Applied Stochastic Analysis

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EDITORIAL COMMITTEE

To our families

> *Hongjun, Jane, and Ilene*
> *Xueqing, Baitian, and Baile*
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Contents

Part 2. Advanced Topics

Introduction
to the Series

It is fairly well accepted that to learn pure mathematics, a student has to take analysis, algebra, geometry, and topology. Until now there has not been an equally well-accepted curriculum for applied mathematics. There are many reasons one can think of. For one thing, applied mathematics is truly very diverse. Traditional subjects such as numerical analysis, statistics, operational research, etc., can all be regarded as part of applied mathematics. Beyond that, a huge amount of applied mathematics is practiced in other scientific and engineering disciplines. For example, a large part of fluid dynamics research has become computational. The same can be said about theoretical chemistry, biology, material science, etc. The algorithmic issues that arise in these disciplines are at the core of applied mathematics. Machine learning, a subject that deals with mathematical models and algorithms for complex data, is, at its heart, a very mathematical discipline, although at the moment it is much more commonly practiced in computer science departments.

In 2002, David Cai, Shi Jin, Eric Vanden-Eijnden, Pingwen Zhang, and I started the applied mathematics summer school in Beijing, with the objective of creating a systematic and unified curriculum for students in applied mathematics. Since then, this summer school has been repeated every year at Peking University. The main theme of the summer school has also evolved. But in the early years, the main topics were applied stochastic analysis, differential equations, numerical algorithms, and a mathematical introduction to physics. In recent years, a mathematical introduction to

machine learning has also been added to the list. In addition to the summer school, these courses have also been taught from time to time during regular terms at New York University, Peking University, and Princeton University. The lecture notes from these courses are the main origin of this textbook series. The early participants, including some of the younger people who were students or teaching assistants early on, have also become contributors to this book series.

After many years, this series of courses has finally taken shape. Obviously, this has not come easy and is the joint effort of many people. I would like to express my sincere gratitude to Tiejun Li, Pingbing Ming, Shi Jin, Eric Vanden-Eijnden, Pingwen Zhang, and other collaborators involved for their commitment and dedication to this effort. I am also very grateful to Mrs. Yanyun Liu, Baomei Li, Tian Tian, Yuan Tian for their tireless efforts to help run the summer school. Above all, I would like to pay tribute to someone who dedicated his life to this cause, David Cai. David had a passion for applied mathematics and its applications to science. He believed strongly that one has to find ways to inspire talented young people to go into applied mathematics and to teach them applied mathematics in the right way. For many years, he taught a course on introducing physics to applied mathematicians in the summer school. To create a platform for practicing the philosophy embodied in this project, he cofounded the Institute of Natural Sciences at Shanghai Jiaotong University, which has become one of the most active centers for applied mathematics in China. His passing away last year was an immense loss, not just for all of us involved in this project, but also for the applied mathematics community as a whole.

This book is the first in this series, covering probability theory and stochastic processes in a style that we believe is most suited for applied mathematicians. Other subjects covered in this series will include numerical algorithms, the calculus of variations and differential equations, a mathematical introduction to machine learning, and a mathematical introduction to physics and physical modeling. The stochastic analysis and differential equations courses summarize the most relevant aspects of pure mathematics, the algorithms course presents the most important technical tool of applied mathematics, and the learning and physical modeling courses provide a bridge to the real world and to other scientific disciplines. The selection of topics represents a possibly biased view about the true fundamentals of applied mathematics. In particular, we emphasize three themes throughout this textbook series: learning, modeling, and algorithms. Learning is about data and intelligent decision making. Modeling is concerned with physics-based models. The study of algorithms provides the practical tool for building and interrogating the models, whether machine learning–based

or physics-based. We believe that these three themes should be the major pillars of applied mathematics, the applied math analog of algebra, analysis, and geometry.

While physical modeling and numerical algorithms have been the dominating driving force in applied mathematics for years, machine learning is a relatively new comer. However, there are very good reasons to believe that machine learning will not only change AI but also the way we do physical modeling. With this last missing component in place, applied mathematics will become the natural platform for integrating machine learning and physical modeling. This represents a new style for doing scientific research, a style in which the data-driven Keplerian paradigm and the first principle-driven Newtonian paradigm are integrated to give rise to unprecedented technical power. It is our hope that this series of textbooks will be of some help for making that a reality!

Weinan E, Princeton, 2018

Preface

This book is written for students and researchers in applied mathematics with an interest in science and engineering. Our main purpose is to provide a mathematically solid introduction to the basic ideas and tools in probability theory and stochastic analysis. Starting from the basics of random variables and probability theory, we go on to discuss limit theorems, Markov chains, diffusion processes, and random fields. Since the kind of readers we have in mind typically have some background in differential equations, we put more weight on the differential equation approach. In comparison, we have neglected entirely martingale theory even though it is a very important part of stochastic analysis. The diffusion process occupies a central role in this book. We have presented three different ways of looking at the diffusion process: the approach of using stochastic differential equations, the Fokker-Planck equation approach, and the path integral approach. The first allows us to introduce stochastic calculus. The second approach provides a link between differential equations and stochastic analysis. The path integral approach is very much preferred by physicists and is also suited for performing asymptotic analysis. In addition, it can be extended to random fields.

In choosing the style of the presentation, we have tried to strike a balance between rigor and the heuristic approach. We have tried to give the reader an idea about the kind of mathematical construction or mathematical argument that goes into the subject matter, but at the same time, we often stop short of proving all the theorems we state or we prove the theorems under stronger assumptions. Whenever possible, we have tried to give the intuitive picture behind the mathematical constructions.

Another emphasis is on numerical algorithms, including Monte Carlo methods, numerical schemes for solving stochastic differential equations, and the stochastic simulation algorithm. The book ends with a discussion on two application areas, statistical mechanics and chemical kinetics, and a discussion on rare events, which is perhaps the most important manifestation of the effect of noise.

The material contained in this book has been taught in various forms at Peking University, Princeton University, and New York University since 2001. It is now a required course for the special applied mathematics program at Peking University.

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Notation

(1) Geometry notation:
  (a) $\mathbb{N}$: Natural numbers, $\mathbb{N} = \{0, 1, \ldots\}$.
  (b) $\mathbb{Z}$: Integers.
  (c) $\mathbb{Q}$: Rational numbers.
  (d) $\mathbb{R}$: Real numbers.
  (e) $\bar{\mathbb{R}}$: Extended real numbers, $\bar{\mathbb{R}} = [-\infty, \infty]$.
  (f) $\mathbb{R}_+$: Nonnegative real numbers.
  (g) $\bar{\mathbb{R}}_+$: Extended nonnegative real numbers, $\bar{\mathbb{R}}_+ = [0, \infty]$.
  (h) $\mathbb{S}^{n-1}$: $(n-1)$-dimensional unit sphere in $\mathbb{R}^n$.
  (i) $\mathbb{R}^{\mathbf{T}}$: Collection of all real functions on time domain $\mathbf{T}$.

(2) Probability notation:
  (a) $\mathbb{P}$: Probability measure.
  (b) $\mathbb{E}$: Mathematical expectation.
  (c) $\mathbb{P}^i$, $\mathbb{P}^x$, or $\mathbb{P}^\mu$: Probability distribution conditioned on $X_0 = i$, $X_0 = x$, or $X_0 \sim \mu$.
  (d) $\mathbb{E}^i$, $\mathbb{E}^x$, $\mathbb{E}^\mu$: Mathematical expectation with respect to $\mathbb{P}^i$, $\mathbb{P}^x$, or $\mathbb{P}^\mu$.
  (e) $\mathbb{E}^{x,t}$: Mathematical expectation conditioned on $X_t = x$.
  (f) Ω: Sample space.
  (g) $\mathcal{F}$: σ-algebra in probability space.
  (h) $\mathcal{R}, \mathcal{R}^d$: The Borel σ-algebra on $\mathbb{R}$ or $\mathbb{R}^d$.
  (i) $\sigma(\mathcal{B})$: The smallest σ-algebra generated by sets in $\mathcal{B}$.
  (j) $\mathcal{R}^{\mathbf{T}}$: The product Borel σ-algebra on $\mathbb{R}^{\mathbf{T}}$.
  (k) $\mathcal{U}(A)$: Uniform distribution on set A.

(l) $\mathcal{P}(\lambda)$: Poisson distribution with mean λ.

(m) $\mathcal{E}(\lambda)$: Exponential distribution with mean λ^{-1}.

(n) $[X, X]_t$: Quadratic variation process of X.

(o) $X \sim \mathcal{P}(\lambda)$: Distribution of X. The right-hand side can be distributions like $\mathcal{P}(\lambda)$ or $N(\mu, \sigma^2)$, etc.

(3) Function spaces:

   (a) $C_c^\infty(\mathbb{R}^d)$ or $C_c^k(\mathbb{R}^d)$: Smooth or C^k-functions with compact support in $\mathbb{R}^d$.

   (b) $C_0(\mathbb{R}^d)$: Continuous functions in $\mathbb{R}^d$ that vanish at infinity.

   (c) $C_b(\mathbb{R}^d)$: Bounded continuous functions in $\mathbb{R}^d$.

   (d) L_t^p or $L^p([0, T])$: L^p-functions as a function of t.

   (e) L_ω^p or $L^p(\Omega)$: L^p-functions as a function of ω.

   (f) $\mathscr{B}, \mathscr{H}$: Banach or Hilbert spaces.

   (g) $\mathscr{B}^*$: Dual space of $\mathscr{B}$.

(4) Operators: $\mathcal{I}, \mathcal{P}, \mathcal{Q}, \mathcal{K}$, etc.

(5) Functions:

   (a) $\lceil \cdot \rceil$: The ceil function. $\lceil x \rceil = m+1$ if $x \in [m, m+1)$ for $m \in \mathbb{Z}$.

   (b) $\lfloor \cdot \rfloor$: The floor function. $\lfloor x \rfloor = m$ if $x \in [m, m+1)$ for $m \in \mathbb{Z}$.

   (c) $|\boldsymbol{x}|$: ℓ^2-modulus of a vector $\boldsymbol{x} \in \mathbb{R}^d$: $|\boldsymbol{x}| = (\sum_{i=1}^d x_i^2)^{\frac{1}{2}}$.

   (d) $\|f\|$: Norm of function f in some function space.

   (e) $a \vee b$: Maximum of a and b: $a \vee b = \max(a, b)$.

   (f) $a \wedge b$: Minimum of a and b: $a \wedge b = \min(a, b)$.

   (g) $\langle f \rangle$: The average of f with respect to a measure μ: $\langle f \rangle = \int f(x)\mu(dx)$.

   (h) $(\boldsymbol{x}, \boldsymbol{y})$: Inner product for $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$: $(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}^T \boldsymbol{y}$.

   (i) (f, g): Inner product for L^2-functions f, g: $(f, g) = \int f(x)g(x)dx$.

   (j) $\langle f, g \rangle$: Dual product for $f \in \mathscr{B}^*$ and $g \in \mathscr{B}$.

   (k) $A : B$: Twice contraction for second-order tensors, i.e., $A : B = \sum_{ij} a_{ij} b_{ji}$.

   (l) $|S|$: The cardinality of set S.

   (m) $|\Delta|$: The subdivision size when Δ is a subdivision of a domain.

   (n) $\chi_A(x)$: Indicator function, i.e., $\chi_A(x) = 1$ if $x \in A$ and 0 otherwise.

   (o) $\delta(x - a)$: Dirac's delta-function at $x = a$.

   (p) $\mathrm{Range}(\mathcal{P})$, $\mathrm{Null}(\mathcal{P})$: The range and null space of operator $\mathcal{P}$, i.e., $\mathrm{Range}(\mathcal{P}) = \{y | y = \mathcal{P}x\}$, $\mathrm{Null}(\mathcal{P}) = \{x | \mathcal{P}x = 0\}$.

   (q) $^\perp \mathscr{C}$: Perpendicular subspace, i.e., $^\perp \mathscr{C} = \{x | x \in \mathscr{B}^*, \langle x, y \rangle = 0, \forall y \in \mathscr{C}\}$ where $\mathscr{C} \subset \mathscr{B}$.

(6) Symbols:
   (a) $c_\varepsilon \asymp d_\varepsilon$: Logrithmic equivalence, i.e., $\lim_{\varepsilon \to 0} \log c_\varepsilon / \log d_\varepsilon = 1$.
   (b) $c_\varepsilon \sim d_\varepsilon$ or $c_n \sim d_n$: Equivalence, i.e., $\lim_{\varepsilon \to 0} c_\varepsilon / d_\varepsilon = 1$ or $\lim_{n \to \infty} c_n / d_n = 1$.
   (c) $\mathcal{D}x$: Formal infinitesimal element in path space, $\mathcal{D}x = \prod_{0 \le t \le T} dx_t$.

Part 1

Fundamentals

Random Variables

1.1. Elementary Examples

We will start with some elementary examples of probability. The most well-known example is that of a fair coin: if flipped, the probability of getting a head or tail both equal to $1/2$. If we perform n independent tosses, then the probability of obtaining n heads is equal to $1/2^n$: among the 2^n equally possible outcomes only one gives the result that we look for. More generally, let $S_n = X_1 + X_2 + \cdots + X_n$, where

$$X_j = \begin{cases} 1, & \text{if the result of the } n\text{th trial is a head,} \\ 0, & \text{if the result of the } n\text{th trial is a tail.} \end{cases}$$

Then the probability that we get k heads out of n tosses is equal to

$$\text{Prob}(S_n = k) = \frac{1}{2^n} \binom{n}{k}.$$

Applying Stirling's formula

$$n! \sim \sqrt{2\pi n} \left(\frac{n}{e}\right)^n, \quad n \to \infty,$$

we can calculate, for example, the asymptotic probability of obtaining heads exactly half of the time:

$$\text{Prob}(S_{2n} = n) = \frac{1}{2^{2n}} \binom{2n}{n} = \frac{1}{2^{2n}} \frac{(2n)!}{(n!)^2} \sim \frac{1}{\sqrt{\pi n}} \to 0,$$

as $n \to \infty$.

On the other hand, since we have a fair coin, we do expect to obtain heads roughly half of the time; i.e.,

$$\frac{S_{2n}}{2n} \approx \frac{1}{2},$$

for large n. Such a statement is indeed true and is embodied in the law of large numbers that we will discuss in the next chapter. For the moment let us simply observe that while the probability that S_{2n} equals n goes to zero as $n \to \infty$, the probability that S_{2n} is close to n goes to 1 as $n \to \infty$. More precisely, for any $\epsilon > 0$,

$$\text{Prob}\left(\left|\frac{S_{2n}}{2n} - \frac{1}{2}\right| > \epsilon\right) \to 0,$$

as $n \to \infty$. This can be seen as follows. Noting that the distribution $\text{Prob}\{S_{2n} = k\}$ is unimodal and symmetric around the state $k = n$, we have

$$\text{Prob}\left(\left|\frac{S_{2n}}{2n} - \frac{1}{2}\right| > \epsilon\right) \leq 2 \cdot \frac{1}{2^{2n}} \sum_{k > n + 2n\epsilon} \frac{(2n)!}{k!(2n-k)!}$$

$$\leq 2(n - 2n\epsilon) \cdot \frac{1}{2^{2n}} \frac{(2n)!}{\lceil n + 2n\epsilon \rceil! \lfloor n - 2n\epsilon \rfloor!}$$

$$\sim \frac{2\sqrt{1 - 2\epsilon}}{\sqrt{\pi(1 + 2\epsilon)}} \cdot \frac{\sqrt{n}}{(1 - 2\epsilon)^{n(1-2\epsilon)}(1 + 2\epsilon)^{n(1+2\epsilon)}} \to 0$$

for sufficiently small ϵ and $n \gg 1$, where $\lceil \cdot \rceil$ and $\lfloor \cdot \rfloor$ are the ceil and floor functions, respectively, defined by $\lceil x \rceil = m+1$ and $\lfloor x \rfloor = m$ if $x \in [m, m+1)$ for $m \in \mathbb{Z}$. This is the *weak law of large numbers* for this particular example.

In the example of a fair coin, the number of outcomes in an experiment is finite. In contrast, the second class of examples involves a continuous set of possible outcomes. Consider the orientation of a unit vector $\boldsymbol{\tau}$. Denote by $\mathbb{S}^2$ the unit sphere in $\mathbb{R}^3$. Define $\rho(\boldsymbol{n})$, $\boldsymbol{n} \in \mathbb{S}^2$, as the orientation distribution density; i.e., for $A \subset \mathbb{S}^2$,

$$\text{Prob}(\boldsymbol{\tau} \in A) = \int_A \rho(\boldsymbol{n}) dS,$$

where dS is the surface area element on $\mathbb{S}^2$. If $\boldsymbol{\tau}$ does not have a preferred orientation, i.e., it has equal probability of pointing at any direction, then

$$\rho(\boldsymbol{n}) = \frac{1}{4\pi}.$$

In this case, we say that $\boldsymbol{\tau}$ is isotropic. On the other hand, if $\boldsymbol{\tau}$ does have a preferred orientation, say $\boldsymbol{n}_0$, then we expect $\rho(\boldsymbol{n})$ to be peaked at $\boldsymbol{n}_0$.

1.2. Probability Space

It is useful to put these intuitive notions of probability on a firm mathematical basis, as was done by Kolmogorov. For this purpose, we need the notion of *probability space*, often written as a triplet $(\Omega, \mathcal{F}, \mathbb{P})$, defined as follows.

Definition 1.1 (Sample space)**.** The sample space Ω is the set of all possible outcomes. Each element $\omega \in \Omega$ is called a sample point.

Definition 1.2 (σ-algebra)**.** A σ-algebra (or σ-field) $\mathcal{F}$ is a collection of subsets of Ω that satisfies the following conditions:

   (i) $\Omega \in \mathcal{F}$;
   (ii) if $A \in \mathcal{F}$, then $A^c \in \mathcal{F}$, where $A^c = \Omega \backslash A$ is the complement of A in Ω;
   (iii) if $A_1, A_2, \ldots \in \mathcal{F}$, then $\bigcup_{n=1}^{\infty} A_n \in \mathcal{F}$.

Each set A in $\mathcal{F}$ is called an event. Let $\mathcal{B}$ be a collection of subsets of Ω. We denote by $\sigma(\mathcal{B})$ the smallest σ-algebra generated by the sets in $\mathcal{B}$, i.e., the smallest σ-algebra that contains $\mathcal{B}$. The pair $(\Omega, \mathcal{F})$ with the above properties is called a *measurable space.*

Definition 1.3 (Probability measure)**.** The probability measure $\mathbb{P} : \mathcal{F} \to [0, 1]$ is a set function defined on $\mathcal{F}$ which satisfies

   (a) $\mathbb{P}(\emptyset) = 0$, $\mathbb{P}(\Omega) = 1$;
   (b) if $A_1, A_2, \ldots \in \mathcal{F}$ are pairwise disjoint, i.e., $A_i \cap A_j = \emptyset$ if $i \neq j$, then

$$(1.1) \qquad \mathbb{P}\left(\bigcup_{n=1}^{\infty} A_n \right) = \sum_{n=1}^{\infty} \mathbb{P}(A_n).$$

(1.1) is called countable additivity or σ-additivity.

Example 1.4 (Fair coin)**.** The probability space for the outcome of one trial can be defined as follows. The sample space $\Omega = \{H, T\}$ where H and T represent head and tail, respectively. The σ-algebra

$$\mathcal{F} = \text{ all subsets of } \Omega = \{\emptyset, \{H\}, \{T\}, \Omega\}$$

and

$$\mathbb{P}(\emptyset) = 0, \qquad \mathbb{P}(\{H\}) = \mathbb{P}(\{T\}) = \frac{1}{2}, \qquad \mathbb{P}(\Omega) = 1.$$

For n independent tosses, we can take $\Omega = \{H, T\}^n$, $\mathcal{F} = $ all subsets of Ω, and

$$\mathbb{P}(A) = \frac{1}{2^n} |A|,$$

where $|A|$ is the cardinality of the set A.

Example 1.5 (Uniform orientation distribution on $\mathbb{S}^2$)**.** In this case, the sample space $\Omega = \mathbb{S}^2$. Let $\mathcal{B}$ be the set of all open sets of $\mathbb{S}^2$, defined as the intersection of any open set $B \subset \mathbb{R}^3$ and $\mathbb{S}^2$. Then we can take the σ-algebra to be $\mathcal{F} = \sigma(\mathcal{B})$ and

$$\mathbb{P}(U) = \frac{\text{surface area}(U)}{4\pi} \quad \text{for any } U \in \mathcal{F}.$$

Within this framework, the standard rules of set theory are used to answer probability questions. For instance, if both $A, B \in \mathcal{F}$, the probalility that both A and B occurs is given by $\mathbb{P}(A \cap B)$, the probability that either A or B occurs is given by $\mathbb{P}(A \cup B)$, the probability that A but not B occurs is given by $\mathbb{P}(A \backslash B)$, etc. It is easy to check that

$$(1.2) \qquad\qquad A \subseteq B \Rightarrow \mathbb{P}(A) \leq \mathbb{P}(B).$$

This is because $B = A \cup (B \backslash A)$; therefore, $\mathbb{P}(B) = \mathbb{P}(A) + \mathbb{P}(B \backslash A) \geq \mathbb{P}(A)$. We also have

$$(1.3) \qquad\qquad \mathbb{P}(A \cup B) \leq \mathbb{P}(A) + \mathbb{P}(B)$$

since $A = A \cup (B \cap A^c)$, and $\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B \cap A^c) \leq \mathbb{P}(A) + \mathbb{P}(B)$. This last inequality is known as *Boole's inequality*.

1.3. Conditional Probability

Let $A, B \in \mathcal{F}$ and assume that $\mathbb{P}(B) \neq 0$. Then the *conditional probability* of A given B is defined as

$$(1.4) \qquad\qquad \mathbb{P}(A|B) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(B)}.$$

This is the proportion of events that both A and B occur given that B occurs. For instance, the probability to obtain two tails in two tosses of a fair coin is $1/4$, but the conditional probability to obtain two tails is $1/2$ given that the first toss is a tail, and it is zero given that the first toss is a head.

Since $\mathbb{P}(A \cap B) = \mathbb{P}(A|B)\mathbb{P}(B)$ by definition, we also have

$$\mathbb{P}(A \cap B \cap C) = \mathbb{P}(A|B \cap C)\mathbb{P}(B|C)\mathbb{P}(C),$$

and so on. It is straightforward to obtain

$$(1.5) \qquad\qquad \mathbb{P}(A|B) = \frac{\mathbb{P}(A)\mathbb{P}(B|A)}{\mathbb{P}(B)}$$

from the definition of conditional probability. This is called *Bayes's rule*.

Proposition 1.6 (Bayes's theorem)**.** *If* $A_1, A_2, \ldots$ *are disjoint sets such that* $\bigcup_{j=1}^{\infty} A_j = \Omega$, *then we have*

$$(1.6) \qquad \mathbb{P}(A_j|B) = \frac{\mathbb{P}(A_j)\mathbb{P}(B|A_j)}{\sum_{n=1}^{\infty} \mathbb{P}(A_n)\mathbb{P}(B|A_n)} \qquad \text{for any } j \in \mathbb{N}.$$

This is useful in Bayesian statistics where A_j corresponds to the hypothesis and $\mathbb{P}(A_j)$ is the prior probability of the hypothesis A_j. The conditional probability $\mathbb{P}(A_j|B)$ is the posterior probability of A_j given that the event B occurs.

1.4. Discrete Distributions

If the elements in Ω are finite or enumerable, say, $\Omega = \{\omega_1, \omega_2, \ldots\}$, we have a situation of discrete probability space and discrete distribution. In this case, let $X(\omega_j) = x_j$ and

$$p_j = \mathbb{P}(X = x_j), \qquad j = 0, 1, \ldots.$$

Of course, we have to have

$$0 \le p_j \le 1, \qquad \sum_j p_j = 1.$$

Given a function f of X, its *expectation* is given by

$$(1.7) \qquad \mathbb{E}f(X) = \sum_j f(x_j)p_j$$

if the sum is well-defined. In particular, the pth moment of the distribution is defined as

$$m_p = \sum_j x_j^p p_j.$$

When $p = 1$, it is called the *mean* of the random variable and is also denoted by $\text{mean}(X)$. Another important quantity is its *variance*, defined as

$$(1.8) \qquad \text{Var}(X) = m_2 - m_1^2 = \sum_j (x_j - m_1)^2 p_j.$$

Example 1.7 (Bernoulli distribution)**.** The Bernoulli distribution has the form

$$\mathbb{P}(X = j) = \left\{ \begin{array}{ll} p, & j = 1, \\ q, & j = 0, \end{array} \right.$$

$p + q = 1$ and $p, q \ge 0$. When $p = q = 1/2$, it corresponds to the toss of a fair coin. The mean and variance can be calculated directly:

$$\mathbb{E}X = p, \quad \text{Var}(X) = pq.$$

Example 1.8 (Binomial distribution $B(n, p)$)**.** The binomial distribution $B(n, p)$ has the form

$$(1.9) \qquad \mathbb{P}(X = k) = \binom{n}{k} p^k q^{n-k}, \quad k = 0, 1, \dots, n.$$

It is straightforward to obtain

$$\mathbb{E}X = np, \quad \text{Var}(X) = npq.$$

The binomial distribution $B(n, p)$ can be obtained from the sum of n independent Bernoulli trials (Exercise 1.1).

Example 1.9 (Poisson distribution $\mathcal{P}(\lambda)$)**.** The Poisson distribution $\mathcal{P}(\lambda)$ has the form

$$(1.10) \qquad \mathbb{P}(X = k) = \frac{\lambda^k}{k!} e^{-\lambda}, \quad k = 0, 1, \dots.$$

The mean and variance are, respectively,

$$\mathbb{E}X = \text{Var}(X) = \lambda.$$

This is often used to model the number of events during a time interval or the number of points that fall in a given set.

The Poisson distribution $\mathcal{P}(\lambda)$ may be viewed as the limit of the binomial distribution in the sense that

$$C_n^k p^k q^{n-k} \longrightarrow \frac{\lambda^k}{k!} e^{-\lambda} \ \text{ as } n \to \infty, p \to 0, np = \lambda.$$

The proof is simple and is left as an exercise.

1.5. Continuous Distributions

Consider now the general case when Ω is not necessarily enumerable. Let us begin with the definition of a *random variable*. Denote by $\mathcal{R}$ the Borel σ-algebra on $\mathbb{R}$, the smallest σ-algebra containing all open sets.

Definition 1.10. A random variable X is an $\mathcal{F}$-measurable real-valued function $X : \Omega \to \mathbb{R}$; i.e., for any $B \in \mathcal{R}$, $X^{-1}(B) \in \mathcal{F}$.

Definition 1.11. The *distribution* of the random variable X is a probability measure μ on $\mathbb{R}$, defined for any set $B \in \mathcal{R}$ by

$$(1.11) \qquad \mu(B) = \mathbb{P}(X \in B) = \mathbb{P} \circ X^{-1}(B).$$

In particular, we define the *distribution function* $F(x) = \mathbb{P}(X \le x)$ when $B = (-\infty, x]$.

If there exists an integrable function $\rho(x)$ such that

$$(1.12) \qquad \mu(B) = \int_B \rho(x)dx$$

for any $B \in \mathcal{R}$, then ρ is called the *probability density function* (PDF) of X. Here $\rho(x) = d\mu/dm$ is the Radon-Nikodym derivative of $\mu(dx)$ with respect to the Lebesgue measure $m(dx)$ if $\mu(dx)$ is absolutely continuous with respect to $m(dx)$; i.e., for any set $B \in \mathcal{R}$, if $m(B) = 0$, then $\mu(B) = 0$ (see also Section C of the appendix) [**Bil79**]. In this case, we write $\mu \ll m$.

Definition 1.12. The *expectation* of a random variable X is defined as

$$(1.13) \qquad \mathbb{E}X = \int_\Omega X(\omega)\mathbb{P}(d\omega) = \int_\mathbb{R} x\mu(dx)$$

if the integrals are well-defined.

The *variance* of X is defined as

$$(1.14) \qquad \mathrm{Var}(X) = \mathbb{E}(X - \mathbb{E}X)^2.$$

For two random variables X and Y, we can define their *covariance* as

$$(1.15) \qquad \mathrm{Cov}(X, Y) = \mathbb{E}(X - \mathbb{E}X)(Y - \mathbb{E}Y).$$

X and Y are called *uncorrelated* if $\mathrm{Cov}(X, Y) = 0$.

All of the above definitions can be extended to the vectorial case in which $\boldsymbol{X} = (X_1, X_2, \ldots, X_d)^T \in \mathbb{R}^d$ is a *random vector* and each component X_k is a random variable. In this case, the *covariance matrix* of $\boldsymbol{X}$ is defined as

$$(1.16) \qquad \mathrm{Cov}(\boldsymbol{X}) = \mathbb{E}(\boldsymbol{X} - \mathbb{E}\boldsymbol{X})(\boldsymbol{X} - \mathbb{E}\boldsymbol{X})^T.$$

Definition 1.13. For any $p \geq 1$, the space $L^p(\Omega)$ (or L^p_ω) consists of random variables whose pth-order moment is finite:

$$(1.17) \qquad L^p(\Omega) = \{\boldsymbol{X}(\omega) : \mathbb{E}|\boldsymbol{X}|^p < \infty\}.$$

For $\boldsymbol{X} \in L^p(\Omega)$, let

$$(1.18) \qquad \|\boldsymbol{X}\|_p = (\mathbb{E}|\boldsymbol{X}|^p)^{1/p}, \quad p \geq 1.$$

Theorem 1.14.

(i) *Minkowski inequality.*

$$\|\boldsymbol{X} + \boldsymbol{Y}\|_p \leq \|\boldsymbol{X}\|_p + \|\boldsymbol{Y}\|_p, \qquad p \geq 1, \ \boldsymbol{X}, \boldsymbol{Y} \in L^p(\Omega)$$

(ii) *Hölder inequality.*

$$\mathbb{E}|(\boldsymbol{X}, \boldsymbol{Y})| \leq \|\boldsymbol{X}\|_p \|\boldsymbol{Y}\|_q, \quad p > 1, \ 1/p + 1/q = 1, \ \boldsymbol{X} \in L^p(\Omega), \ \boldsymbol{Y} \in L^q(\Omega),$$

where $(\boldsymbol{X}, \boldsymbol{Y})$ *denotes the standard scalar product in* $\mathbb{R}^d$.

(iii) *Schwartz inequality.*

$$\mathbb{E}|(\boldsymbol{X}, \boldsymbol{Y})| \leq \|\boldsymbol{X}\|_2 \|\boldsymbol{Y}\|_2.$$

Obviously Schwartz inequality is a special case of Hölder inequality when $p = q = 2$.

The proof of these inequalities can be found, for example, in Chapter 2 of [**Shi96**].

It also follows that $\|\cdot\|_p$ is a norm. One can further prove that $L^p(\Omega)$ is a Banach space and $L^2(\Omega)$ is a Hilbert space with inner product

$$(1.19) \qquad\qquad (\boldsymbol{X}, \boldsymbol{Y})_{L^2_\omega} = \mathbb{E}(\boldsymbol{X}, \boldsymbol{Y}).$$

Lemma 1.15 (Chebyshev's inequality). *Let $\boldsymbol{X}$ be a random variable such that $\mathbb{E}|\boldsymbol{X}|^p < \infty$ for some $p > 0$. Then*

$$(1.20) \qquad\qquad \mathbb{P}\{|\boldsymbol{X}| \geq \lambda\} \leq \frac{1}{\lambda^p} \mathbb{E}|\boldsymbol{X}|^p,$$

for any positive constant λ.

Proof. For any $\lambda > 0$,

$$\mathbb{E}|\boldsymbol{X}|^p = \int_{\mathbb{R}^d} |\boldsymbol{x}|^p \mu(d\boldsymbol{x}) \geq \int_{|\boldsymbol{x}| \geq \lambda} |\boldsymbol{x}|^p \mu(d\boldsymbol{x}) \geq \lambda^p \int_{|\boldsymbol{x}| \geq \lambda} \mu(d\boldsymbol{x}) = \lambda^p \mathbb{P}(|\boldsymbol{X}| \geq \lambda).$$

$\square$

It is straightforward to generalize the above estimate to any nonnegative increasing function $f(x)$, which gives $\mathbb{P}(|\boldsymbol{X}| \geq \lambda) \leq \mathbb{E}f(|\boldsymbol{X}|)/f(\lambda)$ if $f(\lambda) > 0$.

Lemma 1.16 (Jensen's inequality). *Let $\boldsymbol{X}$ be a random variable such that $\mathbb{E}|\boldsymbol{X}| < \infty$ and $\phi : \mathbb{R} \to \mathbb{R}$ is a convex function such that $\mathbb{E}|\phi(\boldsymbol{X})| < \infty$. Then*

$$(1.21) \qquad\qquad \mathbb{E}\phi(\boldsymbol{X}) \geq \phi(\mathbb{E}\boldsymbol{X}).$$

This follows directly from the definition of convex functions. Readers can also refer to [**Chu01**] for the details.

Below we list some typical continuous distributions.

Example 1.17 (Uniform distribution). The uniform distribution on a domain B (in $\mathbb{R}^d$) is defined by the probability density function:

$$\rho(x) = \begin{cases} \frac{1}{\text{vol}(B)}, & \text{if } \boldsymbol{x} \in B, \\ 0, & \text{otherwise.} \end{cases}$$

In one dimension if $B = [0, 1]$ (denoted as $\mathcal{U}[0, 1]$ later), this reduces to

$$\rho(x) = \begin{cases} 1, & \text{if } x \in [0, 1], \\ 0, & \text{otherwise.} \end{cases}$$

For the uniform distribution on $[0, 1]$, we have

$$\mathbb{E}X = \frac{1}{2}, \quad \text{Var}(X) = \frac{1}{12}.$$

Example 1.18 (Exponential distribution)**.** The exponential distribution $\mathcal{E}(\lambda)$ is defined by the probability density function:

$$\rho(x) = \begin{cases} 0, & \text{if } x < 0, \\ \lambda e^{-\lambda x}, & \text{if } x \geq 0. \end{cases}$$

The mean and variance of $E(\lambda)$ are

$$(1.22) \qquad \mathbb{E}X = \frac{1}{\lambda}, \quad \text{Var}(X) = \frac{1}{\lambda^2}.$$

As an example, the waiting time of a Poisson process with rate λ is exponentially distributed with parameter λ.

Example 1.19 (Normal distribution)**.** The one-dimensional normal distribution (also called Gaussian distribution) $N(\mu, \sigma^2)$ is defined by the probability density function:

$$(1.23) \qquad \rho(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x - \mu)^2\right)$$

with mean μ and variance σ^2.

If $\boldsymbol{\Sigma}$ is an $n \times n$ symmetric positive definite matrix and $\boldsymbol{\mu}$ is a vector in $\mathbb{R}^n$, we can also define the n-dimensional normal distribution $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ through the density

$$(1.24) \qquad \rho(\boldsymbol{x}) = \frac{1}{(2\pi)^{n/2}(\det \boldsymbol{\Sigma})^{1/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu})\right).$$

In this case, we have

$$\mathbb{E}\boldsymbol{X} = \boldsymbol{\mu}, \quad \text{Cov}(\boldsymbol{X}) = \boldsymbol{\Sigma}.$$

The normal distribution is the most important probability distribution. It is also called the Gaussian distribution. Random variables with normal distribution are also called Gaussian random variables. In the case of degeneracy, i.e., the covariance matrix $\boldsymbol{\Sigma}$ is not invertible, which corresponds to the case that some components are in the subspace spanned by other components, we need to define the Gaussian distribution via characteristic functions (see Section 1.9).

Example 1.20 (Gibbs distribution). In equilibrium statistical mechanics, we are concerned with a probability distribution π over a state space S. In the case of an n-particle system with continuous states, we have $\boldsymbol{x} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n, \boldsymbol{p}_1, \ldots, \boldsymbol{p}_n) \in S = \mathbb{R}^{6n}$, where $\boldsymbol{x}_k$ and $\boldsymbol{p}_k$ are the position and momentum of the kth particle, respectively. The PDF $\pi(\boldsymbol{x})$, called the *Gibbs distribution*, has a specific form:

$$(1.25) \qquad \pi(\boldsymbol{x}) = \frac{1}{Z} e^{-\beta H(\boldsymbol{x})}, \qquad \boldsymbol{x} \in \mathbb{R}^{6n}, \ \beta = (k_B T)^{-1},$$

where H is the energy of the considered system, T is the absolute temperature, k_B is the Boltzmann constant, and

$$(1.26) \qquad Z = \int_{\mathbb{R}^{6n}} e^{-\beta H(\boldsymbol{x})} d\boldsymbol{x}$$

is called the partition function. Let $f(\boldsymbol{x})$ be a function defined on the configuration space S. Then its thermodynamic average $\langle f \rangle$, i.e., the expectation of f, is given by

$$(1.27) \qquad \mathbb{E}f = \langle f \rangle = \int_{\mathbb{R}^{6n}} f(\boldsymbol{x}) \pi(\boldsymbol{x}) d\boldsymbol{x}.$$

A similar definition holds for the discrete space setting by replacing the integral with summation.

Another important notion is the distribution function of a random variable X:

$$(1.28) \qquad F(x) = \mathbb{P}(X < x).$$

One can easily see that if the distribution of X is absolutely continuous with respect to the Lebesgue measure, then the density ρ and the distribution function F of X are related by

$$(1.29) \qquad \rho(x) = \frac{d}{dx} F(x).$$

1.6. Independence

We now come to one of the most distinctive notions in probability theory, the notion of independence. Let us start by defining the independence of events. Two events $A, B \in \mathcal{F}$ are *independent* if

$$\mathbb{P}(A \cap B) = \mathbb{P}(A)\mathbb{P}(B).$$

Definition 1.21. Two random variables X and Y are said to be independent if for any two Borel sets A and B, $X^{-1}(A)$ and $Y^{-1}(B)$ are independent; i.e.,

$$(1.30) \qquad \mathbb{P}\left(X^{-1}(A) \cap Y^{-1}(B)\right) = \mathbb{P}\left(X^{-1}(A)\right)\mathbb{P}\left(Y^{-1}(B)\right).$$

The joint distribution of the two random variables X and Y is defined to be the distribution of the random vector (X, Y). Let μ_1 and μ_2 be the probability distribution of X and Y, respectively, and let μ be their joint distribution. If X and Y are independent, then for any two Borel sets A and B, we have

$$(1.31) \qquad \mu(A \times B) = \mu_1(A)\mu_2(B).$$

Consequently, we have

$$(1.32) \qquad \mu = \mu_1\mu_2;$$

i.e., the joint distribution of two independent random variables is the product distribution. If both μ_1 and μ_2 are absolutely continuous, with densities p_1 and p_2, respectively, then μ is also absolutely continuous, with density given by

$$(1.33) \qquad p(x, y) = p_1(x)p_2(y).$$

One can also understand independence from the viewpoint of expectations. Let f_1 and f_2 be two continuous functions. If X and Y are two independent random variables, then

$$(1.34) \qquad \mathbb{E}f_1(X)f_2(Y) = \mathbb{E}f_1(X)\mathbb{E}f_2(Y).$$

In fact, this can also be used as the definition of independence.

This discussion can be readily generalized to multiple events and multiple random variables. A sequence of events $\{A_k\}_{k=1}^n$ are independent if for $k = 1, 2 \ldots, n$ and $1 \le i_1 < i_2 < \cdots < i_k \le n$

$$\mathbb{P}\left(\bigcap_{j=1}^{k} A_{i_j}\right) = \prod_{j=1}^{k} \mathbb{P}(A_{i_j}).$$

Note that pairwise independence does not imply independence (see Exercise 1.9).

Definition 1.22. The random variables $X_1, \ldots, X_n$ are said to be independent if for any Borel sets $B_j \in \mathcal{R}$,

$$(1.35) \qquad \mathbb{P}\left(\bigcap_{j=1}^{n} X_j^{-1}(B_j)\right) = \prod_{j=1}^{n} \mathbb{P}(X_j^{-1}(B_j)).$$

If the random variables are independent, then their joint distribution is the product measure of their distributions.

1.7. Conditional Expectation

Let X and Y be two discrete random variables, not necessarily independent, with joint distribution

$$p(i,j) = \mathbb{P}(X = i, Y = j).$$

Since $\sum_i p(i,j) = \mathbb{P}(Y = j)$, the *probability* that $X = i$ conditioned on $Y = j$ is given by

$$p(i|j) = \frac{p(i,j)}{\sum_i p(i,j)} = \frac{p(i,j)}{\mathbb{P}(Y = j)}$$

if $\sum_i p(i,j) > 0$. The convention is to set $p(i|j) = 0$ if $\sum_i p(i,j) = 0$. Now let f be a continuous function. It is natural to define the *conditional expectation* of $f(X)$ given that $Y = j$ by

$$(1.36) \qquad \mathbb{E}(f(X)|Y = j) = \sum_i f(i)p(i|j).$$

A difficulty arises when one tries to generalize this to continuous random variables. Indeed, given two continuous random variables X and Y, the probability that $Y = y$ is zero for most values of y. Therefore, we need to proceed differently.

Let $\mathcal{G}$ be a sub-σ-algebra of $\mathcal{F}$. Let X be a random variable such that $\mathbb{E}|X| < \infty$.

Definition 1.23 (Conditional expectation)**.** The conditional expectation Z of X given $\mathcal{G}$ is defined by the following conditions:

(i) Z is measurable with respect to $\mathcal{G}$;

(ii) for any set $A \in \mathcal{G}$,

$$\int_A Z(\omega)\mathbb{P}(d\omega) = \int_A X(\omega)\mathbb{P}(d\omega).$$

The existence of $Z = \mathbb{E}(X|\mathcal{G})$ follows from the Radon-Nikodym theorem if we consider the measure μ on $\mathcal{G}$ defined by $\mu(A) = \int_A X(\omega)\mathbb{P}(d\omega)$ (see [**Bil79**]). One can easily see that μ is absolutely continuous with respect to the measure $\mathbb{P}|_{\mathcal{G}}$, the restriction of $\mathbb{P}$ to $\mathcal{G}$. Thus Z exists and is unique up to almost sure equivalence in $\mathbb{P}|_{\mathcal{G}}$.

In addition, we have

Theorem 1.24 (Properties of conditional expectation)**.** *Assume that X, Y are random variables with $\mathbb{E}|X|, \mathbb{E}|Y| < \infty$. Let $a, b \in \mathbb{R}$. Then:*

(i) $\mathbb{E}(aX + bY|\mathcal{G}) = a\mathbb{E}(X|\mathcal{G}) + b\mathbb{E}(Y|\mathcal{G})$.

(ii) $\mathbb{E}(\mathbb{E}(X|\mathcal{G})) = \mathbb{E}(X)$.

(iii) $\mathbb{E}(X|\mathcal{G}) = X$ *if X is $\mathcal{G}$-measurable.*

(iv) $\mathbb{E}(X|\mathcal{G}) = \mathbb{E}X$ *if X is independent of $\mathcal{G}$.*

(v) $\mathbb{E}(XY|\mathcal{G}) = Y\mathbb{E}(X|\mathcal{G})$ *if Y is $\mathcal{G}$-measurable.*

(vi) *If $\mathcal{H}$ is a sub-σ-algebra of $\mathcal{G}$, then $\mathbb{E}(X|\mathcal{H}) = \mathbb{E}(\mathbb{E}(X|\mathcal{H})|\mathcal{G})$.*

Similar to Lemma 1.16 we have

Lemma 1.25 (Conditional Jensen inequality)**.** *Let X be a random variable such that $\mathbb{E}|X| < \infty$ and let $\phi : \mathbb{R} \to \mathbb{R}$ be a convex function such that $\mathbb{E}|\phi(X)| < \infty$. Then*

$$(1.37) \qquad \mathbb{E}(\phi(X)|\mathcal{G}) \geq \phi(\mathbb{E}(X|\mathcal{G})).$$

These statements are straightforward. The reader may also consult [**Chu01**] for the details of the proof.

Given two random variables X and Y, the conditional expectation of X with respect to Y is defined as the conditional expectation of X with respect to the σ-algebra $\mathcal{G} = \sigma(Y)$ generated by Y

$$\mathcal{G} = \sigma(Y) := \{Y^{-1}(B), B \in \mathcal{R}\}.$$

To see that this definition reduces to the previous one for the case of discrete random variables, let $\Omega_j = \{\omega : Y(\omega) = j\}$ and

$$\Omega = \bigcup_{j=1}^{n} \Omega_j.$$

The σ-algebra $\mathcal{G}$ is simply the set of all possible unions of the Ω_j's. The measurability condition of $\mathbb{E}(X|Y)$ with respect to $\mathcal{G}$ means $\mathbb{E}(X|Y)$ is constant on each Ω_j, which is exactly $\mathbb{E}(X|Y = j)$ as we will see. By definition, we have

$$(1.38) \qquad \int_{\Omega_j} \mathbb{E}(X|Y)\mathbb{P}(d\omega) = \int_{\Omega_j} X(\omega)\mathbb{P}(d\omega),$$

which implies

$$(1.39) \qquad \mathbb{E}(X|Y) = \frac{1}{\mathbb{P}(\Omega_j)} \int_{\Omega_j} X(\omega)\mathbb{P}(d\omega).$$

This is exactly $\mathbb{E}(X|Y = j)$ in (1.36) when $f(X) = X$.

