Classics in Mathematics

Richard S. Ellis

Entropy, Large Deviations, and Statistical Mechanics

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For Alison, Melissa, and Michael
my wife and children
who make it all worthwhile

Preface

This book has two main topics: large deviations and equilibrium statistical mechanics. I hope to convince the reader that these topics have many points of contact and that in being treated together, they enrich each other. Entropy, in its various guises, is their common core.

The large deviation theory which is developed in this book focuses upon convergence properties of certain stochastic systems. An elementary example is the weak law of large numbers. For each positive ε, $P\{|S_n/n| \geq \varepsilon\}$ converges to zero as $n \to \infty$, where S_n is the nth partial sum of independent identically distributed random variables with zero mean. Large deviation theory shows that if the random variables are exponentially bounded, then the probabilities converge to zero exponentially fast as $n \to \infty$. The exponential decay allows one to prove the stronger property of almost sure convergence ($S_n/n \to 0$ a.s.). This example will be generalized extensively in the book. We will treat a large class of stochastic systems which involve both independent and dependent random variables and which have the following features: probabilities converge to zero exponentially fast as the size of the system increases; the exponential decay leads to strong convergence properties of the system. The most fascinating aspect of the theory is that the exponential decay rates are computable in terms of entropy functions. This identification between entropy and decay rates of large deviation probabilities enhances the theory significantly.

Entropy functions have their roots in statistical mechanics. They originated in the work of L. Boltzmann, who in the 1870's studied the relation between entropy and probability in physical systems. Thus statistical mechanics has a strong historical connection with large deviation theory. It also provides a natural context in which the theory can be applied. Applications of large deviations to models in equilibrium statistical mechanics are presented in Chapters III–V. These applications illustrate convincingly the power of the theory.

Equilibrium statistical mechanics is an exciting area of mathematical physics but one which remains inaccessible to many mathematicians. Some texts on the subject provide an introduction to the physics but do not develop the mathematics in much detail or with great rigor. Other texts treat mathematical problems in statistical mechanics with complete rigor but assume an extensive background in the physics. The uninitiated reader has difficulty understanding how concepts like ensemble, free energy, or entropy connect up with more familiar concepts in mathematics. My approach in this book is to emphasize strongly the connections between statistical mechanics on the one hand and probability and large deviations on the other. I hope that in so doing, I have succeeded in providing a readable treatment of statistical mechanics which is accessible to a general mathematical audience. My large deviation approach to statistical mechanics was inspired in part by the article of O. E. Lanford (1973).

In recent years, the scope of large deviations has been greatly expanded by M. D. Donsker and S. R. S. Varadhan. This book contains an introduction to their theory. I illustrate the main features in the context of independent identically distributed random vectors taking values in $\mathbb{R}^d$. I also present my own large deviation results, which are particularly suited for applications to statistical mechanics. Since readability rather than completeness has been my goal, the large deviation theorems are not stated in the greatest generality.

There are two parts to the book, Part I consisting of Chapters I–V. Chapter I introduces large deviations by means of elementary examples involving combinatorics and Stirling's formula. Chapter II presents the Donsker–Varadhan theory as well as my own large deviation results. The proofs of the theorems in this chapter are detailed and are postponed until Part II. Postponing proofs allows the reader to reach, as soon as possible, interesting applications of large deviations to statistical mechanics in Chapters III–V. Chapter III gives a large deviation analysis of a discrete gas model. Chapters IV–V discuss the Ising model of ferromagnetism and related spin systems. The emphasis in these two chapters is upon properties of Gibbs states. While large deviation theory provides a terminology and a set of results that are useful for treating Gibbs states, the book also develops other tools that are needed. These include convexity and moment inequalities.

Part II consists of Chapters VI–IX. Chapter VI is a summary of the theory of convex functions on $\mathbb{R}^d$. Chapters VII–IX prove the large deviation results stated in Chapter II without proof. The prerequisite for these chapters is a good working knowledge of probability and measure theory. The essential definitions and theorems in probability are listed in Appendix A. The appendix is intended to be a review or an outline for study rather than a detailed exposition.

This book can be used as a text. It contains over 100 problems, many of which have hints. Chapters I and II and VI–IX are a self-contained treatment of large deviations and convex functions. Readers primarily interested in spin systems can concentrate upon Chapters IV and V and refer to the statements and proofs of large deviation results as needed. Those portions of Chapters IV and V which do not rely on large deviations are self-contained. Chapters IV and V can be completely understood without reading Chapter III.

This book contains new results and new proofs of known theorems. These include the following: exponential convergence properties of Gibbs states

[Theorems IV.5.5, IV.6.6, and V.6.1]; a large deviation proof of the Gibbs variational formula [Theorem IV.7.3(a)]; a proof of the central limit theorem for spin systems [Theorem V.7.2(a)]; a level-3 large deviation theorem for i.i.d. random variables with a finite state space [Theorem IX.1.1]; a level-3 large deviation theorem for Markov chains with a finite state space [Problems IX.6.10–IX.6.15]; the solution of the Gibbs variational formula for finite-range interactions on $\mathbb{Z}$ via large deviations [Appendix C.6]. Many of the large deviation results and applications in the book depend upon my large deviation theorem, Theorem II.6.1. The proof of the level-3 theorem in Chapter IX was inspired by statistical mechanics [see Appendix C.6] and information theory.

I have had the good fortune of interacting with a number of special people. Todd Baker edited the manuscript with creativity and care. The book benefited greatly from his involvement. Peg Bombardier was my superb typist. She was always cheerful and patient, despite the numerous revisions, and was a pleasure to work with. Alan Sokal read portions of the manuscript and was a big help with the statistical mechanics. I owe a special debt of gratitude to Srinivasa Varadhan. He answered my many questions about large deviations patiently and with insight and showed a strong interest in the book. The encouragement of my family and friends was greatly appreciated. Above all, I thank my wife Alison. Her love is a blessing.

I am grateful to Alejandro de Acosta, Hans-Otto Georgii, Joseph Horowitz, Jonathan Machta, Charles Newman, and R. Tyrrell Rockafellar for reading portions of the manuscript and suggesting improvements. I am also indebted to the many other people, too numerous to mention by name, with whom I have consulted. While writing the book, I received support from the University of Massachusetts, the National Science Foundation, and the Lady Davis Fellowship Trust. Their support is gratefully acknowledged.

Richard S. Ellis

Comments on the Use of This Book

At the end of each chapter, there is a Notes section, followed by a Problems section. References to the Notes are indicated by superscripted integers; e.g., entropy[4] refers to Note 4. Near the end of the book, there is a list of frequently used symbols.

The main large deviation theorems are stated in Chapter II and are proved in Chapters VI–IX. Readers interested primarily in large deviations may read Chapters I, II, VI–IX while those interested primarily in statistical mechanics may read Chapters I–V.

Contents

Part I

Large Deviations and Statistical Mechanics