

Preface

Stochastic processes and diffusion theory are the mathematical underpinnings of many scientific disciplines, including statistical physics, physical chemistry, molecular biophysics, communications theory, and many more. Many books, reviews, and research articles have been published on this topic, from the purely mathematical to the most practical. Some are listed below in alphabetical order, but a Web search reveals many more.

- Mathematical theory of stochastic processes [14], [25], [46], [47], [53], [58], [57], [72], [76], [74], [82], [206], [42], [101], [106], [115], [116], [117], [150], [153], [161], [208], [234], [241]
- Stochastic dynamics [5], [80], [84], [171], [193], [204], [213]
- Numerical analysis of stochastic differential equations [207], [59], [132], [131], [103], [174], [206], [4]
- Large deviations theory [32], [52], [54], [68], [77], [110], [55]
- Statistical physics [38], [82], [100], [98], [99], [185], [206], [196], [242]
- Electrical engineering [108], [148], [199]

This book offers an analytical approach to stochastic processes that are most common in the physical and life sciences. Its aim is to make probability theory in function space readily accessible to scientists trained in the traditional methods of applied mathematics, such as integral, ordinary, and partial differential equations and asymptotic methods, rather than in probability and measure theory.

The book presents the basic notions of stochastic processes, mostly diffusions, including fundamental concepts from measure theory in the space of continuous functions (the space of random trajectories). The rudiments of the Wiener measure in function space are introduced not for the sake of mathematical rigor, but rather as a tool for counting trajectories, which are the elementary events in the probabilistic description of experiments. The Wiener measure turns out to be appropriate for the statistical description of nonequilibrium systems and replaces the equilibrium Boltzmann distribution in configuration space. The relevant stochastic processes are mainly stochastic differential equations driven by Einstein's white or the Ornstein–Uhlenbeck (OU) colored noise, but include also continuous-time Markovian jump

processes and discrete-time semi-Markovian processes, such as renewal processes. Continuous- or discrete-time jump processes often contain more information about the origin of randomness in a given system than diffusion (white noise) models. Approximations of the more microscopic discrete models by their continuum limits (diffusions) are the cornerstone of modeling random systems.

The analytical approach relies heavily on initial and boundary value problems for partial differential equations that describe important probabilistic quantities, such as probability density functions, mean first passage times, density of the mean time spent at a point, survival probability, probability flux density, and so on. Green's function and its derivatives play a central role in expressing these quantities analytically and in determining their interrelationships. The most prominent equations are the Fokker–Planck and Kolmogorov equations for the transition probability density, which are the well-known transport–diffusion partial differential equations of continuum theory, the Kolmogorov and Feynman–Kac representation formulas for solutions of initial boundary value problems in terms of conditional probabilities, the Andronov–Vitt–Pontryagin equation for the conditional mean first passage time, and more.

Computer simulations are the numerical realizations of stochastic dynamics and are ubiquitous in computational physics, chemistry, molecular biophysics, and communications theory. The behavior of random trajectories near boundaries of the simulation impose a variety of boundary conditions on the probability density and its functionals. The quite intricate connection between the random trajectories and the boundary conditions for the partial differential equations is treated here with special care. The Wiener path integral and Wiener measure in function space are used extensively for determining these connections. Some of the simulation-oriented topics are discussed in one dimension only, because the book is not about simulations. Special topics that arise in Brownian dynamics simulations and their analysis, such as simulating trajectories between constant concentrations, connecting a simulation to the continuum, the albedo problem, behavior of trajectories at higher-dimensional partially reflecting boundaries, the estimate of rare events due to escape of random trajectories through small openings, the analysis of simulations of interacting particles and more are discussed in [214]. The important topic of nonlinear optimal filtering theory and performance evaluation of optimal phase trackers is discussed in [215].

The extraction of useful information about stochastic processes requires the solution of the basic equations of the theory. Numerical solutions of integral and partial differential equations or computer simulations of stochastic dynamics are often inadequate for the exploration of the parameter space or for studying rare events. The methods and tricks of the trade of applied mathematics are used extensively to obtain explicit analytical approximations to the solutions of complicated equations. The methods include singular perturbation techniques such as the WKB expansion, borrowed from quantum mechanics, boundary layer theory, borrowed from continuum theory, the Wiener–Hopf method, and more. These methods are the main analytical tools for the analysis of systems driven by small noise (small relative to the drift). In particular, they provide analytical expressions for the mean exit time of

a random trajectory from a given domain, a problem often encountered in physics, physical chemistry, molecular and cellular biology, and in other applications. The last chapter, on stochastic stability, illustrates the power of the analytical methods for establishing the stochastic stability, or even for stabilizing unstable structures by noise.

The book contains exercises and worked-out examples. The hands-on training in stochastic processes, as my long teaching experience shows, consists of solving the exercises, without which understanding is only illusory. The book is based on lecture notes from a one- or two-semester course on stochastic processes and their applications that I taught many times to graduate students of mathematics, applied mathematics, physics, chemistry, computer science, electrical engineering, and other disciplines. My experience shows that mathematical rigor and applications cannot coexist in the same course; excessive rigor leaves no room for in-depth development of modeling methodology and turns off students interested in scientific and engineering applications. Therefore the book contains only the minimal mathematical rigor required for understanding the necessary measure-theoretical concepts and for enabling the students to use their own judgment of what is correct and what requires further theoretical study. The student should be familiar with basic measure and integration theory as well as with rudiments of functional analysis, as taught in most graduate analysis courses (see, e.g., [79]). More intricate measure-theoretical problems are discussed in theoretical texts, as mentioned in the first list of references above. The first course can cover the fundamental concepts presented in the first six chapters and either Chapter 8 on Markov processes and their diffusion approximations, or Chapters 7 or 11, which develop some of the mentioned methods of applied mathematics and apply them to the study of systems driven by small noise. Chapters 7 and 9–12, which develop and apply the analytical tools to the study of the equations developed in Chapters 1–6 and 8, can be chosen for the second semester. A well-paced course can cover most of the book in a single semester. The two books [214], on Brownian dynamics and simulations, and [215], on optimal filtering and phase tracking, can be used for one-semester special topics followup courses.

It is recommended that students of Chapters 7 and 9–12 acquire some independent training in singular perturbation methods, for example, from classical texts such as [194], [121], [20], [195], [251]. These chapters require the basic knowledge of Chapters 1–6 and a solid training in partial differential equations of mathematical physics and in the asymptotic methods of applied mathematics.

Acknowledgment. Much of the material presented in this book is based on my collaboration with many scientists and students, whose names are listed next to mine in the author index. Much of the work done in the nearly 30 years since my first book appeared [213], was initiated in the Department of Applied Mathematics and Engineering Science at Northwestern University and in the Department of Molecular Biophysics and Physiology at Rush Medical Center in Chicago, for whose hospitality I am grateful. The scientific environment provided by Tel-Aviv University, my home institution, was conducive to interdisciplinary cooperation. Its double-major undergraduate program in mathematics and physics, as well as its M.Sc. program in E.E. produced my most brilliant graduate students and collaborators in applied mathematics.

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