The conditional expectation is the optimal approximation in $L^2(\Omega)$ among all $\mathcal{G}$-measurable functions.

Proposition 1.26. *Let g be a measurable function. Then*

$$(1.40) \qquad \mathbb{E}(X - \mathbb{E}(X|Y))^2 \leq \mathbb{E}(X - g(Y))^2.$$

Proof. We have

$$\mathbb{E}(X - g(Y))^2 = \mathbb{E}(X - E(X|Y))^2 + \mathbb{E}(E(X|Y) - g(Y))^2$$
$$+ 2\mathbb{E}\Big[(X - E(X|Y))(E(X|Y) - g(Y))\Big]$$

and

$$\mathbb{E}\Big[(X - \mathbb{E}(X|Y))(\mathbb{E}(X|Y) - g(Y))\Big]$$
$$= \mathbb{E}\Big[\mathbb{E}\big[(X - \mathbb{E}(X|Y))(E(X|Y) - g(Y))|Y\big]\Big]$$
$$= \mathbb{E}\Big[(\mathbb{E}(X|Y) - \mathbb{E}(X|Y))(E(X|Y) - g(Y))\Big] = 0,$$

which implies (1.40). □

1.8. Notions of Convergence

Let $\{X_n\}_{n=1}^{\infty}$ be a sequence of random variables defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, and let μ_n be the distribution of X_n. Let X be another random variable with distribution μ. We will discuss four notions of convergence: almost sure convergence, convergence in probability, convergence in distribution, and convergence in L^p.

Definition 1.27 (Almost sure convergence)**.** X_n converges to X almost surely if

$$(1.41) \qquad \mathbb{P}(\omega : X_n(\omega) \to X(\omega)) = 1.$$

We write almost sure convergence as $X_n \to X$, a.s.

Definition 1.28 (Convergence in probability)**.** X_n converges to X in probability if for any $\epsilon > 0$,

$$(1.42) \qquad \mathbb{P}(\omega : |X_n(\omega) - X(\omega)| > \epsilon) \to 0,$$

as $n \to \infty$.

Definition 1.29 (Convergence in distribution)**.** X_n converges to X in distribution if for any $f \in C_b(\mathbb{R})$,

$$(1.43) \qquad \mathbb{E}f(X_n) \to \mathbb{E}f(X).$$

This is denoted as $X_n \xrightarrow{d} X$ or $\mu_n \xrightarrow{d} \mu$ or $\mu_n \Rightarrow \mu$.

Definition 1.30 (Convergence in L^p)**.** X_n converges to X in L^p $(0 < p < \infty)$ if

$$(1.44) \qquad \mathbb{E}|X_n - X|^p \to 0.$$

For $p = 1$, this is also referred to as convergence in mean; for $p = 2$, this is referred to as convergence in mean square.

Remark 1.31. Note that the power p does not need to be greater than 1 since it still gives a metric for the random variables. But only when $p \geq 1$ do we get a norm. The statements in this section hold when $0 < p < \infty$.

We have the following relations between different notions of convergence.

Theorem 1.32.

(i) *Almost sure convergence implies convergence in probability.*

(ii) *Convergence in probability implies almost sure convergence along a subsequence.*

(iii) *If $p < q$, then convergence in L^q implies convergence in L^p.*

(iv) *Convergence in L^p implies convergence in probability.*

(v) *Convergence in probability implies convergence in distribution.*

Proof. (i) Note that

$$\mathbb{P}(|X_n(\omega) - X(\omega)| > \epsilon) = \int_\Omega \chi_{\{|X_n - X| > \epsilon\}}(\omega)\mathbb{P}(d\omega) \to 0$$

by the almost sure convergence and dominated convergence theorems.

(ii) The proof will be deferred to Section 1.11.

(iii) This is a consequence of the Hölder inequality:

$$\mathbb{E}|X_n - X|^p \leq \left(\mathbb{E}(|X_n - X|^p)^{\frac{q}{p}}\right)^{\frac{p}{q}} = (\mathbb{E}|X_n - X|^q)^{\frac{p}{q}}, \quad p < q.$$

(iv) This is a consequence of the Chebyshev inequality:

$$\mathbb{P}(\omega : |X_n(\omega) - X(\omega)| > \epsilon) \leq \frac{1}{\epsilon^p}\mathbb{E}|X_n - X|^p$$

for any $\epsilon > 0$.

(v) Argue by contradiction. Suppose there exist a bounded continuous function $f(x)$ and a subsequence X_{n_k} such that

(1.45) $$\mathbb{E}f(X_{n_k}) \not\to \mathbb{E}f(X), \quad k \to \infty.$$

From assertion (ii), there exists a further subsequence of $\{X_{n_k}\}$ (still denoted as $\{X_{n_k}\}$) such that X_{n_k} converges to X almost surely. This contradicts (1.45) by the dominated convergence theorem. $\square$

1.9. Characteristic Function

The *characteristic function* of a random variable X is defined as

(1.46) $$f(\xi) = \mathbb{E}e^{i\xi X} = \int_\mathbb{R} e^{i\xi x}\mu(dx).$$

Proposition 1.33. *The characteristic function has the following properties:*

(1) $\forall \xi \in \mathbb{R}$, $|f(\xi)| \leq 1$, $f(\xi) = \overline{f(-\xi)}$, $f(0) = 1$;

(2) f *is uniformly continuous on* $\mathbb{R}$.

Proof. The proof of the first statements is straightforward. For the second statement, we have

$$|f(\xi_1) - f(\xi_2)| = |\mathbb{E}(e^{i\xi_1 X} - e^{i\xi_2 X})| = |\mathbb{E}(e^{i\xi_1 X}(1 - e^{i(\xi_2 - \xi_1)X}))|$$
$$\leq \mathbb{E}|1 - e^{i(\xi_2 - \xi_1)X}|.$$

Since the integrand $|1 - e^{i(\xi_2 - \xi_1)X}|$ depends only on the difference between ξ_1 and ξ_2 and since it tends to 0 almost surely as the difference goes to 0, uniform continuity follows immediately from the dominated convergence theorem. $\qquad\square$

Example 1.34. Here are the characteristic functions of some typical distributions:

(1) Bernoulli distribution.
$$f(\xi) = q + pe^{i\xi}.$$

(2) Binomial distribution $B(n, p)$.
$$f(\xi) = (q + pe^{i\xi})^n.$$

(3) Poisson distribution $\mathcal{P}(\lambda)$.
$$f(\xi) = e^{\lambda(e^{i\xi} - 1)}.$$

(4) Exponential distribution $\mathcal{E}(\lambda)$.
$$f(\xi) = (1 - \lambda^{-1} i\xi)^{-1}.$$

(5) Normal distribution $N(\mu, \sigma^2)$.

(1.47)
$$f(\xi) = \exp\left(i\mu\xi - \frac{\sigma^2 \xi^2}{2}\right).$$

(6) Multivariate normal distribution $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

(1.48)
$$f(\boldsymbol{\xi}) = \exp\left(i\boldsymbol{\mu}^T \boldsymbol{\xi} - \frac{1}{2}\boldsymbol{\xi}^T \boldsymbol{\Sigma} \boldsymbol{\xi}\right).$$

The property (1.48) is also used to define degenerate multivariate Gaussian distributions.

The following result gives an explicit characterization of the weak convergence of probability measures in terms of their characteristic functions. This is the key ingredient in the proof of the central limit theorem.

Theorem 1.35 (Lévy's continuity theorem). *Let $\{\mu_n\}_{n\in\mathbb{N}}$ be a sequence of probability measures, and let $\{f_n\}_{n\in\mathbb{N}}$ be their corresponding characteristic functions. Assume that:*

(1) *f_n converges everywhere on $\mathbb{R}$ to a limiting function f.*

(2) *f is continuous at $\xi = 0$.*

Then there exists a probability distribution μ such that $\mu_n \overset{d}{\to} \mu$. Moreover f is the characteristic function of μ.

Conversely, if $\mu_n \overset{d}{\to} \mu$, where μ is some probability distribution, then f_n converges to f uniformly on every finite interval, where f is the characteristic function of μ.

For a proof, see [**Chu01**].

As for Fourier transforms, one can also define the inverse transform

$$\rho(x) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{-i\xi x} f(\xi) d\xi.$$

An interesting question arises as to when this gives the density of a probability measure. To address this, we introduce the following notion.

Definition 1.36. A function f is called positive semidefinite if for any finite set of values $\{\xi_1, \ldots, \xi_n\}$, $n \in \mathbb{N}$, the matrix $(f(\xi_i - \xi_j))_{i,j=1}^n$ is positive semidefinite; i.e.,

$$(1.49) \qquad \sum_{i,j} f(\xi_i - \xi_j) v_i \bar{v}_j \geq 0,$$

for every set of values $v_1, \ldots, v_n \in \mathbb{C}$.

Theorem 1.37 (Bochner's theorem). *A function f is the characteristic function of a probability measure if and only if it is positive semidefinite and continuous at 0 with $f(0) = 1$.*

Proof. We only prove the necessity part. The other part is less trivial and readers may consult [**Chu01**]. Assume that f is a characteristic function. Then

$$(1.50) \qquad \sum_{i,j=1}^n f(\xi_i - \xi_j) v_i \bar{v}_j = \int_{\mathbb{R}} \Big| \sum_{i=1}^n v_i e^{i\xi_i x} \Big|^2 dx \geq 0. \qquad \square$$

1.10. Generating Function and Cumulants

For a discrete random variable, its *generating function* is defined as

$$(1.51) \qquad G(x) = \sum_{k=0}^{\infty} P(X = x_k) x^k.$$

One immediately has

$$P(X = x_k) = \frac{1}{k!} G^{(k)}(x)\Big|_{x=0}.$$

Definition 1.38. The convolution of two sequences $\{a_k\}$, $\{b_k\}$, $\{c_k\} = \{a_k\} * \{b_k\}$, is defined by

(1.52)
$$c_k = \sum_{j=0}^{k} a_j b_{k-j}.$$

It is easy to show that the generating functions defined by

$$A(x) = \sum_{k=0}^{\infty} a_k x^k, \quad B(x) = \sum_{k=0}^{\infty} b_k x^k, \quad C(x) = \sum_{k=0}^{\infty} c_k x^k$$

with $\{c_k\} = \{a_k\} * \{b_k\}$ satisfy $C(x) = A(x)B(x)$. The following result is more or less obvious.

Theorem 1.39. *Let X and Y be two independent random variables with probability distribution*

$$P(X = j) = a_j, \quad P(Y = k) = b_k,$$

respectively, and let A and B be the corresponding generating functions. Then the generating function of $X + Y$ is $C(x) = A(x)B(x)$.

This can be used to compute some generating functions.

  (a) Bernoulli distribution: $G(x) = q + px$.
  (b) Binomial distribution: $G(x) = (q + px)^n$.
  (c) Poisson distribution: $G(x) = e^{-\lambda + \lambda x}$.

The moment generating function of a random variable X is defined for all values of t by

(1.53)
$$M(t) = \mathbb{E}e^{tX} = \begin{cases} \displaystyle\sum_{x} p(x)e^{tx}, & X \text{ is discrete-valued}, \\ \displaystyle\int_{\mathbb{R}} p(x)e^{tx}dx, & X \text{ is continuous}, \end{cases}$$

provided that e^{tX} is integrable. It is obvious that $M(0) = 1$.

Once $M(t)$ is defined, one can show $M(t) \in C^{\infty}$ in its domain and its relation to the nth moment

(1.54) $M^{(n)}(t) = \mathbb{E}(X^n e^{tX})$ and $\mu_n := \mathbb{E}X^n = M^{(n)}(0), \ n \in \mathbb{N}.$

This gives

$$(1.55) \qquad M(t) = \sum_{n=0}^{\infty} \mu_n \frac{t^n}{n!},$$

which explains why $M(t)$ is called the moment generating function.

Theorem 1.40. *Denote $M_X(t), M_Y(t)$, and $M_{X+Y}(t)$ the moment generating functions of the random variables X, Y, and $X + Y$, respectively. If X, Y are independent, then*

$$(1.56) \qquad M_{X+Y}(t) = M_X(t) M_Y(t).$$

Proof. The proof is straightforward by noticing

$$M_{X+Y}(t) = \mathbb{E} e^{t(X+Y)} = \mathbb{E} e^{tX} \mathbb{E} e^{tY} = M_X(t) M_Y(t). \qquad \square$$

The following can be obtained by direct calculation.

  (a) Binomial distribution: $M(t) = (pe^t + 1 - p)^n$.
  (b) Poisson distribution: $M(t) = \exp[\lambda(e^t - 1)]$.
  (c) Exponential distribution: $M(t) = \lambda/(\lambda - t)$ for $t < \lambda$.
  (d) Normal distribution $N(\mu, \sigma^2)$: $M(t) = \exp\left(\mu t + \frac{1}{2}\sigma^2 t^2\right)$.

The cumulant generating function $K(t)$ is defined by

$$(1.57) \qquad \Lambda(t) = \log M(t) = \log \mathbb{E} e^{tX} = \sum_{n=1}^{\infty} \kappa_n \frac{t^n}{n!}.$$

With such a definition, we have $\kappa_0 = 0$ and

$$(1.58) \qquad \kappa_n = \frac{d^n}{dt^n} \Lambda(0), \quad n \in \mathbb{N}.$$

It is straightforward to define moment and cumulant generating functions for random vectors:

$$M(\boldsymbol{t}) = \mathbb{E} e^{\boldsymbol{t} \cdot \boldsymbol{X}}, \ \Lambda(\boldsymbol{t}) = \log M(\boldsymbol{t}), \quad \boldsymbol{t} \in \mathbb{R}^d.$$

These notions are useful, for example, in statistical physics [**TKS95**], [**KTH95**].

1.11. The Borel-Cantelli Lemma

We now turn to a technical tool that will be useful in the next chapter. Given a sequence of events $\{A_n\}_{n=1}^{\infty}$, we are interested in the event that A_n occurs infinitely often, i.e.,

$$\{A_n \text{ i.o.}\} = \{\omega : \omega \in A_n \text{ i.o.}\} = \limsup_{k \to \infty} A_n = \bigcap_{n=1}^{\infty} \bigcup_{k=n}^{\infty} A_k.$$

The probability of such an event can be characterized by the Borel-Cantelli lemma.

Lemma 1.41.

(1) *If $\sum_{n=1}^{\infty} \mathbb{P}(A_n) < \infty$, then $\mathbb{P}\left(\{A_n \ i.o.\}\right) = 0$.*

(2) *If $\sum_{n=1}^{\infty} \mathbb{P}(A_n) = \infty$ and the A_n's are mutually independent, then $\mathbb{P}\left(\{A_n \ i.o.\}\right) = 1$.*

Proof. (1) We have

$$
\mathbb{P}\left(\Big\{\bigcap_{n=1}^{\infty}\bigcup_{k=n}^{\infty} A_k\Big\}\right) \leq \mathbb{P}\left(\Big\{\bigcup_{k=n}^{\infty} A_k\Big\}\right) \leq \sum_{k=n}^{\infty} \mathbb{P}(A_k)
$$

for any n. The last term goes to 0 as $n \to \infty$ since $\sum_{k=1}^{\infty} \mathbb{P}(A_k) < \infty$ by assumption.

(2) Using independence, one has

$$
\mathbb{P}\left(\bigcup_{k=n}^{\infty} A_k\right) = 1 - \mathbb{P}\left(\bigcap_{k=n}^{\infty} A_k^c\right) = 1 - \prod_{k=n}^{\infty} \mathbb{P}(A_k^c) = 1 - \prod_{k=n}^{\infty}(1 - \mathbb{P}(A_k)).
$$

Using $1 - x \leq e^{-x}$, this gives

$$
\mathbb{P}\left(\bigcup_{k=n}^{\infty} A_k\right) \geq 1 - \prod_{k=n}^{\infty} e^{-\mathbb{P}(A_k)} = 1 - e^{-\sum_{k=n}^{\infty} \mathbb{P}(A_k)} = 1.
$$

The result follows immediately. $\qquad\square$

As an example of the application of this result, we prove

Lemma 1.42. *Let $\{X_n\}_{n\in\mathbb{N}}$ be a sequence of identically distributed (not necessarily independent) random variables, such that $\mathbb{E}|X_n| < \infty$. Then*

$$
\lim_{n\to\infty} \frac{X_n}{n} = 0 \qquad a.s.
$$

Proof. For any $\epsilon > 0$, define

$$
A_n^\epsilon = \{\omega \in \Omega : |X_n(\omega)/n| > \epsilon\}.
$$

Then

$$\sum_{n=1}^{\infty} \mathbb{P}(A_n^{\epsilon}) = \sum_{n=1}^{\infty} \mathbb{P}(|X_n| > n\epsilon) = \sum_{n=1}^{\infty} \mathbb{P}(|X_1| > n\epsilon)$$

$$= \sum_{n=1}^{\infty} \sum_{k=n}^{\infty} \mathbb{P}\left(k\epsilon < |X_1| \le (k+1)\epsilon\right)$$

$$= \sum_{k=1}^{\infty} k \mathbb{P}\left(k\epsilon < |X_1| \le (k+1)\epsilon\right)$$

$$= \sum_{k=1}^{\infty} k \int_{k\epsilon < |X_1| \le (k+1)\epsilon} \mathbb{P}(d\omega)$$

$$\le \frac{1}{\epsilon} \sum_{k=1}^{\infty} \int_{k\epsilon < |X_1| \le (k+1)\epsilon} |X_1| \mathbb{P}(d\omega)$$

$$= \frac{1}{\epsilon} \int_{\epsilon < |X_1|} |X_1| \mathbb{P}(d\omega) \le \frac{1}{\epsilon} \mathbb{E}|X_1| < \infty.$$

Therefore if we define

$$B_{\epsilon} = \{\omega \in \Omega : \omega \in A_n^{\epsilon} \text{ i.o.}\},$$

then $\mathbb{P}(B_{\epsilon}) = 0$. Let $B = \bigcup_{n=1}^{\infty} B_{\frac{1}{n}}$. Then $\mathbb{P}(B) = 0$, and

$$\lim_{n \to \infty} \frac{X_n(\omega)}{n} = 0 \quad \text{if } \omega \notin B.$$

The proof is complete.   □

With the Borel-Cantelli lemma, we can give the proof of (ii) in Theorem 1.32.

Proof. Without loss of generality, we may assume that $X = 0$. By the condition of convergence in probability we can take $n_k \in \mathbb{N}$ which is increasing in k such that

$$\mathbb{P}\left(|X_{n_k}| \ge \frac{1}{k}\right) \le \frac{1}{2^k}$$

for each $k \in \mathbb{N}$. For any fixed ϵ, there exists an integer k_0 such that $k_0^{-1} \le \epsilon$ and we have

$$\sum_{k=1}^{\infty} \mathbb{P}(|X_{n_k}| \ge \epsilon) \le \sum_{k=1}^{k_0} \mathbb{P}(|X_{n_k}| \ge \epsilon) + \sum_{k=k_0+1}^{\infty} \mathbb{P}\left(|X_{n_k}| \ge \frac{1}{k}\right)$$

$$\le \sum_{k=1}^{k_0} \mathbb{P}(|X_{n_k}| \ge \epsilon) + \sum_{k=k_0+1}^{\infty} \frac{1}{2^k} < \infty.$$

By the Borel-Cantelli lemma we obtain

$$\mathbb{P}(|X_{n_k}| \geq \epsilon, \text{ i.o.}) = 0.$$

Thus the subsequence X_{n_k} converges to 0 almost surely by the same argument as the example above. $\qquad\square$

Exercises

In the following, i.i.d. stands for independent, identically distributed.

1.1. Let $X = \sum_{j=1}^{n} X_j$, where the X_j are i.i.d. random variables with Bernoulli distribution with parameter p. Prove that $X \sim B(n, p)$.

1.2. Let S_n be the number of heads in the outcome of n independent tosses for a fair coin. Its distribution is given by

$$p_j = \mathbb{P}(S_n = j) = \frac{1}{2^n} \binom{n}{j}.$$

Show that the mean and the variance of this random variable are

$$\mathbb{E}S_n = \frac{n}{2}, \qquad \text{Var}(S_n) = \frac{n}{4}.$$

This implies that $\text{Var}(S_n)/(\mathbb{E}S_n)^2 \to 0$ as $n \to \infty$.

1.3. Prove that

$$C_n^k p^k q^{n-k} \longrightarrow \frac{\lambda^k}{k!} e^{-\lambda} \text{ for any fixed } k$$

as $n \to \infty, p \to 0$, and $np = \lambda$. This is the classical Poisson approximation to the binomial distribution.

1.4. Numerically investigate the limit processes

   Binomial $B(n, p) \longrightarrow$ Poisson $\mathcal{P}(\lambda) \longrightarrow$ Normal $N(\lambda, \lambda)$

when $\lambda = np$, $n \gg 1$, and $\lambda \gg 1$, by comparing the plots for different distributions. Find the parameter regimes such that the approximation is valid.

1.5. Suppose $X \sim \mathcal{P}(\lambda)$, $Y \sim \mathcal{P}(\mu)$ are two independent Poisson random variables.
   (a) Prove that $Z = X + Y \sim \mathcal{P}(\lambda + \mu)$.
   (b) Prove that the conditional distribution of X (or Y), conditioning on $X + Y$ being fixed, i.e., $X + Y = N$, is a binomial distribution with parameter $n = N$ and $p = \lambda/(\lambda + \mu)$ (or $p = \mu/(\lambda + \mu)$).

1.6. Prove the following statements:

(a) (Memoryless property of exponential distribution) Suppose $X \sim \mathcal{E}(\lambda)$. Prove that

$$\mathbb{P}(X > s + t | X > s) = \mathbb{P}(X > t) \quad \text{for all } s, t > 0.$$

(b) Let $X \in (0, \infty)$ be a random variable such that

$$\mathbb{P}(X > s + t) = \mathbb{P}(X > s)\mathbb{P}(X > t) \quad \text{for all } s, t > 0.$$

Prove that there exists $\lambda > 0$ such that $X \sim \mathcal{E}(\lambda)$.

1.7. Let $X = (X_1, \ldots, X_n)$ be an n-dimensional Gaussian random variable and let $Y = c_1 X_1 + c_2 X_2 + \cdots + c_n X_n$, where $c_1, \ldots, c_n$ are constants. Show that Y is also Gaussian.

1.8. Suppose that the multivariate Gaussian variable

$$\begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix} \sim N\left(\begin{pmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{pmatrix}, \begin{pmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{pmatrix} \right).$$

Prove that the conditional distribution of $\boldsymbol{X}$ given $\boldsymbol{Y} = \boldsymbol{y}$ is Gaussian with mean $\tilde{\boldsymbol{\mu}}$ and covariance $\tilde{\boldsymbol{\Sigma}}$:

$$\tilde{\boldsymbol{\mu}} = \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}_y), \quad \tilde{\boldsymbol{\Sigma}} = \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}\boldsymbol{\Sigma}_{yx}.$$

1.9. Pairwise independence does not imply independence. Let X, Y be two independent random variables such that

$$\mathbb{P}(X = \pm 1) = \mathbb{P}(Y = \pm 1) = \frac{1}{2},$$

and let $Z = XY$. Check that X, Y, Z are pairwise independent but not independent.

1.10. Independence does not imply conditional independence. Construct a concrete example such that

$$p(x, y) = p(x)p(y) \quad \text{for any } x, y$$

but $p(x, y|z) \neq p(x|z)p(y|z)$ for some x, y, and z, where x, y, z are the values of random variables X, Y, and Z.

1.11. Let $\mathcal{R}$ be the Borel σ-algebra on $\mathbb{R}$. For any random variable X, prove that the sets $\mathcal{B} = X^{-1}(\mathcal{R})$ form a σ-algebra.

1.12. If X_j $(j = 1, \ldots, n)$ are independent random variables and f_j $(j = 1, \ldots, n)$ are Borel measurable functions, i.e., $f_j^{-1}(B) \in \mathcal{R}$ for any $B \in \mathcal{R}$, then $f_j(X_j)$ $(j = 1, \ldots, n)$ are independent.

1.13. Prove that if the σ-algebra $\mathcal{F}$ has finite members, then there exist nonempty sets $B_1, \ldots, B_K \in \mathcal{F}$ such that $\Omega = \bigcup_{j=1}^{K} B_j$, $B_i \cap B_j = \emptyset$ for $i, j = 1, \ldots, K$, and any $B \in \mathcal{F}$ can be represented as a finite union of the sets in $\{B_j\}$.

1.14. (*Variance identity*) Suppose the random variable $\boldsymbol{X}$ has the partition $\boldsymbol{X} = (\boldsymbol{X}^{(1)}, \boldsymbol{X}^{(2)})$. Prove the variance identity for any integrable function f:

$$\operatorname{Var}(f(\boldsymbol{X})) = \operatorname{Var}(\mathbb{E}(f(\boldsymbol{X})|\boldsymbol{X}^{(2)})) + \mathbb{E}(\operatorname{Var}(f(\boldsymbol{X})|\boldsymbol{X}^{(2)})).$$

1.15. Prove Theorem 1.24.

1.16. Let X be a discrete random variable and let $p_i = \mathbb{P}(X = i)$ for $i = 1, 2, \ldots, n$. Define the *Shannon entropy* of X by

$$H(X) = -\sum_{i=1}^{n} p_i \log p_i.$$

Prove that $H(X) \geq 0$ and that the equality holds only when X is reduced to a deterministic variable; i.e., $p_i = \delta_{ik_0}$, for some fixed integer k_0 in $\{1, 2, \ldots, n\}$. Here we take the convention $0 \log 0 = 0$.

1.17. Let $\boldsymbol{X} = (X_1, X_2, \ldots, X_n)$ be i.i.d. continuous random variables with common distribution function F and density $\rho(x) = F'(x)$. $(X_{(1)}, X_{(2)}, \ldots, X_{(n)})$ are called the *order statistics* of $\boldsymbol{X}$ if $X_{(k)}$ is the kth smallest of these random variables. Prove that the density of the order statistics is given by

$$p(x_1, x_2, \ldots, x_n) = n! \prod_{k=1}^{n} \rho(x_k), \quad x_1 < x_2 < \cdots < x_n.$$

1.18. (*Stable laws*) A one-dimensional distribution $\mu(dx)$ is stable if given any two independent random variables X and Y with distribution $\mu(dx)$, there exists a and b such that

$$a(X + Y - b)$$

has distribution $\mu(dx)$. Show that $f(\xi) = e^{-|\xi|^\alpha}$ is the characteristic function of a stable distribution for $0 < \alpha \leq 2$ and that it is not a characteristic function for other values of α.

1.19. Prove that if the moment generating function $M(t)$ can be defined on an open set U, then $M \in C^\infty(U)$.

1.20. (*Wick's theorem*) For multivariate Gaussian random variables X_1, X_2, ..., X_n with mean 0, prove

$$\mathbb{E}(X_1 X_2 \cdots X_k) = \begin{cases} \sum \prod \mathbb{E}(X_i X_j), & k \text{ is even}, \\ 0, & k \text{ is odd}, \end{cases}$$

where the notation $\sum\prod$ means summing of the products over all possible partitions of $X_1,\ldots,X_k$ into pairs; e.g., if (X,Y,Z) is jointly Gaussian, we have

$$(1.59) \quad \mathbb{E}(X^2Y^2Z^2) = (\mathbb{E}X^2)(\mathbb{E}Y^2)(\mathbb{E}Z^2) + 2(\mathbb{E}YZ)^2\mathbb{E}X^2 + 2(\mathbb{E}XY)^2\mathbb{E}Z^2$$
$$+ 2(\mathbb{E}XZ)^2\mathbb{E}Y^2 + 8(\mathbb{E}XY)(\mathbb{E}YZ)(\mathbb{E}XZ).$$

Each term in (1.59) can be schematically mapped to some graph, as shown below:

The coefficient of each term is the combinatorial number for generating the corresponding schematic combinations. This is essentially the so-called Feynman diagrams.

1.21. Suppose that the events $\{A_n\}$ are mutually independent with

$$\mathbb{P}\Big(\bigcup_n A_n\Big) = 1 \quad \text{and} \quad \mathbb{P}(A_n) < 1$$

for each n. Prove that $\mathbb{P}(A_n \text{ i.o.}) = 1$.

1.22. (*Girko's circular law*) If the $n \times n$ matrix $\boldsymbol{A}$ has i.i.d. entries with mean zero and variance σ^2, then the eigenvalues of $\boldsymbol{A}/\sqrt{n}\sigma$ are asymptotically uniformly distributed in the unit disk in the complex plane when $n \to \infty$. Investigate this numerically.

Notes

The axiomatic approach to probability theory starts with Kolmogorov's masterpiece [**Kol56**]. There are already lots of excellent textbooks on the introduction to elementary probability theory [**Chu01**, **Cin11**, **Dur10**, **KS07**, **Shi96**]. To know more about the measure theory approach to probability theory, please consult [**Bil79**]. More on the practical side of probability theory can be found in the classic book by Feller [**Fel68**] or the books by some applied mathematicians and scientists [**CH13**, **CT06**, **Gar09**, **VK04**].

Limit Theorems

Let $\{X_j\}_{j=1}^\infty$ be a sequence of independent and identically distributed (abbreviated as i.i.d.) random variables. Let $\eta = \mathbb{E}X_1$ and $S_n = \sum_{j=1}^n X_j$. We will be interested in three classes of limit theorems:

a) *The law of large numbers*, which states how the empirical average S_n/n approaches the real average η as $n \to \infty$.

b) *The central limit theorem*, which states that the suitably rescaled error between the empirical average and the real average has the standard Gaussian distribution.

c) *The large deviation theorem*, which estimates the probability that the empirical average approaches a value other than the real average. Such events are rare but important for a lot of applications.

At the end of this chapter, we will also discuss extreme statistics, i.e., the distribution of the maximum or minimum of a sequence of random variables.

2.1. The Law of Large Numbers

Theorem 2.1 (Weak law of large numbers (WLLN))**.** *Let $\{X_j\}_{j=1}^\infty$ be a sequence of i.i.d. random variables such that $\mathbb{E}|X_j| < \infty$. Then*

$$\frac{S_n}{n} \to \eta \qquad in\ probability.$$

Proving this result under the stated assumption is quite involved. We will give a proof of the WLLN under the stronger assumption that $\mathbb{E}|X_j|^2 < \infty$.

Proof. Without loss of generality, we can assume $\eta = 0$. From the Chebyshev inequality, we have

$$\mathbb{P}\left(\left|\frac{S_n}{n}\right| > \epsilon\right) \leq \frac{1}{\epsilon^2}\mathbb{E}\left|\frac{S_n}{n}\right|^2$$

for any $\epsilon > 0$. Using independence, we have

$$\mathbb{E}|S_n|^2 = \sum_{i,j=1}^{n} \mathbb{E}(X_i X_j) = n\mathbb{E}|X_1|^2.$$

Hence

$$\mathbb{P}\left(\left|\frac{S_n}{n}\right| > \epsilon\right) \leq \frac{1}{n\epsilon^2}\mathbb{E}|X_1|^2 \to 0,$$

as $n \to \infty$. $\square$

Theorem 2.2 (Strong law of large numbers (SLLN)). *Let $\{X_j\}_{j=1}^{\infty}$ be a sequence of i.i.d. random variables such that $\mathbb{E}|X_j| < \infty$. Then*

$$\frac{S_n}{n} \to \eta \quad a.s.$$

Proof. We will only give a proof of the SLLN under the stronger assumption that $\mathbb{E}|X_j|^4 < \infty$. The proof under the stated assumption can be found in [**Chu01**].

Without loss of generality, we can assume $\eta = 0$. Using the Chebyshev inequality, we have

$$\mathbb{P}\left(\left|\frac{S_n}{n}\right| > \epsilon\right) \leq \frac{1}{\epsilon^4}\mathbb{E}\left|\frac{S_n}{n}\right|^4.$$

Using independence, we get

$$\mathbb{E}|S_n|^4 = \sum_{i,j,k,l=1}^{n} \mathbb{E}(X_i X_j X_k X_l) = n\mathbb{E}|X_j|^4 + 3n(n-1)(\mathbb{E}|X_j|^2)^2.$$

Using Hölder's inequality, we have $(\mathbb{E}|X_j|^2)^2 \leq \mathbb{E}|X_j|^4 < \infty$. Hence

$$\mathbb{P}\left(\left|\frac{S_n}{n}\right| > \epsilon\right) \leq \frac{\mathbb{E}|X_j|^4}{n^2\epsilon^4}.$$

Now we are in a situation to use the Borel-Cantelli lemma, since the series $1/n^2$ is summable. This gives us

$$\mathbb{P}\left(\left|\frac{S_n}{n}\right| > \epsilon, \text{ i.o.}\right) = 0.$$

Hence $S_n/n \to 0$ a.s. $\square$

The weak and strong laws of large numbers may not hold if the moment condition is not satisfied.

Example 2.3 (Cauchy-Lorentz distribution)**.** For the distribution with PDF

$$(2.1) \qquad p(x) = \frac{1}{\pi(1 + x^2)}, \quad x \in \mathbb{R},$$

we have $\mathbb{E}|X_j| = \infty$. For a sequence of i.i.d. random variables $\{X_j\}_{j=1}^{\infty}$ with Cauchy-Lorentz distribution, one can easily check that S_n/n also has the Cauchy-Lorentz distribution. Thus both the weak and strong laws of large numbers are violated.

In fact, the converse statement for SLLN is also true: If $S_n/n \to a < \infty$ a.s. holds, then $\mathbb{E}|X_j| < \infty$. The proof can be found in [**Chu01**].

2.2. Central Limit Theorem

The following result explains why Gaussian noises (i.e., normal random variables) are so prevalent in nature.

Theorem 2.4 (Lindeberg-Lévy central limit theorem (CLT))**.** *Let $\{X_j\}_{j=1}^{\infty}$ be a sequence of i.i.d. random variables. Assume that $\mathbb{E}X_j^2 < \infty$ and let $\sigma^2 = \text{Var}(X_j)$. Then*

$$\frac{S_n - n\eta}{\sqrt{n\sigma^2}} \to N(0, 1)$$

in the sense of distribution.

Outline of proof. Assume without loss of generality that $\eta = 0$ and $\sigma = 1$; otherwise we can shift and rescale X_j. Let f be the characteristic function of X_1 and let g_n be the characteristic function of $S_n/\sqrt{n}$. Then

$$g_n(\xi) = \mathbb{E}e^{i\xi S_n/\sqrt{n}} = \prod_{j=1}^{n} \mathbb{E}e^{i\xi X_j/\sqrt{n\sigma^2}} = \prod_{j=1}^{n} f\left(\frac{\xi}{\sqrt{n}}\right) = f\left(\frac{\xi}{\sqrt{n}}\right)^n.$$

Using Taylor expansion and the properties of characteristic functions we obtain

$$f\left(\frac{\xi}{\sqrt{n}}\right) = f(0) + \frac{\xi}{\sqrt{n}}f'(0) + \frac{1}{2}\left(\frac{\xi}{\sqrt{n}}\right)^2 f''(0) + o\left(\frac{1}{n}\right)$$

$$= 1 - \frac{\xi^2}{2n} + o\left(\frac{1}{n}\right).$$

Hence

$$(2.2) \quad g_n(\xi) = f\left(\xi/\sqrt{n}\right)^n = \left(1 - \frac{\xi^2}{2n} + o\left(\frac{1}{n}\right)\right)^n \to e^{-\frac{1}{2}\xi^2} \qquad \text{as } n \to \infty$$

for every $\xi \in \mathbb{R}$. Using Theorem 1.35, we obtain the stated result. $\qquad \square$

Remark 2.5. Equation (2.2) can be made more accurate by including higher-order terms. In fact we have

$$G_n(x) = \Phi(x) - \phi(x)\left(\frac{\gamma(x^2-1)}{6\sqrt{n}}\right) + O\left(\frac{1}{n}\right),$$

where $G_n(x)$, $\Phi(x)$ are distribution functions of $S_n/\sqrt{n}$ and $N(0,1)$ random variable, respectively, $\phi(x)$ is the PDF of $N(0,1)$, and $\gamma = \mathbb{E}X_j^3$. This is called the Edgeworth expansion in the literature.

The CLT gives an estimate for the rate of convergence in the law of large numbers. Since by the CLT we have

$$\frac{S_n}{n} - \eta \approx \frac{\sigma}{\sqrt{n}}N(0,1),$$

the rate of convergence of S_n/n to η is $O(n^{-\frac{1}{2}})$. This is the reason why most Monte Carlo methods has a rate of convergence of $O(n^{-\frac{1}{2}})$ where n is the sample size.

Remark 2.6 (Stable laws)**.** Theorem 2.4 requires that the variance of X_j be finite. For random variables with unbounded variances, one can show that the following generalized central limit theorem holds: If there exist $\{a_n\}$ and $\{b_n\}$ such that

$$\mathbb{P}(a_n(S_n - b_n) \le x) \to G(x) \quad \text{as } n \to \infty,$$

then the distribution $G(x)$ must be a stable law. A probability distribution is said to be a *stable law* if any linear combination of two independent random variables with that distribution has again the same distribution, up to a shift and rescaling. One simple instance of the stable law is the Cauchy distribution considered in Example 2.3, for which we can take $a_n = 1/n$ and $b_n = 0$ and the limit $G(x)$ is exactly the distribution function of the Cauchy-Lorentz distribution (the limit process is in fact an identity in this case). For more details about the generalized central limit theorem and stable law see [**Bre92**, **Dur10**].

2.3. Cramér's Theorem for Large Deviations

Let $\{X_j\}_{j=1}^n$ be a sequence of i.i.d. random variables and let $\eta = \mathbb{E}X_j$. The laws of large numbers says that for any $\epsilon > 0$, with probability close to 1, $|S_n/n - \eta| < \epsilon$ for large enough n; conversely if $y \ne \eta$, then the probability that S_n/n is close to y goes to zero as $n \to \infty$. Events of this type, i.e., $\{|S_n/n - y| < \epsilon\}$ for $y \ne \eta$, are called *large deviation events*.

To estimate the precise rate at which $\mathbb{P}\left(|S_n/n - y| < \epsilon\right)$ goes to zero, we assume that the distribution μ of the X_j's has finite *exponential moments*.

Define the moment and cumulant generating functions as in Section 1.10:

$$(2.3) \qquad M(\lambda) = \mathbb{E}e^{\lambda X_j}, \quad \Lambda(\lambda) = \log M(\lambda).$$

The Legendre-Fenchel transform of $\Lambda(\lambda)$ is

$$(2.4) \qquad I(x) = \sup_\lambda \{x\lambda - \Lambda(\lambda)\}.$$

Let $\mu_n(\Gamma) = \mathbb{P}(S_n/n \in \Gamma)$. We have the following important characterization for μ_n.

Theorem 2.7 (Cramér's theorem). *$\{\mu_n\}$ satisfies the large deviation principle:*

(i) *For any closed set $F \in \mathcal{R}$*

$$(2.5) \qquad \overline{\lim_{n\to\infty}} \frac{1}{n} \log \mu_n(F) \leq -\inf_{x\in F} I(x).$$

(ii) *For any open set $G \in \mathcal{R}$*

$$(2.6) \qquad \underline{\lim_{n\to\infty}} \frac{1}{n} \log \mu_n(G) \geq -\inf_{x\in G} I(x).$$

Taking the two bounds together, this theorem suggests that

$$\mu_n(\Gamma) \asymp \exp\left(-n \inf_{x\in\Gamma} I(x)\right).$$

Here the symbol $\asymp$ means logarithmic equivalence; i.e., $\lim_{\varepsilon\to 0} \log c_\varepsilon / \log d_\varepsilon = 1$ if $c_\varepsilon \asymp d_\varepsilon$.

This is the large deviation theorem (LDT) for i.i.d. random variables. It states roughly that the probability of large deviation events converges to 0 exponentially fast. $I(x)$ is called the rate function.

To study the properties of the rate function, we need some results on the Legendre-Fenchel transform.

Lemma 2.8. *Assume that $f : \mathbb{R}^d \to \bar{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$ is a lower semicontinuous convex function. Let F be its conjugate function (the Legendre-Fenchel transform):*

$$F(\boldsymbol{y}) = \sup_{\boldsymbol{x}} \{(\boldsymbol{x}, \boldsymbol{y}) - f(\boldsymbol{x})\}.$$

Then:

(i) *F is also a lower semicontinuous convex function.*

(ii) *The Fenchel inequality holds:*

$$(\boldsymbol{x}, \boldsymbol{y}) \leq f(\boldsymbol{x}) + F(\boldsymbol{y}).$$

(iii) *The conjugacy relation holds:*

$$f(\boldsymbol{x}) = \sup_{\boldsymbol{y}} \{(\boldsymbol{x}, \boldsymbol{y}) - F(\boldsymbol{y})\}.$$

Here we need to adopt the following arithmetic rules on the extended reals $\bar{\mathbb{R}}$:

$$\alpha + \infty = \infty, \ \alpha - \infty = -\infty \quad \text{for } \alpha \text{ finite}.$$

(2.7) $$\alpha \cdot \infty = \infty, \ \alpha \cdot (-\infty) = -\infty \quad \text{for } \alpha > 0.$$

$$0 \cdot \infty = 0 \cdot (-\infty) = 0, \quad \inf \emptyset = \infty, \ \sup \emptyset = -\infty.$$

Readers may refer to [**RW09**, **Roc70**] for a proof.

To see why the rate function takes the particular form in (2.8), assume for the moment that Cramér's theorem holds. Then we have roughly

$$\mu_n(dx) \propto \exp(-nI(x))dx.$$

By Laplace asymptotics (cf. Section A of the appendix)

$$\lim_{n\to\infty} \frac{1}{n} \log \mathbb{E}^{\mu_n}(\exp(n\Phi(x))) := \lim_{n\to\infty} \frac{1}{n} \log \int_{\mathbb{R}} \exp(n\Phi(x))\mu_n(dx)$$

(2.8) $$= \sup_x \{\Phi(x) - I(x)\}.$$

Take $\Phi(x) = \lambda x$. We then have

$$\mathbb{E}^{\mu_n}(\exp(n\lambda x)) = \mathbb{E} \exp \left(\lambda \sum_{j=1}^{n} X_j \right) = [\mathbb{E}\exp(\lambda X_j)]^n = \left(M(\lambda) \right)^n.$$

Equation (2.8) leads to

$$\Lambda(\lambda) = \sup_x \{\lambda x - I(x)\}.$$

Since I is convex, I must be the Legendre transform of Λ.

Lemma 2.9. *The rate function $I(x)$ has the following properties:*

(i) *$I(x)$ is convex and lower semicontinuous.*

(ii) *$I(x)$ is nonnegative and $I(\eta) = 0$.*

(iii) *$I(x)$ is nondecreasing in $[\eta, \infty)$ and nonincreasing in $(-\infty, \eta]$.*

(iv) *If $x > \eta$, then $I(x) = \sup_{\lambda>0}\{\lambda x - \Lambda(\lambda)\}$, and if $x < \eta$, then $I(x) = \sup_{\lambda<0}\{\lambda x - \Lambda(\lambda)\}$.*

Proof. (i) The convexity of $\Lambda(\lambda)$ follows from Hölder's inequality. For any $0 \le \theta \le 1$,

$$\Lambda(\theta\lambda_1 + (1-\theta)\lambda_2) = \log \mathbb{E}\Big(\exp(\theta\lambda_1 X_j) \exp((1-\theta)\lambda_2 X_j) \Big)$$
$$\le \log \Big((\mathbb{E}\exp(\lambda_1 X_j))^\theta (\mathbb{E}\exp(\lambda_2 X_j))^{(1-\theta)} \Big)$$
$$= \theta\Lambda(\lambda_1) + (1-\theta)\Lambda(\lambda_2).$$

Thus $\Lambda(\lambda)$ is a convex function. The rest is a direct application of Lemma 2.8.

(ii) Taking $\lambda = 0$, we obtain $x \cdot 0 - \Lambda(0) = 0$. Thus $I(x) \geq 0$. On the other hand, we have

$$\Lambda(\lambda) = \log \mathbb{E} \exp(\lambda X_j) \geq \log \exp(\lambda \eta) = \lambda \eta$$

by Jensen's inequality. This gives $I(\eta) \leq 0$. Combined with the fact that $I(x) \geq 0$, we get $I(\eta) = 0$.

(iii) From the convexity of I and the fact that it achieves minimum at $x = \eta$, we immediately obtain the desired monotonicity property.

(iv) If $x > \eta$, then when $\lambda \leq 0$

$$\lambda x - \Lambda(\lambda) \leq \lambda \eta - \Lambda(\lambda) \leq 0.$$

Since $I \geq 0$, the supremum is only achieved when $\lambda > 0$. The case when $x < \eta$ can be dealt with similarly. $\qquad\square$

Proof of Theorem 2.7. We will only consider the one-dimensional case here. Without loss of generality, we assume $\eta = 0$.

