

SpringerBriefs in Physics

Series Editors

Balasubramanian Ananthanarayan, Centre for High Energy Physics, Indian Institute of Science, Bangalore, India

Egor Babaev, Physics Department, University of Massachusetts Amherst, Amherst, MA, USA

Malcolm Bremer, H H Wills Physics Laboratory, University of Bristol, Bristol, UK

Xavier Calmet, Department of Physics and Astronomy, University of Sussex, Brighton, UK

Francesca Di Lodovico, Department of Physics, Queen Mary University of London, London, UK

Pablo D. Esquinazi, Institute for Experimental Physics II, University of Leipzig, Leipzig, Germany

Maarten Hoogerland, University of Auckland, Auckland, New Zealand

Eric Le Ru, School of Chemical and Physical Sciences, Victoria University of Wellington, Kelburn, Wellington, New Zealand

Dario Narducci, University of Milano-Bicocca, Milan, Italy

James Overduin, Towson University, Towson, MD, USA

Vesselin Petkov, Montreal, QC, Canada

Stefan Theisen, Max-Planck-Institut für Gravitationsphysik, Golm, Germany

Charles H.-T. Wang, Department of Physics, The University of Aberdeen, Aberdeen, UK

James D. Wells, Physics Department, University of Michigan, Ann Arbor, MI, USA

Andrew Whitaker, Department of Physics and Astronomy, Queen's University Belfast, Belfast, UK

SpringerBriefs in Physics are a series of slim high-quality publications encompassing the entire spectrum of physics. Manuscripts for SpringerBriefs in Physics will be evaluated by Springer and by members of the Editorial Board. Proposals and other communication should be sent to your Publishing Editors at Springer.

Featuring compact volumes of 50 to 125 pages (approximately 20,000–45,000 words), Briefs are shorter than a conventional book but longer than a journal article. Thus, Briefs serve as timely, concise tools for students, researchers, and professionals.

Typical texts for publication might include:

- A snapshot review of the current state of a hot or emerging field
- A concise introduction to core concepts that students must understand in order to make independent contributions
- An extended research report giving more details and discussion than is possible in a conventional journal article
- A manual describing underlying principles and best practices for an experimental technique
- An essay exploring new ideas within physics, related philosophical issues, or broader topics such as science and society

Briefs allow authors to present their ideas and readers to absorb them with minimal time investment.

Briefs will be published as part of Springer's eBook collection, with millions of users worldwide. In addition, they will be available, just like other books, for individual print and electronic purchase.

Briefs are characterized by fast, global electronic dissemination, straightforward publishing agreements, easy-to-use manuscript preparation and formatting guidelines, and expedited production schedules. We aim for publication 8–12 weeks after acceptance.

More information about this series at <http://www.springer.com/series/8902>

Anosh Joseph

Markov Chain Monte Carlo Methods in Quantum Field Theories

A Modern Primer

 Springer

Anosh Joseph
Department of Physical Sciences
Indian Institute of Science Education
and Research (IISER) Mohali
SAS Nagar, Punjab, India

ISSN 2191-5423

SpringerBriefs in Physics

ISBN 978-3-030-46043-3

<https://doi.org/10.1007/978-3-030-46044-0>

ISSN 2191-5431 (electronic)

ISBN 978-3-030-46044-0 (eBook)

© The Author(s), under exclusive license to Springer Nature Switzerland AG 2020

This work is subject to copyright. All rights are solely and exclusively licensed by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

*To my parents Ouseppachan and Elyakutty
Velliyamkandathil with gratitude*

Foreword

This book may well be the most concise and pedagogical introduction to Monte Carlo methods in Quantum Field Theory available in the market today. Beginning with simple examples of how to numerically integrate ordinary functions in a small number of dimensions, the book gradually warms up the reader to the idea of using random numbers to estimate integrals. These ‘Monte Carlo’ ideas are easily tested in low-dimensional cases, but they stand without competition when the dimensionality becomes large.

Quantum Field Theory in its path-integral formulation is an example of where even infinitely-dimensional integrals can be needed in order to compute. The trick is to return to the very definition of the path integral, chop up space and time in small discretized intervals and enclose everything in a finite volume. The result is very large-dimensional integral that can be evaluated approximately by Monte Carlo techniques. This sounds simple, but the reader is warned along the way regarding potential difficulties or even misleading estimates. Methods are tested in great detail on analytically solvable cases, drawing on modern examples that also include supersymmetry. The book ends with the most important example for relativistic field theories: that of gauge fields defined on a space-time lattice. In an outlook, the reader is given a peek at what may lie ahead of new developments based on machine learning. Finally, a full set of C++ programs are included so that no student will be lost.

