self-avoiding walk (Madras and Slade (1993), Chapter 9). The interested reader is invited to consult these and other references for a fuller picture of current research in Monte Carlo methods.

I am grateful to Peter Peskun, Irwin Pressman, Donna Salopek, Soonok You, and Zhongrong Zheng for their feedback on an initial draft of these lectures. Dean Slonowsky provided valuable assistance in the early typing of these notes. It is a pleasure to record my thanks to Don Dawson, Tom Salisbury, and Gordon Slade, my co-organizers of the 1998–99 theme year in Probability and Its Applications at the Fields Institute. I also wish to thank the staff at the Fields Institute, especially Alesia Zuccala, who helped in the organization of the theme year as well as of this book. Finally, I happily acknowledge the continued support of the Natural Sciences and Engineering Research Council of Canada.

Neal Madras
Toronto, July 2001

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Monte Carlo methods form an experimental branch of mathematics that employs simulations driven by random number generators. These methods are often used when others fail, since they are much less sensitive to the "curse of dimensionality", which plagues deterministic methods in problems with a large number of variables. Monte Carlo methods are used in many fields: mathematics, statistics, physics, chemistry, finance, computer science, and biology, for instance.

This book is an introduction to Monte Carlo methods for anyone who would like to use these methods to study various kinds of mathematical models that arise in diverse areas of application. The book is based on lectures in a graduate course given by the author. It examines theoretical properties of Monte Carlo methods as well as practical issues concerning their computer implementation and statistical analysis. The only formal prerequisite is an undergraduate course in probability.

The book is intended to be accessible to students from a wide range of scientific backgrounds. Rather than being a detailed treatise, it covers the key topics of Monte Carlo methods to the depth necessary for a researcher to design, implement, and analyze a full Monte Carlo study of a mathematical or scientific problem. The ideas are illustrated with diverse running examples. There are exercises sprinkled throughout the text. The topics covered include computer generation of random variables, techniques and examples for variance reduction of Monte Carlo estimates, Markov chain Monte Carlo, and statistical analysis of Monte Carlo output.

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