(i) *Upper bound.* Suppose $x > 0$, $J_x := [x, \infty)$. For $\lambda > 0$,

$$\mu_n(J_x) = \int_x^\infty \mu_n(dy) \leq e^{-\lambda x} \int_x^\infty e^{\lambda y} \mu_n(dy)$$
$$\leq e^{-\lambda x} \int_{-\infty}^\infty e^{\lambda y} \mu_n(dy) = e^{-\lambda x} \Big[M(\frac{\lambda}{n}) \Big]^n.$$

Replacing λ by $n\lambda$, we obtain

$$\frac{1}{n} \log \mu_n(J_x) \leq -(\lambda x - \Lambda(\lambda)).$$

Thus, we have

$$\frac{1}{n} \log \mu_n(J_x) \leq - \sup_{\lambda > 0} \{\lambda x - \Lambda(\lambda)\} = -I(x).$$

If $x < 0$, we can define $\tilde{J}_x = (-\infty, x]$. Similarly we get

$$\frac{1}{n} \log \mu_n(\tilde{J}_x) \leq -I(x).$$

For a closed set $F \in \mathcal{R}$, if $0 \in F$, $\inf_{x \in F} I(x) = 0$. The upper bound obviously holds in this case. Otherwise, let (x_1, x_2) be the maximal interval satisfying the conditions $(x_1, x_2) \cap F = \emptyset$ and $0 \in (x_1, x_2)$. Then $x_1, x_2 \in F$, $F \subset \tilde{J}_{x_1} \cup J_{x_2}$. From the monotonicity of I on $(-\infty, 0]$ and $[0, \infty)$, we obtain

$$\varlimsup_{n \to \infty} \frac{1}{n} \log \mu_n(F) \leq \max \left(\varlimsup_{n \to \infty} \frac{1}{n} \log \mu_n(\tilde{J}_{x_1}), \varlimsup_{n \to \infty} \frac{1}{n} \log \mu_n(J_{x_2}) \right)$$
$$\leq - \min(I(x_1), I(x_2)) = - \inf_{x \in F} I(x).$$

(ii) *Lower bound.* Let G be a nonempty open set. It suffices to prove that for any $x \in G$

$$\varliminf_{n \to \infty} \frac{1}{n} \log \mu_n(G) \geq -I(x).$$

Now fix x and assume that $I(x) < \infty$.

Case 1. If x is such that the supremum in

$$I(x) = \sup_\lambda \{\lambda x - \Lambda(\lambda)\}$$

cannot be achieved, then $x \neq 0$. Suppose $x > 0$. There exists $\lambda_n \to \infty$ such that

$$I(x) = \lim_{n \to \infty} (\lambda_n x - \Lambda(\lambda_n)).$$

We have

$$\int_{-\infty}^{x-0} \exp(\lambda_n(y - x))\mu(dy) \to 0 \text{ as } n \to \infty$$

by the dominated convergence theorem. On the other hand

$$\lim_{n \to \infty} \int_x^\infty \exp(\lambda_n(y - x))\mu(dy) = \lim_{n \to \infty} \int_{-\infty}^\infty \exp(\lambda_n(y - x))\mu(dy)$$
$$= \exp(-I(x)) < \infty.$$

Thus $\mu((x, \infty)) = 0$ and

$$\exp(-I(x)) = \lim_{n \to \infty} \int_x^\infty \exp(\lambda_n(y - x))\mu(dy) = \mu(\{x\}).$$

Since

$$\mu_n(G) \geq \mu_n(\{x\}) \geq (\mu(\{x\}))^n = \exp(-nI(x)),$$

we get

$$\frac{1}{n} \log \mu_n(G) \geq -I(x).$$

A similar argument can be applied to the case when $x < 0$.

Case 2. Assume that the supremum in the definition of $I(x)$ is attained at λ_0:

$$I(x) = \lambda_0 x - \Lambda(\lambda_0).$$

Then $x = \Lambda'(\lambda_0) = M'(\lambda_0)/M(\lambda_0)$. Define a new probability measure:

$$\tilde{\mu}(dy) = \frac{1}{M(\lambda_0)} \exp(\lambda_0 y)\mu(dy).$$

Its expectation is given by

$$\int_{\mathbb{R}} y\tilde{\mu}(dy) = \frac{1}{M(\lambda_0)} \int_{\mathbb{R}} y \exp(\lambda_0 y)\mu(dy) = \frac{M'(\lambda_0)}{M(\lambda_0)} = x.$$

If $x \geq 0$, then $\lambda_0 \geq 0$. For sufficiently small $\delta > 0$, we have $(x - \delta, x + \delta) \subset G$,

$$\mu_n(G) \geq \mu_n(x - \delta, x + \delta)$$

$$= \int_{\left\{ \left| \frac{1}{n} \sum\limits_{j=1}^{n} y_j - x \right| < \delta \right\}} \mu(dy_1) \cdots \mu(dy_n)$$

$$\geq e^{-n\lambda_0(x+\delta)} \int_{\left\{ \left| \frac{1}{n} \sum\limits_{j=1}^{n} y_j - x \right| < \delta \right\}} \exp(\lambda_0 y_1 + \cdots + \lambda_0 y_n) \mu(dy_1) \cdots \mu(dy_n)$$

$$= e^{-n\lambda_0(x+\delta)} M(\lambda_0)^n \int_{\left\{ \left| \frac{1}{n} \sum\limits_{j=1}^{n} y_j - x \right| < \delta \right\}} \tilde{\mu}(dy_1) \cdots \tilde{\mu}(dy_n).$$

By the WLLN, we have

$$\int_{\left\{ \left| \frac{1}{n} \sum\limits_{j=1}^{n} y_j - x \right| < \delta \right\}} \tilde{\mu}(dy_1) \cdots \tilde{\mu}(dy_n) \to 1 \text{ as } n \to \infty.$$

Thus

$$\varliminf_{n \to \infty} \frac{1}{n} \log \mu_n(G) \geq -\lambda_0(x + \delta) + \Lambda(\lambda_0) = -I(x) - \lambda_0 \delta \text{ for all } 0 < \delta \ll 1.$$

A similar argument can be applied to the case when $x < 0$. $\qquad \square$

Example 2.10 (Cramér's theorem applied to the Bernoulli distribution with parameter p $(0 < p < 1)$)**.** We have $\Lambda(\lambda) = \log(pe^\lambda + q)$ where $q = 1 - p$. The rate function

$$(2.9) \qquad I(x) = \begin{cases} x \log \frac{x}{p} + (1 - x) \log \frac{1-x}{q}, & x \in [0, 1], \\ \infty, & \text{otherwise.} \end{cases}$$

It is obvious that $I(x) \geq 0$, and $I(x)$ achieves its global minimum 0 at $x^* = p$. The function I is a special case of the so-called relative entropy, or Kullback-Leibler distance, defined between two (discrete) distributions μ and ν:

$$(2.10) \qquad D(\boldsymbol{\mu} \| \boldsymbol{\nu}) = \sum_{i=1}^{r} \mu_i \log \frac{\mu_i}{\nu_i},$$

where $\boldsymbol{\mu} = (\mu_1, \mu_2, \ldots, \mu_r)$, $\boldsymbol{\nu} = (\nu_1, \nu_2, \ldots, \nu_r)$.

The above discussion can be easily generalized to the case of finitely many states. Suppose that $X_1, X_2, \ldots, X_n$ are i.i.d. samples from the state space $S = \{a_1, a_2, \ldots, a_r\}$ with probability $\boldsymbol{\nu} = (\nu_1, \nu_2, \ldots, \nu_r)$. We are interested in the empirical distribution $\boldsymbol{p} = (p_1, p_2, \ldots, p_r)$ of X as

$$p_i = \frac{1}{n} \sum_{k=1}^{n} \delta(X_k = a_i), \quad i = 1, 2, \ldots, r.$$

Here the Boolean function $\delta(X_k = a_i) = 1$ if $X_k = a_i$ and 0 otherwise. It can be put into the large deviation framework by mapping X_k to the kth canonical basis vector $\boldsymbol{e}_k = (0, \ldots, 1, \ldots, 0)$ in the Euclidean space. By the multidimensional version of Cramérs theorem we have $\Lambda(\lambda) = \log \sum_{i=1}^{r} \nu_i e^{\lambda_i}$ and the rate function

$$I(\boldsymbol{x}) = D(\boldsymbol{x}||\boldsymbol{\nu}).$$

The corresponding estimate of the form (2.5) and (2.6) now reads

$$\lim_{n \to \infty} \frac{1}{n} \log \mathbb{P}(\boldsymbol{p} \in \Gamma) = -\min_{\boldsymbol{\mu} \in \Gamma} D(\boldsymbol{\mu}||\boldsymbol{\nu}),$$

where $\Gamma \subset \{\boldsymbol{x} | x_i \geq 0,\ \sum_{i=1}^{r} x_i = 1\}$ is assumed to be a closed set. This is a special form of the so-called Sanov theorem and has many applications in information theory [**CT06**].

Connection with Statistical Mechanics. The large deviation theory is intimately related to equilibrium statistical mechanics [**Ell85**]. As an example we show that the rate function $I(x)$ has a direct connection to Boltzmann's entropy in statistical mechanics.

Consider a system with n independent spins, each being up or down with equal probability $1/2$. If it is up, we label it 1, and 0 otherwise. We define the set of microstates as

$$\Omega = \{\omega : \omega = (s_1, s_2, \ldots, s_n), s_i = 1 \text{ or } 0\}.$$

For each microstate ω, we define its mean energy as

$$h_n(\omega) = \frac{1}{n} \sum_{i=1}^{n} s_i.$$

In thermodynamics, the entropy is a function of the macrostate energy. In statistical mechanics, the Boltzmann entropy is defined by

$$(2.11) \qquad\qquad S(E) = k_B \log W(E),$$

where k_B is the Boltzmann constant and $W(E)$ is the number of the microstates corresponding to the fixed energy E. From large deviation theory we have

$$I(E) = \lim_{n \to \infty} -\frac{1}{n} \log \mathbb{P}(h_n \in [E, E + dE]),$$

where dE is an infinitesimal quantity and thus

$$
\begin{aligned}
I(E) &= \lim_{n \to \infty} -\frac{1}{n} \log \frac{W(h_n \in [E, E + dE])}{2^n} \\
&= \log 2 - \frac{1}{k_B} \lim_{n \to \infty} \frac{1}{n} S_n(E).
\end{aligned}
$$

Here $S_n(E)$ is the Boltzmann entropy for the system with n spins. Denote by $S(E)$ the limit of $S_n(E)/n$ as $n \to \infty$. We get

(2.12) $$k_B I(E) = k_B \log 2 - S(E).$$

So we obtain that *the rate function is the negative entropy (with factor $1/k_B$) up to an additive constant* in this simplest setup. In fact this is a general statement.

In the canonical ensemble in statistical mechanics (the number of spins n and the temperature T are fixed in this setup), let us investigate the physical meaning of Λ. The logarithmic moment generating function of $H_n(\omega) = n h_n(\omega)$ with normalization $1/n$ is

$$\Lambda(\lambda) = \lim_{n \to \infty} \frac{1}{n} \log \mathbb{E} e^{\lambda H_n},$$

where we take H_n instead of $n h_n$ since it admits more general interpretation. Take $\lambda = -\beta = -(k_B T)^{-1}$. We have

$$\Lambda(-\beta) = \lim_{n \to \infty} \frac{1}{n} \log \Big(\sum_\omega e^{-\beta H_n(\omega)} \Big) - \log 2.$$

Define the partition function

$$Z_n(\beta) = \sum_\omega e^{-\beta H_n(\omega)}$$

and Helmholtz free energy

$$F_n(\beta) = -\beta^{-1} \log Z_n(\beta).$$

We have

$$\Lambda(-\beta) = -\beta \lim_{n \to \infty} \frac{1}{n} F_n(\beta) - \log 2 = -\beta F(\beta) - \log 2.$$

Thus *the free energy $F(\beta)$ is the negative logarithmic moment generating function up to a constant.*

According to the large deviation theory we have

$$-\beta F(\beta) - \log 2 = \sup_E \{-\beta E - \log 2 + k_B^{-1} S(E)\};$$

i.e.,

$$F(\beta) = \inf_E \{E - T S(E)\}.$$

The infimum is achieved at the critical point E^* such that

$$\frac{\partial S(E)}{\partial E}\Big|_{E=E^*} = \frac{1}{T},$$

which is exactly a thermodynamic relation between S and T. Here E^* is called the internal energy U. Readers may referd to [**Cha87**, **Ell85**] for more details.

2.4. Statistics of Extrema

In many cases we are interested in estimating the maximum or minimum of a set of random variables. Let $\{X_j\}_{j=1}^n$ be a sequence of i.i.d. random variables, and let

$$M_n = \max\{X_1, X_2, \ldots, X_n\}.$$

We would like to study the distribution of M_n as $n \to \infty$. The statistics of the minimum $m_n = \min\{X_1, X_2, \ldots, X_n\}$ can be obtained similarly based on the fact that

(2.13) $\qquad \min\{X_1, X_2, \ldots, X_n\} = -\max\{-X_1, -X_2, \ldots, -X_n\}.$

Example 2.11. Assume that X_j is exponentially distributed; i.e., if we denote by $\rho(x)$ the probability density function of X_j, then

$$\rho(x) = \begin{cases} e^{-x}, & \text{if } x > 0, \\ 0, & \text{if } x \le 0. \end{cases}$$

Then $\mathbb{P}(X_j < x) = 1 - e^{-x}$ for $x > 0$ and

$$\mathbb{P}(M_n \le x) = \mathbb{P}(X_j \le x \text{ for all } j = 1, 2, \ldots, n)$$

$$= \prod_{j=1}^n \mathbb{P}(X_j \le x) = (1 - e^{-x})^n.$$

This remains true even if x depends on n. We will choose $x = x_n$ such that $(1 - e^{-x_n})^n$ has a nontrivial limit. For this purpose, we let

$$x_n = -\log(e^{-x}) + \log n = x + \log n.$$

Then

$$\mathbb{P}(M_n \le x_n) = (1 - e^{-x_n})^n = \left(1 - \frac{e^{-x}}{n}\right)^n \to e^{-e^{-x}}$$

as $n \to \infty$. In other words,

$$\mathbb{P}\{M_n \le x + \log n\} \to e^{-e^{-x}}.$$

In particular, M_n grows like $\log n$ as $n \to \infty$.

Example 2.12. Assume that X_j is uniformly distributed on $[0, 1]$; i.e.,

$$\rho(x) = \begin{cases} 1, & \text{if } x \in [0, 1], \\ 0, & \text{otherwise.} \end{cases}$$

We expect that $M_n \to 1$ as $n \to \infty$. The question is how $1 - M_n$ behaves. Notice that if we let $x_n = 1 - x/n$, then

$$\mathbb{P}(M_n \le x_n) = \left(1 - \frac{x}{n}\right)^n \to e^{-x}$$

as $n \to \infty$, or equivalently

$$\mathbb{P}(n(M_n - 1) \le x) \to e^{-|x|} \qquad \text{for } x \le 0.$$

This implies that $1 - M_n = O(1/n)$ as $n \to \infty$.

For the general case, we have

Theorem 2.13 (Fisher-Tippett-Gnedenko theorem). *If there exist $\{a_n\}$ and $\{b_n\}$, such that*

$$\mathbb{P}(a_n(M_n - b_n) \le x) \to G(x) \qquad \text{as } n \to \infty,$$

then $G(x)$ must be one of the following types:

  (i) *Type I (Gumbel):* $G(x) = e^{-e^{-x}}$.

  (ii) *Type II (Fréchet):* $G(x) = \begin{cases} 0, & x \le 0, \\ e^{-x^{-\alpha}}, & x > 0, \ \alpha > 0. \end{cases}$

  (iii) *Type III (Weibull):* $G(x) = \begin{cases} e^{-|x|^{\alpha}}, & x \le 0, \ \alpha > 0, \\ 1, & x > 0. \end{cases}$

In the examples above, we have $b_n = \log n$, $a_n = 1$ for the exponential distribution which is a type I situation, and $b_n = 1$, $a_n = n$ for the uniform distribution which is a type III situation with $\alpha = 1$. According to the relation (2.13), the statistics of minima m_n has the universal limit $g(x) = 1 - G(-x)$ as $n \to \infty$.
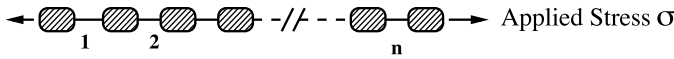
Figure 2.1. Schematics of the weakest link model.

The Weakest Link Model in Fracture Mechanics. Consider the failure of a chain of length L with n links (see Figure 2.1). Assume that the failure probability of an element of length $\delta L \ll 1$ has the form

$$P(\delta L, \sigma) = \lambda \delta L (\sigma/s_0)^p, \quad p > 0.$$

Here σ is the applied stress, s_0 is a scale parameter, $\lambda = n/L$ is the density of links, $(\sigma/s_0)^p$ is the failure probability for a single link [**BP06**]. The survival probability of the whole chain is given by

$$(2.14) \qquad F(\sigma) = 1 - (1 - P(\delta L, \sigma))^m \longrightarrow 1 - e^{-n(\sigma/s_0)^p}, \quad m\delta L = L,$$

as $m \to \infty$. This corresponds to the Weibull type of statistics.

Exercises

2.1. Let X_j be i.i.d. $\mathcal{U}[0,1]$ random variables. Prove that

$$\lim_{n\to\infty} \frac{n}{X_1^{-1} + \cdots + X_n^{-1}}, \quad \lim_{n\to\infty} \sqrt[n]{X_1 X_2 \cdots X_n}, \quad \lim_{n\to\infty} \sqrt{\frac{X_1^2 + \cdots + X_n^2}{n}}$$

exist almost surely and find the limits.

2.2. Consider the queuing service problem. Suppose that the service time for the jth customer is a random variable $X_j < \infty$ ($j = 1, 2, \ldots$) and the $\{X_j\}$'s are independent and identically distributed. Define

$$T_n = \sum_{j=1}^{n} X_j \quad \text{and} \quad N_t = \sup_n \{n | T_n \leq t\}.$$

Prove that under the condition $\mathbb{E}X_j = \mu < \infty$, we have the service rate of the queue

$$\lim_{t\to\infty} \frac{N_t}{t} = \frac{1}{\mu} \quad \text{a.s.}$$

2.3. The fact that the "central limit" of i.i.d. random variables must be Gaussian can be understood from the following viewpoint. Let $X_1, X_2, \ldots$ be i.i.d. random variables with mean 0. Let

(2.15) $$Z_n = \frac{X_1 + \cdots + X_n}{\sqrt{n}} \xrightarrow{d} X \quad \text{and} \quad Z_{2n} = \frac{X_1 + \cdots + X_{2n}}{\sqrt{2n}} \xrightarrow{d} X.$$

Let the characteristic function of X be $f(\xi)$.
   (a) Prove that $f(\xi) = f^2(\xi/\sqrt{2})$.
   (b) Prove that $f(\xi)$ is the characteristic function of a Gaussian random variable if $f \in C^2(\mathbb{R})$.
   (c) Investigate the situation when the scaling $1/\sqrt{n}$ in (2.15) is replaced with $1/n$. Prove that X corresponds to the Cauchy-Lorentz distribution under the symmetry condition $f(\xi) = f(-\xi)$, or $f(\xi) \equiv 1$.
   (d) If the scaling $1/\sqrt{n}$ is replaced by $1/n^\alpha$, what can we infer about the characteristic function $f(\xi)$ if we assume $f(\xi) = f(-\xi)$? What is the correct range of α?

2.4. Prove the assertion in Example 2.3.

2.5. (*Single-sided Laplace lemma*) Suppose that $h(x)$ attains the only maximum at $x = 0$, $h' \in C^1(0, +\infty), h'(0) < 0$, $h(x) < h(0)$ for $x > 0$. Here $h(x) \to -\infty$ as $x \to \infty$, and $\int_0^\infty e^{h(x)} dx$ converges.

Prove that, to leading order,

$$\int_0^\infty e^{th(x)}\,dx \sim (-th'(0))^{-1} e^{th(0)}$$

as $t \to \infty$.

2.6. Compute the large deviation rate function $I(x)$ for the following distributions:

(a) Gaussian distribution $N(\mu, \sigma^2)$.

(b) Poisson distribution with the parameter $\lambda > 0$.

(c) Exponential distribution with the parameter $\lambda > 0$.

2.7. (*Asymptotic Equipartition Principle* in information theory) Consider a document D with N letters $D = \{X_1 X_2 \ldots X_N\}$, where the $\{X_j\}$'s are from the alphabet $S = \{a_1, \ldots, a_r\}$. Assume that the $\{X_j\}$'s are i.i.d. random variables with the distribution

$$\mathbb{P}(X_j = a_k) = p(k) > 0, \quad k = 1, \ldots, r; \quad \sum_{k=1}^r p(k) = 1.$$

(a) Define the information content of the document as $-\log \mathbb{P}(D) = -\log(\prod_{j=1}^N p(X_j))$. Prove that the average information content

$$\lim_{N \to \infty} \frac{1}{N} \log \frac{1}{\mathbb{P}(D)} = H = -\sum_{k=1}^r p(k) \log p(k) \quad a.s.$$

where H is called Shannon's entropy.

(b) Define the set $B_j = \{k | X_k = a_j, X_k \in D, k = 1, \ldots, N\}$ and the typical set

$$T_N = \left\{ D \in S^N : \left| \frac{1}{N} |B_j| - p(j) \right| < \delta(\epsilon), \quad j = 1, \ldots, r \right\},$$

where $|B_j|$ is the number of elements in set B_j. Prove that for any fixed $\delta > 0$

$$\lim_{N \to \infty} \mathbb{P}(T_N) = 1.$$

(c) For any $\epsilon > 0$, there exists $\delta(\epsilon) > 0$ such that for sufficiently large N

$$e^{N(H-\epsilon)} \le |T_N| \le e^{N(H+\epsilon)}$$

and for any $D \in T_N$, we have

$$e^{-N(H+\epsilon)} \le \mathbb{P}(D) \le e^{-N(H-\epsilon)}.$$

This property is called the *asymptotic equipartition principle* for the elements in a typical set.

2.8. Let $\{X_j\}$ be i.i.d. random variables. Suppose that the variance of X_j is finite. Then by the CLT the distribution $G(x)$ in Remark 2.6 is Gaussian for $b_n = \text{mean}(X_1)$, $a_n = \sqrt{\text{Var}(X_1)}$. Show that one also recovers WLLN for a different choice of $\{a_n\}$ and $\{b_n\}$. What is the stable distribution $G(x)$ in this case?

2.9. For the statistics of extrema, verify that

$$a_n = \sqrt{2 \log n}, \qquad b_n = \sqrt{2 \log n}(\log \log n + \log 4\pi)$$

for the normal distribution $N(0, 1)$.

Notes

Rigorous mathematical work on the law of large numbers for general random variables starts from that of Chebyshev in the 1860s. The strong law of large numbers stated in this chapter is due to Kolmogorov [**Shi92**]. The fact that the Gaussian distribution and stable laws are the scaling limit of empirical averages of i.i.d. random variables can also be understood using renormalization group theory [**ZJ07**]. A brief introduction to the LDT can be found in [**Var84**].

Markov Chains

So far we have discussed random variables. We next discuss random processes, i.e., random functions of time. These random functions are defined on a set, called the index set. The index set can be discrete, as in the case of discrete time Markov chains, or continuous, as in the case of Poisson processes and diffusion processes.

There is not much one can say about general random processes since it is too large a class of objects. We therefore need to focus on random processes with some special features. The most important feature studied so far is Markov property. Roughly speaking, a random process is a Markov process if knowing the present state of the process, its future is independent of the past. Markov processes are much easier to deal with since we may use ideas related to differential equations or semigroup theory, such as the idea of generators.

For continuous time random processes, an important issue is the continuity of the sample paths. A particularly interesting class of random process is Markov processes with continuous sample paths. These are called diffusion processes. It turns out that they can be represented as solutions of stochastic differential equations, a topic that we will take up later.

There are certain mathematical subtleties associated with random processes, having to do with measurability and σ-algebras. We will try to avoid this as much as we can, without significantly compromising the mathematical content. We will start with the simplest case, the case of Markov chains, for which these mathematical subtleties largely disappear. We will postpone discussions of general random processes to Chapter 5.

3.1. Discrete Time Finite Markov Chains

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be the probability space. A Markov chain is a sequence of parameterized random variables $\{X_t\}_{t\in\mathbf{T}}$ with the so-called Markov property, to be introduced below, where $\mathbf{T}$ is the index set. When $\mathbf{T} = \mathbb{N}$, we denote the random variables as $\{X_n\}_{n\in\mathbb{N}}$, and this is the case that we will consider in this chapter. We assume that X_n takes values in the state space S.

Example 3.1 (Symmetric random walk)**.** Consider the sequence of random variables $\{\xi_j\}_{j=1}^{\infty}$, where the $\{\xi_j\}$'s are i.i.d and $\xi_j = \pm 1$ with probability $1/2$. Let

$$X_n = \sum_{j=1}^{n} \xi_j.$$

$\{X_n\}_{n\in\mathbb{N}}$ is a symmetric random walk on $\mathbb{Z}$, the set of integers.

Given $X_n = i$, we have

$$\mathbb{P}(X_{n+1} = i \pm 1 | X_n = i) = \mathbb{P}(\xi_{n+1} = \pm 1) = \frac{1}{2}$$

and $\mathbb{P}(X_{n+1} = \text{anything else} | X_n = i) = 0$. We see that, knowing X_n, the distribution of X_{n+1} is completely determined. In other words,

$$(3.1) \qquad \mathbb{P}(X_{n+1} = i_{n+1} | \{X_m = i_m\}_{m=0}^{n}) = \mathbb{P}(X_{n+1} = i_{n+1} | X_n = i_n);$$

i.e., the probability of X_{n+1} conditional on the whole past history of the sequence, $\{X_m\}_{m=0}^{n}$, is equal to the probability of X_{n+1} conditional on the latest value alone, X_n. The sequence (or process) $\{X_n\}_{n\in\mathbb{N}}$ is called a *Markov process*. In contrast, instead we consider

$$Y_n = \sum_{j=1}^{n} \frac{1}{2}(\xi_j + 1)\xi_{j+1}.$$

$\{Y_n\}_{n\in\mathbb{N}}$ is also a kind of random walk on $\mathbb{Z}$, but with a bias: the walk stops if the last move was to the left, and it remains there until some subsequent $\xi_j = +1$. It is easy to see that

$$\mathbb{P}(Y_{n+1} = i_{n+1} | \{Y_m = i_m\}_{m=0}^{n}) \neq \mathbb{P}(Y_{n+1} = i_{n+1} | Y_n = i_n)$$

and the sequence $\{Y_n\}_{n\in\mathbb{N}}$ is not a Markov process.

Example 3.2 (Ehrenfest's diffusion model)**.** Consider a container separated by a permeable membrane in the middle and filled with a total of K particles. At each time $n = 1, 2\ldots$, pick one particle in random among the K particles and place it into the other part of the container. Let X_n be the number of particles in the left part of the container. Then we have

$$\mathbb{P}(X_{n+1} = i_{n+1} | \{X_m = i_m\}_{m=0}^{n}) = \mathbb{P}(X_{n+1} = i_{n+1} | X_n = i_n),$$

for $i_k \in \{0, 1, \ldots, K\}$, and this is also a Markov process.

Example 3.3 (Autoregressive model). The autoregressive process $\{Y_n\}_{n\in\mathbb{N}}$ of order k is defined as follows. For each $n \geq 1$,

$$Y_n = \alpha_1 Y_{n-1} + \alpha_2 Y_{n-2} + \cdots + \alpha_k Y_{n-k} + R_n,$$

where $\alpha_1, \ldots, \alpha_k \in \mathbb{R}$, and $\{R_n\}_{n=1}^{\infty}$ is a prescribed random sequence with independent components. The initial values are specified for $Y_0, \ldots, Y_{-k+1}$.

In this example, Y_n itself is not Markovian since Y_n depends not only on Y_{n-1}, but also on $Y_{n-2}, \ldots, Y_{n-k}$. But if we introduce the new variable

$$\boldsymbol{X}_n = (Y_n, \ldots, Y_{n-k+1})^T, \quad n = 0, 1, \ldots,$$

then we obtain a Markov process on $\mathbb{R}^k$:

$$\boldsymbol{X}_n = \begin{pmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_k \\ 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 \end{pmatrix} \boldsymbol{X}_{n-1} + \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} R_n.$$

There are two important ingredients for discrete time Markov chains, the state space, i.e., the space in which the chain takes its values, and the transition probability. For simplicity, we will focus on the case when the state space is finite.

Without loss of generality, we let the state space be $S = \{1, 2, \ldots, I\}$.

Define the *transition probabilities*, i.e., the probabilities that the process is in state j at time $n + 1$ conditional on it being in state k at time n,

$$p_{kj}^{(n)} = \mathbb{P}(X_{n+1} = j | X_n = k).$$

The Markov chain is called *stationary* if $p_{kj}^{(n)}$ is independent of n. From now on we will discuss only stationary Markov chains and let $p_{kj} = p_{kj}^{(n)}$. We also denote $\boldsymbol{P} = (p_{ij})_{i,j\in S}$. Here $\boldsymbol{P}$ is a *stochastic matrix* in the sense that

$$(3.2) \qquad\qquad p_{ij} \geq 0, \qquad \sum_{j\in S} p_{ij} = 1.$$

A basic property of Markov chains is the following:

Proposition 3.4 (Chapman-Kolmogorov equation)**.**

$$\mathbb{P}(X_n = j | X_0 = i)$$
$$= \sum_{k\in S} \mathbb{P}(X_n = j | X_m = k)\mathbb{P}(X_m = k | X_0 = i), \quad 1 \leq m \leq n - 1.$$

The proof is a straightforward application of Bayes's rule and the Markov property.

Using the Chapman-Kolmogorov equation, we get

$$\mathbb{P}(X_0 = i_0, X_1 = i_1, \ldots, X_n = i_n) = \mu_{0,i_0} p_{i_0 i_1} p_{i_1 i_2} \ldots p_{i_{n-1} i_n},$$

where $\boldsymbol{\mu}_0 = (\mu_{0,1}, \ldots, \mu_{0,I})$ is the initial distribution and its component

$$\mu_{0,i_0} = \mathbb{P}(X_0 = i_0).$$

From this we get

$$\mathbb{P}(X_n = i_n | X_0 = i_0) = \sum_{i_1, \ldots, i_{n-1} \in S} p_{i_0 i_1} p_{i_1 i_2} \ldots p_{i_{n-1} i_n} = (\boldsymbol{P}^n)_{i_0 i_n}.$$

The last quantity is the (i_0, i_n)th entry of the matrix $\boldsymbol{P}^n$.

3.2. Invariant Distribution

Given the initial distribution of the Markov chain $\boldsymbol{\mu}_0$, the distribution of X_n is then given by

$$\boldsymbol{\mu}_n = \boldsymbol{\mu}_0 \boldsymbol{P}^n.$$

We call a distribution $\boldsymbol{\pi}$ an *invariant distribution* or *stationary distribution* if

$$(3.3) \qquad\qquad\qquad\qquad \boldsymbol{\pi} = \boldsymbol{\pi} \boldsymbol{P}.$$

If the initial distribution is an invariant distribution, then the distribution of the Markov chain will be invariant in time. It is also useful to define the *invariant measure* or *stationary measure* $\boldsymbol{\pi}$ of a Markov chain if (3.3) holds and $\pi_i \geq 0$ for any $i \in S$, but $\boldsymbol{\pi}$ need not be normalized.

One can represent a finite Markov chain by a directed graph, as shown in Figure 3.1. The arrows and real numbers show the transition probability of the Markov chain. The transition probability matrix corresponding to the left side of the figure is

$$(3.4) \qquad\qquad\qquad \boldsymbol{P} = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 1 \end{bmatrix},$$

which is a reducible matrix (see Definition 3.6) and has two linearly independent invariant distributions $\boldsymbol{\pi}_1 = (1, 0, 0)$ and $\boldsymbol{\pi}_2 = (0, 0, 1)$. The transition probability matrix corresponding to the right side of the figure is

$$(3.5) \qquad\qquad\qquad \boldsymbol{P} = \begin{bmatrix} 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \end{bmatrix}.$$

which is irreducible and has only one invariant distribution $\boldsymbol{\pi} = (1/4, 1/2, 1/4)$.
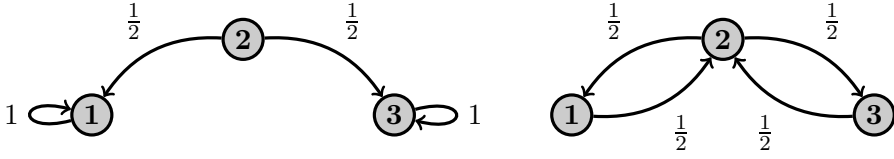
Figure 3.1. Graphical representation of two Markov chains in (3.4) and (3.5).

The following questions are of special interest for a given Markov chain.

(i) Existence: Is there an invariant distribution?

This is equivalent to asking whether there exists a nonnegative left eigenvector of $\boldsymbol{P}$ with eigenvalue equal to 1. Note that 1 is always an eigenvalue of $\boldsymbol{P}$ since it always has the right eigenvector $\mathbf{1} = (1, \ldots, 1)^T$ by the second property in (3.2).

(ii) Uniqueness: When is the invariant distribution unique?

The answer of these questions is closely related to the spectral structure of the matrix $\boldsymbol{P}$. We begin with the following preliminary result.

Lemma 3.5. *The spectral radius of $\boldsymbol{P}$ is equal to 1:*

$$\rho(\boldsymbol{P}) = \max_{\lambda} |\lambda| = 1,$$

where the maximum is taken over the eigenvalues of $\boldsymbol{P}$.

Proof. We already know that 1 is an eigenvalue of $\boldsymbol{P}$. To show it is the maximum eigenvalue, denote by $\boldsymbol{u}$ the left eigenvector of $\boldsymbol{P}$ with eigenvalue λ. Then

$$\lambda u_i = \sum_{j \in S} u_j p_{ji},$$

which implies that

$$|\lambda| \sum_{i \in S} |u_i| = \sum_{i \in S} \left| \sum_{j \in S} u_j p_{ji} \right| \leq \sum_{i,j \in S} |u_j| p_{ji} = \sum_{j \in S} |u_j|.$$

Hence $|\lambda| \leq 1$. $\qquad\qquad\square$

Definition 3.6 (Irreducibility)**.** If there exists a permutation matrix $\boldsymbol{R}$ such that

$$(3.6) \qquad\qquad \boldsymbol{R}^T \boldsymbol{P} \boldsymbol{R} = \begin{pmatrix} \boldsymbol{A}_1 & \boldsymbol{B} \\ 0 & \boldsymbol{A}_2 \end{pmatrix},$$

then $\boldsymbol{P}$ is called *reducible*. Otherwise $\boldsymbol{P}$ is called *irreducible*.

Besides the above characterization, irreducibility can also be checked by studying the *communication* between each pair of nodes. We say that state j is *accessible* from state i if

$$p_{k_0 k_1} p_{k_1 k_2} \cdots p_{k_{s-1} k_s} > 0, \qquad k_0 = i, k_s = j,$$

for some $s \geq 1$ and $(k_1, \ldots, k_{s-1})$, and the pair (i, j) *communicates* if j is accessible from i and i is also accessible from j.

Lemma 3.7. *Irreducibility is equivalent to the property that every pair of nodes in the state space communicates with each other.*

The proof is left as an exercise for the readers.

The following important theorem gives an affirmative answer to the existence and uniqueness of the invariant distribution under the irreducibility condition.

Theorem 3.8 (Perron-Frobenius theorem)**.** *Let $\boldsymbol{A}$ be an irreducible non-negative matrix, and let $\rho(\boldsymbol{A})$ be its spectral radius: $\rho(\boldsymbol{A}) = \max_\lambda |\lambda(\boldsymbol{A})|$. Then:*

(1) *There exist positive right and left eigenvectors x and y of $\boldsymbol{A}$, such that*

$$\boldsymbol{A}\boldsymbol{x} = \rho(\boldsymbol{A})\boldsymbol{x}, \quad x_j > 0; \qquad \boldsymbol{y}^T \boldsymbol{A} = \rho(\boldsymbol{A})\boldsymbol{y}^T, \quad y_j > 0.$$

(2) $\lambda = \rho(\boldsymbol{A})$ *is an eigenvalue of multiplicity 1.*

We refer to [**HJ85**] for the proof.

From the viewpoint of the graphical representation of a Markov chain, the action of a permutation matrix $\boldsymbol{R}$ corresponds to a relabeling of the nodes. Irreducibility means that there does not exist a subgroup of nodes which forms a connected subgraph with no arrows pointing to the rest of the nodes. Violation of irreducibility may lead to nonuniqueness of the invariant distribution as shown for the Markov chain (3.4). However, irreducibility is by no means necessary for uniqueness.

Example 3.9. Consider the Markov chain with the transition probability matrix

$$(3.7) \qquad \boldsymbol{P} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0.3 & 0.4 & 0.3 & 0 & 0 \\ 0.3 & 0 & 0.4 & 0.3 & 0 \\ 0 & 0 & 0 & 0.5 & 0.5 \\ 0 & 0 & 0 & 0.5 & 0.5 \end{bmatrix}.$$

This is reducible. But one can verify that the chain has a unique invariant distribution

$$\boldsymbol{\pi} = (0, 0, 0, 0.5, 0.5).$$

Sharp conditions for uniqueness and delicate characterization of the invariant distribution require the concepts of recurrence and transience. More can be found in [**Dur10**, **Nor97**].

3.3. Ergodic Theorem for Finite Markov Chains

As we have seen, irreducibility itself is enough to guarantee the convergence of the time average to the ensemble average. However, irreducibility is not enough to guarantee strong ergodicity; namely

$$\boldsymbol{\mu}_n = \boldsymbol{\mu}_0 \boldsymbol{P}^n \to \boldsymbol{\pi}$$

for any initial distribution $\boldsymbol{\mu}_0$. The simplest counterexample is as follows:

$$\boldsymbol{P} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

We have $\boldsymbol{P}^{2n} = \boldsymbol{I}$ and $\boldsymbol{P}^{2n+1} = \boldsymbol{P}$; thus $\boldsymbol{\mu}_n$ will oscillate instead of converge to some limit. This type of periodicity is a barrier for strong ergodicity. To avoid this, we introduce a stronger condition called the *primitive chain*.

Definition 3.10. A Markov chain is said to be primitive if there exists an $s > 0$ such that $(\boldsymbol{P}^s)_{ij} > 0$ for any pair (i, j).

Theorem 3.11. *Assume that the Markov chain is primitive. Then for any initial distribution $\boldsymbol{\mu}_0$*

$$\boldsymbol{\mu}_n = \boldsymbol{\mu}_0 \boldsymbol{P}^n \to \boldsymbol{\pi} \quad \text{exponentially fast as } n \to \infty,$$

where $\boldsymbol{\pi}$ is the unique invariant distribution.

Proof. Given two distributions, $\boldsymbol{\mu}_0$ and $\tilde{\boldsymbol{\mu}}_0$, we define the *total variation distance* by

$$d(\boldsymbol{\mu}_0, \tilde{\boldsymbol{\mu}}_0) = \frac{1}{2} \sum_{i \in S} |\mu_{0,i} - \tilde{\mu}_{0,i}|.$$

Since

$$0 = \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i}) = \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^+ - \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^-,$$

where $a^+ = \max(a, 0)$ and $a^- = \max(-a, 0)$, we also have

$$d(\boldsymbol{\mu}_0, \tilde{\boldsymbol{\mu}}_0) = \frac{1}{2} \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^+ + \frac{1}{2} \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^-$$

$$= \sum_{i \in S} (\mu_{0,i} - \tilde{\mu}_{0,i})^+ \leq 1.$$

Let $\boldsymbol{\mu}_s = \boldsymbol{\mu}_0 \boldsymbol{P}^s$, $\tilde{\boldsymbol{\mu}}_s = \tilde{\boldsymbol{\mu}}_0 \boldsymbol{P}^s$ and consider $d(\boldsymbol{\mu}_s, \tilde{\boldsymbol{\mu}}_s)$. We have

$$d(\boldsymbol{\mu}_s, \tilde{\boldsymbol{\mu}}_s) = \sum_{i \in S} \left[\sum_{j \in S} \left(\mu_{0,j}(\boldsymbol{P}^s)_{ji} - \tilde{\mu}_{0,j}(\boldsymbol{P}^s)_{ji} \right) \right]^+$$

$$\leq \sum_{j \in S} \left(\mu_{0,j} - \tilde{\mu}_{0,j} \right)^+ \sum_{i \in B_+} (\boldsymbol{P}^s)_{ji},$$

where B_+ is the subset of indices where $\sum_{j \in S} (\mu_{0,j} - \tilde{\mu}_{0,j}) (\boldsymbol{P}^s)_{ji} > 0$. We note that B_+ cannot contain all the elements of S; otherwise one must have $(\boldsymbol{\mu}_0 \boldsymbol{P}^s)_i > (\tilde{\boldsymbol{\mu}}_0 \boldsymbol{P}^s)_i$ for all i and

$$\sum_{i \in S} (\boldsymbol{\mu}_0 \boldsymbol{P}^s)_i > \sum_{i \in S} (\tilde{\boldsymbol{\mu}}_0 \boldsymbol{P}^s)_i,$$

which is impossible since both sides sum to 1. Therefore at least one element is missing in B_+. By assumption, there exists an $s > 0$ and $\alpha \in (0,1)$ such that $(\boldsymbol{P}^s)_{ij} \geq \alpha$ for all pairs (i,j). Hence $\sum_{i \in B_+} (\boldsymbol{P}^s)_{ji} \leq (1-\alpha) < 1$. Therefore

$$d(\boldsymbol{\mu}_s, \tilde{\boldsymbol{\mu}}_s) \leq d(\boldsymbol{\mu}_0, \tilde{\boldsymbol{\mu}}_0)(1-\alpha);$$

i.e., the Markov chain is contractive after every s steps. Similarly for any $m \geq 0$

$$d(\boldsymbol{\mu}_n, \boldsymbol{\mu}_{n+m}) \leq d(\boldsymbol{\mu}_{n-sk}, \boldsymbol{\mu}_{n+m-sk})(1-\alpha)^k \leq (1-\alpha)^k,$$

where k is the largest integer such that $n - sk \geq 0$. If n is sufficiently large, the right-hand side can be made arbitrarily small. Therefore the sequence $\{\boldsymbol{\mu}_n\}_{n=0}^\infty$ is a Cauchy sequence. Hence it has to converge to a limit π, which satisfies

$$\boldsymbol{\pi} = \lim_{n \to \infty} \boldsymbol{\mu}_0 \boldsymbol{P}^{n+1} = \lim_{n \to \infty} (\boldsymbol{\mu}_0 \boldsymbol{P}^n) \boldsymbol{P} = \boldsymbol{\pi} \boldsymbol{P}.$$

The probability distribution satisfying such a property is also unique, for if there were two such distributions, $\boldsymbol{\pi}^{(1)}$ and $\boldsymbol{\pi}^{(2)}$, then

$$d(\boldsymbol{\pi}^{(1)}, \boldsymbol{\pi}^{(2)}) = d(\boldsymbol{\pi}^{(1)} \boldsymbol{P}^s, \boldsymbol{\pi}^{(2)} \boldsymbol{P}^s) < d(\boldsymbol{\pi}^{(1)}, \boldsymbol{\pi}^{(2)}).$$

This implies $d(\boldsymbol{\pi}^{(1)}, \boldsymbol{\pi}^{(2)}) = 0$, i.e $\boldsymbol{\pi}^{(1)} = \boldsymbol{\pi}^{(2)}$. $\qquad\qquad\square$

The following theorem provides a rationale for the famous hypothesis that "time average = ensemble average" in statistical physics [**TKS95**].

Theorem 3.12 (Ergodic theorem). *Let $\{X_m\}$ be an irreducible finite Markov chain and let f be a bounded function from S to $\mathbb{R}$. Then*

$$\frac{1}{n} \sum_{m=0}^{n-1} f(X_m) \to \langle f \rangle_{\boldsymbol{\pi}} = \sum_{i \in S} f(i) \pi_i, \quad a.s.,$$

as $n \to \infty$, where $\boldsymbol{\pi}$ is the unique invariant distribution.

The readers may refer to [**Dur10**, **Nor97**] for proof details.

3.4. Poisson Processes

From now on we will consider the case when $\mathbf{T} = \mathbb{R}_+$. We will focus on finite-state chains. For the case with countably many states, only the constant rate Poisson processes will be considered. We will use the notation X_t to denote the state of X at time t. Note that X_t does not mean time derivative.

Definition 3.13 (Poisson process). Let $\{N_t\}_{t\geq 0}$ be an increasing, right-continuous integer-valued process that satisfies the following properties:

(i) $N_0 = 0$.

(ii) N_t has stationary independent increments; i.e., for any $0 \leq t_1 < t_2 < \cdots < t_n$,

$$N_{t_2} - N_{t_1}, N_{t_3} - N_{t_2}, \ldots, N_{t_n} - N_{t_{n-1}}$$

are independent, and for any $t \geq 0, s \geq 0$ the distribution of

$$N_{t+s} - N_t$$

is independent of t.

(iii) For any $t \geq 0, h > 0$, we have

$$\mathbb{P}(N_{t+h} = N_t + 1 \mid N_t) = \lambda h + o(h),$$
$$\mathbb{P}(N_{t+h} = N_t | N_t) = 1 - \lambda h + o(h),$$
$$\mathbb{P}(N_{t+h} \geq N_t + 2) = o(h),$$

in the limit $h \to 0+$, where λ is a positive real number.