Anosh Joseph has the advantage of coming from the main analytical approach to Quantum Field Theory while having continually worked hand in hand with numerical techniques. This gives him a fresh look on the matter and it enables him

to draw on example that standard practitioners of Monte Carlo methods in, say, lattice gauge theory may not be aware of. The book is delightfully well written and is bound to please students who would like to learn the subject from the scratch.

Copenhagen, Denmark
March 2020

Poul H. Damgaard
Professor Theoretical Physics, Niels
Bohr Institute, Director, Niels Bohr
International Academy

Preface

Quantum field theory is a tool to understand a vast array of perturbative and non-perturbative phenomena found in physical systems. Some of the most interesting features of quantum field theories, such as spontaneous symmetry breaking, phase transitions, and bound states of particles, demand computational tools beyond the machinery of ordinary perturbation theory. Monte Carlo methods using Markov chain based sampling algorithms provide powerful tools for carrying out such explorations.

We can use lattice regularized quantum field theories and simulation algorithms based on Monte Carlo methods to reveal the non-perturbative structure of many interesting quantum field theories, including Quantum Chromodynamics (QCD), the theory of strong interactions. The rapidly developing field of Machine Learning could provide novel tools to find phase structures and order parameters of systems where they are hard to identify.

This book contains 9 chapters. In Chap. 1 we discuss various simple methods of numerical integration, including the rectangle rule, midpoint rule, trapezoidal rule, and Simpson's rule. Random numbers are introduced next. We discuss pseudo-random numbers and how they can be generated on a computer using a seed number. After that, we move on to discuss the Monte Carlo method for numerical integration. We also discuss how to compute the error in Monte Carlo integration, the questions on when Monte Carlo is useful for integration and when it can fail. In Chap. 2 we discuss Monte Carlo with importance sampling and how it reduces the variance of the Monte Carlo estimate of the given integral. In Chap. 3 we introduce Markov chains and discuss their properties and convergence to the unique equilibrium distribution when the chain is irreducible and aperiodic. In Chap. 4 we introduce Markov chain Monte Carlo. Concepts such as Metropolis algorithm and thermalization of Markov chains are introduced. In Chap. 5 we discuss the connection between Markov chain Monte Carlo and Feynman path integrals of Euclidean quantum field theories. We also numerically study a zero-dimensional quantum field theory that undergoes dynamical supersymmetry breaking, one-dimensional simple harmonic oscillator, and a unitary matrix model that undergoes Gross-Witten-Wadia phase transition. In Chap. 6 we discuss the

reliability of Monte Carlo simulations and introduce the idea of auto-correlation time in the observables. The method of Hybrid (Hamiltonian) Monte Carlo is discussed next in Chap. 7. There, we look at the properties of Hamiltonian dynamics and how the Leapfrog integration method can be used to evolve the system in simulation time. We then apply Hamiltonian Monte Carlo to a Gaussian model and a zero-dimensional supersymmetric model. In Chap. 8 we briefly discuss how Markov chain Monte Carlo can be used to extract physics from quantum field theories formulated on a spacetime lattice. In Chap. 9 we discuss how Machine Learning and quantum field theory can work together to further our understanding of the nature of the physical systems we are interested in. This book ends with several appendices containing various C++ programs that were used to generate data and numerical results provided in this book.

Mohali, India
February 2020

Anosh Joseph

Acknowledgements

This book benefits from various dialogues with colleagues and students in research conferences, seminars, and classroom discussions. I would like to thank the following people for influencing and shaping the way I look at the mesmerizing world of quantum fields on a lattice: Felix Bahr, Debasish Banerjee, Pallab Basu, Tanmoy Bhattacharya, Mattia Dalla Brida, Mattia Bruno, Simon Catterall, Vincenzo Cirigliano, Saul Cohen, Poul Damgaard, N. D. Hari Dass, Saumen Datta, Sanatan Digal, Gerald Dunne, Daniel Ferrante, Richard Galvez, Rajiv Gavai, Dimitrios Giataganas, Joel Giedt, Rajan Gupta, Sourendu Gupta, Masanori Hanada, Prasad Hegde, Ron Horgan, Karl Jansen, Vishnu Jejjala, Raghav Jha, David B. Kaplan, Liam Keegan, Nilmani Mathur, Robert de Mello Koch, Huey-Wen Lin, Stefano Lottini, So Matsuura, Dhagash Mehta, Jun Nishimura, Apoorva Patel, Joao Rodrigues, Alberto Ramos, Stefan Schaefer, David Schaich, Jonathan Shock, Rainer Sommer, Fumihiko Sugino, Christopher Thomas, David Tong, Giacomo Torlai, Mithat Unsal, Aarti Veernala, Matthew Wingate, Toby Wiseman, Ulli Wolff, Boram Yoon, and Konstantinos Zoubos.