Then $\{N_t\}_{t\geq 0}$ is called a Poisson process with rate λ.

Poisson processes are often used to model the number of telephone calls received at a phone booth, or the number of customers waiting in a queue, etc.

Theorem 3.14. *For any fixed time t, the distribution of N_t is Poisson with parameter λt.*

Proof. Let $p_m(t) = \mathbb{P}(N_t = m)$. Taking $h \ll 1$ we have

$$p_0(t + h) = p_0(t)(1 - \lambda h) + o(h),$$

or equivalently

$$\frac{p_0(t + h) - p_0(t)}{h} = \lambda p_0(t) + o(1).$$

As $h \to 0+$, we obtain

$$\frac{dp_0(t)}{dt} = -\lambda p_0(t), \quad p_0(0) = 1.$$

The solution is given by

$$p_0(t) = e^{-\lambda t}.$$

For $m \geq 1$, we have

$$p_m(t + h) = p_m(t)(1 - \lambda h) + p_{m-1}(t)\lambda h + o(h).$$

Following the same procedure as before and taking the limit as $h \to 0$, we get

$$\frac{dp_m(t)}{dt} = -\lambda p_m(t) + \lambda p_{m-1}(t).$$

Using the fact that $p_m(0) = 0$ for $m \geq 1$, we get

(3.8) $$p_m(t) = \frac{\lambda^m t^m}{m!} e^{-\lambda t}$$

by induction. $\square$

Waiting Time Distribution. Define the waiting time

(3.9) $$\tau = \inf\{t : t > 0, N_t \neq N_0\}$$

and the waiting time distribution

(3.10) $$\nu(t) = \mathbb{P}(\tau \geq t).$$

Then $\nu(0) = 1$ and

$$\nu(t) - \nu(t + h) = \nu(t)\lambda h + o(h), \quad h \ll 1.$$

Letting $h \to 0$ we obtain

$$\frac{d\nu}{dt} = -\lambda \nu(t).$$

This leads to $\nu(t) = e^{-\lambda t}$, which means that the waiting times are exponentially distributed with rate λ. This characterization gives an explicit strategy to generate sample trajectories of a Poisson process.

3.5. Q-processes

Now let us turn to a type of continuous time Markov chains called Q-processes. We assume that the trajectory $\{X_t\}_{t \in \mathbb{R}_+}$ is right-continuous and the state space S is finite, i.e., $S = \{1, 2, \ldots, I\}$. Let the transition probability

$$p_{ij}(t) = \mathbb{P}(X_{t+s} = j | X_s = i).$$

Here we have assumed that the Markov chain is stationary; i.e., the right-hand side is independent of s. By definition we have

$$p_{ij}(t) \geq 0, \qquad \sum_{j \in S} p_{ij}(t) = 1.$$

In addition we require that in the limit $h \to 0+$

(3.11) $$p_{ii}(h) = 1 - \lambda_i h + o(h), \quad \lambda_i > 0,$$

(3.12) $$p_{ij}(h) = \lambda_{ij} h + o(h), \quad j \neq i.$$

(3.13) $$p_{jj}(0) = 1.$$

Equation (3.11) is a statement about the regularity in time of the Markov chain. Equation (3.12) states that if the process is in state j at time t and a change occurs between t and $t + h$, the process must have jumped to some other state $i \neq j$; λ_{ij} is the rate of switching from state i to state j. From the nonnegativity and normalization conditions, we have

(3.14) $$\lambda_{ij} \geq 0, \qquad \sum_{j \in S, j \neq i} \lambda_{ij} = \lambda_i.$$

The Markov property of the process implies the Chapman-Kolmogorov equation

(3.15) $$p_{ij}(t + s) = \sum_{k \in S} p_{ik}(t) p_{kj}(s).$$

Using matrix notation

$$\boldsymbol{P}(t) = (p_{ij}(t))_{i,j \in S},$$

we can express the Chapman-Kolmogorov equation as

$$\boldsymbol{P}(t + s) = \boldsymbol{P}(t)\boldsymbol{P}(s) = \boldsymbol{P}(s)\boldsymbol{P}(t).$$

If we define

(3.16) $$\boldsymbol{Q} = \lim_{h \to 0+} \frac{1}{h}(\boldsymbol{P}(h) - \boldsymbol{I})$$

and denote $\boldsymbol{Q} = (q_{ij})$, (3.11), (3.12), and (3.14) can be stated as

$$q_{ii} = -\lambda_i, \qquad q_{ij} = \lambda_{ij} \quad (i \neq j), \qquad \sum_{j \in S} q_{ij} = 0.$$

$\boldsymbol{Q}$ is called the *generator* of the Markov chain. For simplicity, we also define $q_i = -q_{ii} \geq 0$.

Since

(3.17) $$\frac{\boldsymbol{P}(t + h) - \boldsymbol{P}(t)}{h} = \frac{\boldsymbol{P}(h) - \boldsymbol{I}}{h}\boldsymbol{P}(t)$$

as $s \to 0+$, we get the well-known *forward equation* for $\boldsymbol{P}(t)$

(3.18) $$\frac{d\boldsymbol{P}(t)}{dt} = \boldsymbol{P}(t)\boldsymbol{Q}.$$

Since $\boldsymbol{P}(h)$ and $\boldsymbol{P}(t)$ commute, we also get from (3.17) the *backward equation*

(3.19) $$\frac{d\boldsymbol{P}(t)}{dt} = \boldsymbol{Q}\boldsymbol{P}(t).$$

Both the solutions of the forward and the backward equations are given by

$$\boldsymbol{P}(t) = e^{\boldsymbol{Q}t}\boldsymbol{P}(0) = e^{\boldsymbol{Q}t}$$

since $\boldsymbol{P}(0) = \boldsymbol{I}$.

Next we discuss how the distribution of the Markov chain evolves in time. Let $\boldsymbol{\mu}(t)$ be the distribution of X_t. Then

$$\mu_j(t + dt) = \sum_{i \neq j} \mu_i(t) p_{ij}(dt) + \mu_j(t) p_{jj}(dt)$$

$$= \sum_{i \neq j} \mu_i(t) q_{ij} dt + \mu_j(t)(1 + q_{jj} dt) + o(dt)$$

for infinitesimal dt. This gives

$$(3.20) \qquad \frac{d\boldsymbol{\mu}(t)}{dt} = \boldsymbol{\mu}(t)\boldsymbol{Q},$$

which is called the forward Kolmogorov equation for the distribution. Its solution is given by

$$\mu_j(t) = \sum_{i \in S} \mu_{0,i} p_{ij}(t),$$

or, in matrix notation,

$$\boldsymbol{\mu}(t) = \boldsymbol{\mu}_0 e^{\boldsymbol{Q}t}.$$

It is natural to consider the invariant distribution for Q-processes. From the forward Kolmogorov equation (3.20), the invariant distribution $\boldsymbol{\pi}$ must satisfy

$$\boldsymbol{\pi}\boldsymbol{Q} = 0, \quad \boldsymbol{\pi} \cdot \mathbf{1} = 1,$$

where $\mathbf{1} = (1, 1, \ldots, 1)^T$. It is also obvious that the invariant distribution $\boldsymbol{\pi}$ satisfies

$$\boldsymbol{\pi}\boldsymbol{P}(t) = \boldsymbol{\pi}$$

for any t.

Waiting Time Distribution. Consider the waiting time distribution $\boldsymbol{\nu}$ for each initial state j,

$$\nu_j(t) = \mathbb{P}(\tau \geq t | X_0 = j),$$

where τ is defined as in (3.9). The same procedure as in the previous subsection leads to

$$(3.21) \qquad \frac{d\nu_j(t)}{dt} = q_{jj}\nu_j(t), \qquad \nu_j(0) = 1.$$

Thus the waiting time at state j is exponentially distributed with rate $q_j = -q_{jj}$. From the memoryless property of exponential distribution, the waiting time can be counted from any starting point.

It is interesting to study the probability

$$p(\theta, j | 0, i) d\theta := \mathbb{P}^i(\text{the jump time } \tau \text{ is in } [\theta, \theta + d\theta) \text{ and } X_\tau = j),$$

where $\mathbb{P}^i$ is the distribution when the chain starts from state i. We have

$$p(\theta, j | 0, i) d\theta = \mathbb{P}(\text{no jump occurs in } [0, \theta) \text{ given } X_0 = i)$$
$$\times \mathbb{P}(\text{one jump occurs from } i \text{ to } j \text{ in } [\theta, \theta + d\theta))$$
$$(3.22) \qquad = \nu_i(\theta) q_{ij} d\theta = \exp(q_{ii}\theta) q_{ij} d\theta.$$

This gives

$$\mathbb{P}^i(X_\tau = j) = p(j | 0, i) = \frac{q_{ij}}{q_i} = \frac{q_{ij}}{\sum_{j \neq i} q_{ij}}$$

where τ is the waiting time. These results are particularly useful for numerical simulation of the trajectories of Q-processes and form the basis for the *stochastic simulation algorithm* (SSA) (or Gillespie's algorithm) in chemical reaction kinetics. We will discuss this in Chapter 13.

3.6. Embedded Chain and Irreducibility

A Q-process with generator $\boldsymbol{Q}$ is nicely connected with a discrete time Markov chain with transition probability matrix $\tilde{\boldsymbol{Q}} = (\tilde{q}_{ij})$ defined by

$$(3.23) \qquad \tilde{q}_{ij} = \begin{cases} q_{ij}/q_i, & \text{if } i \neq j \text{ and } q_i > 0, \\ 0, & \text{if } i \neq j \text{ and } q_i = 0, \end{cases}$$

$$(3.24) \qquad \tilde{q}_{ii} = \begin{cases} 0, & \text{if } q_i > 0, \\ 1, & \text{if } q_i = 0. \end{cases}$$

$\tilde{\boldsymbol{Q}}$ is called the *jump matrix*, and the corresponding Markov chain is called the *embedded chain* or *jump chain* of the original Q-process.

Define the *jump times* of $\{X_t\}_{t \geq 0}$ by

$$J_0 = 0, \quad J_{n+1} = \inf\{t : t \geq J_n, X_t \neq X_{J_n}\}, \quad n \in \mathbb{N},$$

where we take the convention $\inf \emptyset = \infty$. Define the *holding times* by

$$(3.25) \qquad H_n = \begin{cases} J_n - J_{n-1}, & \text{if } J_{n-1} < \infty, \\ \infty, & \text{otherwise,} \end{cases}$$

for $n = 1, 2, \ldots$. We let $X_\infty = X_{J_n}$ if $J_{n+1} = \infty$. The *jump chain* induced by X_t is defined to be

$$Y_n = X_{J_n}, \quad n \in \mathbb{N}.$$

The following result provides a connection between the jump chain and the original Q-process.
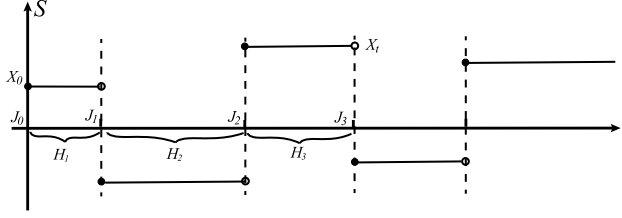
Figure 3.2. Schematics of the jump time and holding time of a Q-process.

Theorem 3.15. *The jump chain $\{Y_n\}$ is a Markov chain with $\tilde{\boldsymbol{Q}}$ as the transition probability matrix, and the holding times $H_1, H_2, \ldots$ are independent exponential random variables with parameters $q_{Y_0}, q_{Y_1}, \ldots$, respectively.*

The proof relies on the strong Markov property of the Q-process. See Section E of the appendix and [**Nor97**].

A state j is said to be *accessible* from i if there exists $t > 0$ such that $p_{ij}(t) > 0$. Similarly to the discrete time case, one can define communication and irreducibility.

Theorem 3.16. *The Q-process X is irreducible if and only if the embedded chain Y is irreducible.*

Proof. First note that for any $i \neq j$, if $q_{ij} > 0$, we have

$$p_{ij}(t) \geq \mathbb{P}^i(J_1 \leq t, Y_1 = j, H_2 > t) = \int_0^t \exp(-q_i u) q_{ij} du \exp(-q_j t)$$
$$= (1 - e^{-q_i t}) \frac{q_{ij}}{q_i} e^{-q_j t} > 0$$

for any $t > 0$. If Y is irreducible, then for any $i \neq j$, there exist $s \geq 1$ and $(k_1, \ldots, k_{s-1})$ such that

$$\tilde{q}_{k_0 k_1} \tilde{q}_{k_1 k_2} \cdots \tilde{q}_{k_{s-1} k_s} > 0, \qquad k_0 = i, k_s = j.$$

Thus we have the corresponding $q_{k_j k_{j+1}} > 0$ $(j = 0, \ldots, s - 1)$ and

$$p_{ij}(t) \geq p_{k_0 k_1}(t/s) p_{k_1 k_2}(t/s) \cdots p_{k_{s-1} k_s}(t/s) > 0.$$

Conversely, suppose $p_{ij}(t) > 0$ for some $t > 0$. From

$$p_{ij}(t) = (e^{\boldsymbol{Q} t})_{ij} = \left(\sum_{n=0}^{\infty} \frac{t^n}{n!} \boldsymbol{Q}^n \right)_{ij} > 0,$$

there exist $n_0 \geq 1$ and $k_1, \ldots, k_{n_0 - 1}$ such that

$$q_{k_0 k_1} q_{k_1 k_2} \cdots q_{k_{n_0 - 1} k_{n_0}} > 0, \qquad k_0 = i, k_{n_0} = j.$$

It follows that j is accessible from i for Y. The proof is complete. $\square$

3.7. Ergodic Theorem for Q-processes

For the Q-process, irreducibility is enough to guarantee the convergence to equilibrium due to the special property revealed by Theorem 3.16.

Theorem 3.17 (Convergence to equilibrium). *Assume that Q is irreducible. Then for any initial distribution $\boldsymbol{\mu}_0$*

$$\boldsymbol{\mu}(t) = \boldsymbol{\mu}_0 \boldsymbol{P}(t) \to \boldsymbol{\pi} \quad \text{exponentially fast as } t \to \infty,$$

where $\boldsymbol{\pi}$ is the unique invariant distribution.

Proof. From irreducibility and Theorem 3.16, we know that $p_{ij}(t) > 0$ for any $i \neq j$ and $t > 0$. It is straightforward to see that

$$p_{ii}(t) \geq \mathbb{P}^i(J_1 > t) = e^{-q_i t} > 0$$

for any $i \in S$ and $t > 0$, where $\mathbb{P}^i$ is the probability distribution conditioned on $X_0 = i$. From this, we conclude that there exist $t_0 > 0$ and $\alpha \in (0, 1)$ such that $p_{ij}(t_0) \geq \alpha$ for any pairs (i, j). By following a similar induction procedure as in the proof of Theorem 3.11, we obtain, for any two initial distributions $\boldsymbol{\mu}(0), \tilde{\boldsymbol{\mu}}(0)$,

$$d(\boldsymbol{\mu}(t), \tilde{\boldsymbol{\mu}}(t)) \leq d\left(\boldsymbol{\mu}(t - kt_0), \tilde{\boldsymbol{\mu}}(t - kt_0)\right)(1 - \alpha)^k, \quad t \geq kt_0, \ k \in \mathbb{N}.$$

This implies the existence and uniqueness of the invariant distribution $\boldsymbol{\pi}$ for the Q process. Furthermore, we have

$$d(\boldsymbol{\mu}(t), \boldsymbol{\pi}) \leq d(\boldsymbol{\mu}(t - kt_0), \boldsymbol{\pi})(1 - \alpha)^k, \quad t \geq kt_0, \ k \in \mathbb{N}.$$

Letting $t, k \to \infty$, we get the desired result. $\qquad\qquad\square$

Theorem 3.18 (Ergodic theorem). *Assume that Q is irreducible. Then for any bounded function f we have*

$$\frac{1}{T} \int_0^T f(X_s)ds \to \langle f \rangle_{\boldsymbol{\pi}}, \qquad a.s.,$$

as $T \to \infty$, where $\boldsymbol{\pi}$ is the unique invariant distribution.

The proof can be found in [**Dur10**, **Nor97**].

3.8. Time Reversal

First let us consider an irreducible discrete time Markov chain $\{X_n\}_{n \geq 0}$ with transition probability matrix $\boldsymbol{P}$ and the unique invariant distribution $\boldsymbol{\pi}$. Assume that the initial distribution is also $\boldsymbol{\pi}$. Define the time-reversed process $\{\hat{X}_n\}_{0 \leq n \leq N}$ by $\hat{X}_n = X_{N-n}$ where N is a fixed positive integer. We want to study the transition rules for the process $\hat{X}$.

Note that

$$
\begin{aligned}
\mathbb{P}(\hat{X}_0 = i_0, &\hat{X}_1 = i_1, \ldots, \hat{X}_N = i_N) \\
&= \mathbb{P}(X_N = i_0, X_{N-1} = i_1, \ldots, X_0 = i_N) \\
&= \pi_{i_N} p_{i_N i_{N-1}} \cdots p_{i_1 i_0} = \pi_{i_0} \hat{p}_{i_0 i_1} \cdots \hat{p}_{i_{N-1} i_N}
\end{aligned}
$$

for any $i_0, i_1, \ldots, i_N \in S$, where the matrix $\hat{\boldsymbol{P}}$ has components

$$
(3.26) \qquad\qquad\qquad \hat{p}_{ij} = \frac{\pi_j}{\pi_i} p_{ji}.
$$

This calculation shows that $(\hat{X}_n)_{0 \leq n \leq N}$ is also an Markov chain with transition probability matrix $\hat{\boldsymbol{P}}$ and invariant distribution $\boldsymbol{\pi}$.

The above construction can also be applied to the Q-processes. For an irreducible Q-process $\{X_t\}_{0 \leq t \leq T}$ with generator $\boldsymbol{Q}$ and invariant distribution $\boldsymbol{\pi}$, we define the time-reversed process $\{\hat{X}_t\}_{0 \leq t \leq T}$ by $\hat{X}_t = X_{T-t}$. The initial distribution is also assumed to be $\boldsymbol{\pi}$. The joint distribution of $\hat{X}$ for any $0 \leq t_0 < t_1 < \cdots < t_N \leq T$ is given by

$$
\begin{aligned}
\mathbb{P}(\hat{X}_{t_0} = i_0, &\hat{X}_{t_1} = i_1, \ldots, \hat{X}_{t_N} = i_N) \\
&= \mathbb{P}(X_{T-t_0} = i_0, X_{T-t_1} = i_1, \ldots, X_{T-t_N} = i_N) \\
&= \pi_{i_N} p_{i_N i_{N-1}}(s_N) \cdots p_{i_1 i_0}(s_1) = \pi_{i_0} \hat{p}_{i_0 i_1}(s_1) \cdots \hat{p}_{i_{N-1} i_N}(s_N),
\end{aligned}
$$

where $s_k = t_k - t_{k-1}$ for $k = 1, 2, \ldots, N$. As before, the time-dependent transition probability matrix $\hat{\boldsymbol{P}}(t)$ is defined by

$$
(3.27) \qquad\qquad\qquad \hat{p}_{ij}(t) = \frac{\pi_j}{\pi_i} p_{ji}(t).
$$

It is straightforward to check that $\hat{\boldsymbol{P}}(t)$ satisfies the Chapman-Kolmogorov equation and

$$
\frac{d\hat{\boldsymbol{P}}(t)}{dt} = \hat{\boldsymbol{Q}}\hat{\boldsymbol{P}}(t) = \hat{\boldsymbol{P}}(t)\hat{\boldsymbol{Q}},
$$

where $\hat{\boldsymbol{Q}}$ is a generator with entries

$$
\hat{q}_{ij} = \frac{\pi_j}{\pi_i} q_{ji}, \qquad i, j \in S.
$$

Ignoring the issue of left-continuity of the path $\hat{X}$, we obtain that $\hat{X}$ is also a Q-process with invariant distribution $\boldsymbol{\pi}$ and generator $\hat{\boldsymbol{Q}}$.

A particularly important class of Markov chains is those that satisfy the condition of *detailed balance*; i.e., $\hat{X}$ obeys the same statistics as X. Depending on the discrete or continuous time setup, the detailed balance condition has the form

$$
(3.28) \qquad \pi_i p_{ij} = \pi_j p_{ji} \quad \text{(discrete time)}, \qquad \pi_i q_{ij} = \pi_j q_{ji} \quad (Q\text{-process}).
$$

In this case, we have $\hat{p}_{ij} = p_{ij}$ or $\hat{q}_{ij} = q_{ij}$. We call the chain *reversible*. A reversible chain can be equipped with a variational structure and has nice spectral properties. In the discrete time setup, define the *Laplacian matrix*

$$\boldsymbol{L} = \boldsymbol{P} - \boldsymbol{I}$$

and correspondingly its action on any function f

$$(\boldsymbol{L}f)(i) = \sum_{j \in S} p_{ij}(f(j) - f(i)).$$

Let $L_{\boldsymbol{\pi}}^2$ be the space of square summable functions f endowed with the $\boldsymbol{\pi}$-weighted scalar product

(3.29)
$$(f, g)_{\boldsymbol{\pi}} = \sum_{i \in S} \pi_i f(i) g(i).$$

Denote the *Dirichlet form*, or energy of a function f, by

$$D(f) = \sum_{i,j \in S} \pi_i p_{ij}(f(j) - f(i))^2.$$

One can show that $D(f) = (f, -\boldsymbol{L}f)_{\boldsymbol{\pi}}$. Similar constructions can be done for Q-processes and more general stochastic processes. These formulations are particularly useful in potential theory for Markov chains [**Soa94**].

3.9. Hidden Markov Model

The hidden Markov model (HMM) is a powerful tool for analyzing time series or even spatially distributed data. It has been widely used in numerous applications such as image processing, speech recognition, data compression, bioinformatics, and pattern recognition, etc. [**EAM95**, **Rab89**]. The fundamental issue in the HMM is to infer the underlying hidden Markov transition rules based on the sequences of observations. In this sense, it can be understood as an inverse problem to the direct problem of generating state sequences from a known Markov chain.

We will limit ourselves to the discrete time setting. The data that is available to us is a time series $\boldsymbol{Y} = (Y_{1:N}) = (Y_1, \ldots, Y_N)$, resulting from the partial observation of a trajectory $\boldsymbol{X} = (X_{1:N}) = (X_1, \ldots, X_N)$ of the underlying Markov chain with initial distribution $\boldsymbol{\mu} = (\mu_i)_{i \in S}$ and transition probability matrix $\boldsymbol{P} = (p_{ij})_{i,j \in S}$. The schematic figure of a hidden Markov model is shown in Figure 3.3. We assume that the observations are in state space O and the probability of the observations is given by the so-called *emission matrix* $\boldsymbol{R} = (r_{ij})_{i \in S, j \in O}$, where r_{ij} is the probability of observing j when the hidden state is i; i.e.,

$$r_{ij} = \mathbb{P}(Y = j | X = i), \quad i \in S \text{ and } j \in O.$$
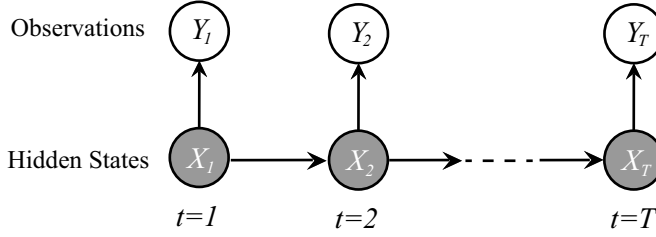
Figure 3.3. Schematics of the hidden Markov model (HMM).

In this setup, both $\boldsymbol{P}$ and $\boldsymbol{R}$ are time independent. The HMM is fully specified by the parameter set:

$$\boldsymbol{\theta} = (\boldsymbol{P}, \boldsymbol{R}, \boldsymbol{\mu}).$$

In this formulation, the probability of observing $\boldsymbol{Y}$ conditional on the hidden states $\boldsymbol{X}$ is

$$(3.30) \qquad \mathbb{P}(\boldsymbol{Y}|\boldsymbol{X}, \boldsymbol{\theta}) = \prod_{n=1}^{N} \mathbb{P}(Y_n|X_n, \boldsymbol{\theta}) = \prod_{n=1}^{N} r_{X_n Y_n},$$

and the probability of generating hidden states $\boldsymbol{X}$ with parameter $\boldsymbol{\theta}$ is

$$(3.31) \qquad \mathbb{P}(\boldsymbol{X}|\boldsymbol{\theta}) = \mu_{X_1} \prod_{n=1}^{N-1} p_{X_n X_{n+1}}.$$

Hence the joint distribution of the states $\boldsymbol{X}$ and observation $\boldsymbol{Y}$ is given by

$$\mathbb{P}(\boldsymbol{X}, \boldsymbol{Y}|\boldsymbol{\theta}) = \mathbb{P}(\boldsymbol{Y}|\boldsymbol{X}, \boldsymbol{\theta}) P(\boldsymbol{X}|\boldsymbol{\theta})$$

$$(3.32) \qquad = \mu_{X_1} r_{X_1 Y_1} \prod_{n=1}^{N-1} \left(p_{X_n X_{n+1}} r_{X_{n+1} Y_{n+1}} \right).$$

The joint distribution $\mathbb{P}(\boldsymbol{X}, \boldsymbol{Y}|\boldsymbol{\theta})$ is also called the *likelihood function* in statistics. We are mainly concerned with the following three types of questions:

i) **Model selection**. Given a sequence of observations $\boldsymbol{Y}$ and a number of possible models, i.e., a set of $\boldsymbol{\theta}_k = (\boldsymbol{P}^{(k)}, \boldsymbol{R}^{(k)}, \boldsymbol{\mu}^{(k)})$ triplets, find out efficiently which model most probably generated the observed sequence.

ii) **Optimal prediction**. Given the observation sequence $\boldsymbol{Y}$ and the HMM $\boldsymbol{\theta}$, find the most probable state sequence $\boldsymbol{X}$ that best explains the observations.

iii) **Parameter estimation**. Given the observation sequence $\boldsymbol{Y}$, find the model parameters $\boldsymbol{\theta} = (\boldsymbol{P}, \boldsymbol{R}, \boldsymbol{\mu})$ that maximize the likelihood function $\mathbb{P}(\boldsymbol{X}, \boldsymbol{Y}|\boldsymbol{\theta})$.

Model Selection. From $\mathbb{P}(\boldsymbol{X}, \boldsymbol{Y}|\boldsymbol{\theta})$, we obtain the marginal distribution

$$(3.33) \qquad \mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta}) = \sum_{\boldsymbol{x}} \mathbb{P}(\boldsymbol{x}, \boldsymbol{Y}|\boldsymbol{\theta})$$

and the posterior distribution for the kth model $\boldsymbol{\theta}_k$ under the observation $\boldsymbol{Y}$

$$(3.34) \qquad \mathbb{P}(\boldsymbol{\theta}_k|\boldsymbol{Y}) = \frac{1}{\mathbb{P}(\boldsymbol{Y})} \mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta}_k) \cdot \mathbb{P}(\boldsymbol{\theta}_k), \quad k = 1, \dots, K$$

where $\mathbb{P}(\boldsymbol{Y}) = \sum_k \mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta}_k) \cdot \mathbb{P}(\boldsymbol{\theta}_k)$. Since the observation $\boldsymbol{Y}$ is given, we have

$$(3.35) \qquad \mathbb{P}(\boldsymbol{\theta}_k|\boldsymbol{Y}) \propto \mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta}_k) \cdot \mathbb{P}(\boldsymbol{\theta}_k).$$

A priori, we assume there is no bias for any choice of the model; thus $\mathbb{P}(\boldsymbol{\theta}_k) = 1/K$ and $\mathbb{P}(\boldsymbol{\theta}_k|\boldsymbol{Y}) \propto \mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta}_k)$. So the most natural way to identify which model is the best for the data can be made by choosing the maximum of $\mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta}_k)$ among all K candidates. However, the naive direct sum via (3.33) requires I^N operations, which is computationally expensive and even infeasible in many cases. Therefore a more efficient algorithm is needed.

The *forward algorithm* in HMM is motivated by ideas from dynamic programming. Consider the forward variable $\alpha_n(i)$ defined by

$$\alpha_n(i) = \mathbb{P}(Y_{1:n} = y_{1:n}, X_n = i|\boldsymbol{\theta}),$$

which represents the probability of the observation sequence $Y_{1:n}$ and the hidden state at time n, given the model $\boldsymbol{\theta}$. Here $\{\alpha_n(i)\}$ satisfies the dynamic programming principle:

$$(3.36) \qquad \alpha_n(i) = \Big(\sum_{j \in S} \alpha_{n-1}(j) p_{ji} \Big) r_{iy_n}, \quad n = 2, \dots, N; \ i \in S.$$

The distribution $\mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta})$ can be obtained via the following forward algorithm.

Algorithm 1 (Forward procedure)**.** Finding the posterior probability under each model.

  (i) Initialization. Compute $\alpha_1(i) = \mu_i r_{iy_1}$ for $i \in S$.
  (ii) Induction. Compute $\{\alpha_n(i)\}$ via (3.36).
  (iii) Termination. Compute the final a posterior probability $\mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta}) = \sum_{i \in S} \alpha_N(i)$.

Note that the total number of products in the forward algorithm is $O(IN)$. The basic idea of the forward algorithm is to avoid the necessity of enumerating all possible paths by exploiting the recursive relations. Using the forward algorithm, one can compute the a posterior probability for each model and select the one with the highest probability. This is called the *maximum a posteriori* (MAP) estimation in Bayesian statistics.

Optimal Prediction. From the joint distribution $\mathbb{P}(\boldsymbol{X}, \boldsymbol{Y}|\boldsymbol{\theta})$, we have the conditional probability

$$\mathbb{P}(\boldsymbol{X}|\boldsymbol{Y}, \boldsymbol{\theta}) = \frac{1}{\mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta})}\mathbb{P}(\boldsymbol{X}, \boldsymbol{Y}|\boldsymbol{\theta}) \propto \mathbb{P}(\boldsymbol{X}, \boldsymbol{Y}|\boldsymbol{\theta})$$

since the parameter $\boldsymbol{\theta}$ and the observation $\boldsymbol{Y}$ are already known. Thus given $\boldsymbol{\theta}$ and $\boldsymbol{Y}$, the optimal state sequence $\boldsymbol{X}$ can be defined as the most probable path that maximizes the probability $\mathbb{P}(\boldsymbol{X}, \boldsymbol{Y}|\boldsymbol{\theta})$ in the path space S^N. Again, naive enumeration and maximization are not feasible. The *Viterbi algorithm* is designed for this task.

The Viterbi algorithm also uses ideas from dynamic programming to decompose the optimization problem into many subproblems. First, let us define the partial probability $\delta_n(i)$:

$$\delta_n(i) = \max_{x_{1:n-1}} \left\{ \mathbb{P}(X_{1:n-1} = x_{1:n-1}, X_n = i, Y_{1:n} = y_{1:n}|\boldsymbol{\theta}) \right\},$$

which corresponds to the subproblem with partial observation sequence and final state $X_n = i$ until time n. By induction we have

$$(3.37) \qquad \delta_{n+1}(j) = \left(\max_{i \in S}(\delta_n(i)p_{ij}) \right) r_{jy_{n+1}}, \quad n = 1, \ldots, N-1; \; j \in S.$$

To retrieve the state sequence, we need to keep track of the argument that maximizes $\delta_n(j)$ for each n and j. This can be done by recording the maximizer in step n in (3.37) in an array, denoted by ψ_n. The complete Viterbi algorithm is as follows.

Algorithm 2 (Viterbi algorithm). Finding the optimal state sequence $\hat{\boldsymbol{X}} = (\hat{X}_{1:N})$ given $\boldsymbol{\theta}$ and $\boldsymbol{Y}$.

   (i) Initialization. Compute $\delta_1(i) = \mu_i r_{iy_1}$ for $i \in S$.

   (ii) Induction. Compute

$$\psi_n(j) = \arg \max_{i \in S}\{\delta_n(i)p_{ij}\}, \quad n = 1, \ldots, N-1; \; j \in S.$$

$$\delta_n(j) = \left(\max_{i \in S}\{\delta_{n-1}(i)p_{ij}\} \right) r_{jy_n}, \quad n = 2, \ldots, N; \; j \in S.$$

   (iii) Termination. Obtain the maximum probability and record the maximizer in the final step

$$P^* = \max_{i \in S}\{\delta_N(i)\}, \quad \hat{X}_N = \arg \max_{i \in S}\{\delta_N(i)\}.$$

   (iv) Backtracking. Obtain the optimal state sequence through backtracking

$$\hat{X}_n = \psi_n(\hat{X}_{n+1}), \quad n = N-1, \ldots, 1.$$

Except for the backtracking step, the implementation of the Viterbi algorithm is very similar to the forward algorithm. The main difference is that maximization over previous states is used instead of summation.

Parameter Estimation. In statistics, a common approach to parameter estimation is the *maximum likelihood* approach, i.e., to perform the optimization with respect to the parameters:

$$(3.38) \qquad \max_{\boldsymbol{\theta}} \mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta})$$

given the observation $\boldsymbol{Y}$, where $\mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta})$ is defined in (3.33). This maximization is nontrivial since it is generally nonconvex and involves hidden variables. Below we introduce a very simple iterative method that gives rise to a local maximizer, the well-known *Baum-Welch algorithm* proposed in the 1970s [**BE67**].

To do this let us first introduce the backward procedure. We define the backward variable $\beta_n(i)$, which represents the probability of the observation sequence from time $n + 1$ to N, given that the hidden state at time n is at state i and the model $\boldsymbol{\theta}$

$$(3.39) \qquad \beta_n(i) = \mathbb{P}(Y_{n+1:N} = y_{n+1:N}|X_n = i, \boldsymbol{\theta}), \quad n = N - 1, \ldots, 1.$$

The calculation of $\{\beta_n(i)\}$ can be simplified using the dynamic programming principle:

$$(3.40) \qquad \beta_n(i) = \sum_{j \in S} p_{ij} r_{j y_{n+1}} \beta_{n+1}(j), \quad n = N - 1, \ldots, 1.$$

Similarly to the forward procedure, we have

Algorithm 3 (Backward procedure)**.** Evaluation of the backward variables β_n.

    (i) Initialization. Set $\beta_N(i) = 1$ for $i \in S$.

    (ii) Induction. Compute $\{\beta_n(i)\}$ via (3.40).

Moreover, let us define

$$(3.41) \qquad \xi_n(i, j) = \mathbb{P}(X_n = i, X_{n+1} = j|\boldsymbol{Y}, \boldsymbol{\theta}), \quad n = 1, \ldots, N - 1,$$

the probability of being at state i at time n and at state j at time $n+1$, given $\boldsymbol{Y}$ and $\boldsymbol{\theta}$. Using the definition of the forward and the backward variables, we can represent $\xi_n(i, j)$ as

$$\begin{aligned} \xi_n(i, j) \;\; &= \;\; \frac{\mathbb{P}(X_n = i, X_{n+1} = j, \boldsymbol{Y}|\boldsymbol{\theta})}{\mathbb{P}(\boldsymbol{Y}|\boldsymbol{\theta})} \\[2mm] &= \;\; \frac{\alpha_n(i) p_{ij} r_{j y_{n+1}} \beta_{n+1}(j)}{\sum_{i,j \in S} \alpha_n(i) p_{ij} r_{j y_{n+1}} \beta_{n+1}(j)} \end{aligned}$$

by the Markov property. Furthermore, we define the marginal of ξ_n at time n

$$\gamma_n(i) = \mathbb{P}(X_n = i | \boldsymbol{Y}, \boldsymbol{\theta}) = \sum_{j \in S} \xi_n(i, j), \quad n = 1, \ldots, N - 1.$$

Summing $\gamma_n(i)$ and $\xi_n(i, j)$ over n, we get two quantities:

$$\sum_{n=1}^{N-1} \gamma_n(i): \text{ expected number of transitions from state } i \text{ given } (\boldsymbol{Y}, \boldsymbol{\theta}),$$

$$\sum_{n=1}^{N-1} \xi_n(i, j): \text{ expected number of transitions from state } i \text{ to } j \text{ given } (\boldsymbol{Y}, \boldsymbol{\theta}).$$

Note that the above equivalence is up to a constant, e.g., the number of transitions starting from state i in the whole observation time series.

Algorithm 4 (Baum-Welch algorithm). Parameter estimation of the HMM.

(i) Set up an initial HMM $\boldsymbol{\theta} = (\boldsymbol{P}, \boldsymbol{R}, \boldsymbol{\mu})$.

(ii) Update the parameter $\boldsymbol{\theta}$ through

$$(3.42) \qquad \qquad \mu^* = \gamma_1(i),$$

$$(3.43) \qquad \qquad p_{ij}^* = \frac{\sum_{n=1}^{N-1} \xi_n(i, j)}{\sum_{n=1}^{N-1} \gamma_n(i)},$$

$$(3.44) \qquad \qquad r_{jk}^* = \frac{\sum_{n=1, Y_n=k}^{N} \gamma_n(j)}{\sum_{n=1}^{N} \gamma_n(j)}.$$

(iii) Repeat the above procedure until convergence.

The iteration formulas are quite intuitive. If we simply understand $\sum_n \gamma_n(i)$ as the number of transitions starting from state i and $\sum_n \xi_n(i, j)$ as the number of transitions starting from state i to state j in the observation $\boldsymbol{Y}$, (3.43) is then simply an empirical estimation of p_{ij} from the data. Equations (3.42) and (3.44) can be explained similarly. The difference between the direct empirical estimate and the updating rule is that the iteration algorithm takes into account the underlying parameters $\boldsymbol{\theta}$ rather than the data itself.

Application to Speech Recognition. The HMM has been widely used in various fields, such as speech recognition [**Jel97**, **Rab89**], natural language processing [**JM09**, **MS99**], and the analysis of biological sequences [**BB01**], etc. Below we will illustrate application of the HMM in speech recognition on a specific task: isolated word recognition.

The objective is to identify a single word from a given vocabulary V of $|V|$ words according to its digitized speech signal. We assume that for each word in the vocabulary we have already collected a training set of

speech data. In practice, the recognition procedure consists of two steps: i) preprocessing and ii) recognition. In the preprocessing step, the digitized speech data for each spoken word is sliced into N consecutive frames. These frames are then processed into a discrete observation sequence $\{Y_j\}_{j=1:N}$ according to a finite codebook O generated from these frames using the vector quantization technique. Typically, the codebook size is $O(10^2)$. So, after preprocessing, we have a time series $\{Y_j\}_{j=1:N}$ for each spoken word.

The recognition step can be decomposed into three substeps.

(1) *Training.* In this substep, we build an HMM with parameter $\boldsymbol{\theta}_k = (\boldsymbol{P}^{(k)}, \boldsymbol{R}^{(k)}, \boldsymbol{\mu}^{(k)})$ for each word in the vocabulary according to the quantized training data. The number of the hidden states for each word model is chosen roughly as the number of sounds within the word, which is $O(10)$ in general. This corresponds to the parameter estimation problem in the HMM, and the Baum-Welch algorithm can be used.

(2) *Analysis and model improvement.* Based on the training result, we can obtain the most probable hidden states $\{X_i\}_{i=1:N}$ by finding the optimal state sequence using the Viterbi algorithm. These hidden states are then used to perform segmentation analysis of the speech data. The number of hidden state can also be adjusted to achieve better model performance.

(3) *Identification.* For each unknown word to be recognized, we identify it from the vocabulary via a model selection procedure. That is, we obtain its index

$$k^* = \arg \max_{k \in V} P(\boldsymbol{Y}|\boldsymbol{\theta}_k)$$

by the MAP estimate. This is implemented through the forward algorithm.

The HMM has played a key role in the speech recognition problem. Interested readers may refer to [**Jel97**, **JM09**] and the references therein for more details.

3.10. Networks and Markov Chains

As another example of the application of Markov chains, we take a brief look at networks, which provide a general setting for analyzing interactions between agents in social, biological, and other settings.

A network is a directed or undirected weighted graph G. Its structure is specified by a set of nodes, here denoted by S, and the set of weights W, $G = (S, W)$. We assume that the network has I nodes with $S = \{1, 2, \ldots, I\}$. The weight matrix $W = \{e_{ij}\}_{i,j \in S}$, where e_{ij} is the weight for the edge from

node i to node j. The simplest example of the weight matrix is given by the adjacency matrix: $e_{ij} = 0$ or 1, depending on whether i and j are connected. Below we will focus on the situation when the network is undirected; i.e., W is symmetric.

Given a network, one can define naturally a discrete time Markov chain, with the transition probability matrix $\boldsymbol{P} = (p_{ij})_{i,j \in S}$ given by

$$(3.45) \qquad p_{ij} = \frac{e_{ij}}{d_i}, \qquad d_i = \sum_{k \in S} e_{ik}.$$

Here d_i is the degree of the node i [**Chu97**, **Lov96**]. Let

$$(3.46) \qquad \pi_i = \frac{d_i}{\sum_{k \in S} d_k}.$$

Then it is easy to see that

$$(3.47) \qquad \sum_{i \in S} \pi_i p_{ij} = \pi_j;$$

i.e., $\boldsymbol{\pi}$ is an invariant distribution of this Markov chain. Furthermore, one has the detailed balance relation:

$$(3.48) \qquad \pi_i p_{ij} = \pi_j p_{ji}.$$

For $\boldsymbol{u} = (u_i)_{i \in S}, \boldsymbol{v} = (v_i)_{i \in S}$ defined on S, introduce the inner product

$$(\boldsymbol{u}, \boldsymbol{v})_\pi = \sum_{i \in S} u_i v_i \pi_i.$$

With this inner product, $\boldsymbol{P}$ is selfadjoint in the sense that

$$(\boldsymbol{P} \boldsymbol{u}, \boldsymbol{v})_{\boldsymbol{\pi}} = (\boldsymbol{u}, \boldsymbol{P} \boldsymbol{v})_{\boldsymbol{\pi}}.$$

Denote by $\{\lambda_k\}_{k=0,\dots,I-1}$ the eigenvalues of $\boldsymbol{P}$, $\{\boldsymbol{\varphi}_k\}_{k=0}^{I-1}$ and $\{\boldsymbol{\psi}_k\}_{k=0}^{I-1}$ the corresponding right and left eigenvectors. We have $(\boldsymbol{\varphi}_j, \boldsymbol{\varphi}_k)_{\boldsymbol{\pi}} = \delta_{jk}$, $\psi_{k,i} = \varphi_{k,i} \pi_i$, and

$$(3.49) \qquad \boldsymbol{P} \boldsymbol{\varphi}_k = \lambda_k \boldsymbol{\varphi}_k, \quad \boldsymbol{\psi}_k^T \boldsymbol{P} = \lambda_k \boldsymbol{\psi}_k^T, \qquad k = 0, 1, \dots, I - 1.$$

Moreover, one can easily see that 1 is an eigenvalue and all other eigenvalues lie in the interval $[-1, 1]$. We will order them according to $1 = \lambda_0 \geq |\lambda_1| \geq \cdots \geq |\lambda_{I-1}|$. Note that $\boldsymbol{\psi}_0 = \boldsymbol{\pi}$ and $\boldsymbol{\varphi}_0$ is a constant vector. The spectral decomposition of $\boldsymbol{P}^t$ is then given by

$$(3.50) \qquad (\boldsymbol{P}^t)_{ij} = \sum_{k=0}^{I-1} \lambda_k^t \varphi_{k,i} \psi_{k,j}.$$

An interesting problem is to infer the structural and dynamic properties of the network from that of the random walkers on the network. As an example, we will discuss the connection between the community structure of the network and the lumpability properties of the Markov chain just defined.

A network has *community structure* if it can be partitioned into the union of subnetworks with no edges across the different subnetworks. A Markov chain is *lumpable* if the state space can be decomposed into the union of subsets and the chain can be equivalently defined as a chain between the subsets. These two notions obviously correspond to each other. However, they are both too restrictive. So in applications we are often faced with the situation of approximate community structure and approximate lumpability. We will start with the precise notion of lumpability.

Given a Markov chain on the state space S and a partition of S: $S = \bigcup_{k=1}^{K} C_k$ with $C_k \cap C_l = \emptyset$ if $k \neq l$, define the lumped process through the joint probability:

$$(3.51) \qquad p_{i_0 i_1 \cdots i_m} = \mathbb{P}\{X_m \in C_{i_m} | X_{m-1} \in C_{i_{m-1}}, \ldots, X_0 \in C_{i_0}\}.$$

Definition 3.19 (Lumpability). A Markov chain is said to be lumpable with respect to the partition $S = \bigcup_{k=1}^{K} C_k$ if for every initial distribution $\boldsymbol{\mu}_0$ the lumped process defined through (3.51) is a Markov chain and the transition probabilities do not depend on the choice of $\boldsymbol{\mu}_0$.

The following result gives an equivalent characterization of lumpablity [**KS76**].

Theorem 3.20. *A Markov chain with transition matrix $\boldsymbol{P}$ is lumpable with respect to the partition $S = \bigcup_{k=1}^{K} C_k$ if and only if for any $k, l \in \{1, 2 \ldots, K\}$*

$$p_{i,C_l} := \sum_{j \in C_l} p_{ij}$$

is a piecewise constant with respect to the partition $S = \bigcup_{k=1}^{K} C_k$. These constants form the components $(\hat{p}_{kl})$ of the lumped transition probability matrix for $k, l \in \{1, 2 \ldots, K\}$.

A closely related concept is spectral clustering. In this context, one has the following result [**MS01**, **SM00**].

Theorem 3.21. *Assume that the transition matrix $\boldsymbol{P}$ has I independent eigenvectors. Let $S = \bigcup_{k=1}^{K} C_k$ be a partition of S. Then the Markov chain is lumpable with respect to this partition and the corresponding lumped matrix $\{\hat{p}_{kl}\}_{k,l=1}^{K}$ is nonsingular if and only if $\boldsymbol{P}$ has K eigenvectors that are piecewise constant with respect to the partition and corresponding eigenvalues are nonzero.*

For applications of this result to image segmentation, please see [**MS01**, **SM00**].

We finish with an approximate coarse-graining procedure for Markov chains [**ELVE08**]. For this purpose, we define a metric in the space of

Markov chains (stochastic matrices) on S with invariant distribution $\boldsymbol{\pi}$. Let $\boldsymbol{Q} = (q_{ij})_{i,j \in S}$ be a stochastic matrix with invariant distribution $\boldsymbol{\pi}$. We define its norm by

$$(3.52) \qquad \|\boldsymbol{Q}\|_{\boldsymbol{\pi}}^2 = \sum_{i,j \in S} \frac{\pi_i}{\pi_j} q_{ij}^2.$$

It is easy to see that if $\boldsymbol{Q}$ satisfies the condition of detailed balance, this norm is in fact the sum of the squares of the eigenvalues of $\boldsymbol{Q}$.

Given a partition of S: $S = \bigcup_{k=1}^{K} C_k$ with $C_k \cap C_l = \emptyset$ if $k \neq l$, let $\hat{\boldsymbol{P}} = (\hat{p}_{kl})_{k,l=1}^{K}$ be a stochastic matrix on the state space $C = \{C_1, \ldots, C_K\}$. This matrix can be naturally lifted to the space of stochastic matrices on the original state space S by

$$(3.53) \qquad \tilde{p}_{ij} = \frac{\pi_j \hat{p}_{kl}}{\sum\limits_{k \in C_l} \pi_k} \qquad \text{if } i \in C_k, j \in C_l.$$

Equation (3.53) says that the probability of jumping from any state in C_k is the same and the walker enters C_l according to the invariant distribution. This is consistent with the idea of coarsening the original dynamics onto the new state space $C = \{C_1, \ldots, C_K\}$ and ignoring the details of the dynamics within the sets C_k. Note that $\tilde{\boldsymbol{P}}$ is a stochastic matrix on S with invariant distribution $\boldsymbol{\pi}$ if $\hat{\boldsymbol{P}}$ is a stochastic matrix on C with invariant distribution $\hat{\boldsymbol{\pi}}$.
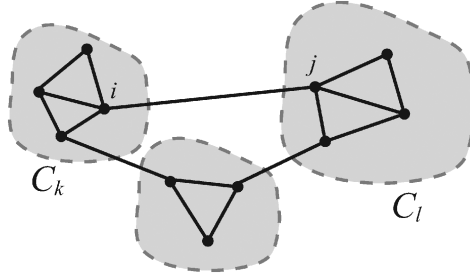
Figure 3.4. Schematics of the network partition and community structure.

Given a Markov chain $\boldsymbol{P}$ and predefined partition C, finding the optimal coarse-grained chain $\tilde{\boldsymbol{P}}$ is a useful problem and can be investigated under the framework of optimal prediction [**Cho03**] with respect to the norm (3.52)

$$\min_{\hat{\boldsymbol{P}} \cdot \mathbf{1} = 1, \hat{\boldsymbol{P}} \geq 0} \|\tilde{\boldsymbol{P}} - \boldsymbol{P}\|_{\boldsymbol{\pi}}.$$

One can ask further about the optimal partition, and this can be approached by minimizing the approximation error with respect to all possible partitions. Algebraically, the existence of community structure or clustering property of

a network corresponds to the existence of a spectral gap in the eigenvalues of $\boldsymbol{P}$; i.e., $\lambda_k = 1 - \eta_k \delta$ for $k = 0, \ldots, K - 1$ and $|\lambda_k| < \lambda^* < 1$ for $k = K, \ldots, I - 1$ where $0 < \delta \ll 1$, $\eta_k > 0$. See [**ELVE08**] for more details.

Exercises

3.1. Write down the transition probability matrix $\boldsymbol{P}$ of Ehrenfest's diffusion model and analyze its invariant distribution.

3.2. Suppose $\{X_n\}_{n \in \mathbb{N}}$ is a Markov chain on a finite state space S. Prove that

$$\mathbb{P}(A \cap \{X_{m+1} = i_{m+1}, \ldots, X_{m+n} = i_{m+n}\} | X_m = i_m)$$
$$= \mathbb{P}(A | X_m = i_m) \mathbb{P}^i(\{X_1 = i_{m+1}, \ldots, X_n = i_{m+n}\}),$$

where the set A is an arbitrary union of elementary events like $\{(X_0, \ldots, X_{m-1}) = (i_0, \ldots, i_{m-1})\}$.

3.3. Prove Lemma 3.7.

3.4. Show that the exponent s in $\boldsymbol{P}^s$ in Theorem 3.11 necessarily satisfies $s \leq I - 1$, where $I = |S|$ is the number of states of the chain.

3.5. Show that the recurrence relation $\boldsymbol{\mu}_n = \boldsymbol{\mu}_{n-1} \boldsymbol{P}$ can be written as

$$\mu_{n,i} = \mu_{n-1,i} \Big(1 - \sum_{j \in S, j \neq i} p_{ij} \Big) + \sum_{j \in S, j \neq i} \mu_{n-1,j} p_{ji}.$$

The first term on the right-hand side gives the total probability of not making a transition from state i, while the last term is the probability of transition from one of states $j \neq i$ to state i.

3.6. Prove (3.8) by mathematical induction.

3.7. Derive (3.8) through the moment generating function

$$g(t, z) = \sum_{m=0}^{\infty} p_m(t) z^m.$$

3.8. Let f be a function defined on the state space S, and let

$$h_i(t) = \mathbb{E}^i f(X_t), \quad i \in S.$$

Prove that $d\boldsymbol{h}/dt = \boldsymbol{P}\boldsymbol{h}$ for $\boldsymbol{h} = (h_1(t), \ldots, h_I(t))^T$.

3.9. Let $\{N_t^1\}$ and $\{N_t^2\}$ be two independent Poisson processes with parameters λ_1 and λ_2, respectively. Prove that $N_t = N_t^1 + N_t^2$ is a Poisson process with parameter $\lambda_1 + \lambda_2$.

3.10. Let $\{N_t\}$ be a Poisson process with rate λ and let $\tau \sim \mathcal{E}(\mu)$ be an independent random variable. Prove that

$$\mathbb{P}(N_\tau = m) = (1 - p)^m p, \quad m \in \mathbb{N},$$

where $p = \mu/(\lambda + \mu)$.

3.11. Let $\{N_t\}$ be a Poisson process with rate λ. Show that the distribution of the arrival time τ_k between k successive jumps is a gamma distribution with probability density

$$p(t) = \frac{\lambda^k t^{k-1}}{\Gamma(k)} e^{-\lambda t}, \quad t > 0,$$

where $\Gamma(k) = (k-1)!$ is the gamma function.

3.12. Consider the Poisson process $\{N_t\}$ with rate λ. Given that $N_t = n$, prove that the n arrival times $J_1, J_2, \ldots, J_n$ have the same distribution as the order statistics corresponding to n independent random variables uniformly distributed in $(0, t)$. That is, $(J_1, \ldots, J_n)$ has the probability density

$$p(x_1, x_2, \ldots, x_n | N_t = n) = \frac{n!}{t^n}, \quad 0 < x_1 < \cdots < x_n < t.$$

3.13. The compound Poisson process $\{X_t\}$ ($t \in \mathbb{R}^+$) is defined by

$$X_t = \sum_{k=1}^{N_t} Y_k$$

where $\{N_t\}$ is a Poisson process with rate λ and $\{Y_k\}$ are i.i.d. random variables on $\mathbb{R}$ with probability density function $q(y)$. Derive the equation for the probability density function $p(x, t)$ of X_t.

3.14. Suppose that $\{N_t^{(k)}\}$ ($k = 1, 2, \ldots$) are independent Poisson processes with rate λ_k, respectively, $\lambda = \sum_{k=1}^{\infty} \lambda_k < \infty$. Prove that $\{X_t = \sum_{k=1}^{\infty} k N_t^{(k)}\}$ is a compound Poisson process.

3.15. Prove (3.36) and (3.40).

3.16. Consider an irreducible Markov chain $\{X_n\}_{n \in \mathbb{N}}$ on a finite state space S. Let $H \subset S$. Define the first passage time $T_H = \inf\{n | X_n \in H, n \in \mathbb{N}\}$ and

$$h_i = \mathbb{P}^i(T_H < \infty), \quad i \in S.$$

Prove that $\boldsymbol{h} = (h_i)_{i \in S}$ satisfies the equation

$$(\boldsymbol{I} - \boldsymbol{P}) \cdot \boldsymbol{h} = 0 \quad \text{with boundary condition } h_i = 1, i \in H,$$

where $\boldsymbol{P}$ is the transition probability matrix.

3.17. Connection between resistor networks and Markov chains.

 (a) Consider a random walk $\{X_n\}_{n \in \mathbb{N}}$ on a one-dimensional lattice S with states $\{1, 2, \ldots, I\}$. Assume that the transition probability $p_{ij} > 0$ for $|i - j| = 1$ and $\sum_{|j-i|=1} p_{ij} = 1$, where $i, j \in S$. Let $x_L = 1$, $x_R = N$. Define the first passage times

$$T_L = \inf\{n | X_n = x_L, n \in \mathbb{N}\}, \quad T_R = \inf\{n | X_n = x_R, n \in \mathbb{N}\}$$

and the probability

$$h_i = \mathbb{P}^i(T_R < T_L).$$

Prove that $\boldsymbol{h} = (h_i)_{i \in S}$ satisfies the equation

$$(\boldsymbol{I} - \boldsymbol{P}) \cdot \boldsymbol{h} = 0 \quad \text{with boundary condition } h_1 = 0, h_I = 1.$$

(b) Apply 1 volt on the resistor network formed by the resistors with conductance $C_{ij} = 1/R_{ij}$ between $i, j \in S$, where R_{ij} is the resistance ($R_{ij} := \infty$ if i, j are not connected). Assume that x_L is connected to ground. We assume $C_{ij} > 0$ only for $|i - j| = 1$ as in the random walk setting. Define the transition probability matrix $\boldsymbol{P}$ by $p_{ij} = C_{ij}/C_i$, where $C_i = \sum_j C_{ij}$. Denote the voltage at state i by v_i. Prove that $\boldsymbol{v}$ satisfies the same equation as $\boldsymbol{h}$.

(c) Generalize the above result to general finite resistor networks.

Notes

The finite state Markov chain is one of the most commonly used stochastic models in practice. More refined notions, such as recurrence and transience, can be found in [**Dur10**, **Nor97**]. Ergodicity for Markov chains with countable or continuous states is discussed in [**MT93**]. Our discussion of the hidden Markov model follows [**Rab89**]. The Baum-Welch algorithm is essentially the EM (expectation-maximimization) algorithm applied to the HMM [**DLR77**, **Wel03**]. However, it was proposed long before the EM algorithm.

More theoretical studies about the random walk on graphs can be found in [**Chu97**, **Lov96**]. One very interesting application is the PageRank algorithm for ranking webpages [**BP98**].

Monte Carlo Methods

From a practical viewpoint, one most important aspect of the probability theory is how to sample a probability distribution. Sampling can be used to:

(i) Compute expectations

$$(4.1) \qquad \mathbb{E}f(X) = \int f(x)\mu(dx) \approx \frac{1}{N}\sum_{j=1}^{N} f(X_j),$$

where $\mu(\cdot)$ is the probability distribution of the random variable X and $\{X_1, \ldots, X_N\}$ are independent samples of μ.

(ii) Find the maximum or minimum of a function. For example, let U be a smooth function defined on $\mathbb{R}^d$ bounded from below, and let $Z_\beta = \int_{\mathbb{R}^d} e^{-\beta U(\boldsymbol{x})} d\boldsymbol{x}$ be the normalization constant associated with U. Then as $\beta = T^{-1} \to \infty$,

$$(4.2) \qquad \frac{1}{Z_\beta} e^{-\beta U(\boldsymbol{x})} \longrightarrow \delta(\boldsymbol{x} - \boldsymbol{x}^*),$$

where $\boldsymbol{x}^*$ is the global minimum of U. For this reason, sampling can be viewed as a "finite temperature" version of optimization. This analogy between sampling and optimization can be used in at least two ways. The first is that ideas used in optimization algorithms, such as the Gauss-Seidel and the multigrid methods, can be adopted in the sampling setting. The second is a way of performing global optimization, by sampling the probability distribution on the left-hand side of (4.2), in the "low temperature" limit when $\beta \to \infty$. This idea is the essence of one of the best known global minimization technique, the simulated annealing method.

(iii) Perform parameter estimation in statistical models. A typical example is the expectation-maximization (EM) algorithm where sampling strategies are often used in the expectation step.

Two most notable areas where sampling plays a crucial role are statistical mechanics and statistics. A typical problem in statistical mechanics is the sampling of a Gibbs or other distributions. This is a direct problem. A typical problem in statistics is to find the underlying distribution that gives rise to the observed data. This is an inverse problem. In technical terms the two fields are closely related.

Sampling methods are broadly called Monte Carlo methods. In this chapter, we discuss the basic concepts and techniques that can be used to sample a probability distribution.

4.1. Numerical Integration

Let f be a continuous function on $[0, 1]$. We would like to compute $I(f) = \int_0^1 f(x)dx$ approximately. The traditional approach is to divide $[0, 1]$ into small subintervals and then use numerical quadrature formulas such as the trapezoidal rule or Simpson's rule. Here we would like to explore a probabilistic approach, which is generally more efficient for high-dimensional problems. This is based on the law of large numbers. If $\{X_i\}_{i=1}^N$ is a sequence of i.i.d. random samples that are uniformly distributed on $[0, 1]$, then

$$(4.3) \qquad \int_0^1 f(x)dx = \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^N f(X_i).$$

This suggests approximating $I(f)$ by the sample average

$$(4.4) \qquad I_N(f) = \frac{1}{N} \sum_{i=1}^N f(X_i).$$

The error $e_N = I_N(f) - I(f)$ can be estimated as

$$(4.5) \quad \mathbb{E}|e_N|^2 = \frac{1}{N^2} \sum_{i,j=1}^N \mathbb{E}\Big[(f(X_i) - I(f))(f(X_j) - I(f))\Big] = \frac{1}{N} \text{Var}(f)$$

by using independence, where $\text{Var}(f) = \int_0^1 (f(x) - I(f))^2 dx$. Therefore, we conclude that

$$(4.6) \qquad I_N(f) - I(f) \approx \frac{\sigma_f}{\sqrt{N}},$$

where $\sigma_f = \sqrt{\mathrm{Var}(f)}$ is the standard deviation. We can compare this with the error bound for the trapezoidal rule [**HNW08**] with N points

$$(4.7) \qquad e_N \approx \frac{1}{12}h^2 \max_{x\in[0,1]} |f''(x)|$$

where h is the size of the grid spacing. In one dimension, $h = N^{-1}$. We see that the trapezoidal rule clearly has an advantage if f is sufficiently smooth.

The real interest on the probablistic approach comes from high-dimensional problems. Let d be the dimension, and let f be a continuous function on $[0,1]^d$. If we pick N random points uniformly distributed on $[0,1]^d$ and define $I_N(f)$ in the same way as above, then the same error bound holds. In particular, the error still decays as $1/\sqrt{N}$ for large N. For the trapezoidal rule, the error still has the form (4.7), but now $h \sim N^{-1/d}$ if N quadrature points are used and they are distributed evenly in each direction. Hence the error decreases as $N^{-2/d}$ for large N. Therefore the Monte Carlo method should have a smaller error asymptotically when $d > 4$. Though higher-order methods can be applied to improve the accuracy of the deterministic quadrature methods, the Monte Carlo method still outperforms when the dimension is high enough.

An area where high-dimensional integration problems often show up is statistical physics, where one is interested in computing averages of the type

$$\langle f \rangle = \int_{R^{6n}} f(\boldsymbol{x})\pi(\boldsymbol{x})d\boldsymbol{x},$$

where $\pi(\boldsymbol{x}) = \frac{1}{Z}e^{-\beta H(\boldsymbol{x})}$ is the Gibbs distribution defined in Example 1.20. This is also one of the areas where Monte Carlo methods have received the most attention [**FS02**].

4.2. Generation of Random Variables

To apply Monte Carlo method, we need to generate random numbers. In computer simulatons, one has to be content with generating the so-called pseudo-random numbers. These numbers are not truly random. If one waits long enough, the sequence of numbers generated will repeat itself. However, we can make sure that the period is long enough and within the required accuracy; these numbers behave like desired random numbers.

The starting point is usually to generate (pseudo-)random number with uniform distribution $\mathcal{U}[0,1]$. Here we will discuss some of the simplest algorithms for this purpose. Readers are referred to [**PTVF95**] for codes that can be used in practice.

Uniform Distribution. The most commonly used pseudo-random number generator for $\mathcal{U}[0, 1]$ is the linear congruential generator (LCG). It has the simple form

(4.8) $$X_{n+1} \equiv aX_n + b \ (\text{mod } m)$$

where a, b, and m are some carefully chosen natural numbers and X_0 is the seed. The sequence $\{X_n/m\}$ gives the desired pseudo-random numbers in $[0, 1]$. Of particular interest is the period of such a recursion relation. The following result addresses this issue (cf. [**Knu98**]).

Theorem 4.1. *The period of an LCG is m if and only if*

  (i) *b and m are relatively prime;*
  (ii) *every prime factor of m divides $a - 1$;*
  (iii) *if $4 \mid m$, then $4 \mid (a - 1)$.*

If one chooses $m = 2^k$, $a = 4c + 1$, and b odd, then these conditions are satisfied. One can also use the LCG when $b = 0$. In 1969, Lewis, Goodman and Miller proposed the following pseudo-random number generator

$$X_{n+1} \equiv aX_n \ (\text{mod } m),$$

with $a = 7^5 = 16807, m = 2^{31} - 1$. The function `ran0()` in *Numerical Recipes* is based on this generator [**PTVF95**]. The period of `ran0()` is about 2.1×10^9. One can further combine sequences with different periods (the shuffling algorithm) to obtain more desirable pseudo-random number generators. `ran2()` in *Numerical Recipes* was constructed this way and its period is about 2.3×10^{18}.

A more general form of the LCG is given by

$$X_{n+1} = a_0 X_n + a_1 X_{n-1} + \cdots + a_j X_{n-j} + b \ (\text{mod } m).$$

One important fact about the LCG is that it shows very poor behavior for the s-tuples, i.e., the vectors $(X_n, X_{n+1}, \ldots, X_{n+s-1})$. In [**Mar68**], Marsaglia proved the following:

Theorem 4.2. *Let $\{Y_n\}$ be a sequence generated by (4.8) and let $X_n = Y_n/m$. Then the s-tuples $(X_n, X_{n+1}, \ldots, X_{n+s-1})$ lie on a maximum of $(s!m)^{\frac{1}{s}}$ equidistant parallel hyperplanes within the s-dimensional hypercube $[0, 1]^s$.*

The deviation from the uniform distribution over $[0, 1]^s$ is apparent when s is large. Inspite of this, the LCG is still one of the most widely used pseudo-random number generators. There are also nonlinear generators which aim to overcome this problem [**RC04**]. Some very recent mathematical software

packages adopted the so-called *Mersenne Twister* generator, which avoids the linear congruential steps and has a period of up to $2^{19937} - 1$ [**MN98**].

Various statistical tests have been proposed to calibrate the quality of random number generators by checking the validity of the null hypothesis:

(H0): The generated sequence of random variables $\{X_1, \ldots, X_N\}$ is i.i.d. $\mathcal{U}[0,1]$ distributed.

The most commonly used tests include:

(1) Equidistribution test: The interval $[0,1]$ is divided into K subintervals. Given a sequence $\{X_1, \ldots, X_N\}$, let N_j be the number of points that fall into the jth interval. A χ^2-test is then performed to check the uniformity of the points.

(2) Serial test: Consider the s-vector
$$\boldsymbol{X}_n = (X_n, X_{n+1}, \ldots, X_{n+s-1})$$
in s-dimensional space ($s > 2$). The s-hypercube is partitioned into the union of equal sized subcubes. The number of points in each subcube is computed and a χ^2-test is then performed. This is the high-dimensional version of the test above.

(3) Run test: Consider a short sequence $X_{n-1} > X_n < X_{n+1} > X_{n+2} < X_{n+3}$. We have a run-up of length 1 followed by two run-ups of length 2 since it has three increasing subsequences $X_{n-1}|X_n$, $X_{n+1}|X_{n+2}, X_{n+3}$. For a sequence of pseudo-random numbers, we can count the number of run-ups of length 1, length 2, ... and denote them by R_1, R_2, etc. It can be shown that $\{R_k\}$ is normally distributed when the sample size goes to infinity. Various statistical tests can be used to test such distributions.

The readers may consult Knuth's book [**Knu98**] or the document [**Rea10**] by the National Institute of Standards and Technology for more details about statistical tests for pseudo-random number generators.

The Inverse Transformation Method. Once we know how to generate uniformly distributed random numbers, we may in principle obtain random numbers with other distributions by the following strategy.

Proposition 4.3 (Inverse transformation method)**.** *Let F be the distribution function of X; i.e., $F(x) = \mathbb{P}(X \leq x)$. Let U be a $\mathcal{U}[0,1]$ random variable. Define the generalized inverse of F by*
$$F^-(u) = \inf\{x : F(x) \geq u\}, \quad u \in (0,1).$$
Then $X := F^-(U)$ is a random variable with distribution function F for $U \in (0,1)$.

Proof. If F is continuous and strictly increasing, we have $F^-(u) = F^{-1}(u)$ and

$$\mathbb{P}(X \leq x) = \mathbb{P}(F^{-1}(U) \leq x) = \mathbb{P}(U \leq F(x)) = F(x).$$

In the general case, we have that for any $u \in (0,1)$ and $x \in F^-(0,1)$, the generalized inverse satisfies

$$F(F^-(u)) \geq u \quad \text{and} \quad F^-(F(x)) \leq x.$$

We have $\{(u,x) : F^-(u) \leq x\} = \{(u,x) : F(x) \geq u\}$ and therefore

$$\mathbb{P}(F^-(U) \leq x) = \mathbb{P}(U \leq F(x)) = F(x).$$

The cases $U = 0$ or 1 can be neglected since they have zero probability. $\quad\square$

See Figure 4.1 for an illustration of inverse transformation method.
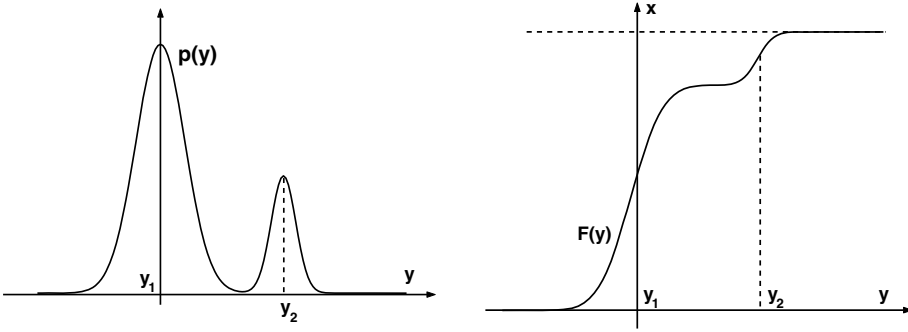
Figure 4.1. Left panel: The PDF of Y. Right panel: The distribution function $F(y)$.

Some straightforward applications of the inverse transformation method are:

(1) Uniform distribution on the interval $[a,b]$: $\mathcal{U}[a,b]$. The distribution function is given by

$$F(y) = \frac{y-a}{b-a}, \qquad y \in [a,b].$$

Thus $F^{-1}(x) = (b-a)x + a$. We can generate $Y \sim \mathcal{U}[a,b]$ by setting $Y = (b-a)X + a$ where $X \sim \mathcal{U}[0,1]$.

(2) Exponential distribution: $\mathcal{E}(\lambda)$. The distribution function is given by $F(y) = 1 - e^{-\lambda y}$. Then $F^{-1}(x) = -\log(1-x)/\lambda$, $x \in [0,1]$. We can generate $Y \sim \mathcal{E}(\lambda)$ by setting

$$Y = -\frac{1}{\lambda} \log X$$

since $1 - X \sim \mathcal{U}[0,1]$ if $X \sim \mathcal{U}[0,1]$.

To generate the Gaussian random variable with distribution $N(0,1)$, note that

$$F(x) = \int_{-\infty}^{x} p(y)dy = \frac{1}{2} + \frac{1}{2}\text{erf}\left(\frac{x}{\sqrt{2}}\right),$$

where $\text{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt$ is the error function. Therefore $F^{-1}(x) = \sqrt{2}\text{erf}^{-1}(2x-1)$. This is inefficient since it involves the solution of transcendental equations. A much more efficient way of generating Gaussian random variables is presented next.

The Box-Muller Method. The basic idea is to use the strategy presented above in two dimensions instead of one. Consider a two-dimensional Gaussian random vector with independent components. Using polar coordinates $x_1 = r\cos\theta$, $x_2 = r\sin\theta$, we have

$$\frac{1}{2\pi}e^{-\frac{x_1^2+x_2^2}{2}}dx_1dx_2 = \left(\frac{1}{2\pi}d\theta\right)\cdot(e^{-\frac{r^2}{2}}rdr).$$

This means that θ and r^2 are also independent, θ is uniformly distributed over the interval $[0,2\pi]$, and r^2 is exponentially distributed. Hence if $X, Y \sim \mathcal{U}[0,1]$ i.i.d. and we let $R = \sqrt{-2\log X}$, $\Theta = 2\pi Y$, then

$$Z_1 = R\cos\Theta, \quad Z_2 = R\sin\Theta$$

are independent and have the desired distribution $N(0,1)$.

Composition of Random Variables. Some distributions can be obtained by the composition of simple random variables instead of the direct application of the methods discussed above. Here are some examples.

(1) The hat probability distribution function. Let

$$f(z) = \left\{ \begin{array}{ll} z, & 0 < z < 1, \\ 2-z, & 1 \le z < 2. \end{array} \right.$$

Observe that if X and Y are i.i.d. with distribution $\mathcal{U}[0,1]$, then the distribution of $Z = X + Y$ is f.

(2) Sampling the mixture model. Let

$$f(x) = \sum_{i=1}^{K} \alpha_i g_i(x), \quad \alpha_i \ge 0, \ g_i(x) \ge 0.$$

We can rewrite it as

$$f(x) = \sum_{i=1}^{K} \beta_i h_i(x), \quad \beta_i = \alpha_i \int g_i(x)dx, \quad h_i(x) = \frac{g_i(x)}{\int g_i(x)dx},$$

where

$$\int h_i(x)dx = 1, \quad \sum_{i=1}^{K} \beta_i = 1.$$

To produce random variables with PDF f, we can proceed as follows. First we sample an index I from the integers $\{1, \ldots, K\}$ according to the distribution $(\beta_1, \beta_2, \ldots, \beta_K)$. Then we sample according to the PDF $h_I(x)$. The fact that this produces the desired distribution is a consequence of the definition of conditional probability.

The Acceptance-Rejection Method. We have seen that the inverse transformation method is only suited for the situation when the inverse function of the distribution function has a simple analytic form. We now present an alternative strategy for generating random variables with fairly general distributions.

The idea is shown in Figure 4.2. Assume that we want to generate random variables with density $0 \leq p(x) \leq d$, $a \leq x \leq b$. Suppose we can sample a uniformly distributed two-dimensional random variable (X, Y) in the shaded domain A, where

$$A := \{(x, y) \ : \ x \in [a, b], y \in [0, p(x)]\}.$$

The PDF of this random variable is the characteristic function of the domain A, $\chi_A(x, y)$. Its X-marginal distribution is

$$p_X(x) = \int_0^{p(x)} \chi_A(x, y) dy = \int_0^{p(x)} 1 dy = p(x).$$

The uniform distribution on domain A can be easily obtained from the uniform distribution in $[a, b] \times [0, d]$ by an acceptance-rejection procedure. This leads to the following *acceptance-rejection* algorithm:

Algorithm 5 (Acceptance-rejection method)**.**

Step 1. Generate $X_i \sim \mathcal{U}[a, b]$.

Step 2. Generate a decision-making random variable $Y_i \sim \mathcal{U}[0, d]$.

Step 3. If $0 \leq Y_i < p(X_i)$, accept; otherwise, reject.

Step 4. Back to Step 1.

For unbounded random variables, we can introduce more general *comparison functions*. Let f be such that $p < f$ holds everywhere. Such an f is called a comparison function. Assume that

$$\int_{-\infty}^{\infty} f(x) dx = Z$$

and we have an analytic expression for $F^{-1}(x)$, where

$$F(x) = \int_{-\infty}^{x} f(x) dx.$$
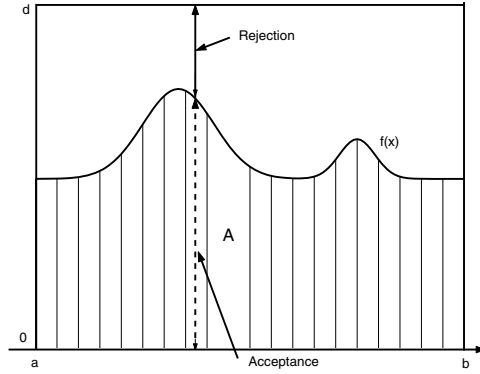
Figure 4.2. Schematics of the acceptance-rejection method.

Write the uniform measure on the set bounded by the graph of f, $x \in (-\infty, \infty), y \in [0, f(x)]$, as

$$\frac{1}{Z} f(x)dx \frac{1}{f(x)} dy.$$

This suggests a strategy for generating the two-dimensional uniform distribution on the set below the graph of f by conditional sampling.

Algorithm 6 (Acceptance-rejection with general comparison function)**.**

　　Step 1. Generate $X_i = F^{-1}(ZW_i)$, where $W_i \sim \mathcal{U}([0,1])$.

　　Step 2. Generate decision-making random variables $Y_i \sim \mathcal{U}[0, f(X_i)]$.

　　Step 3. If $0 \le Y_i < p(X_i)$, accept; otherwise, reject.

　　Step 4. Back to Step 1.

　　If p is bell-shaped, we commonly use the Cauchy distribution (or Lorentzian function) as a comparison function

$$f(y) = \frac{1}{\pi(1 + y^2)}.$$

The inverse function for the indefinite integral F is simply the tangent function. More generally, one can use

$$f(x) = \frac{c_0}{1 + (x - x_0)^2/a_0^2}$$

with suitable values of x_0, a_0, and c_0.

4.3. Variance Reduction

We see from (4.6) that there are two factors that affect the error of the Monte Carlo method: the sampling size N and the variance of f. Here N is

clearly limited by the computational cost we are willing to afford. But the variance can be manipulated in order to reduce the size of the error.

Importance Sampling. Consider for example the numerical evaluation of $\int_{-10}^{10} e^{-\frac{1}{2}x^2} dx$. Straightforward application of (4.4) would give

$$\int_{-10}^{10} e^{-\frac{1}{2}x^2} dx \approx \frac{20}{N} \sum_{i=1}^{N} e^{-\frac{1}{2}X_i^2},$$

where $\{X_i\}_{i=1}^{N}$ are i.i.d. random variables that are uniformly distributed on $[-10, 10]$. However, notice that the integrand $e^{-\frac{1}{2}x^2}$ is an extremely nonuniform function: Its value is very small everywhere except in a small neighborhood of $x = 0$. This means that most of the samples are wasted in the region with little contribution to the integral. The idea of *importance sampling* is to take the size of the integrand into account when sampling. This is schematically shown in Figure 4.3.
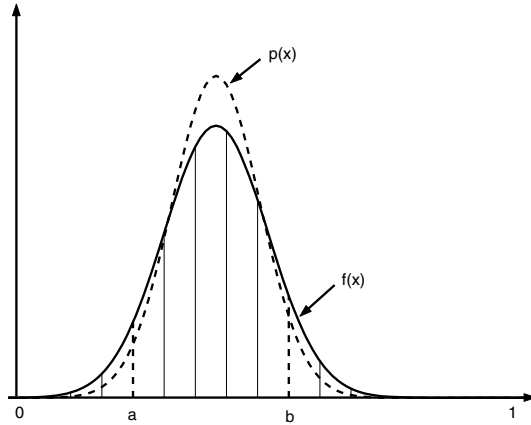
Figure 4.3.　Schematics of importance sampling.

If the $\{X_i\}$'s are sampled according to a different distribution, say with density function $p(x)$, then since

$$\int f(x)dx = \int \frac{f(x)}{p(x)} p(x)dx = \mathbb{E}\Big(\frac{f}{p}(X)\Big)$$

$$= \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \frac{f(X_i)}{p(X_i)},$$

we should approximate $\int f(x)dx$ by

$$I_N^p(f) = \frac{1}{N} \sum_{i=1}^{N} \frac{f(X_i)}{p(X_i)}.$$

The error can be estimated in the same way as before, and we get

$$\mathbb{E}(I(f) - I_N^p(f))^2 = \frac{1}{N} \text{Var}\left(\frac{f}{p}\right) = \frac{1}{N}\left(\int \frac{f^2(x)}{p(x)} dx - I^2(f)\right).$$

From this, we see that an ideal importance function is

$$p(x) = Z^{-1} f(x)$$

if f is nonnegative, where Z is the normalization factor $Z = \int f(x) dx$. In this case

$$I(f) = I_N^p(f).$$

This is not a miracle since all the necessary work has gone into computing Z, which was our original task.

Nevertheless, this suggests how the sample distribution should be constructed. For the example discussed earlier, we can pick $p(x)$ that behaves like $e^{-\frac{1}{2}x^2}$ and at the same time can be sampled with a reasonable cost. This is the basic idea behind importance sampling. One should note that importance sampling bears a lot of similarity with preconditioning in linear algebra.

A slight variant of these ideas is as follows [**Liu04**]. To compute

$$I = \int f(x)\pi(x) dx,$$

where π is a PDF, here is what we do:

(1) Draw $X_1, \ldots, X_N$ i.i.d. from a distribution g.

(2) Calculate the weight

$$w_j = \frac{\pi(X_j)}{g(X_j)}, \quad \text{for } j = 1, 2, \ldots, N.$$

(3) Approximate the integral by

(4.9)
$$\hat{I} = \frac{\sum_{i=1}^N w_i f(X_i)}{\sum_{i=1}^N w_i}.$$

We call $\hat{I}$ a *biased estimator* of I since $\mathbb{E}\hat{I} \neq I$. By the SLLN

$$\tilde{I} = \frac{1}{N}\sum_{i=1}^N w_i f(X_i) \to \mu \qquad \text{and} \qquad \frac{1}{N}\sum_{i=1}^N w_i \to 1$$

and hence

$$\hat{I} \to I \qquad \text{as } N \to \infty.$$

A major advantage of using (4.9) instead of $\tilde{I}$ is that we only need to compute weight function $\pi(x)/g(x)$ up to a multiplicative constant. This constant will be canceled between the denominator and the numerator in (4.9). If we use the estimator $\tilde{I}$, this constant needs to be computed.

Control Variates. Consider another form of $I(f)$:

$$I(f) = \int f(\boldsymbol{x})d\boldsymbol{x} = \int (f(\boldsymbol{x}) - g(\boldsymbol{x}))d\boldsymbol{x} + \int g(\boldsymbol{x})d\boldsymbol{x}.$$

The idea of *control variates* is quite simple. If $g(\boldsymbol{x})$ is very similar to $f(\boldsymbol{x})$, and $I(g)$ is known or can be approximated with good accuracy, then $\text{Var}(f-g) < \text{Var}(f)$ and we can obtain a variance reduced estimator of $I(f)$. Here g is called the control variates. The ideal control variates would be f itself if only we knew $I(f)$!

Example 4.4. Consider the integral

$$I(f) = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}}(1+r)^{-1}e^{-\frac{x^2}{2}}dx,$$

where $r = e^{\sigma x}$, $\sigma \gg 1$.

Notice that

$$(1+r)^{-1} \approx h(x) = \begin{cases} 1, & x \leq 0, \\ 0, & x > 0. \end{cases}$$

We have

$$I(f) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left((1+r)^{-1} - h(x)\right)e^{-\frac{x^2}{2}}dx + \frac{1}{2}.$$

Here $h(x)$ is the control variates.

Rao-Blackwellization. Suppose we have n independent samples $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$ drawn from the PDF $\pi(\boldsymbol{x})$ and we are interested in evaluating $I = \int f(\boldsymbol{x})\pi(\boldsymbol{x})d\boldsymbol{x}$. A straightforward estimator is

$$\hat{I} = \frac{1}{N} \sum_{i=1}^{N} f(\boldsymbol{X}_i).$$

Suppose that $\boldsymbol{x}$ can be decomposed into two parts $(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)})$ and the conditional expectation $\mathbb{E}(f(\boldsymbol{X})|\boldsymbol{x}^{(2)})$ can be approximated with good accuracy and low cost. We can define another unbiased estimator of I by

$$\tilde{I} = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}(f(\boldsymbol{X})|\boldsymbol{X}_i^{(2)}).$$

If the computational effort for obtaining the two estimates is similar, then $\tilde{I}$ should be preferred. This is because [**Dur10**]

$$(4.10) \qquad \text{Var}(f(\boldsymbol{X})) = \text{Var}(\mathbb{E}(f(\boldsymbol{X})|\boldsymbol{X}^{(2)})) + \mathbb{E}(\text{Var}(f(\boldsymbol{X})|\boldsymbol{X}^{(2)})),$$

which implies

$$\text{Var}(\hat{I}) = \frac{\text{Var}(f(\boldsymbol{X}))}{N} \geq \frac{\text{Var}(\mathbb{E}(f(\boldsymbol{X})|\boldsymbol{X}^{(2)}))}{N} = \text{Var}(\tilde{I}).$$

The above procedure is called Rao-Blackwellization. Readers are referred to [**Liu04**] for more details.

4.4. The Metropolis Algorithm

Another general strategy for sampling a distribution is to construct a Markov chain whose invariant distribution is the desired one. Denote by $\boldsymbol{\pi}$ the desired distribution and by $\boldsymbol{P}$ the transition matrix of the Markov chain that we would like to construct. Then $\boldsymbol{P}$ must satisfy

$$(4.11) \qquad\qquad \boldsymbol{\pi P} = \boldsymbol{\pi}.$$

For an n-state Markov chain, $\boldsymbol{P}$ has n^2 unknowns and (4.11) only gives n linear equations. This is an underdetermined problem. Therefore, it is convenient to impose the additional constraint, the detailed balance condition,

$$(4.12) \qquad\qquad \pi_i p_{ij} = \pi_j p_{ji},$$

which is stronger than the global balance condition (4.11).

For the case when $\boldsymbol{\pi}$ is a Gibbs distribution, i.e., $\pi_i = \frac{1}{Z} e^{-\beta H_i}$, (4.12) implies that

$$\frac{p_{ij}}{p_{ji}} = \frac{\pi_j}{\pi_i} = e^{-\beta \Delta H_{ij}},$$

where $\Delta H_{ij} = H_j - H_i$. The Metropolis algorithms are a class of Markov chain Monte Carlo methods (MCMC) that respect the detailed balance condition. They consist of two steps:

a) *Proposal step:* propose a new configuration.

b) *Decision step:* accept or reject this new configuration.

Accordingly, $\boldsymbol{P} = (p_{ij})$ is designed to have the form

$$p_{ij} = \begin{cases} Q_{ij} A_{ij}, & \text{for } i \neq j, \\ 1 - \sum_{j \neq i} p_{ij}, & \text{for } i = j, \end{cases}$$

where $\boldsymbol{Q} = (Q_{ij})$ is a transition probability matrix with Q_{ij} being the probability of generating state j from state i and A_{ij} is the probability of accepting state j. We will call $\boldsymbol{Q}$ the *proposal matrix* and $\boldsymbol{A}$ the *decision matrix*. We will require $\boldsymbol{Q}$ to be symmetric for the moment:

$$Q_{ij} = Q_{ji}.$$

Then the detailed balance condition is reduced to

$$\frac{A_{ij}}{A_{ji}} = e^{-\beta \Delta H_{ij}}.$$

Two popular choices of A_{ij} are:

- The Metropolis strategy.

(4.13) $$A_{ij} = \min(1, e^{-\beta \Delta H_{ij}}).$$

- Glauber dynamics.

(4.14) $$A_{ij} = \left(1 + e^{\beta \Delta H_{ij}}\right)^{-1}.$$

Both choices satisfy the detailed balance condition. Usually the Metropolis strategy results in faster convergence since its off-diagonal elements are larger than those of the Glauber dynamics [**Liu04**]. Note that in the Metropolis strategy, we accept the new configuration if its energy is lower than that of the current state. But if the energy of the new configuration is higher, we still accept it with some positive probability.

The choice of $\boldsymbol{Q}$ depends on the specific problem. To illustrate this, we consider the one-dimensional Ising model as an example.

Example 4.5. Shown in Figure 4.4 is a one-dimensional model for the magnetization of a ferromagnet. The lattice has M sites, the state space $S = \{\boldsymbol{x}\} = \{+1, -1\}^M$. It has 2^M states in total. The states at the sites are called spins. The microscopic configurations are described by

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_M),$$

where $x_i = +1$ or -1 for $i = 1, \ldots, M$, when the state of the ith spin is ↑ or ↓, respectively.
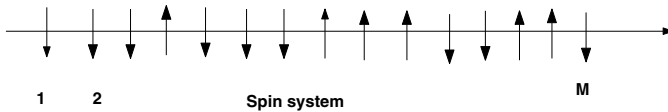
Figure 4.4. One-dimensional Ising model with M sites.

The behavior of the system is determined by its Hamiltonian, which is a function of the spin configuration. For the Ising model, the Hamiltonian is given by

$$H(\boldsymbol{x}) = -J \sum_{\langle i,j \rangle} x_i x_j - h \sum_{i=1}^{M} x_i, \quad J > 0, h > 0,$$

where $\boldsymbol{x}$ is a specific microscopic state, J is an interaction parameter, h is the strength of the external magnetic field, $\langle i, j \rangle$ means that the summation

is taken over all nearest neighbor spins, i.e., $|i - j| = 1$. The magnetization of the system at a specific state $\boldsymbol{x}$ is defined by

$$M_a(\boldsymbol{x}) = \sum_{i=1}^{M} x_i.$$

The average magnetization (i.e., magnetization per site) is $m(\boldsymbol{x}) = M_a(\boldsymbol{x})/M$.

In equilibrium statistical mechanics, we are interested in the thermodynamic average of some function $f(\boldsymbol{x})$ given by

$$(4.15) \qquad \langle f \rangle = \sum_{\boldsymbol{x} \in S} f(\boldsymbol{x}) \pi(\boldsymbol{x}) \qquad \text{or} \qquad \int_S f(\boldsymbol{x}) \pi(\boldsymbol{x}) d\boldsymbol{x},$$

where $\pi(\boldsymbol{x})$ is the Gibbs distribution. In particular, the thermodynamic average magnetization of the Ising model is

$$(4.16) \qquad m = \sum_{\boldsymbol{x}} m(\boldsymbol{x}) \frac{\exp(-\beta H(\boldsymbol{x}))}{Z_M} = \sum_{\boldsymbol{x}} m(\boldsymbol{x}) \pi(\boldsymbol{x}).$$

With the Metropolis algorithm, we will approximate these thermodynamic averages by using

$$(4.17) \qquad \langle f \rangle \approx \langle f \rangle_N := \frac{1}{N} \sum_{j=1}^{N} f(X_j),$$

where $\{X_j\}$ is the time series generated according to the Markov chain $\boldsymbol{P}$. The ergodic Theorem 3.12 ensures the convergence of the empirical average (4.17) if the chain $\boldsymbol{P}$ satisfies the irreducibility and primitivity conditions.

Coming back to the choice of $\boldsymbol{Q}$, let $N_t = 2^M$, the total number of microscopic configurations. The following are two simple options:

Proposal 1. Equiprobability proposal.

$$Q(\boldsymbol{x} \to \boldsymbol{y}) = \begin{cases} \frac{1}{N_t - 1}, & \boldsymbol{x} \neq \boldsymbol{y}, \\ 0, & \boldsymbol{x} = \boldsymbol{y}. \end{cases}$$

Proposal 2. Single flip proposal (Gibbs sampling).

$$(4.18) \qquad Q(\boldsymbol{x} \to \boldsymbol{y}) = \begin{cases} \frac{1}{M}, & \boldsymbol{x} \neq \boldsymbol{y} \text{ only at one site,} \\ 0, & \text{otherwise.} \end{cases}$$

Here $Q(\boldsymbol{x} \to \boldsymbol{y})$ denotes the proposal probability from the configuration $\boldsymbol{x}$ to $\boldsymbol{y}$. Proposal 1 may seem to be more straightforward but it is more difficult to implement since it needs to order the $2^M - 1$ states in each step.