I would like to thank Navdeep Singh Dhindsa, Roshan Kaundinya, Arpith Kumar, and Vamika Longia for providing valuable suggestions on improving the manuscript.

I am indebted to the organizers, the lecturers, and the students of the *2019 Joburg School in Theoretical Physics: Aspects of Machine Learning*, at the Mandelstam Institute for Theoretical Physics, The University of the Witwatersrand, Johannesburg, South Africa, for an inspiring atmosphere at the School. This book started taking shape there.

Last but not least, I would like to thank Lisa Scalone, B Ananthanarayan, and Christian Caron for their guidance on preparing this book in its current form.

The work on this book was supported in part by the Start-up Research Grant (No. SRG/2019/002035) from the Science and Engineering Research Board (SERB), Department of Science and Technology, Government of India, and in part by a Seed Grant from the Indian Institute of Science Education and Research (IISER) Mohali.

Contents

1 Monte Carlo Method for Integration	1
1.1 Numerical Integration	1
1.2 Composite Formulas for Numerical Integration	4
1.2.1 Composite Rectangle Rule	4
1.2.2 Composite Midpoint Rule	4
1.2.3 Composite Trapezoidal Rule	5
1.2.4 Composite Simpson’s Rule	5
1.3 Random Numbers	6
1.3.1 Physical Random Numbers	7
1.3.2 Pseudo-random Numbers	7
1.3.3 Random Numbers Using UNIX Function Drand48()	9
1.3.4 Random Numbers Using a Seed	9
1.3.5 Random Numbers from Non-uniform Distributions	9
1.4 Monte Carlo Method	13
1.4.1 Worked Example—Composite Midpoint Rule	14
1.4.2 Worked Example—Composite Simpson’s Rule	15
1.4.3 Worked Example—Monte Carlo Integration	16
1.5 Error in Monte Carlo Integration	17
1.6 When is Monte Carlo Good for Integration?	17
1.7 When does Monte Carlo Fail?	18
2 Monte Carlo with Importance Sampling	21
2.1 Naive Sampling and Importance Sampling	21
2.2 Worked Example—Importance Sampling	24
2.3 When does Importance Sampling Fail?	26

3	Markov Chains	29
3.1	Properties of Markov Chains	31
3.1.1	Irreducibility	32
3.1.2	Aperiodicity	32
3.2	Convergence of Markov Chains	33
4	Markov Chain Monte Carlo	37
4.1	Metropolis-Hastings Algorithm	37
4.2	Metropolis Algorithm	38
4.3	Worked Example—Metropolis for Gaussian Integral	40
4.4	Thermalization in Markov Chain Monte Carlo	41
5	MCMC and Feynman Path Integrals	43
5.1	Transition Amplitudes	43
5.2	Feynman Path Integrals	45
5.3	Worked Example—Supersymmetry Breaking	47
5.4	Worked Example—Simple Harmonic Oscillator	49
5.5	Worked Example—Unitary Matrix Model	53
6	Reliability of Simulations	55
6.1	Auto-correlation Time	55
6.2	Error Analysis	58
7	Hybrid (Hamiltonian) Monte Carlo	59
7.1	Hamilton’s Equations	60
7.2	Properties of Hamiltonian Dynamics	60
7.3	Leapfrog Method	61
7.4	MCMC from Hamiltonian Dynamics	62
7.4.1	Joint Probability Distribution	62
7.4.2	Tuning HMC Algorithm	63
7.4.3	HMC Algorithm—Step by Step	64
7.5	Worked Example—HMC for Gaussian Model	65
7.6	Worked Example—HMC for Supersymmetric Model	67
8	MCMC and Quantum Field Theories on a Lattice	71
9	Machine Learning and Quantum Field Theories	75
	Appendix: C++ Programs	77
	References	125