In summary, having generated the sequence of configurations $X_1, X_2, \ldots,$ X_n, the new configuration X_{n+1} is generated via the following steps.

Algorithm 7 (Metropolis algorithm).

  Step 1. Generate a new configuration $Y = j$ from $X_n = i$ according to proposal $\boldsymbol{Q}$.

  Step 2. Compute the acceptance probability A_{ij} according to (4.13).

  Step 3. Generate a random variable $R \sim \mathcal{U}[0, 1]$.

  Step 4. If $R \leq A_{ij}$, then $X_{n+1} = Y = j$; otherwise $X_{n+1} = X_n = i$, and return to Step 1.

We should remark that the symmetry condition for the proposal matrix $\boldsymbol{Q}$ can also be relaxed, and this leads to the *Metropolis-Hastings* algorithm:

$$(4.19) \qquad A_{ij} = \min\left(1, \frac{Q_{ji}\pi_j}{Q_{ij}\pi_i}\right).$$

There is an obvious balance between the proposal step and the decision step. One would like the proposal step to be more aggresive since this will allow us to sample larger parts of the configuration space. However, this may also result in more proposals being rejected.

Regarding the issue of convergence, we refer the readers to [**Liu04**, **Win03**].

Application to Bayesian Statistics. In statistical inference, one is required to establish statistical models to interpret the available data $\boldsymbol{X} = \{X_i\}_{i=1:n}$. Assume that the distribution density of the chosen model is $p(\boldsymbol{x}|\boldsymbol{\theta})$, where $\boldsymbol{\theta}$ is the parameter to be estimated from the data. Then the joint distribution for the observed data, assumed to be i.i.d., has the form

$$(4.20) \qquad L(\boldsymbol{\theta}|\boldsymbol{X}) = \prod_{i=1}^{n} p(X_i|\boldsymbol{\theta}).$$

$L(\boldsymbol{\theta}|\boldsymbol{X})$ is called the *likelihood function*. The determination of the parameter $\boldsymbol{\theta}$ can be done through the maximum likelihood estimate; i.e.,

$$\theta^* = \arg\max_{\boldsymbol{\theta}} L(\boldsymbol{\theta}|\boldsymbol{X}).$$

On the other hand, in Bayesian statistics, the parameter $\boldsymbol{\theta}$ is considered as a random variable with prior distribution $\mu(\boldsymbol{\theta})$. The philosophy is that our prior knowledge on $\boldsymbol{\theta}$ will be improved by integrating the data. With Bayes's rule, we get the posterior distribution

$$(4.21) \qquad \pi(\boldsymbol{\theta}|\boldsymbol{X}) = \frac{L(\boldsymbol{\theta}|\boldsymbol{X})\mu(\boldsymbol{\theta})}{\int L(\boldsymbol{\theta}|\boldsymbol{X})\mu(\boldsymbol{\theta})d\boldsymbol{\theta}} = \frac{1}{Z}L(\boldsymbol{\theta}|\boldsymbol{X})\mu(\boldsymbol{\theta}),$$

where $Z = \int L(\boldsymbol{\theta}|\boldsymbol{X})\mu(\boldsymbol{\theta})d\boldsymbol{\theta}$ is simply a normalization constant that only depends on the data $\boldsymbol{X}$. One can sample the posterior distribution of $\boldsymbol{\theta}$ according to (4.21) or extract the posterior mean by

$$\bar{\boldsymbol{\theta}} = \mathbb{E}\boldsymbol{\Theta} = \int \boldsymbol{\theta}\pi(\boldsymbol{\theta}|\boldsymbol{X})d\boldsymbol{\theta}$$

using the Metropolis algorithm. The Markov chain Monte Carlo method is perfect here for computing $\bar{\boldsymbol{\theta}}$ since it does not need the actual value of Z.

4.5. Kinetic Monte Carlo

Kinetic Monte Carlo (KMC) is the extension of the Metropolis type of algorithms for simulating dynamic processes such as growth processes. The first such algorithm, the BKL algorithm proposed by Bortz, Kalos, and Lebowitz [**BKL75**], was also motivated by trying to develop a rejection-free Monte Carlo method.

To illustrate the idea, we still use the one-dimensional Ising model as an example. Given any configuration, we divide its sites into six different types according to the local environment of each spin, as shown in Table 4.1. If the spin at a site is flipped, the energy difference between the new and the old configurations depends only on the type of that site. We denote these flipping probabilities by $P_j = \min(1, \exp(-\beta\Delta H_j))$ for $j = 1, \ldots, 6$, where ΔH_j is the energy difference between the flipped and previous states if the flipped site is of the jth type before flipping.

Table 4.1. Classification of sites according to the spins at the site and neighboring sites.

Class	Spin	Number of neighboring spin ups
1	↑	2
2	↑	1
3	↑	0
4	↓	2
5	↓	1
6	↓	0

For each given state $\boldsymbol{x}$, let n_j be the number of sites in the jth class, and define

$$Q_i = \sum_{j=1}^{i} n_j P_j, \quad i = 1, \ldots, 6,$$

and $Q_0 = 0$. The BKL algorithm works as follows.

Algorithm 8 (BKL algorithm). Kinetic Monte Carlo method.

   Step 1. Generate $R \sim \mathcal{U}[0, Q_6)$.

   Step 2. Identify the index K, such that $Q_{K-1} \leq R < Q_K$, where $K \in \{1, 2, \ldots, 6\}$.

   Step 3. Randomly choose a site to flip in the Kth class of sites.

   This algorithm is obviously rejection free.

   The weight of each configuration, i.e., the time increment between configurations, is determined as follows. Suppose on the average there is a physical time T_a during which each site attempts to make a flip. Then the probability for a site to succeed in flipping in a unit time is given by Q_6/T_a. Similar to the derivation of (3.10), the waiting time between two flips is exponentially distributed and can be sampled according to

$$\tau = -\frac{T_a}{Q_6} \log R, \quad R \sim \mathcal{U}[0, 1].$$

It then follows from Theorem 3.18 that instead of (4.17), one should use

(4.22) $$\langle f \rangle_{\boldsymbol{\pi}} \approx \frac{1}{\sum_j \tau_j} \sum_j f(X_j) \tau_j.$$

However note that if the aim is to compute some thermodynamic averages, then the value of T_a does not matter since it is cancelled between the numerator and the denominator in (4.22). One can simply choose $T_a = 1$ in the simulation.

   From a mathematical viewpoint, we can also view KMC as being the result of replacing the discrete time Markov chain in Markov chain Monte Carlo with a continuous time Q-process with the $\boldsymbol{Q}$-matrix

$$\begin{cases} q_{ij} &= 1_{Q_{ij}} A_{ij}, \quad \text{for} \quad i \neq j, \\ q_{ii} &= -\sum_{j \neq i} q_{ij}, \end{cases}$$

where $1_{Q_{ij}} = 1$ if $Q_{ij} > 0$ and $1_{Q_{ij}} = 0$ otherwise. A_{ij} is the Metropolis acceptance probability.

4.6. Simulated Tempering

When we sample the Gibbs distribution

$$\pi(x) \propto \exp\left(-\frac{U(x)}{T}\right), \quad x \in \mathcal{X},$$

or compute the ensemble average like $\langle f \rangle_\pi$ via the MCMC algorithm, the Metropolis acceptance probability will generally be very small when climbing a barrier in the energy landscape at low temperature T. This feature implies a low mixing rate, i.e., low efficiency to explore the whole energy landscape

of $U(x)$. This issue becomes quite severe when we have multiple peaks in $\pi(x)$, which is very common in real applications (see Figure 4.5).

To improve the mixing rate of the MCMC algorithm in the low temperature regime, Marinari and Parasi [**MP92**] and Geyer and Thompson [**GT95**] proposed the simulated tempering technique, by varying the temperature during the simulation. The idea of simulated tempering is to utilize the virtue of the fast exploration on the overall energy landscape at high temperature and the fine resolution of local details at low temperature, thus reducing the chances that the simulation gets trapped at local metastable states.
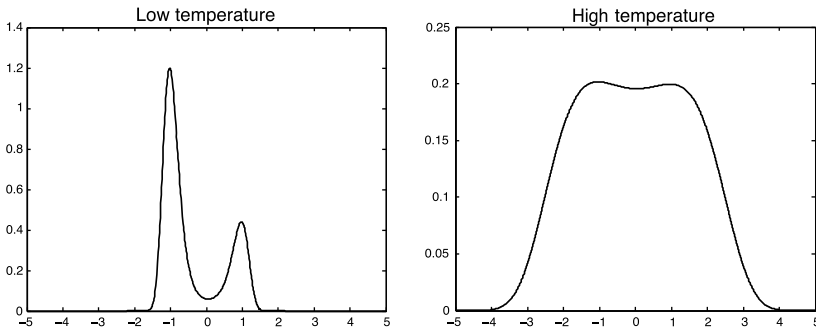
Figure 4.5. The Gibbs distribution at low temperature (left panel) and high temperature (right panel).

For the mathematical formulation of simulated tempering, consider a stationary distribution on the augmented space $\mathcal{X} \times I$:

$$(4.23) \qquad \pi_{\mathrm{st}}(x, i) \propto \pi_i \exp\Big(- \frac{U(x)}{T_i} \Big), \quad (x, i) \in \mathcal{X} \times I,$$

where π_i is called a pseudo-prior and is set up a priori and the set I and T_i are defined as

$$I = \{1, 2, \ldots, L\}, \quad T_1 < T_2 < \cdots < T_L.$$

Here $T_1 = T$, $T_L = T_{\mathrm{high}}$.

With this definition, we have the conditional distribution

$$\pi_{\mathrm{st}}(x|i) \propto \exp\Big(- \frac{U(x)}{T_i} \Big)$$

which is the standard Gibbs distribution at the temperature T_i. The marginal distribution

$$\pi_{\mathrm{st}}(i) \propto \int \pi_i \exp\Big(- \frac{U(x)}{T_i} \Big) dx = \pi_i Z_i.$$

To make the transition in different temperatures more uniform, the best choice for the parameters should satisfy $\pi_i \propto 1/Z_i$. Unfortunately this is

not feasible in real applications and one only obtains some guidance through some pilot studies [**GT95**].

To perform the MCMC in the augmented space, here we present a mixture-type conditional sampling instead of a deterministic alternating approach.

Algorithm 9 (Simulated tempering). Set mixture weight $\alpha_0 \in (0, 1)$.

    Step 1. Given $(x_n, i_n) = (x, i)$, draw $u \sim \mathcal{U}[0, 1]$.

    Step 2. If $u < \alpha_0$, let $i_{n+1} = i$ and sample x_{n+1} with the MCMC for the Gibbs distribution $\pi_{\text{st}}(x|i)$ from the current state x_n.

    Step 3. If $u \geq \alpha_0$, let $x_{n+1} = x$ and sample i_{n+1} with the MCMC for the distribution $\pi_{\text{st}}(i|x)$ from the current state i_n.

In Step 3, we also generate a proposal with transition probability $\alpha(i, j)$ from index i to j and then the Metropolis type decision step in the MCMC sampling. A commonly used strategy for $\alpha(i, j)$ is the random walk proposal with reflecting barrier; that is,

$$\alpha(i, i \pm 1) = 1/2, \quad i = 2, \ldots, L - 1,$$

and $\alpha(1, 2) = \alpha(L, L - 1) = 1$. This is easy to implement and increases the acceptance probability.

4.7. Simulated Annealing

Global optimization is among the most important and most challenging problems in scientific computing. In fact, almost all optimization algorithms such as the gradient decent methods or quasi-Newton methods are only able to find local minima of the objective function. For many practical problems, the objective function has many local minima and only the global minimum or local minima with the values of the objective function close to that of the global minimum are of real interest.

To find the global minimum, the algorithm needs to be able to do two things:

    Task 1. Find local minima.

    Task 2. Overcome the barriers between different local minima.

Deterministic methods are often effective in performing the first task but not the second. Stochastic algorithms are often effective in performing the second task but less so for the first. Simulated annealing is a stochastic algorithm but the amplitude of the noise is tuned so that ideally, it is large at the barrier-crossing stage but small when seeking minima.

Let H be the objective function. The idea of simulated annealing is to associate the optimization problem $\min_{x \in \mathcal{X}} H(x)$ with a parameterized Gibbs distribution

$$(4.24) \qquad \pi_\beta(x) = \frac{1}{Z_\beta} e^{-\beta H(x)}, \qquad Z_\beta = \sum_{x \in \mathcal{X}} \exp(-\beta H(x)),$$

where $\beta > 0$ resembles the inverse temperature in statistical physics. Define the global minimizers of H by

$$\mathcal{M} = \{x_0 \ : \ H(x_0) = \min_{x \in \mathcal{X}} H(x)\}.$$

Theorem 4.6. *The Gibbs distribution has the limit*

$$\lim_{\beta \to +\infty} \pi_\beta(x) = \begin{cases} \frac{1}{|\mathcal{M}|}, & \text{if } x \in \mathcal{M}, \\ 0, & \text{othewise,} \end{cases}$$

where $|\mathcal{M}|$ is the number of elements in the set $\mathcal{M}$. If $x \in \mathcal{M}$, then for sufficiently large β, $\pi_\beta(x)$ is monotonically increasing as a function of β. If $x \notin \mathcal{M}$, then for sufficiently large β, $\pi_\beta(x)$ is monotonically decreasing as a function of β.

Proof. Define $m = \min_x H(x)$. Then

$$\pi_\beta(x) \quad = \quad \frac{e^{-\beta(H(x)-m)}}{\sum_{z \in \mathcal{M}} e^{-\beta(H(z)-m)} + \sum_{z \notin \mathcal{M}} e^{-\beta(H(z)-m)}}$$

$$\xrightarrow{\beta \to +\infty} \begin{cases} 1/|\mathcal{M}|, & x \in \mathcal{M}, \\ 0, & x \notin \mathcal{M}. \end{cases}$$

If $x \in \mathcal{M}$, we have

$$\pi_\beta(x) = \frac{1}{|\mathcal{M}| + \sum_{z \notin \mathcal{M}} e^{-\beta(H(z)-m)}};$$

hence $\pi_\beta(x)$ monotonically increases with β.

If $x \notin \mathcal{M}$, we have

$$\frac{\partial \pi_\beta(x)}{\partial \beta} = \frac{1}{\tilde{Z}_\beta^2} \Big(e^{-\beta(H(x)-m)} \Big[(m - H(x))\tilde{Z}_\beta - \sum_{z \in \mathcal{X}} e^{-\beta(H(z)-m)}(m - H(z)) \Big] \Big),$$

where $\tilde{Z}_\beta := \sum_{z \in \mathcal{X}} \exp(-\beta(H(z) - m))$. Note that

$$\lim_{\beta \to +\infty} \Big[(m - H(x))\tilde{Z}_\beta - \sum_{z \in \mathcal{X}} e^{-\beta(H(z)-m)}(m - H(z)) \Big]$$

$$= |\mathcal{M}|(m - H(x)) < 0.$$

Hence $\pi_\beta(x)$ is monotonically decreasing in β. $\qquad \square$

Physically, $\beta \to \infty$ corresponds to the limit as the temperature goes to 0. This procedure is called *annealing.* One may imagine the following process: One starts at a very high temperature, which allows the algorithm to explore the configuration space. One then decreases the temperature slowly until the temperature is close to 0. This allows the system to settle down to the minimum. This is the physical intuition behind simulated annealing.

Let

$$P_\beta(x, y) = \begin{cases} Q(x, y) \frac{\pi_\beta(y)}{\pi_\beta(x)}, & \pi_\beta(y) < \pi_\beta(x) \text{ and } x \neq y, \\ Q(x, y), & \pi_\beta(y) \geq \pi_\beta(x) \text{ and } x \neq y, \\ 1 - \sum_{z \neq x} P_\beta(x, z), & x = y, \end{cases}$$

where $Q(x, y)$ is the proposal matrix, assumed to be symmetric. During annealing, the temperature gradually changes: At the nth step, $\beta = \beta(n)$. A key question is how to choose $\beta(n)$.

Theorem 4.7 (Convergence of simulated annealing). *Assume that H is defined over a finite set $\mathcal{X}$ and Q is a symmetric irreducible proposal matrix. If the annealing procedure is chosen such that $\beta(n) \leq C \log n$, where C only depends on the structure of Q and function H, then for any initial distribution μ_0 we have*

$$\lim_{n \to +\infty} \|\mu_0 P_{\beta(1)} \cdots P_{\beta(n)} - \pi_\infty\| = 0,$$

where $\|\mu_1 - \mu_2\| := \sum_x |\mu_1(x) - \mu_2(x)|$ is the total variation norm.

The proof of this theorem can be found in [**Win03**].

The above theorem requires an extremely slow annealing rate: $n \sim O(\exp(N_0))$ if $\beta(n) = N_0 \gg 1$. This means an exponentially long computing time. In practice, one often uses a faster cooling rate such as $\beta(n) \sim p^{-n}$ with $p \lesssim 1$. The theoretical analysis of these kinds of situations is still largely open.

Exercises

4.1. For different choices of N, apply the simple Monte Carlo method and importance sampling to approximate the integral

$$I(f) = \int_{-10}^{10} e^{-\frac{1}{2}x^2} dx.$$

Test the half-order convergence $|I_N(f) - I(f)| \sim C N^{-\frac{1}{2}}$ and compare the error constant C.

4.2. Construct at least two algorithms for sampling the uniform distribution on the two-dimensional unit sphere: $\mathcal{U}(\mathbb{S}^2)$. Implement them and make a comparison on their efficiency.

4.3. Derive the overall rejection probability of Algorithms 5 and 6.

4.4. Suppose that the PDF $p(x)$ of X has the bounds $0 \leq g_l(x) \leq p(x) \leq Mg_u(x)$, where M is a positive constant and $g_u(x)$ is a PDF. Show that the following *squeeze* acceptance-rejection algorithm generates $X_i \sim p(x)$ and compare it with Algorithm 6.
   (a) Step 1. Generate $X_i \sim g_u(x)$, $Y_i \sim \mathcal{U}[0,1]$.
   (b) Step 2. Accept X_i if $Y_i \leq g_l(X_i)/Mg_u(X_i)$.
   (c) Step 3. Otherwise accept X_i if $Y_i \leq p(X_i)/Mg_u(X_i)$.

4.5. (*Antithetic variables*) The following is an example of the variance reducation method for estimating $I(f) = \int_0^1 f(x)dx$. Define

$$I_{2N}(f) = \frac{1}{2N} \sum_{i=1}^{N} (f(X_i) + f(1 - X_i)), \qquad X_i \sim \text{i.i.d. } \mathcal{U}[0,1].$$

Prove that if $X \sim \mathcal{U}[0,1]$ and f is monotone, then

$$\text{Cov}(f(X), f(1 - X)) \leq 0.$$

Prove that the estimator $I_{2N}(f)$ has a smaller variance compared with the estimator obtained by straightforward averaging using $2N$ samples.

4.6. (*Stratified sampling*) We are interested in computing

$$I = \int_0^1 f(x)dx.$$

Divide $S = [0,1]$ into M equipartitions $S_k = [(k-1)/M, k/M]$ ($k = 1, 2, \ldots, M$) and sample $N_k = N/M$ points uniformly in S_k, denoted as $X_i^{(k)}$, $i = 1, \ldots, N_k$. Define the estimator

$$I_N = \frac{1}{N} \sum_{k=1}^{M} \sum_{i=1}^{N_k} f(X_i^{(k)}).$$

Prove that the variance is reduced with this uniformization; i.e.,

$$\text{Var}(I_N) \leq \text{Var}(I) = \int_S (f(x) - I)^2 dx.$$

4.7. Prove that both the Metropolis strategy (4.13) and Glauber dynamics (4.14) satisfy the detailed balance condition.

4.8. Prove that when the proposal matrix $\boldsymbol{Q}$ is not symmetric, the detailed balance condition can be preserved by choosing the *Metropolis-Hastings* decision matrix (4.19).

4.9. Prove that the Markov chain set up by the Gibbs sampling (4.18) and Metropolis strategy (4.13) is primitive for the one-dimensional Ising model.

4.10. Consider the two-dimensional Ising model on the $M \times M$ periodic lattice.

(a) Prove that the Gibbs distribution

$$\pi(\boldsymbol{x}) \propto \exp\left(\beta J \sum_{\langle i,j \rangle} x_i x_j\right) \propto \prod_{\langle i,j \rangle} \exp\left\{\beta J(1 + x_i x_j)\right\}.$$

(b) Define the bond variable $\boldsymbol{u} = (u_{ij})$ on each edge and the extended Gibbs distribution

$$\pi(\boldsymbol{x}, \boldsymbol{u}) \propto \prod_{\langle i,j \rangle} \chi_{\{0 \le u_{ij} \le \exp\{\beta J(1+x_i x_j)\}\}}(\boldsymbol{x}, \boldsymbol{u}).$$

Show that the marginal distribution of $\boldsymbol{x}$ is simply $\pi(\boldsymbol{x})$, and derive the conditional distributions $\pi(\boldsymbol{u}|\boldsymbol{x})$ and $\pi(\boldsymbol{x}|\boldsymbol{u})$.

4.11. Describe a Metropolis Monte Carlo algorithm to compute

$$\frac{\int_{-10}^{10} e^{-x^2/a} dx}{\int_{-10}^{10} e^{-x^2/b} dx},$$

where a and b are positive constants. Make an computational test when $a = 10$ and $b = 12$.

4.12. Consider a function H on $\mathbb{R}^d$ such that $H \in C^2(\mathbb{R}^d)$, $H(\boldsymbol{x}) \to \infty$ as $|\boldsymbol{x}| \to \infty$. Let

$$\mathcal{M} = \{\boldsymbol{x}_0 : H(\boldsymbol{x}_0) = \min H(\boldsymbol{x})\}.$$

Assume that $|\mathcal{M}|$ is finite and the Hessian $\nabla^2 H(\boldsymbol{x}_0)$ is positive definite for all $\boldsymbol{x}_0 \in \mathcal{M}$. Study the limit of the Gibbs distribution

$$\pi_\beta(\boldsymbol{x}) = \frac{1}{Z_\beta} e^{-\beta H(\boldsymbol{x})}$$

as $\beta \to \infty$, where Z_β is assumed to be finite for any positive β.

Notes

Buffon's needle problem is considered as the most primitive form of the Monte Carlo methods [**Ram69**]. The modern Monte Carlo method begins from the pioneering work of von Neumann, Ulam, Fermi, Metropolis, et al. in the 1950s [**And86**, **Eck87**].

A more detailed discussion on variance reduction can be found in [**Gla04**]. In practical applications, the choice of the proposal is essential for the efficiency of the Markov chain Monte Carlo method. In this regard, we mention Gibbs sampling which is easy to implement, but its efficiency for high-dimensional problems is questionable. More global moves like the Swendsen-Wang algorithm have been proposed [**Tan96**]. Other

developments for multilevel sampling include parallel tempering [**Gey91**], equienergy sampler [**KZW06**], and the infinite swapping method [**YLAVE16**]. For practical applications of the MC, we refer to [**FS02**, **Gla04**, **KW08**, **LB05**, **Liu04**].

Stochastic Processes

Before going further, we discuss briefly the general features of two most important classes of stochastic processes, the Markov process and the Gaussian process.

There are two ways to think about stochastic processes:

(1) As random functions of one variable. In this picture, we think about the properties of the paths which are individual realizations of the random function. Events are sets of paths. One particularly interesting issue is whether typical paths are continuous.

   The natural extension would be random functions of more than one variable. These are called random fields. We will come to this topic later in the book.

(2) As a probability distribution on the path spaces, i.e., spaces of functions of one variable. Path spaces are often infinite-dimensional spaces. Measure theory tells us that there are no analogs of the Lebesgue measure, i.e., translation invariant measure, on such spaces. Therefore constructing nontrivial measures on such spaces is itself a very nontrivial task.

   If we observe a stochastic process at a fixed finite set of points, we get a random vector whose distribution is of course on a finite-dimensional space. Obviously this family of distributions, parametrized by the set of points, is determined by the original stochastic process. Kolmogorov's extension theorem tells us that the converse is also true, as long as the measures in this family satisfy

obvious consistency conditions. This gives us a starting point for constructing stochastic processes, by specifying a family of consistent finite-dimensional distributions.

5.1. Axiomatic Construction of Stochastic Process

Example 5.1. Consider the independent fair coin tossing process described by the sequence

$$X = (X_1, X_2, \ldots, X_n, \ldots) \in \{0,1\}^{\mathbb{N}},$$

where $X_n = 0$ or 1 if the nth output is "Tail" (T) or "Head" (H), respectively. Different trials are assumed to be independent and $\mathbb{P}(X_n = 0) = \mathbb{P}(X_n = 1) = 1/2$.

Notice that for this process the number of all possible outputs is uncountable. We cannot just define the probability of an event by summing up the probabilities of every atom in the event, as for the case of discrete random variables. In fact, if we define $\Omega = \{H, T\}^{\mathbb{N}}$, the probability of an *atom* $\omega = (\omega_1, \omega_2, \ldots, \omega_n, \ldots) \in \{H, T\}^{\mathbb{N}}$ is 0; i.e.,

$$\mathbb{P}(X_1(\omega) = k_1, X_2(\omega) = k_2, \ldots, X_n(\omega) = k_n, \ldots)$$
$$= \lim_{n \to \infty} \left(\frac{1}{2}\right)^n = 0, \qquad k_j \in \{0,1\}, \ j = 1, 2, \ldots$$

and events such as $\{X_n(\omega) = 1\}$ involve uncountably many elements.

To set up a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ for this process, it is natural to take $\Omega = \{H, T\}^{\mathbb{N}}$ and the σ-algebra $\mathcal{F}$ as the smallest σ-algebra containing all events of the form

$$(5.1) \qquad C = \left\{\omega | \omega \in \Omega, \omega_{i_k} = a_k \in \{H, T\}, \ k = 1, 2, \ldots, m\right\}$$

for any $1 \le i_1 < i_2 < \cdots < i_m$ and $m \in \mathbb{N}$. These are sets whose finite time projections are specified. They are called *cylinder sets*, which form an algebra in $\mathcal{F}$. We denote them generically by C. The probability of an event of the form (5.1) is given by

$$\mathbb{P}(C) = \frac{1}{2^m}.$$

It is straightforward to check that for any cylinder set $F \in \mathcal{C}$, the probability $\mathbb{P}(F)$ coincides with the one defined in Example 5.1 for the independent coin tossing process. From the extension theorem of measures, this probability measure $\mathbb{P}$ is uniquely defined on $\mathcal{F}$ since it is well-defined on $\mathcal{C}$ [**Bil79**].

Another natural way is to take $\Omega = \{0,1\}^{\mathbb{N}}$, $\mathcal{F}$ being the smallest σ-algebra containing all cylinder sets in Ω, and $\mathbb{P}$ is defined in the same way as above. With this choice we have

$$X_n(\omega) = \omega_n, \quad \omega \in \Omega = \{0,1\}^{\mathbb{N}},$$

which is called a *coordinate process* in the sense that $X_n(\omega)$ is just the nth coordinate of ω.

In general, a stochastic process is a parameterized random variable $\{X_t\}_{t \in \mathbf{T}}$ defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ taking values in $\mathbb{R}$; the parameter set $\mathbf{T}$ can be $\mathbb{N}$, $[0, +\infty)$, or some finite interval. For any fixed $t \in \mathbf{T}$, we have a random variable

$$X_t : \Omega \to \mathbb{R}, \qquad \omega \rightarrowtail X_t(\omega).$$

For any fixed $\omega \in \Omega$, we have a real-valued measurable function on $\mathbf{T}$

$$X_.(\omega) : \mathbf{T} \to \mathbb{R}, \qquad t \rightarrowtail X_t(\omega).$$

This is called a trajectory or sample path of X. As a bivariate function, a stochastic process can also be viewed as a measurable function from $\Omega \times \mathbf{T}$ to $\mathbb{R}$

$$(\omega, t) \rightarrowtail X(\omega, t) := X_t(\omega),$$

with the σ-algebra in $\Omega \times \mathbf{T}$ chosen as $\mathcal{F} \times \mathcal{T}$ and where $\mathcal{T}$ is the Borel σ-algebra on $\mathbf{T}$.

The largest probability space that one can take is the infinite product space $\Omega = \mathbb{R}^{\mathbf{T}}$; i.e., Ω is the space of all real-valued functions on $\mathbf{T}$. Here $\mathcal{F}$ can be taken as the infinite product σ-algebra $\mathcal{R}^{\mathbf{T}}$, which is the smallest σ-algebra containing all cylinder sets

$$C = \{\omega \in \mathbb{R}^{\mathbf{T}} | (\omega(t_1), \omega(t_2), \ldots, \omega(t_k)) \in A\}, \quad A \in \mathcal{R}^k, \ t_i \in \mathbf{T} \text{ for } i = 1, \ldots, k,$$

where $\mathcal{R}, \mathcal{R}^k$ are the Borel σ-algebras on $\mathbb{R}$ and $\mathbb{R}^k$, respectively. When $\mathbf{T} = \mathbb{N}$ and X_t takes values in $\{0, 1\}$, we are back to the setting of Example 5.1.

Finite-dimensional distributions are particularly interesting for a stochastic process since they are the ones we can really observe. Let

$$\mu_{t_1, \ldots, t_k}(F_1 \times F_2 \times \cdots \times F_k) = \mathbb{P}[X_{t_1} \in F_1, \ldots, X_{t_k} \in F_k]$$

for all $F_1, F_2, \ldots, F_k \in \mathcal{R}$. Here $\mu_{t_1, \ldots, t_k}$ are called the finite-dimensional distributions of $\{X_t\}_{t \in \mathbf{T}}$ at the time slice $(t_1, \ldots, t_k)$, where $t_i \in \mathbf{T}$ for $i = 1, 2, \ldots, k$.

The following theorem of Kolmogorov states that an abstract probability space $(\Omega, \mathcal{F}, \mathbb{P})$ can be established for a stochastic process X by knowing all its finite-dimensional distributions with suitable consistency conditions.

Theorem 5.2 (Kolmogorov's extension theorem). *Let $\{\mu_{t_1,\ldots,t_k}\}$ be a family of finite-dimensional distributions that satisfy the following consistency conditions for arbitrary sets of $t_1, t_2, \ldots, t_k \in \mathbf{T}$ and $F_1, \ldots, F_k \in \mathcal{R}$, $k \in \mathbb{N}$.*

(i) *For any permutation σ of $\{1, 2, \ldots, k\}$,*

$$\mu_{t_{\sigma(1)},\ldots,t_{\sigma(k)}}(F_1 \times F_2 \times \cdots \times F_k)$$
$$= \mu_{t_1,\ldots,t_k}(F_{\sigma^{-1}(1)} \times F_{\sigma^{-1}(2)} \times \cdots \times F_{\sigma^{-1}(k)}).$$

(ii) *For any $m \in \mathbb{N}$,*

$$\mu_{t_1,\ldots,t_k}(F_1 \times F_2 \times \cdots \times F_k)$$
$$= \mu_{t_1,\ldots,t_k,t_{k+1},\ldots,t_{k+m}}(F_1 \times \cdots \times F_k \times \mathbb{R} \times \cdots \times \mathbb{R}).$$

Then there exists a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and a stochastic process $\{X_t\}_{t\in\mathbf{T}}$ such that

$$\mu_{t_1,\ldots,t_k}(F_1 \times F_2 \times \cdots \times F_m) = \mathbb{P}(X_{t_1} \in F_1, X_{t_2} \in F_2, \ldots, X_{t_m} \in F_m)$$

for any $t_1, t_2, \ldots, t_m \in \mathbf{T}$, $m \in \mathbb{N}$.

The proof of the Kolmogorov extension theorem can be found in [**KS91**, **Lam77**]. The advantage of this result is that it is very general. The problem is that the probability space Ω is too big, so big that we cannot say anything about features of paths in this space. Indeed, the specification of all finite-dimensional distributions is not sufficient to determine the regularity of sample paths. Therefore the real challenge is to define probability measures on smaller spaces with the desired behavior for the paths. Kolmogorov's approach is to start with such an abstract construction and use features of the specific families of the finite-dimensional distributions to infer almost sure properties of their paths, i.e., to conclude that the measure can be defined on smaller spaces. One such example is the Wiener process that we will discuss in the next chapter. In that case, we are able to conclude that the paths are C^α almost surely for $\alpha \in [0, 1/2)$.

5.2. Filtration and Stopping Time

The more we observe about a stochastic process, the more information we have at our disposal. This gives rise to a family of increasingly larger σ-algebras, which we call the *filtration* associated with the stochastic process. The filtration is the main conceptual difference between the random variables and stochastic processes.

Definition 5.3 (Filtration). Given the probability space $(\Omega, \mathcal{F}, \mathbb{P})$, the filtration is a nondecreasing family of σ-algebras $\{\mathcal{F}_t\}_{t\geq 0}$ such that $\mathcal{F}_s \subset \mathcal{F}_t \subset \mathcal{F}$ for any $0 \leq s < t$.

A stochastic process $\{X_t\}$ is called $\mathcal{F}_t$-*adapted* if X_t is $\mathcal{F}_t$-measurable; i.e., $X_t^{-1}(B) \in \mathcal{F}_t$, for any $t \geq 0$ and $B \in \mathcal{R}$. Given a stochastic process $\{X_t\}$, one can define the filtration generated by this process by $\mathcal{F}_t^X = \sigma(X_s, s \leq t)$, which is the smallest σ-algebra such that the $\{X_s\}_{s \leq t}$ are measurable. $\mathcal{F}_t^X$ is the smallest filtration such that the process $\{X_t\}$ is adapted. To avoid technical issues, we often assume that $\mathcal{F}_t$ contains $\mathcal{F}_t^X$ and all sets of measure zero in $\mathcal{F}$, i.e., the augmented filtration of $\{\mathcal{F}_t^X\}$ [**KS91**]. The filtration $\mathcal{F}_t^X$ can be thought of as the information supplied by the process up to time t. Taking again independent coin tossing as the example, let $\Omega = \{H, T\}^{\mathbb{N}}$. In this case, $\mathbf{T} = \mathbb{N}$ and the filtration is $\{\mathcal{F}_n^X\}_{n \geq 0}$. When $n = 0$, the σ-algebra is trivial,

$$\mathcal{F}_0^X = \{\emptyset, \Omega\},$$

which means that we do not know any information about the output of the coin tossing. When $n = 1$, the σ-algebra is

$$\mathcal{F}_1^X = \{\emptyset, \Omega, \{H\}, \{T\}\}$$

since the first output gives either Head or Tail and we only know this information about the first output. When $n = 2$, we have

$$\mathcal{F}_2^X = \Big\{ \emptyset, \Omega, \{HH\}, \{HT\}, \{TH\}, \{TT\}, \{H\cdot\}, \{T\cdot\}, \{\cdot H\}, \{\cdot T\},$$
$$\{HH\} \cup \{TT\}, \{HT\} \cup \{TH\}, \{T\cdot\} \cup \{HT\}, \{T\cdot\} \cup \{HH\},$$
$$\{H\cdot\} \cup \{TT\}, \{H\cdot\} \cup \{TH\} \Big\},$$

which contains all possible combinations of the outputs for the first two rounds of experiments. Sets like

$$\{HH \cdots T\} \quad \text{or} \quad \{HH \cdots H\}$$

are not contained in $\mathcal{F}_0^X$, $\mathcal{F}_1^X$, or $\mathcal{F}_2^X$ since the first two outputs do not give such information. It is obvious that $\mathcal{F}_n^X$ becomes finer and finer as n increases.

Next we introduce the notion of *stopping time* (or *Markov time*) associated with a filtration.

Definition 5.4 (Stopping time for discrete time stochastic processes). A random variable T taking values in $\{1, 2, \ldots\} \cup \{\infty\}$ is said to be a stopping time if for any $n < \infty$

$$\{T \leq n\} \in \mathcal{F}_n.$$

One simple example of stopping time for the coin tossing process is

$$T = \inf \big\{ n : \text{ there exist three consecutive 0's in } \{X_k\}_{k \leq n} \big\}.$$

It is easy to show that the condition $\{T \leq n\} \in \mathcal{F}_n$ is equivalent to $\{T = n\} \in \mathcal{F}_n$ for discrete time processes.

Proposition 5.5 (Properties of stopping times). *For the Markov process* $\{X_n\}_{n\in\mathbb{N}}$, *we have:*

(1) *If* T_1, T_2 *are stopping times, then* $T_1 \wedge T_2$, $T_1 \vee T_2$, *and* $T_1 + T_2$ *are also stopping times.*

(2) *If* $\{T_k\}_{k\geq 1}$ *are stopping times, then*

$$\sup_k T_k, \quad \inf_k T_k, \quad \limsup_k T_k, \quad \liminf_k T_k$$

are stopping times.

Next consider continuous time Markov processes.

Definition 5.6 (Stopping time for continuous time stochastic processes). A random variable T taking values in $\bar{\mathbb{R}}^+$ is said to be a stopping time if for any $t \in \mathbb{R}^+$

$$\{T \leq t\} \in \mathcal{F}_t.$$

In this case we no longer have the equivalence between $\{T \leq t\} \in \mathcal{F}_t$ and $\{T = t\} \in \mathcal{F}_t$. Proposition 5.5 also holds for the continuous time case if the filtration is right continuous; i.e., $\mathcal{F}_t = \mathcal{F}_{t+} := \bigcap_{s>t} \mathcal{F}_s$.

5.3. Markov Processes

We have already encountered discrete time finite Markov chains and Q-processes in Chapter 3. Now we briefly introduce the setup for more general Markov processes in continuous time and space. Given the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and the filtration $\{\mathcal{F}_t\}_{t\geq 0}$, a stochastic process X_t is called a Markov process with respect to $\mathcal{F}_t$ if

(i) X_t is $\mathcal{F}_t$-adapted,

(ii) for any $t \geq s$ and $B \in \mathcal{R}$,

(5.2) $$\mathbb{P}(X_t \in B | \mathcal{F}_s) = \mathbb{P}(X_t \in B | X_s).$$

Here $\mathbb{P}(X_t \in B | \mathcal{F}_s)$ and $\mathbb{P}(X_t \in B | X_s)$ are understood as the conditional expectation with respect to $\mathcal{F}_s$ and the σ-algebra $\sigma(X_s)$, respectively. The distribution of X_0 will be denoted by μ_0. We can associate a family of probability measures $\{\mathbb{P}^x\}_{x\in\mathbb{R}}$ for the processes starting from x, by letting μ_0 be the point mass at x. The expectation of X_t with respect to $\mathbb{P}^x$ will be denoted by $\mathbb{E}^x$. With this definition we still have

$$\mathbb{P}^x(X_t \in B | \mathcal{F}_s) = \mathbb{P}^x(X_t \in B | X_s), \quad t \geq s,$$

and $\mathbb{E}^x f(X_0) = f(x)$ for any function $f \in C(\mathbb{R})$.

The *transition function* $p(B, t | x, s)$ $(t \geq s)$ of the Markov process X_t is defined to be

$$p(B, t | x, s) := \mathbb{P}(X_t \in B | X_s = x).$$

We have that $p : \mathcal{R} \times [0, \infty) | \mathbb{R} \times [0, \infty) \to \mathbb{R}^+$ has the properties [**CW05**]:

(i) For any $t \geq s$ and $x \in \mathbb{R}$, $p(\cdot, t|x, s)$ is a probability measure on $\mathcal{R}$.

(ii) For any $t \geq s$ and $B \in \mathcal{R}$, $p(B, t|\cdot, s)$ is a measurable function on $\mathbb{R}$.

(iii) p satisfies the important relation

$$p(B, t|x, s) = \int_{\mathbb{R}} p(B, t|y, u) p(dy, u|x, s), \quad s \leq u \leq t.$$

Property (iii) is the continuous analog of the Chapman-Kolmogorv equation defined in Proposition 3.4. With this definition, we have $\mathbb{P}^x(X_t \in B) = p(B, t|x, 0)$ and

$$\mathbb{E}^x f(X_{t_1}, X_{t_2}, \ldots, X_{t_n}) = \int_{\mathbb{R}} \cdots \int_{\mathbb{R}} f(x_1, x_2, \ldots, x_n) p(dx_n, t_n|x_{n-1}, t_{n-1})$$
$$\cdot \cdots \cdot p(dx_2, t_2|x_1, t_1) p(dx_1, t_1|x, 0)$$

for $0 < t_1 < \cdots < t_n$.

If the transition function $p(B, t|x, s)$ as a probability measure on $\mathcal{R}$ has a density,

$$p(B, t|x, s) = \int_B p(y, t|x, s) dy,$$

$p(y, t|x, s)$ is called the *transition density function* of X.

A stochastic process is called *stationary* if the joint distributions are translation invariant in time; i.e., the distribution of $(X_{t_1+s}, X_{t_2+s}, \ldots, X_{t_m+s}, \ldots)$ is the same as that of $(X_{t_1}, X_{t_2}, \ldots, X_{t_m}, \ldots)$ for any s. Correspondingly if the transition function depends only on the time difference, the Markov process is called *homogeneous* in time. We denote the simplified transition function as

$$(5.3) \qquad p(t, x, B) := p(B, s + t|x, s), \quad s, t \geq 0,$$

for homogeneous Markov processes. Here $p(t, x, B)$ is called the *transition kernel* of X_t.

We can also study the homogeneous Markov processes using semigroup theory. For $t \geq 0$, define the operator T_t on the bounded measurable function f as

$$T_t f(x) = \mathbb{E}^x f(X_t) = \int_{\mathbb{R}} f(y) p(t, x, dy).$$

By definition T_0 is the identity operator. Here T_t has the following semigroup property for any $t, s \geq 0$:

$$
\begin{aligned}
T_t \circ T_s f(x) &= \int_{\mathbb{R}} p(t, x, dy) \int_{\mathbb{R}} f(z) p(s, y, dz) \\
&= \int_{\mathbb{R}} f(z) \int_{\mathbb{R}} p(t, x, dy) p(s, y, dz) \\
&= \int_{\mathbb{R}} f(z) p(t+s, x, dz) = T_{t+s} f(x)
\end{aligned}
$$

from the Chapman-Kolmogorov equation. These parameterized operators $\{T_t\}_{t \geq 0}$ are called operator semigroup.

For the operator semigroup $\{T_t\}_{t \geq 0}$ on a suitable Banach space $\mathscr{B}$, one can define its *infinitesimal generator* $\mathcal{A}$ (see [**Yos95**] for more details on the abstract setup) as

$$
(5.4) \qquad \mathcal{A}f = \lim_{t \to 0+} \frac{T_t f - f}{t}
$$

on a suitable subspace of $\mathscr{B}$ which is the domain of definition of $\mathcal{A}$. Here the convergence is understood as the norm convergence

$$
\lim_{t \to 0+} \| t^{-1}(T_t f - f) - \mathcal{A}f \| = 0.
$$

Example 5.7 (*Q*-process). Consider the Q-process X_t on $S = \{1, 2, \ldots, I\}$ with generator $\boldsymbol{Q}$ defined as in (3.16). We have

$$
\begin{aligned}
(\mathcal{A}f)(i) &= \lim_{t \to 0+} \frac{\mathbb{E}^i f(X_t) - f(i)}{t} = \lim_{t \to 0+} \frac{1}{t} \Big(\sum_{j \in S} (P_{ij}(t) - \delta_{ij}) f(j) \Big) \\
&= \sum_{j \in S} q_{ij} f(j), \quad i \in S,
\end{aligned}
$$

from (3.16). Thus the generator $\boldsymbol{Q}$ is exactly the infinitesimal generator of X_t. Furthermore, we have that for $\boldsymbol{u} = (u_1, u_2, \ldots, u_I)^T$ and $u_i(t) = \mathbb{E}^i f(X_t)$,

$$
(5.5) \qquad \frac{d\boldsymbol{u}}{dt} = \boldsymbol{Q}\boldsymbol{u} = \mathcal{A}\boldsymbol{u},
$$

which is called the backward Kolomgorov equation. The distribution $\boldsymbol{\nu} = (\nu_1, \nu_2, \ldots, \nu_I)$ satisfies the equation

$$
(5.6) \qquad \frac{d\boldsymbol{\nu}}{dt} = \boldsymbol{\nu}\boldsymbol{Q}, \quad \text{or equivalently} \quad \frac{d\boldsymbol{\nu}^T}{dt} = \boldsymbol{Q}^T \boldsymbol{\nu}^T = \mathcal{A}^* \boldsymbol{\nu}^T,
$$

where the operator $\mathcal{A}^*$ is the adjoint operator of $\mathcal{A}$ defined as

$$
(\mathcal{A}^* g, f) = (g, \mathcal{A}f) \quad \text{for any } f \in \mathscr{B}, g \in \mathscr{B}^*.
$$

Equation (5.6) is called the forward Kolmogorov equation. For the case when $\mathcal{A} = \boldsymbol{Q}$ and $\mathscr{B} = L^2(S)$, it is easy to see that $\mathcal{A}^* = \boldsymbol{Q}^T$.

Example 5.8 (Poisson process)**.** Consider the Poisson process X_t on $\mathbb{N}$ with rate λ. We have

$$(\mathcal{A}f)(n) = \lim_{t\to 0+} \frac{\mathbb{E}^n f(X_t) - f(n)}{t} = \lim_{t\to 0+} \frac{1}{t}\Big(\sum_{k=n}^{\infty} f(k)\frac{(\lambda t)^{k-n}}{(k-n)!}e^{-\lambda t} - f(n)\Big)$$

$$= \lim_{t\to 0+} \frac{1}{t}\Big(f(n)(e^{-\lambda t} - 1) + f(n+1)\lambda t e^{-\lambda t} + \sum_{k=n+2}^{\infty} f(k)\frac{(\lambda t)^{k-n}}{(k-n)!}e^{-\lambda t}\Big)$$

$$= \lambda(f(n+1) - f(n)).$$

It is straightforward to see that

$$\mathcal{A}^* f(n) = \lambda(f(n-1) - f(n)).$$

For $u(t, n) = \mathbb{E}^n f(X_t)$, we have

$$(5.7) \quad \frac{du}{dt} = \frac{d}{dt}\Big(\sum_{k=n}^{\infty} f(k)\frac{(\lambda t)^{k-n}}{(k-n)!}e^{-\lambda t}\Big) = \lambda(u(n+1) - u(n)) = \mathcal{A}u(t, n).$$

The distribution $\boldsymbol{\nu}(t) = (\nu_0(t), \nu_1(t), \dots)$ satisfies

$$(5.8) \quad \frac{d\nu_n(t)}{dt} = \frac{d}{dt}\Big(\frac{(\lambda t)^{k-n}}{(k-n)!}e^{-\lambda t}\Big) = \lambda(\nu_{n-1}(t) - \nu_n(t)) = (\mathcal{A}^*\boldsymbol{\nu}(t))_n.$$

The facts that the equation for the expectation of a given function has the form of backward Kolmogorov equations (5.5) and (5.7) and the distribution satisfies the form of forward Kolmogorov equations (5.6) and (5.8) are general properties of Markov processes. This will be seen again when we study the diffusion processes in Chapter 8.

These discussions can be easily generalized to the multidimensional setting when $X_t \in \mathbb{R}^d$.

5.4. Gaussian Processes

Definition 5.9. A stochastic process $\{X_t\}_{t\geq 0}$ is called a Gaussian process if its finite-dimensional distributions $\mu_{t_1,\dots,t_k}$ are consistent Gaussian measures for any $0 \leq t_1 < t_2 < \cdots < t_k$.

Below we will show that a Gaussian process is determined once its mean and covariance function

$$(5.9) \quad m(t) = \mathbb{E}X_t, \quad K(s, t) = \mathbb{E}(X_s - m(s))(X_t - m(t))$$

are specified. Given these two functions, a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ can be constructed and $\mu_{t_1,\dots,t_k}$ is exactly the finite-dimensional distribution of $(X_{t_1}, \dots, X_{t_k})$ under $\mathbb{P}$.

It is well known that a Gaussian random vector $\boldsymbol{X} = (X_1, X_2, \ldots, X_n)^T$ is completely characterized by its first and second moments

$$\boldsymbol{m} = \mathbb{E}\boldsymbol{X}, \quad \boldsymbol{K} = \mathbb{E}(\boldsymbol{X} - \boldsymbol{m})(\boldsymbol{X} - \boldsymbol{m})^T,$$

or, in component form, $m_i = \mathbb{E}X_i$ and $K_{ij} = \mathbb{E}(X_i - m_i)(X_j - m_j)$. Using $\boldsymbol{m}$ and $\boldsymbol{K}$, one can represent $\boldsymbol{X}$ via its characteristic function

$$\mathbb{E}e^{i\boldsymbol{\xi}\cdot\boldsymbol{X}} = e^{i\boldsymbol{\xi}\cdot\boldsymbol{m} - \frac{1}{2}\boldsymbol{\xi}^T\boldsymbol{K}\boldsymbol{\xi}}.$$

For this reason, given any $0 \le t_1 < t_2 < \cdots < t_k$, the finite-dimensional distribution $\mu_{t_1,\ldots,t_k}$ of a Gaussian process is uniquely determined by the mean $\boldsymbol{m} = (m(t_1), \ldots, m(t_k))$ and covariance matrix $\boldsymbol{K} = (K(t_i, t_j))_{i,j=1}^k$. It is not difficult to check that the consistency conditions in Theorem 5.2 trivially hold if $m(t)$ and $K(s, t)$ are well-defined. The Kolmogorov extension theorem thus ensures the existence of the probability space $(\Omega, \mathcal{F}, \mathbb{P})$.

The covariance function K is obviously symmetric; i.e., $K(t, s) = K(s, t)$. In addition, K must satisfy semipositivity in the following sense.

Theorem 5.10. *Assume the stochastic process $\{X_t\}_{t\in[0,T]}$ satisfies the condition*

$$\mathbb{E}\int_0^T X_t^2 dt < \infty.$$

Then $m \in L_t^2$ in the sense that

$$\int_0^T m^2(t)dt < \infty.$$

Furthermore, the operator

$$\mathcal{K}f(s) := \int_0^T K(s, t)f(t)dt, \quad s \in [0, T],$$

is a nonnegative compact operator on L_t^2.

Proof. First, we have

$$\int_0^T m^2(t)dt = \int_0^T (\mathbb{E}X_t)^2 dt \le \int_0^T \mathbb{E}X_t^2 dt < \infty.$$

In addition, we have

$$\int_0^T \int_0^T K^2(s, t)dsdt = \int_0^T \int_0^T \left(\mathbb{E}(X_t - m(t))(X_s - m(s))\right)^2 dsdt$$

$$\le \int_0^T \int_0^T \mathbb{E}(X_t - m(t))^2 \mathbb{E}(X_s - m(s))^2 dsdt \le \left(\int_0^T \mathbb{E}X_t^2 dt\right)^2,$$

which means $K \in L^2([0, T] \times [0, T])$. Thus $\mathcal{K}$ is a compact operator on L_t^2 (cf. [**Lax02**]).

It is easy to see that the adjoint operator of $\mathcal{K}$ is

$$\mathcal{K}^* f(s) := \int_0^T K(t,s)f(t)dt, \quad s \in [0,T].$$

From the symmetry of $K(s,t)$, we know that $\mathcal{K}$ is selfadjoint.

To show the positivity of $\mathcal{K}$, we have

$$(\mathcal{K}f, f) = \int_0^T \int_0^T \mathbb{E}(X_t - m(t))(X_s - m(s))f(t)f(s)dsdt$$

$$= \mathbb{E}\Big(\int_0^T (X_t - m(t))f(t)dt \Big)^2 \geq 0.$$

The proof is completed. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Formally, one can represent a Gaussian process via its characteristic functional defined on the Hilbert space L_t^2 by mimicking the finite-dimensional characteristic function

$$\mathbb{E}e^{i(\xi, X)} = e^{i(\xi, m) - \frac{1}{2}(\xi, \mathcal{K}\xi)}, \quad \xi \in L_t^2$$

where $(\xi, m) = \int_a^b \xi(t)m(t)dt$ and $\mathcal{K}\xi(t) = \int_a^b K(t,s)\xi(s)ds$. This formulation is useful when studying stochastic processes in the infinite-dimensional setting [**DPZ92**].

Theorem 5.11. *Assume that $X_1, X_2, \ldots$ is a sequence of Gaussian random variables that converges to X in probability. Then X is also Gaussian.*

Proof. Let us denote

$$m_k = \mathbb{E}X_k, \quad \sigma_k^2 = \operatorname{Var} X_k.$$

Then from part (v) of the Theorem 1.32 and Lévy's continuity theorem, we have

$$e^{i\xi m_k - \frac{1}{2}\sigma_k^2 \xi^2} = \mathbb{E}e^{i\xi X_k} \to \mathbb{E}e^{i\xi X} \quad \text{for any } \xi \in \mathbb{R}.$$

For the above to hold, there must exist numbers m and σ^2 such that

$$m = \lim_k m_k, \quad \sigma^2 = \lim_k \sigma_k^2$$

and correspondingly $\mathbb{E}e^{i\xi X} = e^{i\xi m - \frac{1}{2}\sigma^2 \xi^2}$. This gives the desired result. $\quad\square$

The following theorem is fundamental in the construction of the Gaussian process via spectral type expansion [**Loè77**].

Theorem 5.12 (Mercer's theorem). *Let $K : [0,T] \times [0,T] \to \mathbb{R}^+$ be a symmetric, continuous, nonnegative definite function in the sense that the associated operator*

$$(5.10) \qquad \mathcal{K}\phi(s) := \int_0^T K(s,t)\phi(t)dt, \quad s \in [0,T],$$

is a nonnegative operator. Then $K(s,t)$ has the expansion

$$K(s,t) = \sum_{k=1}^{\infty} \lambda_k \phi_k(s)\phi_k(t), \quad (s,t) \in [0,T] \times [0,T],$$

in the $L^{\infty}([0,T] \times [0,T])$ sense, where $\{\lambda_k, \phi_k(t)\}_k$ is the eigensystem of the operator $\mathcal{K}$.

Theorem 5.13 (Karhunen-Loève expansion)**.** *Let $(X_t)_{t \in [0,1]}$ be a Gaussian process with mean 0 and covariance function $K(s,t)$. Assume that K is continuous. Let $\{\lambda_k\}, \{\phi_k\}$ be the sequence of eigenvalues and eigenfunctions for the eigenvalue problem*

$$\int_0^1 K(s,t)\phi_k(t)dt = \lambda_k \phi_k(s), \qquad k = 1, 2, \ldots,$$

with the normalization condition $\int_0^1 \phi_k \phi_j dt = \delta_{kj}$. Then X_t has the representation

$$(5.11) \qquad\qquad X_t = \sum_{k=1}^{\infty} \alpha_k \sqrt{\lambda_k} \phi_k(t),$$

in the sense that the series

$$(5.12) \qquad X_t^N = \sum_{k=1}^{N} \alpha_k \sqrt{\lambda_k} \phi_k(t) \rightarrow X_t \qquad in\ L_t^{\infty} L_{\omega}^2;$$

i.e., we have

$$\lim_{N \to \infty} \sup_{t \in [0,1]} \mathbb{E}|X_t^N - X_t|^2 = 0.$$

Here the α_k are i.i.d. $N(0,1)$ random variables.

Proof. We need to show that the random series is well-defined and that it is a Gaussian process with the desired mean and covariance function.

First consider the operator $\mathcal{K} : L^2([0,1]) \to L^2([0,1])$ defined as in (5.10). Thanks to Theorem 5.10, we know that $\mathcal{K}$ is nonnegative and compact. Therefore it has countably many real eigenvalues, for which 0 is the only possible accumulation point [**Lax02**]. From Mercer's theorem, we have

$$\sum_{k=1}^{N} \lambda_k \phi_k(s)\phi_k(t) \to K(s,t), \quad s,t \in [0,1],\ N \to \infty,$$

uniformly [**RSN56**]. Therefore we have for $N > M$

$$\mathbb{E}|X_t^N - X_t^M|^2 = \sum_{k=M+1}^{N} \lambda_k \phi_k^2(t) \to 0$$

uniformly when $N, M \to \infty$. This implies that $\{X_t^N\}$ is a Cauchy sequence in the Banach space $L_t^\infty L_\omega^2$, which means

$$\sup_{t \in [0,1]} \mathbb{E}|X_t^N - X_t^M|^2 \to 0, \quad \text{as } M, N \to \infty.$$

We denote the unique limit by X_t. For any $t_1, t_2, \ldots, t_m \in [0, 1]$, the mean square convergence of the Gaussian random vector $(X_{t_1}^N, X_{t_2}^N, \ldots, X_{t_m}^N)$ to $(X_{t_1}, X_{t_2}, \ldots, X_{t_m})$ implies the convergence in probability. From Theorem 5.11, we have that the limit X_t is indeed a Gaussian process. Since X^N converges to X in $L_t^\infty L_\omega^2$, we have

$$\mathbb{E}X_t = \lim_{N \to \infty} \mathbb{E}X_t^N = 0,$$

$$\mathbb{E}X_s X_t = \lim_{N \to \infty} \mathbb{E}X_s^N X_t^N = \sum_{k=1}^\infty \lambda_k \phi_k(s) \phi_k(t) = K(s, t).$$

The proof is completed. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad \square$

Exercises

5.1. Prove that in Definition 5.4 the condition $\{T \leq n\} \in \mathcal{F}_n$ is equivalent to $\{T = n\} \in \mathcal{F}_n$ for discrete time stochastic processes.

5.2. Prove Proposition 5.5.

5.3. Let T be a stopping time for the filtration $\{\mathcal{F}_n\}_{n \in \mathbb{N}}$. Define the σ-algebra generated by T as

$$\mathcal{F}_T = \{A : A \in \mathcal{F}, \ A \cap \{T \leq n\} \in \mathcal{F}_n \text{ for any } n \in \mathbb{N}\}.$$

Prove that $\mathcal{F}_T$ is indeed a σ-algebra and T is $\mathcal{F}_T$-measurable. Generalize this result to the continuous time case.

5.4. Let S and T be two stopping times. Prove that:
   (i) If $S \leq T$, then $\mathcal{F}_S \subset \mathcal{F}_T$.
   (ii) $\mathcal{F}_{S \wedge T} = \mathcal{F}_S \cap \mathcal{F}_T$, and the events

   $$\{S < T\}, \ \{T < S\}, \ \{S \leq T\}, \ \{T \leq S\}, \ \{T = S\}$$

   all belong to $\mathcal{F}_S \cap \mathcal{F}_T$.

5.5. Consider the compound Poisson process X_t defined in Exercise 3.13. Find the generator of $\{X_t\}$.

5.6. Find the generator of the following Gaussian processes.
   (i) *Brownian bridge* with the mean and covariance function

   $$m(t) = 0, \quad K(s, t) = s \wedge t - st, \quad s, t \in [0, 1].$$

   (ii) *Ornstein-Uhlenbeck process* with the mean and covariance function

   $$m(t) = 0, \quad K(s, t) = \sigma^2 \exp(-|t - s|/\eta), \quad \eta > 0, \ s, t \geq 0.$$

5.7. Let $p(t)$ and $q(t)$ be positive functions on $[a, b]$ and assume that p/q is strictly increasing. Prove that the covariance function defined by

$$K(s, t) = \begin{cases} p(s)q(t), & s \leq t, \\ p(t)q(s), & t < s, \end{cases}$$

is a strictly positive definite function in the sense that the matrix

$$\boldsymbol{K} = \Big(K(t_i, t_j)\Big)_{i,j=1}^n$$

is strictly positive definite for any $t_1, t_2, \ldots, t_n \in [a, b]$.

5.8. Let $\{X_t\}_{t \in [a,b]}$ be a Gaussian process with mean $m(t) = 0$ and continuous strictly positive definite covariance function $K(s, t)$. Prove that X_t is also Markovian if K has the structure as in Exercise 5.7.

5.9. B_t^H is called the *fractional Brownian motion* if it is a Gaussian process with $m(t) = 0$ and covariance function

$$K(s, t) = \frac{1}{2}(t^{2H} + s^{2H} - |t - s|^{2H}), \quad s, t \in [0, T],$$

where $H \in (0, 1)$ is called the *Hurst index*. Prove that B_t^H has the following properties:
  (a) Self-similarity: B_{ct}^H has the same distribution as $c^H B_t^H$ for $c > 0$.
  (b) Stationary increments: $B_t^H - B_t^H$ has the same distribution as B_{t-s}^H for $s < t$.
  (c) Regularity: $\mathbb{E}|B_t^H - B_s^H|^n = C_n |t - s|^{nH}$ for all $n \geq 1$, where C_n is a positive constant.

5.10. Construct a numerical method for generating the finite-dimensional samples of standard stationary Ornstein-Uhlenbeck process, i.e., the Gaussian process with mean 0 and covariance function $K(s, t) = \exp(-|t - s|)$, at instants $(t_1, t_2, \ldots, t_n)$.

Notes

We did not cover martingales in the main text. Instead, we give a very brief introduction in Section D of the appendix. The interested readers may consult [**Chu01**, **KS91**, **Mey66**] for more details.

Our presentation about Markov processes in this chapter is very brief. But the three most important classes of Markov processes are discussed throughout this book: Markov chains, diffusion processes, and jump processes used to describe chemical kinetics. One most important tool for treating Markov processes is the master equations (also referred to as Kolmogorov equations or Fokker-Planck equations), which are either differential or difference equations.

Besides Gaussian processes, the Karhunen-Loève expansion can be defined for general square integrable processes where the natural orthogonal decomposition still holds [**Loè77**].

Wiener Process

We now discuss the most important example of stochastic processes with continuous paths, the Wiener process, commonly referred to as the Brownian motion in the physics literature.

Mathematically, the Wiener process W_t is defined as a stochastic process with the following properties:

(1) It is a Gaussian process.

(2) Its mean function is $m(t) = 0$, and its covariance function is $K(s,t)$ $= s \wedge t = \min(s,t)$.

(3) With probability 1, $t \mapsto W_t$ is continuous.

However as we will see, one can understand the Wiener process in a number of different ways:

(1) As the continuum limit of random walks. This is most succinctly seen in the invariance principle which is a far-reaching extension of the central limit theorems to path space.

(2) As an example of the Markov process. The generator is the Laplace operator and the transition density is the heat kernel.

(3) As an example of Gaussian processes, with mean 0 and covariance function $K(s,t) = s \wedge t = \min(s,t)$. Gaussian processes can be represented using random series. Therefore Wiener processes can also be constructed using random series.

We will discuss the first and third constructions in this chapter.

6.1. The Diffusion Limit of Random Walks

Example 6.1 (Random walk). Let $\{\xi_i\}$ be i.i.d. random variables such that $\xi_i = \pm 1$ with probability $1/2$, and let

$$X_n = \sum_{k=1}^{n} \xi_k, \quad \text{i.e.,} \quad X_0 = 0.$$

Here $\{X_n\}$ is called a symmetric random walk on $\mathbb{Z}$. Given $X_n = i$, we have

$$P(X_{n+1} = i \pm 1 \mid X_n = i) = \frac{1}{2},$$
$$P(X_{n+1} = \text{anything else} \mid X_n = i) = 0.$$

After taking N steps, the particle might be at any of the positions:

$$-N, -N + 2, \ldots, N - 2, N.$$

Let $W(m, N) = \mathbb{P}\{X_N = m\}$, the probability that the particle arrives at the position m after N steps. It is seen that $W(m, N)$ is a binomial distribution

$$W(m, N) = \frac{N!}{(\frac{N+m}{2})!(\frac{N-m}{2})!} \left(\frac{1}{2}\right)^N.$$

The mean position and mean squared deviation are

$$\mathbb{E}X_N = 0, \quad \mathbb{E}X_N^2 = N.$$

The root mean squared displacement is $\sqrt{N}$.

Definition 6.2 (Diffusion coefficient). The diffusion coefficient D is defined as

$$D = \frac{\langle (X_N - X_0)^2 \rangle}{2N}.$$

For the general stochastic process, it is defined as

$$D = \lim_{t \to \infty} \frac{\langle (X_t - X_0)^2 \rangle}{2dt},$$

where d is the space dimension.

It is straightforward to see that $D = 1/2$ for the one-dimensional symmetric random walk.

Next we study the continuum limit of the random walk under suitable scaling. Let us redefine the step length of the random walk to be l and the time between each jump to be τ. Fixing (x, t), consider the following limit:

(6.1) $N, m \to \infty, \quad l, \tau \to 0, \quad \text{and} \quad N\tau = t, \quad ml = x.$

In order to have a nontrivial limit, we also fix the diffusion coefficient

$$D = \frac{\langle (X_{N\tau} - X_0)^2 \rangle}{2N\tau} = \frac{l^2}{2\tau}.$$

In this regime, $N, m \gg 1$, $m/N = x/t \cdot \tau/l \to 0$ and thus $m \ll N$. By Stirling's formula $\log n! = (n + \frac{1}{2}) \log n - n + \frac{1}{2} \log 2\pi + O(n^{-1})$ for $n \gg 1$, we have

$$\log W(m, N) \approx \left(N + \frac{1}{2}\right) \log N - \frac{1}{2}(N + m + 1) \log \left[\frac{N}{2}\left(1 + \frac{m}{N}\right)\right]$$

$$- \frac{1}{2}(N - m + 1) \log \left[\frac{N}{2}\left(1 - \frac{m}{N}\right)\right] - \frac{1}{2} \log 2\pi - N \log 2.$$

Since $m \ll N$, using $\log(1 + x) = x - \frac{1}{2}x^2 + O(x^3)$ for $x \ll 1$, we have

$$\log W(m, N) \approx -\frac{1}{2} \log N + \log 2 - \frac{1}{2} \log 2\pi - \frac{m^2}{2N}.$$

This gives us the the asymptotic formula

(6.2)
$$W(m, N) \approx \left(\frac{2}{\pi N}\right)^{\frac{1}{2}} \exp \left(-\frac{m^2}{2N}\right).$$

Take Δx to be small but much larger than l. We have

$$W(x, t)\Delta x \approx \int_{x - \Delta x/2}^{x + \Delta x/2} W(y, t) dy$$

$$\approx \sum_{\substack{k \in \{m, m \pm 2, m \pm 4, \ldots\} \\ kl \in (x - \Delta x/2, x + \Delta x/2)}} W(k, N) \approx W(m, N) \frac{\Delta x}{2l},$$

where $x = ml$ and the factor $1/2$ in the last equation appears since m can take only even or odd values depending on whether N is even or odd. Combining the results above we obtain

$$W(x, t)\Delta x = \frac{1}{\sqrt{2\pi t \frac{l^2}{\tau}}} \exp \left(-\frac{x^2}{2t\frac{l^2}{\tau}}\right) \Delta x.$$

The limiting probability density at time t is then

$$W(x, t) = \frac{1}{\sqrt{4\pi Dt}} \exp \left(-\frac{x^2}{4Dt}\right).$$

Note that $W(x, t)$ satisfies the partial differential equation:

(6.3)
$$\begin{cases} \dfrac{\partial W}{\partial t} = D \dfrac{\partial^2 W}{\partial x^2}, & x \in \mathbb{R}, \ t \geq 0, \\ W(x, t)|_{t=0} = \delta(x), \end{cases}$$

where $\delta(x)$ is Dirac's delta function.

Many properties of the Wiener process or Brownian motion to be introduced in this chapter can be derived based on the asymptotic analysis of the symmetric random walk. A typical example is the arcsine law for the Brownian trajectories. Let us define $P_{2k,2n}$ to be the probability that during the interval $[0, 2n]$ the particle spends $2k$ units of time on the positive side

(we say that the particle is on the positive side in the interval $[n-1, n]$ if at least one of the values X_{n-1} and X_n is positive). One can prove that

(6.4) $$P_{2k,2n} = u_{2k} \cdot u_{2n-2k},$$

where $u_{2k} = \mathbb{P}(X_{2k} = 0)$. Now let $\gamma(2n)$ be the number of time units that the particle spends on the positive axis in the interval $[0, 2n]$. Then when $x < 1$,

$$\mathbb{P}\Big(\frac{1}{2} < \frac{\gamma(2n)}{2n} \leq x\Big) = \sum_{k, 1/2 < 2k/2n \leq x} P_{2k,2n}.$$

From the asymptotics (6.2), we have

$$u_{2k} \sim \frac{1}{\sqrt{\pi k}}, \quad P_{2k,2n} \sim \frac{1}{\pi\sqrt{k(n-k)}}$$

as $k, n - k \to \infty$. Therefore

$$\sum_{\{k, 1/2 < 2k/2n \leq x\}} P_{2k,2n} - \sum_{k, 1/2 < 2k/2n \leq x} \frac{1}{\pi n} \cdot \Big[\frac{k}{n}\Big(1 - \frac{k}{n}\Big)\Big]^{-\frac{1}{2}} \to 0 \quad \text{as } n \to \infty,$$

and thus

$$\sum_{\{k, 1/2 < 2k/2n \leq x\}} P_{2k,2n} \to \frac{1}{\pi} \int_{\frac{1}{2}}^{x} \frac{dt}{\sqrt{t(1-t)}}, \quad \text{as } n \to \infty.$$

From the symmetry of random walk, we obtain the following theorem.

Theorem 6.3 (Arcsine law)**.** *The probability that the fraction of the time spent by the particle on the positive side is at most x tends to $\frac{2}{\pi} \arcsin\sqrt{x}$; that is,*

(6.5) $$\sum_{\{k, k/n \leq x\}} P_{2k,2n} \to \frac{2}{\pi} \arcsin\sqrt{x} \qquad \text{as } n \to \infty.$$

This theorem tells us a somewhat counterintuitive fact about the symmetric random walk. It shows that we will observe that one player remains on the winning side and the other on the losing side most of the time instead of frequently exchanging winning status in a fair coin-tossing game.

6.2. The Invariance Principle

Let $\{\xi_n\}_{n\in\mathbb{N}}$ be a sequence of i.i.d. random variables such that $\mathbb{E}\xi_n = 0$ and $\mathbb{E}\xi_n^2 = 1$. Define

$$S_0 = 0, \qquad S_N = \sum_{i=1}^{N} \xi_i.$$

Recall that the central limit theorem asserts that

(6.6) $$\frac{S_N}{\sqrt{N}} \xrightarrow{d} N(0, 1)$$

as $N \to \infty$. This suggests rescaling S_n and defining a continuous random function W_t^N on $t \in [0, 1]$ by letting $W_0^N = 0$ and

(6.7)
$$W_t^N = \frac{1}{\sqrt{N}} \left(\theta S_k + (1 - \theta) S_{k+1} \right) \qquad \text{for } Nt \in (k, k+1], \ k = 0, 1, \ldots, N-1,$$

where $\theta = \lceil Nt \rceil - Nt$. The function $W^N \in C[0, 1]$ and its realizations are shown in Figure 6.1 for different N. Let $\Omega = C[0, 1]$, and let $\mathcal{F}$ be the Borel σ-algebra on the metric space $(C[0, 1], \| \cdot \|_\infty)$, i.e., the smallest σ-algebra containing all open sets in $C[0, 1]$. We have:

Theorem 6.4 (Donsker's invariance principle). *As $N \to \infty$, the process W^N converges to a limit W in the sense of distributions on $(\Omega, \mathcal{F})$,*

(6.8)
$$W^N \xrightarrow{d} W.$$

Here W is the Wiener process. The distribution of W on $\Omega = C[0, 1]$ is called the Wiener measure.

We will not prove Theorem 6.4. Rather we will take for granted that the limiting process W exists and we shall study its properties. It is instructive to see that the spatial-temporal rescaling in (6.7) is exactly the same scaling considered in the previous section.
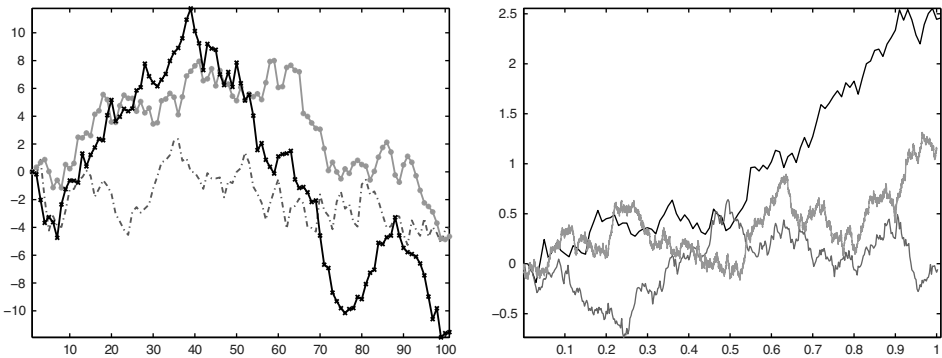
Figure 6.1. Left panel: Three realizations of the (unrescaled) random walk S_N for $N = 100$. Right panel: Realizations of W_t^N for $N = 100$ (top), $N = 400$ (bottom), and $N = 10000$ (middle).

6.3. Wiener Process as a Gaussian Process

The central limit theorem also tells us that the limiting process defined above has to be a Gaussian process. It is straightforward to compute the mean and covariance function for the limiting process. The results are

$$\mathbb{E}W_t = 0, \quad \mathbb{E}(W_t W_s) = \min(t, s) = t \wedge s$$

since $W_{t\vee s}^N - W_{t\wedge s}^N$ is independent of $W_{t\wedge s}^N$ by the construction in the invariance principle. This allows us to construct the Wiener process using the Karhunen-Loève expansion. For this purpose, let us first examine the eigenvalue problem associated with the covariance function.

Consider the eigenvalue problem

$$\int_0^1 (s \wedge t)\phi_k(t)dt = \lambda_k \phi_k(s).$$

One can write this as

(6.9) $$\int_0^s t\phi_k(t)dt + \int_s^1 s\phi_k(t)dt = \lambda_k \phi_k(s).$$

Differentiating with respect to s, we obtain

(6.10) $$\lambda_k \phi_k'(s) = s\phi_k(s) + \int_s^1 \phi_k(t)dt - s\phi_k(s) = \int_s^1 \phi_k(t)dt.$$

Differentiating one more time gives a Sturm-Liouville problem

(6.11) $$\lambda_k \phi_k''(s) = -\phi_k(s).$$

This suggests that $\lambda_k \neq 0$. Taking $s = 0$ in (6.9), we obtain $\phi_k(0) = 0$. Taking $s = 1$ in (6.10), we get $\phi_k'(1) = 0$.

Solving this boundary value problem we obtain

$$\lambda_k = \left(\left(k - \frac{1}{2}\right)\pi\right)^{-2}, \quad \phi_k(s) = \sqrt{2}\sin\left(\left(k - \frac{1}{2}\right)\pi s\right), \quad k = 1, 2, \ldots.$$

Hence we obtain

(6.12) $$W_t = \sum_{k=1}^\infty \alpha_k \frac{\sqrt{2}}{(k - \frac{1}{2})\pi}\sin\left(\left(k - \frac{1}{2}\right)\pi t\right)$$

as the Karhunen-Loève expansion for the Wiener process.

The eigenfunction basis is not the only basis that one can use. A related construction using the Haar basis was invented by Paul Lévy. Let

$$\psi(t) = \begin{cases} 1, & t \in [0, 1/2), \\ -1, & t \in [1/2, 1), \\ 0, & \text{otherwise.} \end{cases}$$

The multilevel Haar functions $\{H_k^{(n)}\}$ are defined by $H_0^{(0)}(t) = 1$ and

$$H_k^{(n)}(t) = 2^{\frac{n-1}{2}}\psi(2^{n-1}t - k), \quad n \geq 1, \ k \in I_n := \{0, 1, \ldots, 2^{n-1} - 1\}$$

for $t \in [0, 1]$. Here we used the convention that $I_0 = \{0\}$. These functions together form the Haar system: $\{H_k^{(n)}\}$ for $n \in \mathbb{N}$ and $k \in I_n$. It is an important fact that the Haar system forms an orthonormal basis in $L^2[0, 1]$ [**Wal02**].

What is relevant in the present context is the following result.

Theorem 6.5. *Let $\{\alpha_k^{(n)}\}$ be a sequence of i.i.d. Gaussian random variables with distribution $N(0,1)$. Then, almost surely,*

$$W_t^N = \sum_{n=0}^{N} \sum_{k\in I_n} \alpha_k^{(n)} \int_0^t H_k^{(n)}(s)ds \longrightarrow W_t, \quad N \to \infty,$$

uniformly for $t \in [0,1]$, where $\{W_t\}$ is the Wiener process.

To get an idea of why this is true, note that

$$(6.13) \qquad \mathbb{E}W_t^N = \sum_{n=0}^{N} \sum_{k\in I_n} \mathbb{E}\alpha_k^{(n)} \int_0^t H_k^{(n)}(s)ds = 0,$$

$$\mathbb{E}W_t^N W_s^N = \sum_{n,m=0}^{N} \sum_{k\in I_n, l\in I_m} \mathbb{E}(\alpha_k^{(n)}\alpha_l^{(m)}) \int_0^t H_k^{(n)}(\tau)d\tau \int_0^s H_l^{(m)}(\tau)d\tau$$

$$= \sum_{n=0}^{N} \sum_{k\in I_n} \int_0^t H_k^{(n)}(\tau)d\tau \int_0^s H_k^{(n)}(\tau)d\tau$$

$$= \sum_{n=0}^{N} \sum_{k\in I_n} \int_0^1 H_k^{(n)}(\tau)\chi_{[0,t]}(\tau)d\tau \int_0^1 H_k^{(n)}(\tau)\chi_{[0,s]}(\tau)d\tau$$

$$(6.14) \qquad \to \int_0^1 \chi_{[0,t]}\chi_{[0,s]}(\tau)d\tau = t \wedge s,$$

where $\chi_{[0,t]}(\cdot)$ is the indicator function of the set $[0,t]$. In the last step, we used Parserval's identity since $\{H_k^{(n)}\}$ is an orthonormal basis.

Proof. First we show that almost surely, W_t^N converges uniformly to some continuous function. For this purpose, we note that for the Gaussian random variable $\xi \sim N(0,1)$,

$$\mathbb{P}(|\xi| > x) = \sqrt{\frac{2}{\pi}} \int_x^{\infty} e^{-\frac{y^2}{2}}dy \le \sqrt{\frac{2}{\pi}} \int_x^{\infty} \frac{y}{x}e^{-\frac{y^2}{2}}dy = \sqrt{\frac{2}{\pi}} \frac{e^{-\frac{x^2}{2}}}{x}, \quad x > 0.$$

Define $a_n = \max_{k\in I_n} |\alpha_k^{(n)}|$. Then

$$\mathbb{P}(a_n > n) = \mathbb{P}\left(\bigcup_{k\in I_n} |\alpha_k^{(n)}| > n\right) \le 2^{n-1}\sqrt{\frac{2}{\pi}}\frac{e^{-\frac{n^2}{2}}}{n}, \quad n \ge 1.$$

Since $\sum_{n=1}^{\infty} 2^{n-1}\sqrt{\frac{2}{\pi}}\frac{e^{-\frac{n^2}{2}}}{n} < \infty$, using the Borel-Cantelli lemma, we conclude that there exists a set $\tilde{\Omega}$ with $\mathbb{P}(\tilde{\Omega}) = 1$ such that for any $\omega \in \tilde{\Omega}$ there
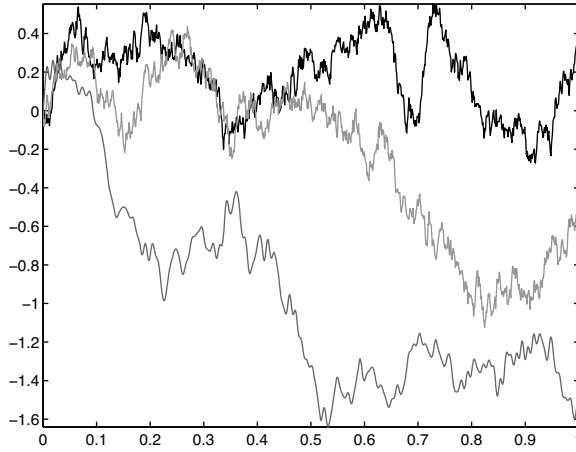
Figure 6.2. Numerical construction of the Wiener process using the invariance principle, the Karhunen-Loève expansion (truncated until 200 terms), and the Haar basis expansion (10 levels).

is an $N(\omega)$ such that $a_m(\omega) \leq m$ for any $m \geq N(\omega)$. For any such ω, we have

$$\left| \sum_{m=N(\omega)}^{\infty} \sum_{k \in I_m} \alpha_k^{(m)} \int_0^t H_k^{(m)}(s)ds \right| \leq \sum_{m=N(\omega)}^{\infty} m \sum_{k \in I_m} \int_0^t H_k^{(m)}(s)ds$$

$$\leq \sum_{m=N(\omega)}^{\infty} m 2^{-\frac{m+1}{2}} < \infty,$$

which implies that W_t^N converges uniformly to a continuous function.

Now we prove that the limit is indeed W_t. From Theorem 5.11, the limit is a Gaussian process. Since the mean and covariance functions are the same as those of W_t, we conclude that the limit is indeed W_t. $\qquad\square$

We now have several representations of the Wiener process. We will see later that different representations are useful for different purposes. For example, the invariance principle is used in the numerical solution of stochastic differential equations; the Karhunen-Loève expansion is often used in finite mode approximation for the Gaussian random field; the construction using the Haar basis or a more general basis is used in the study of stochastic partial differential equations. A realization of the Wiener process with finite cutoff for the three different constructions is shown in Figure 6.2.

Example 6.6. Compute the expectation

$$\mathbb{E} \exp \left(-\frac{1}{2} \int_0^1 W_t^2 dt \right).$$

Solution. This is an example of a Wiener functional. Using the Karhunen-Loève expansion, we get

$$
\int_0^1 W_t^2 dt \;=\; \int_0^1 \sum_{k,l} \sqrt{\lambda_k \lambda_l}\, \alpha_k \alpha_l \phi_k(t)\phi_l(t)dt
$$

$$
=\; \sum_k \int_0^1 \lambda_k \alpha_k^2 \phi_k^2(t)dt = \sum_k \lambda_k \alpha_k^2.
$$

Then

$$
\mathbb{E}\exp\Big(-\frac{1}{2}\int_0^1 W_t^2 dt\Big) \;=\; \mathbb{E}\Big(\prod_k \exp\Big(-\frac{1}{2}\lambda_k \alpha_k^2\Big)\Big) = \prod_k \mathbb{E}\exp\Big(-\frac{1}{2}\lambda_k \alpha_k^2\Big).
$$

From the identity

$$
\mathbb{E}\exp\Big(-\frac{1}{2}\lambda_k \alpha_k^2\Big) = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \cdot e^{-\frac{1}{2}\lambda_k x^2} dx = \sqrt{\frac{1}{1+\lambda_k}}
$$

we obtain

$$
\mathbb{E}\exp\Big(-\frac{1}{2}\int_0^1 W_t^2 dt\Big) \;=\; \prod_k \sqrt{\frac{1}{1+\lambda_k}} := M,
$$

where

$$
M^{-2} = \prod_{k=1}^{\infty}\Big(1 + \frac{4}{(2k-1)^2\pi^2}\Big).
$$

Using the identity

$$
\cosh(x) = \prod_{k=1}^{\infty}\Big(1 + \frac{4x^2}{(2k-1)^2\pi^2}\Big),
$$

we get

$$
M = (\cosh(1))^{-\frac{1}{2}} = \sqrt{\frac{2e}{1+e^2}}. \qquad\qquad \square
$$

6.4. Wiener Process as a Markov Process

From the definition of Wiener process, we can easily obtain that the joint probability distribution density for $(W_{t_1}, W_{t_2}, \ldots, W_{t_n})$ $(t_1 < t_2 < \cdots < t_n)$ is given by

$$
(6.15) \qquad p_n(w_1, w_2, \ldots, w_n) = \frac{1}{\sqrt{2\pi t_1}} e^{-\frac{w_1^2}{2t_1}} \frac{1}{\sqrt{2\pi(t_2 - t_1)}} e^{-\frac{(w_2 - w_1)^2}{2(t_2 - t_1)}}
$$

$$
\cdot \ \cdots \ \cdot \frac{1}{\sqrt{2\pi(t_n - t_{n-1})}} e^{-\frac{(w_n - w_{n-1})^2}{2(t_n - t_{n-1})}}.
$$

In other words,

$$p_n(w_1, w_2, \ldots, w_n) = \frac{1}{Z_n} \exp(-I_n(w)),$$

where

$$I_n(w) = \frac{1}{2} \sum_{j=1}^{n} \left(\frac{w_j - w_{j-1}}{t_j - t_{j-1}} \right)^2 (t_j - t_{j-1}), \quad t_0 := 0, w_0 := 0,$$

$$Z_n = (2\pi)^{\frac{n}{2}} \left[t_1 (t_2 - t_1) \cdots (t_n - t_{n-1}) \right]^{\frac{1}{2}}.$$

From this we see that the Wiener process is a stationary Markov process with transition kernel $p(x, t|y, s)$ given by

$$\mathbb{P}(W_t \in B | W_s = y) = \int_B \frac{1}{\sqrt{2\pi(t-s)}} e^{-\frac{(x-y)^2}{2(t-s)}} dx = \int_B p(x, t|y, s) dx$$

where $s < t$ and B is a Borel set in $\mathbb{R}$. It is also straightforward to see from (6.15) that W_t is a process with independent increments; i.e., for any $t_0 < t_1 < \cdots < t_n$, the random variables $W_{t_0}, W_{t_1} - W_{t_0}, \ldots, W_{t_n} - W_{t_{n-1}}$ are independent, and $W_{s+t} - W_s \sim N(0, t)$ for any $s, t \geq 0$.

The transition probability density $p(x, t|y, s)$ satisfies the stationarity relation $p(x, t|y, s) = p(x - y, t - s|0, 0)$ and $p(x, t|0, 0)$ satisfies the partial differential equation

(6.16) $$\frac{\partial p}{\partial t} = \frac{1}{2} \frac{\partial^2 p}{\partial x^2}, \quad p(x, 0|0, 0) = \delta(x).$$

The generator of the Wiener process can be found by

$$\begin{aligned}
\mathcal{A}f(x) &= \lim_{t \to 0} \frac{1}{t} \left[\mathbb{E}^x f(W_t) - f(x) \right] \\
&= \lim_{t \to 0} \frac{1}{t} \int_0^t \partial_s \left(\int_{\mathbb{R}} f(y) p(y, s|x, 0) dy \right) ds \\
&= \lim_{t \to 0} \frac{1}{t} \int_0^t \int_{\mathbb{R}} f(y) \frac{1}{2} \frac{\partial^2}{\partial y^2} p(y, s|x, 0) dy ds \\
&= \lim_{t \to 0} \frac{1}{t} \int_0^t \int_{\mathbb{R}} \frac{1}{2} \frac{\partial^2}{\partial y^2} f(y) p(y, s|x, 0) dy ds \\
&= \frac{1}{2} \frac{\partial^2 f}{\partial x^2}
\end{aligned}$$

for any $f \in C_0^\infty(\mathbb{R})$.

6.5. Properties of the Wiener Process

We will discuss some basic symmetry properties of the Wiener process and the regularity properties of the paths.

Theorem 6.7. *Wiener process has the following symmetry properties.*

(1) *Time-homogeneity: For any $s > 0$, $W_{t+s} - W_s$, $t \geq 0$, is a Wiener process.*

(2) *Symmetry: The process $-W_t$, $t \geq 0$, is a Wiener process.*

(3) *Scaling: For every $c > 0$, the process cW_{t/c^2}, $t \geq 0$, is a Wiener process.*

(4) *Time-inversion: The process X defined by $X_0 = 0$, $X_t = tW_{1/t}$ for $t > 0$, is a Wiener process.*

The proof is straightforward and is left as an exercise.

From the third statement above, one has

(6.17) $$W_{kt} \sim \sqrt{k}W_t, \quad \dot{W}_{kt} \sim \frac{1}{\sqrt{k}}\dot{W}_t,$$

in distribution, where $\dot{W}_t$ means the formal derivative of W_t with respect to t. This is the white noise process that we will discuss later. This means that from the viewpoint of scaling, W_t behaves like $t^{1/2}$. This is particularly useful when performing the dimensional analysis of stochastic differential equations.

Now, let us turn to the regularity properties of the Wiener paths.

The total variation of a path of the process X on $[a, b]$ is defined by

$$V(X(\omega); [a, b]) = \sup_\Delta \sum_k |X_{t_{k+1}}(\omega) - X_{t_k}(\omega)|,$$

where $\Delta = \bigcup_k [t_k, t_{k+1}]$ is a subdivision of $[a, b]$. The discrete quadratic variation of X on $[0, t]$ for the subdivision Δ is defined by

$$Q_t^\Delta = \sum_k |X_{t_{k+1}}(\omega) - X_{t_k}(\omega)|^2.$$

Let $|\Delta_n|$ be the biggest mesh size of the subdivision Δ_n. If there exists a finite process $[X, X]$ such that

$$Q_t^{\Delta_n} \to [X, X]_t \quad \text{in probability as } |\Delta_n| \to 0,$$

for any t, then $[X, X]$ is called the *quadratic variation process* of X. It is obvious that $[X, X]$ is increasing. The definition can be easily extended to any finite interval $[a, b]$, and one has

$$Q_{[a,b]}^{\Delta_n} \to [X, X]_b - [X, X]_a \quad \text{as } |\Delta_n| \to 0.$$

Proposition 6.8. *Consider the Wiener process. For any t and subdivision Δ of $[0, t]$, we have*

(6.18) $$\mathbb{E}(Q_t^\Delta - t)^2 = 2 \sum_k (t_{k+1} - t_k)^2.$$

Consequently, we have

$$Q_t^\Delta \longrightarrow t \ \text{in} \ L_\omega^2 \quad \text{as} \ |\Delta| \to 0$$

and $[W, W]_t = t$ *a.s.*

The proof of Proposition 6.8 is straightforward and is left as an exercise. This result is sometimes formally stated as $(dW_t)^2 = dt$. We will get back to this formula in Section 7.2.

Theorem 6.9 (Unbounded variation of the Wiener path). *On any finite interval, the total variation of a Wiener path is almost surely infinite.*

Proof. Because of (6.18), there is a subset $\Omega_0 \subset \Omega$ such that $\mathbb{P}(\Omega_0) = 1$, and a subsequence of subdivisions, still denoted as $\{\Delta_n\}$, such that for any pair of rational numbers $(p, q), p < q$,

$$Q_{[p,q]}^{\Delta_n} \to q - p, \quad \text{on} \ \Omega_0.$$

Therefore, we have

$$q - p \leftarrow \sum_k (W_{t_{k+1}} - W_{t_k})^2 \leq \sup_k |W_{t_{k+1}} - W_{t_k}| \cdot V(W(\omega); [p, q]), \qquad \omega \in \Omega_0.$$

From the uniform continuity of W on $[p, q]$, $\sup_k |W_{t_{k+1}} - W_{t_k}| \to 0$. Hence, as a function of t, the total variation of $W_t(\omega)$ is infinite, for $\omega \in \Omega_0$. $\quad\square$

Theorem 6.10 (Smoothness of the Wiener path). *Let Ω_α be the set of functions that are Hölder continuous with exponent α $(0 < \alpha < 1)$:*

$$\Omega_\alpha = \left\{ f \in C[0, 1], \sup_{0 \le s, t \le 1} \frac{|f(t) - f(s)|}{|t - s|^\alpha} < \infty \right\}.$$

Then if $0 \le \alpha < \frac{1}{2}$, $\mathbb{P}(W \in \Omega_\alpha) = 1$; if $\alpha \ge \frac{1}{2}$, $\mathbb{P}(W \in \Omega_\alpha) = 0$.

The proof of Theorem 6.10 relies on the modification concept and the following Kolmogorov continuity theorem, which can be found in [**RY05**].

Definition 6.11 (Modification). Two processes X and $\tilde{X}$ defined on the same probability space Ω are said to be modifications of each other if for each t,

$$X_t = \tilde{X}_t \quad \text{a.s.}$$

They are called indistinguishable if for almost all $\omega \in \Omega$

$$X_t(\omega) = \tilde{X}_t(\omega) \quad \text{for every t.}$$

It is obvious that if X and $\tilde{X}$ are modifications of each other, they have the same finite-dimensional distribution. If X and $\tilde{X}$ are modifications of each other and are almost surely continuous, they are indistinguishable.

Theorem 6.12 (Kolmogorov's continuity theorem). *Let $\{X_t\}$ ($t \in [0,1]^d$) be a stochastic process on probability space Ω. Assume that there exist three positive constants γ, c, ε such that*

$$\mathbb{E}(|X_t - X_s|^\gamma) \le c|t - s|^{d+\varepsilon}.$$

Then there is a modification of X, $\tilde{X}$ such that

$$\mathbb{E}\left(\sup_{s \neq t} \frac{|\tilde{X}_t - \tilde{X}_s|}{|t - s|^\alpha}\right)^\gamma < \infty$$

for every $\alpha \in [0, \varepsilon/\gamma)$. In particular, the paths of $\tilde{X}$ are Hölder continuous with exponent α.

Proof of Theorem 6.10. Since

$$\mathbb{E}|W_t|^{2p} = Ct^p$$

for any $p \in \mathbb{N}$, we can use the theorem above with $\varepsilon = p - 1, \gamma = 2p$. We have $\varepsilon/\gamma = (p-1)/2p = 1/2 - 1/2p$. Thus for $\alpha < 1/2$, $\mathbb{P}(W_t \in \Omega_\alpha) = 1$.

When $\alpha > 1/2$, if there exists a rational interval $[p, q]$ such that $|W_t - W_s| \le c|t - s|^\alpha$ for any $p \le s, t \le q$, then by Proposition 6.8

$$q - p \leftarrow \sum_k (W_{t_{k+1}} - W_{t_k})^2 \le c^2 \sum_k |t_{k+1} - t_k|^{2\alpha-1}|t_{k+1} - t_k|$$
$$\le c^2(q - p) \sup_k |t_{k+1} - t_k|^{2\alpha-1} \to 0,$$

which is a contradiction.

The critical case of $\alpha = 1/2$ is covered by Lévy's modulus of continuity theorem. The reader may refer to [**RY05**] for details. $\square$

The following theorem due to A. Khinchin characterizes the local behavior of W_t as t goes to zero.

Theorem 6.13 (Local law of the iterated logarithm). *We have*

$$\mathbb{P}\left(\limsup_{t \to 0} \frac{W_t}{\sqrt{-2t \log \log t}} = 1\right) = 1,$$

$$\mathbb{P}\left(\liminf_{t \to 0} \frac{W_t}{\sqrt{-2t \log \log t}} = -1\right) = 1.$$

More results of this type can be found in [**KS91**, **MP10**, **RY05**].

6.6. Wiener Process under Constraints

In this section, we consider the Wiener process with constraints that give rise to effective boundary conditions for the paths.

Case 1: Reflecting barrier at $m = m_1$.

The reflecting barrier at $m = m_1$ means that once the particle hits the state m_1 at time n, it will get back to the previous state at time $n + 1$ with probability 1. Without loss of generality we suppose $m_1 > 0$ and ask what the probability $W_r(m, N; m_1)$ is that the particle will arrive at m which is less than m_1 after N steps.
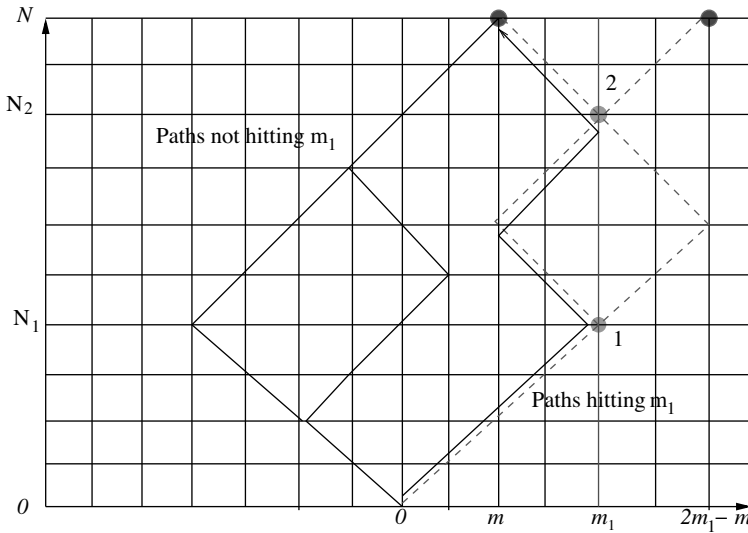
Figure 6.3. Schematics of the reflection principle, where $m = m_1$ is the location of the reflecting barrier. The dashed lines show all of the possible reflected paths.

This problem may be solved very efficiently in the (m-N)-plane in a neat way. As shown in Figure 6.3, the actual sample paths which include the reflected sample are shown with solid lines, and the paths crossing the barrier m_1 in the unrestricted random walk case are shown with dashed lines. These paths can be classified into two classes. One class only contains the paths not hitting m_1 and finally reaching m; the other class contains the paths hitting m_1 before time N and finally reaching m_1 or $2m_1 - m$. We have the following assertions on these paths.

- For the unconstrained random walk, all of the sample paths have equal probability $1/2^N$.
- The probability of the reflected paths which hits m_1 is equal to the sum of the probability of the paths hitting m_1 and reaching m

and the paths reaching $2m_1 - m$. A simple argument to prove this is to observe that the reflecting probability is 1 at the reflection point shown as points 1 and 2 in the figure. From $1 = 1/2 + 1/2$, this decomposition actually decompose the paths into those that go leftward and rightward with equal probability, which corresponds to all the paths just stated.

- The number of the paths hitting m_1 and hitting m finally is equal to that of the paths hitting $2m_1 - m$ finally. This can be understood because these paths have to cross m_1 and we can denote the final hitting time as N_2 as shown in the figure. So after N_2, the paths go leftward or rightward with mirror symmetry to hit m or $2m_1 - m$. Before N_1, the paths can be in either branch.

These assertions are called the *reflection principle*, which is the basis of the following calculations for the reflecting and absorbing barrier problem.

So we have the following identity:

$$W_r(m, N; m_1) = W(m, N) + W(2m_1 - m, N).$$

If we take the same rescaling and asymptotics as before, we have

$$W_r(m, N; m_1) \approx \left(\frac{2}{\pi N} \right)^{\frac{1}{2}} \left[\exp\left(-\frac{m^2}{2N} \right) + \exp\left(-\frac{(2m_1 - m)^2}{2N} \right) \right].$$

Then passing to the continuum limit we have

$$(6.19) \qquad W_r(x, t; x_1) = \frac{1}{\sqrt{4\pi D t}} \left[\exp\left(-\frac{x^2}{4Dt} \right) + \exp\left(-\frac{(2x_1 - x)^2}{4Dt} \right) \right].$$

We remark that in this case $W_r(x, t; x_1)$ satisfies the PDE

$$\begin{cases} \dfrac{\partial W_r}{\partial t} = D\dfrac{\partial^2 W_r}{\partial x^2}, & x \le x_1, \ t \ge 0, \\[2mm] W_r\Big|_{t=0} = \delta(x), \\[2mm] \dfrac{\partial W_r}{\partial x}\Big|_{x=x_1} = 0. \end{cases}$$

Case 2: Absorbing wall at $m = m_1$.

The absorbing wall at $m = m_1$ means that once the particle hits the state m_1 at time n, it will be stuck there forever. We still assume $m_1 > 0$ and obtain the probability $W_a(m, N; m_1)$ that the particle will arrive at m that is less than m_1 after N steps by the reflection principle

$$W_a(m, N; m_1) = W(m, N) - W(2m_1 - m, N).$$

With the same rescaling and asymptotics, we have

$$W_a(m, N; m_1) \approx \left(\frac{2}{\pi N} \right)^{\frac{1}{2}} \left[\exp\left(-\frac{m^2}{2N} \right) - \exp\left(-\frac{(2m_1 - m)^2}{2N} \right) \right],$$

and the continuum limit is

$$(6.20) \quad W_a(x, t; x_1) = \frac{1}{\sqrt{4\pi Dt}} \left[\exp\left(-\frac{x^2}{4Dt} \right) - \exp\left(-\frac{(2x_1 - x)^2}{4Dt} \right) \right],$$

and we again remark that in this case $W_a(x, t; x_1)$ satisfies the PDE

$$\begin{cases} \dfrac{\partial W_a}{\partial t} = D\dfrac{\partial^2 W_a}{\partial x^2}, & x \leq x_1, \ t \geq 0, \\[2mm] W_a\Big|_{t=0} = \delta(x), \\[2mm] W_a\Big|_{x=x_1} = 0. \end{cases}$$

Now let us consider the first hitting probability

$$a(m_1, N) = \mathbb{P}\{X_N = m_1, \text{ and } X_n < m_1, \forall n < N\}$$

that taking N steps the particle will arrive at m_1 without ever hitting $m = m_1$ at any earlier step. Then we have

$$a(m_1, N) = \frac{1}{2}W_a(m_1 - 1, N - 1; m_1) = \frac{m_1}{N}W(m_1, N)$$

by the above formula and the relation $W(m, N) = W(m - 1, N - 1) \cdot N/(N + m)$. In the large N limit we have

$$a(m_1, N) \approx \frac{m_1}{N}\left(\frac{2}{\pi N} \right)^{\frac{1}{2}} \exp\left(-\frac{m_1^2}{2N} \right).$$

The continuous probability density $a(m_1, t)$ becomes

$$a(m_1, t)\Delta t \approx a(m_1, N)\frac{\Delta t}{2\tau},$$

where $t = N\tau$. In the continuum limit one obtains

$$a(x_1, t) = \frac{x_1}{t}\frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x_1^2}{4Dt} \right).$$

6.7. Wiener Chaos Expansion

In this section, we consider functionals of the Wiener process, the Wiener functionals. Specifically, we will discuss the space $L^2(\Omega, \mathcal{F}, \mathbb{P})$, where $\Omega = C[0, T]$, the space of continuous functions on $[0, T]$, and $\mathbb{P}$ is the Wiener measure. Here $T > 0$ is some positive number. We will show that such functionals can be expanded in the Fourier-Hermite series.

Let H_n be the nth-order normalized Hermite polynomial defined by

$$H_n(x) = \frac{(-1)^n}{\sqrt{n!}}e^{x^2/2}\frac{d^n}{dx^n}e^{-x^2/2}.$$

Here $H_n(x)$ satisfies the orthonormality relation

$$\int_{-\infty}^{\infty} H_n(x)H_m(x)\frac{1}{\sqrt{2\pi}}e^{-x^2/2}dx = \delta_{nm}, \quad n, m \geq 0.$$

Let

$$\mathcal{I} = \left\{ \boldsymbol{\alpha} | \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots), \alpha_k \in \{0, 1, \ldots\}, k \in \mathbb{N}, |\boldsymbol{\alpha}| = \sum_{k=1}^{\infty} \alpha_k < \infty \right\}$$

be the set of multi-indices. For any $\boldsymbol{\alpha} \in \mathcal{I}$, define the multivariate Hermite polynomial

$$H_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{k=1}^{\infty} H_{\alpha_k}(\xi_k)$$

where $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots)$. Here $H_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$ is also called the Wick polynomial in the literature.

In the spirit of the series representation of the Wiener process that we discussed earlier, we also have

$$W_t = \sum_{k=1}^{\infty} \xi_k \int_0^t m_k(s)ds, \quad t \leq T,$$

in $L_\omega^2 L_t^2$, where $\{\xi_k\}$ are i.i.d. Gaussian random variables with distribution $N(0, 1)$ and $\{m_k(t)\}$ is any orthonormal basis in $L^2[0, T]$. This establishes another correspondence between the Wiener paths $\omega \in \Omega$ and an infinite sequence of i.i.d. normal random variables $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots)$.

Theorem 6.14 (Wiener chaos expansion). *Let W be a standard Wiener process on $(\Omega, \mathcal{F}, \mathbb{P})$. Let F be a Wiener functional in $L^2(\Omega)$. Then F can be represented as*

(6.21)
$$F[W] = \sum_{\boldsymbol{\alpha} \in \mathcal{I}} f_{\boldsymbol{\alpha}} H_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

in $L^2(\Omega)$, where the coefficients are given by

$$f_{\boldsymbol{\alpha}} = \mathbb{E}\Big(F[W] H_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) \Big).$$

This is an infinite-dimensional analog of the Fourier expansion with weight function $(\sqrt{2\pi})^{-1}e^{-x^2/2}$ in each dimension. Its proof can be found in [**CM47**].

To help appreciate this, let us consider the one-dimensional case $F(\xi)$ where $\xi \sim N(0, 1)$. Then the Wiener chaos expansion reduces to

(6.22)
$$F(\xi) = \sum_{k=0}^{\infty} f_k H_k(\xi) \quad \text{in } L_\omega^2,$$

where $f_k = \mathbb{E}\Big(F(\xi)H_k(\xi)\Big)$. This is simply the probabilistic form of the Fourier-Hermite expansion of F with the weight function $w(x) = (\sqrt{2\pi})^{-1}e^{-x^2/2}$. For the finite-dimensional case $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_K)$, we can define

$$\mathcal{I}_K = \big\{ \boldsymbol{\alpha} | \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_K), \alpha_k \in \{0, 1, 2, \ldots\}, k = 1, 2, \ldots, K \big\}$$

and the finite tensor product of Hermite polynomials

$$H_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \prod_{k=1}^{K} H_{\alpha_k}(\xi_k).$$

Then we have

$$F(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha} \in \mathcal{I}_K} f_{\boldsymbol{\alpha}} H_{\boldsymbol{\alpha}}(\boldsymbol{\xi}). \tag{6.23}$$

The Wiener chaos expansion can be used to numerically solve differential equations involving randomness [**GS12**]. Let us take the simple linear random differential equation

$$\frac{dX_t}{dt} = -\xi X_t, \quad X_t|_{t=0} = X_0, \quad t \in [0, T], \tag{6.24}$$

as an example to illustrate the basic idea, where ξ is assumed to be an $N(0, 1)$ random variable and X_0 is a constant.

We obviously have $X_t \in C_t^\infty L_\omega^2$. Based on (6.22) we have the expansion

$$X_t = \sum_{k=0}^{\infty} x_k(t) H_k(\xi).$$

From (6.24) we obtain

$$\sum_{k=0}^{\infty} \dot{x}_k(t) H_k(\xi) = -\sum_{k=0}^{\infty} \xi H_k(\xi) x_k(t). \tag{6.25}$$

Using the orthogonality of the Wick polynomials in L_ω^2, we get

$$\dot{x}_k(t) = -\sum_{l=0}^{\infty} A_{kl} x_l(t), \tag{6.26}$$

where $A_{kl} = \mathbb{E}(\xi H_k(\xi) H_l(\xi))$. Truncating system (6.25) to order K, we obtain the numerical discretization of (6.24)

$$\dot{x}_k(t) = -\sum_{l=0}^{K} A_{kl} x_l(t), \quad k = 0, 1, \ldots, K, \tag{6.27}$$

with initial conditions $x_0(0) = X_0$ and $x_k(0) = 0$ for $k = 1, 2, \ldots, K$.

The Wiener chaos expansion can also be extended to the so-called generalized polynomial chaos (gPC) expansion when the random variables involved are non-Gaussian [**XK02**]. It is commonly used in uncertainty quantification (UQ) problems [**GHO17**].

Exercises

6.1. Let $\{\xi_n\}_{n=1}^{\infty}$ be a sequence of i.i.d. random variables taking values $+1$ with probability $2/3$ and -1 with probability $1/3$. Consider the (asymmetric) random walk on $\mathbb{Z}$ defined by

$$S_n = \sum_{j=1}^{n} \xi_j.$$

We want to show that there exists $\alpha \in \mathbb{R}$ such that the sequence of piecewise constant functions

$$Z_t^N = \frac{S_{\lfloor Nt \rfloor}}{N^\alpha}$$

converge as $N \to +\infty$ to some nontrivial Z_t. What is the α you need to choose for this to be the case? And what is Z_t?

6.2. Prove that the following definition is an equivalent characterization of the Wiener process:
   (a) For any $t_0 < t_1 < \cdots < t_n$, the random variables $W_{t_0}, W_{t_1} - W_{t_0}, \ldots, W_{t_n} - W_{t_{n-1}}$ are independent.
   (b) For any $s, t \geq 0$, $W_{s+t} - W_s \sim N(0, t)$.
   (c) With probability 1, $t \mapsto W_t$ is continuous.

6.3. Let $\{W_t\}$ be a Wiener process. Compute
   (a) $\mathbb{E}W_t^4$,
   (b) $\mathbb{E}(W_t - W_s + W_z)^2$, $t, s, z \in [0, 1]$.

6.4. Let $\boldsymbol{X} \in \mathbb{R}^d$ be a d-dimensional Gaussian random variable with mean zero and covariance matrix $\boldsymbol{\Sigma}$ (i.e., $\mathbb{E}X_i X_j = \Sigma_{ij}$). Let $\boldsymbol{B}$ be a strictly positive definite symmetric $d \times d$ matrix. Compute

$$\mathbb{E}\exp\left(-\frac{1}{2}\boldsymbol{X}^T \boldsymbol{B}\boldsymbol{X}\right).$$

6.5. Prove the basic properties of the Wiener paths as shown in Theorem 6.7.

6.6. Prove Proposition 6.8. Furthermore, if we choose the dyadic subdivisions $t_k = k2^{-n}t, k = 0, 1, \ldots, 2^n$, and consider the discrete quadrative variation of Wiener process $Q_t^{\Delta_n}$ on $[0, t]$, prove the following sharpened version of Proposition 6.8:

$$Q_t^{\Delta_n} \to t, \quad \text{a.s.} \quad \text{as } n \to \infty.$$

6.7. A standard *Brownian bridge* is a Gaussian process with continuous paths, mean function $m(t) = 0$, and covariance function $K(s,t) = s \wedge t - st$ for $s, t \in [0,1]$. Prove that both $X_t = W_t - tW_1$ and $Y_t = (1-t)W_{t/(1-t)}$ for $0 \le t < 1$, $Y_1 = 0$ give a Brownian bridge.

6.8. Consider a two-dimensional Gaussian random field $B_{(s,t)}$ with mean function $m(s,t) = 0$ and covariance function $K((s,t),(u,v)) = (s \wedge u) \times (t \wedge v)$ where $(s,t), (u,v) \in \mathbb{R}^2_+$.
   (a) Prove that this process has a continuous version. It is called the *Brownian sheet*.
   (b) Prove that if $B_{(s,t)}$ is a Brownian sheet, then the following processes are also Brownian sheets:
        (i) $B_{(a^2 s, b^2 t)}/ab$ where $a, b \in \mathbb{R}^+$.
        (ii) $sB_{(s^{-1},t)}$ and $stB_{(s^{-1},t^{-1})}$.
        (iii) $B_{(s_0+s, t_0+t)} - B_{(s_0, t_0+t)} - B_{(s_0+s, t_0)} + B_{(s_0, t_0)}$.

6.9. Construct the Karhunen-Loève expansion for the Brownian bridge and Ornstein-Uhlenbeck process for $t \in [0,1]$.

6.10. For the standard Wiener process $\{W_t\}$, we can define the conditional distribution of W_t give W_T for $0 \le t \le T$. Prove the following assertions:
   (a) The distribution of $(W_{t_1}, W_{t_2}, \dots, W_{t_k} | W_T)$ is Gaussian.
   (b) The condition mean function
$$\mathbb{E}(W_t | W_T) = \frac{t}{T}W_T.$$
   (c) The conditional covariance function
$$\mathbb{E}(W_s W_t | W_T) = \frac{s(T-t)}{T}.$$

   If $T = 1$ and $W_T = 0$, we obtain exactly the Brownian bridge.

6.11. Consider the *fractional Brownian motion* $\{B_t^{(H)}\}_{t \ge 0}$ with Hurst index $H \in (0,1)$ (defined in Exercise 5.9). Prove that $B_t^{(H)}$ has the following properties:
   (a) $B_0^{(H)} = 0$, and $B_t^{(H)}$ is the standard Brownian motion when $H = 1/2$.
   (b) $B^{(H)}$ admits a version whose sample paths are almost surely C^α for $\alpha \in [0, H)$.

6.12. Let $f(t) = \exp(i\omega_0 t + iW_t)$ represent a wave with random phase W_t. Define the wave detector
$$U = \left| \frac{1}{2\pi} \int_{\mathbb{R}} \psi(\omega) \int_{\mathbb{R}} e^{-i\omega t} f(t)\, dt\, d\omega \right|^2.$$

Compute the mean detecting signal $\mathbb{E}U$ and compare this with the case without random perturbation.

6.13. Prove that the Borel σ-algebra on $(C[0,1], \|\cdot\|_\infty)$ is the same as the product σ-algebra on $C[0,1]$, i.e., the smallest σ-algebra generated by the cylinder sets

$$C = \{\omega : (\omega(t_1), \omega(t_2), \dots, \omega(t_k)) \in \mathcal{R}^k, \text{ for any } k \in \mathbb{N}\}.$$

Notes

Theoretical study of Brownian motion began with Einstein's seminal paper in 1905 [**Ein05**]. The mathematical framework was first established by Wiener [**Wie23**]. More material on Brownian motion can be found in [**KS91**, **MP10**].

Stochastic Differential Equations

We now turn to the most important object in stochastic analysis: the stochastic differential equations (SDEs). Outside of mathematics, SDEs are often written in the form

(7.1) $$\dot{X}_t = b(X_t, t) + \sigma(X_t, t)\dot{W}_t, \quad X|_{t=0} = X_0.$$

The first term on the right-hand side is called the drift term. The second term is called the diffusion term. $\dot{W}_t$ is formally the derivative of the Wiener process, known as the *white noise*. One can think of it as a Gaussian process with mean and covariance functions:

$$m(t) = \mathbb{E}(\dot{W}_t) = \frac{d}{dt}\mathbb{E}(W_t) = 0,$$

$$K(s,t) = \mathbb{E}(\dot{W}_s\dot{W}_t) = \frac{\partial^2}{\partial s \partial t}\mathbb{E}(W_s W_t) = \frac{\partial^2}{\partial s \partial t}(s \wedge t) = \delta(t-s).$$

The name *white noise* comes from its power spectral density $S(\omega)$ defined as the Fourier transform of its autocorrelation function $R(t) = \mathbb{E}(\dot{W}_0\dot{W}_t) = \delta(t)$: $S(\omega) = \widehat{\delta(t)} = 1$. We call it "white" from the analogy with the spectrum of white light. Noises whose spectrum is not a constant are called *colored noises*.

From the regularity theory of the Wiener paths discussed in Section 6.5, $\dot{W}_t$ is not an ordinary function since W_t is not differentiable. It has to be understood in the sense of distribution [**GS66**]. Consequently, defining the product in the last term in (7.1) can be a tricky task.

In the mathematics literature, one often writes (7.1) in the form

(7.2) $$dX_t = b(X_t, t)dt + \sigma(X_t, t)dW_t.$$

This is supposed to be understood in the integral sense:

(7.3) $$X_t = X_0 + \int_0^t b(X_s, s)ds + \int_0^t \sigma(X_s, s)dW_s.$$

To make this precise, the only obvious difficulty is in the last term, which is a stochastic integral. This reduces the problem of the SDEs to that of the stochastic integrals.

It turns out that one cannot use the classical theory of the Lebesgue-Stieltjes integral directly to define stochastic integrals since each Brownian path has unbounded variations on any interval $[t_1, t_2]$. Nevertheless, there are several natural ways of defining stochastic integrals. If we think of approximating the integral by quadrature, then depending on how we pick the quadrature points, we get different limits. This may seem worrisome at first sight. If the stochastic integrals have different meanings, which meaning are we supposed to use in practice? Luckily so far this has not been an issue. It is often quite clear from the context of the problem which version of the stochastic integral one should use. In addition, it is also easy to convert the result of one version to that for another version.

By far the most popular way of defining stochastic integrals is that of Itô.

7.1. Itô Integral

One obvious possibility is to try to define the stochastic integral pathwise as a Riemann-Stieljes integral:

$$\int_0^t \sigma(X_s, s)dW_s = \lim_{|\Delta| \to 0} \sum_j \sigma(X_j, t_j^*)\Big(W_{t_{j+1}} - W_{t_j}\Big),$$

where Δ is a subdivision of $[0, t]$, $X_j = X_{t_j^*}$, and t_j^* is chosen arbitrarily from the interval $[t_j, t_{j+1}]$.

For the ordinary Riemann-Stieljes integral $\int_a^b f(t)dg(t)$, f and g are assumed to be continuous and g is assumed to have bounded variation. In that case the sum

(7.4) $$\sum_j f(t_j^*)\Big(g(t_{j+1}) - g(t_j)\Big)$$

converges to a limit which is independent of the choice of $\{t_j^*\}$. However, for the stochastic integral, the corresponding g does not have bounded variation.

As a result, different choices of $\{t_j^*\}$ lead to different limits. Consider, for example, $\int_0^T W_t dW_t$:

Choice 1. Leftmost endpoint integral: $\quad I_N^L := \sum_j W_{t_j}(W_{t_{j+1}} - W_{t_j})$.

Choice 2. Rightmost endpoint integral: $\quad I_N^R := \sum_j W_{t_{j+1}}(W_{t_{j+1}} - W_{t_j})$.

Choice 3. Midpoint integral: $\quad I_N^M := \sum_j W_{t_{j+\frac{1}{2}}}(W_{t_{j+1}} - W_{t_j})$.

For these choices, we have

$$\mathbb{E}(I_N^L) = \sum_j \mathbb{E} W_{t_j} \mathbb{E}(W_{t_{j+1}} - W_{t_j}) = 0,$$

$$\mathbb{E}(I_N^R) = \sum_j \left[\mathbb{E}(W_{t_{j+1}} - W_{t_j})^2 + \mathbb{E} W_{t_j} \mathbb{E}(W_{t_{j+1}} - W_{t_j}) \right] = \sum_j \delta t_j = T,$$

$$\mathbb{E}(I_N^M) = \mathbb{E}\Big[\sum_j W_{t_{j+\frac{1}{2}}}(W_{t_{j+1}} - W_{t_{j+\frac{1}{2}}}) + \sum_j W_{t_{j+\frac{1}{2}}}(W_{t_{j+\frac{1}{2}}} - W_{t_j}) \Big]$$

$$= \sum_j \mathbb{E}(W_{t_{j+\frac{1}{2}}} - W_{t_j})^2 = \sum_j (t_{j+\frac{1}{2}} - t_j) = \frac{T}{2}.$$

The pathwise results must also be different.

Itô's integral corresponds to the first choice. To rigorously define the Itô integral, we start with *simple functions* which are random functions of the form

$$(7.5) \qquad f(\omega, t) = \sum_{j=1}^n e_j(\omega) \chi_{[t_j, t_{j+1})}(t),$$

where $e_j(\omega)$ is $\mathcal{F}_{t_j}$-measurable and $\chi_{[t_j, t_{j+1})}(t)$ is the indicator function of $[t_j, t_{j+1})$. For technical reason, we always assume that $\{\mathcal{F}_t\}_{t \geq 0}$ is the augmented filtration of $\{\mathcal{F}_t^W\}_{t \geq 0}$; thus W is $\mathcal{F}_t$-adapted. Obviously in this case the Itô integral has to be defined as

$$(7.6) \qquad \int_0^T f(\omega, t) dW_t = \sum_j e_j(\omega)(W_{t_{j+1}} - W_{t_j}).$$

Lemma 7.1. *Assume that $0 \leq S \leq T$. The stochastic integral for the simple functions satisfies*

$$(7.7) \qquad \mathbb{E}\left(\int_S^T f(\omega, t) dW_t \right) = 0,$$

$$(7.8) \qquad \text{(Itô isometry)} \quad \mathbb{E}\Big(\int_S^T f(t, \omega) dW_t \Big)^2 = \mathbb{E}\left(\int_S^T f^2(\omega, t) dt \right).$$

Proof. The first property is straightforward from the independence between $\delta W_j := W_{t_{j+1}} - W_{t_j}$, $e_j(\omega)$, and $\delta W_j \sim N(0, t_{j+1} - t_j)$. For the second property we have

$$\mathbb{E}\left(\int_S^T f(\omega, t)dW_t\right)^2 = \mathbb{E}\left(\sum_j e_j \delta W_j\right)^2 = \mathbb{E}\left(\sum_{j,k} e_j e_k \delta W_j \delta W_k\right)$$

$$= \mathbb{E}\left(\sum_j e_j^2 \delta W_j^2 + 2\sum_{j<k} e_j e_k \delta W_j \delta W_k\right)$$

$$= \sum_j \mathbb{E}e_j^2 \cdot \mathbb{E}\delta W_j^2 + 2\sum_{j<k} \mathbb{E}(e_j e_k \delta W_j) \cdot \mathbb{E}(\delta W_k)$$

$$= \sum_j \mathbb{E}e_j^2 \delta t_j = \mathbb{E}\left(\int_S^T f^2(\omega, t)dt\right),$$

where we have used the independence between δW_k and $e_j e_k \delta W_j$ for $j < k$. $\qquad\square$

Next we approximate general functions by simple functions.

Fix two constants S, T such that $0 \le S < T$. Let $\mathcal{V}[S, T]$ be the class of functions $f(\omega, t)$ that satisfy the following conditions:

(i) f is $(\mathcal{R} \times \mathcal{F})$-measurable as a function from $[S, T] \times \Omega$ to $\mathbb{R}$.

(ii) f is $\mathcal{F}_t$-adapted; i.e., $f(t, \cdot)$ is $\mathcal{F}_t$-measurable for each $t \ge 0$.

(iii) $f \in L_\omega^2 L_t^2$; that is, $\mathbb{E}\left(\int_S^T f^2(\omega, t)dt\right) < \infty$.

It can be shown that if $f \in \mathcal{V}[S, T]$, then there exists a sequence of simple functions $\{\phi_n\}$, such that

$$(7.9) \qquad\qquad \mathbb{E}\left(\int_S^T \left(f(\omega, t) - \phi_n(\omega, t)\right)^2 dt\right) \to 0;$$

i.e., $\phi_n \to f$ in $L_\omega^2 L_t^2$ (cf. [**KS91**, **Oks98**]). Now let

$$(7.10) \qquad \int_S^T f(\omega, t)dW_t = \lim_{n\to\infty} \int_S^T \phi_n(\omega, t)dW_t \qquad \text{in } L_\omega^2.$$

To see that this limit is well-defined, note that from (7.8), $\int_S^T \phi_n(\omega, t)dW_t$ is in L_ω^2 for any simple function $\phi_n(t, \omega)$. Furthermore we have

$$(7.11) \qquad \mathbb{E}\left(\int_S^T \phi_n dW_t - \int_S^T \phi_m dW_t\right)^2 = \mathbb{E}\left(\int_S^T (\phi_n - \phi_m)^2 dt\right).$$

From (7.9), the sequence $\{\phi_n\}$ is a Cauchy sequence in $L_\omega^2 L_t^2$. This implies that $\{\int_S^T \phi_n dW_t\}$ is also a Cauchy sequence in L_ω^2. Therefore it has a unique limit. We can also show that this limit is independent of the choice of the approximating sequence $\{\phi_n\}$. This is left as an exercise.

As a natural extension of Lemma 7.1, we have

Theorem 7.2. *For $f \in \mathcal{V}[S,T]$, the Itô integral satisfies*

$$(7.12) \qquad \mathbb{E}\left(\int_S^T f(\omega, t)dW_t\right) = 0,$$

$$(7.13) \qquad (It\hat{o}\ isometry) \quad \mathbb{E}\left(\int_S^T f(\omega, t)dW_t\right)^2 = \mathbb{E}\left(\int_S^T f^2(\omega, t)dt\right).$$

Proof. Based on Lemma 7.1, we have

$$\left|\mathbb{E}\left(\int_S^T f(\omega, t)dW_t\right)\right| = \left|\mathbb{E}\left(\int_S^T f(\omega, t)dW_t - \int_S^T \phi_n(\omega, t)dW_t\right)\right|$$

$$\leq \left[\mathbb{E}\left(\int_S^T f(\omega, t)dW_t - \int_S^T \phi_n(\omega, t)dW_t\right)^2\right]^{\frac{1}{2}} \to 0.$$

It is a standard result that if $X_n \to X$ in a Hilbert space $\mathscr{H}$, then $\|X_n\| \to \|X\|$ and thus $\|X_n\|^2 \to \|X\|^2$, where $\|\cdot\|$ is the corresponding norm in $\mathscr{H}$. Using this, we have

$$\mathbb{E}\left(\int_S^T \phi_n(\omega, t)dW_t\right)^2 \to \mathbb{E}\left(\int_S^T f(\omega, t)dW_t\right)^2$$

and

$$\mathbb{E}\left(\int_S^T \phi_n^2(\omega, t)dt\right) \to \mathbb{E}\left(\int_S^T f^2(\omega, t)dt\right).$$

From the Itô isometry for simple functions, we obtain (7.13) immediately.
$\square$

The following properties are quite obvious.

Proposition 7.3. *Assume that $f, g \in \mathcal{V}[S,T]$ and $u \in [S,T]$. Then*

(i) $\int_S^T f dW_t = \int_S^u f dW_t + \int_u^T f dW_t$ *a.s.*

(ii) $\int_S^T (f + cg)dW_t = \int_S^T f dW_t + c\int_S^T g dW_t$, *a.s. Here c is a constant.*

(iii) $\int_S^T f dW_t$ *is $\mathcal{F}_T^W$-measurable.*

Lemma 7.4. *Assume that $f \in \mathcal{V}[0,T]$. Then $X_t := \int_0^t f(\omega, s)dW_s$ has continuous trajectories almost surely.*

The proof of this lemma can be found in [**KS91**, **Oks98**, **RY05**].

Example 7.5. For the Itô integral we have

$$(7.14) \qquad \int_0^t W_s dW_s = \frac{W_t^2}{2} - \frac{t}{2} \quad \text{a.s.}$$

Proof. Take the dyadic subdivision with mesh size 2^{-n} on $[0, T]$. From the definition of Itô integral

$$\int_0^t W_s dW_s \approx \sum_j W_{t_j}(W_{t_{j+1}} - W_{t_j}) = \sum_j \frac{2W_{t_j}W_{t_{j+1}} - 2W_{t_j}^2}{2}$$

$$= \sum_j \frac{W_{t_{j+1}}^2 - W_{t_j}^2}{2} - \sum_j \frac{W_{t_{j+1}}^2 - 2W_{t_{j+1}}W_{t_j} + W_{t_j}^2}{2}$$

$$= \frac{W_t^2}{2} - \frac{1}{2}\sum_j (W_{t_{j+1}} - W_{t_j})^2 \to \frac{W_t^2}{2} - \frac{t}{2},$$

where we used the fact that the quadratic variation $[W, W]_t = t$. $\qquad\square$

Multidimensional Itô integrals

$$\int_0^T \boldsymbol{\sigma}(\omega, t) \cdot d\boldsymbol{W}_t,$$

where $\boldsymbol{W}_t$ is an m-dimensional Wiener process, can be defined in a similar way [**KS91**]. Here $\boldsymbol{\sigma} \in \mathbb{R}^{n \times m}$ is assumed to be $\mathcal{F}_t$-adapted. We have

$$\mathbb{E}\left(\int_S^T \sigma(\omega, t)dW_t^j\right) = 0, \ \ \mathbb{E}\Big(\int_S^T \sigma(\omega, t)dW_t^j\Big)^2 = \mathbb{E}\left(\int_S^T \sigma^2(\omega, t)dt\right), \ \ \forall j.$$

Moreover, we also have

$$\mathbb{E}\left(\int_S^T \sigma_1(\omega, t)dW_t^i \cdot \int_S^T \sigma_2(\omega, t)dW_t^j\right) = 0, \qquad \forall i \neq j,$$

$$\mathbb{E}\Big(\int_S^T \sigma_1(\omega, t)dW_t^j \int_S^T \sigma_2(\omega, t)dW_t^j\Big) = \mathbb{E}\left(\int_S^T \sigma_1(\omega, t)\sigma_2(t, \omega)dt\right), \ \ \forall j.$$

7.2. Itô's Formula

One interesting fact about the Itô calculus is that its chain rule takes a somewhat unusual form.

To begin with, note that from (7.14), we have

$$dW_t^2 = 2W_t dW_t + dt,$$

which should be understood in the sense of stochastic integrals. This is different from the usual chain rule in calculus which would suggest $dW_t^2 = 2W_t dW_t$. As another example, we have

Proposition 7.6. *Assume that f is bounded and continuous in t for $t \in [0, T]$ almost surely. Then*

$$\sum_j f(\omega, t_j^*)(W_{t_{j+1}} - W_{t_j})^2 \to \int_0^T f(\omega, s)ds$$

in probability as the size of the subdivision goes to zero. Here $t_j^* \in [t_j, t_{j+1}]$ *but is otherwise arbitrary.*

Proof. A straightforward calculation gives

$$\mathbb{E}\Big(\sum_j f(t_j)\delta W_{t_j}^2 - \sum_j f(t_j)\delta t_j \Big)^2$$

$$= \mathbb{E}\Big(\sum_{j,k} f(t_j)f(t_k)(\delta W_{t_j}^2 - \delta t_j)(\delta W_{t_k}^2 - \delta t_k) \Big)$$

$$= \mathbb{E}\Big(\sum_j f^2(t_j) \cdot \mathbb{E}\Big((\delta W_{t_j}^2 - \delta t_j)^2 | \mathcal{F}_{t_j} \Big) \Big)$$

$$= 2 \sum_j \mathbb{E} f^2(t_j)\delta t_j^2 \to 0.$$

At the same time, we have

$$\Big| \sum_j (f(t_j^*) - f(t_j))\delta W_{t_j}^2 \Big| \le \sup_j |f(t_j^*) - f(t_j)| \cdot \sum_j \delta W_{t_j}^2.$$

The first term on the right-hand side goes to zero almost surely because of the uniform continuity of f on $[0,T]$. The second term converges to the quadratic variation of W_t in probability. $\square$

For this reason, we write formally

$$(dW_t)^2 = dt.$$

Now consider the *Itô process* defined by

(7.15) $$X_t = X_0 + \int_0^t b(\omega, s)ds + \int_0^t \sigma(\omega, s)dW_s,$$

or

(7.16) $$dX_t = b(\omega, t)dt + \sigma(\omega, t)dW_t, \quad X_t|_{t=0} = X_0$$

where

$$\sigma \in \mathcal{V}[0, T], \quad b \text{ is } \mathcal{F}_t\text{-adapted}, \quad \text{and} \quad \int_0^T |b(\omega, t)|dt < \infty \text{ a.s.}$$

Theorem 7.7 (One-dimensional Itô formula)**.** *Let f be a twice differentiable function, and let $Y_t = f(X_t)$ where X_t is an Itô process defined in (7.16). Then Y_t is also an Itô process and*

(7.17) $$dY_t = \Big(b(t,\omega)f'(X_t) + \frac{1}{2}\sigma^2(t,\omega)f''(X_t) \Big) dt + \sigma(\omega, t)f'(X_t)dW_t.$$

Remark 7.8. Equation (7.17) can be derived formally using Taylor expansion and the calculation rules:

$$(7.18) \qquad dt^2 = 0, \quad dt\,dW_t = dW_t\,dt = 0, \quad (dW_t)^2 = dt.$$

First, we have

$$(7.19) \qquad dY_t = f'(X_t)dX_t + \frac{1}{2}f''(X_t)(dX_t)^2$$

by Taylor expanding $Y_t = f(X_t)$ to the second order. Using (7.18), we obtain

$$(dX_t)^2 = (b\,dt + \sigma\,dW_t)^2 = b^2 dt^2 + 2b\sigma\,dt\,dW_t + \sigma^2(dW_t)^2 = \sigma^2 dt.$$

Substituting this into (7.19) yields (7.17).

Sketch of proof. Let us consider the situation when f, f', and f'' are bounded and continuous. If b and σ are simple functions, we have

$$Y_t - Y_0 = \sum_j (f(X_{t_{j+1}}) - f(X_{t_j})) = \sum_j \left(f'(X_{t_j})\delta X_{t_j} + \frac{1}{2}f''(X_{t_j})\delta X_{t_j}^2 + R_j \right),$$

where $\delta X_{t_j} = X_{t_{j+1}} - X_{t_j}$ and $R_j = o(|\delta X_{t_j}|^2)$. Without loss of generality we assume that the discontinuities of the step functions fall into the grid points of the subdivision. Then we have

$$\sum_j f'(X_{t_j})\delta X_{t_j} = \sum_j f'(X_{t_j})b(t_j)\delta t_j + \sum_j f'(X_{t_j})\sigma(t_j)\delta W_{t_j}$$

$$\to \int_0^t b(s)f'(X_s)ds + \int_0^t \sigma(s)f'(X_s)dW_s$$

and

$$\sum_j f''(X_{t_j})\delta X_{t_j}^2 = \sum_j f''(X_{t_j})\left(b^2(t_j)\delta t_j^2 + 2b(t_j)\sigma(t_j)\delta t_j \delta W_{t_j} + \sigma^2(t_j)\delta W_{t_j}^2 \right).$$

Note that

$$\left| \sum_j f''(X_{t_j})b^2(t_j)\delta t_j^2 \right| \le K \sum_j \delta t_j^2 \le KT \sup_j \delta t_j \to 0,$$

$$\left| \sum_j f''(X_{t_j})b(t_j)\sigma(t_j)\delta t_j \delta W_{t_j} \right| \le K \sum_j |\delta t_j \delta W_{t_j}| \le KT \sup_j |\delta W_{t_j}| \to 0$$

as the subdivision size goes to zero, where K is a bound of b, σ, and f''. From Proposition 7.6, we get

$$\sum_j f''(X_{t_j})\sigma^2(t_j)\delta W_{t_j}^2 \to \int_0^t \sigma^2(s)f''(X_s)ds \qquad \text{in } L_\omega^2.$$

The general situation can be handled by approximation using simple functions. $\qquad \square$

The readers are referred to [**IW81**, **KS91**] for the full proof. The above result can be generalized to the multidimensional case.

Theorem 7.9 (Multidimensional Itô formula). *Let $\boldsymbol{X}_t$ be an Itô process defined by $d\boldsymbol{X}_t = \boldsymbol{b}(\omega, t)dt + \boldsymbol{\sigma}(\omega, t)d\boldsymbol{W}_t$, where $\boldsymbol{X}_t \in \mathbb{R}^n$, $\boldsymbol{\sigma} \in \mathbb{R}^{n \times m}$, $\boldsymbol{W} \in \mathbb{R}^m$. Define $Y_t = f(\boldsymbol{X}_t)$, where f is a twice differentiable function. Then*

$$(7.20) \qquad dY_t = \Big(\boldsymbol{b} \cdot \nabla f + \frac{1}{2}\boldsymbol{\sigma}\boldsymbol{\sigma}^T : \nabla^2 f\Big)dt + \nabla f \cdot \boldsymbol{\sigma} \cdot d\boldsymbol{W}_t.$$

Remark 7.10. Equation (7.20) can be derived formally using the calculation rules
$$(7.21)$$
$$dt^2 = 0, \quad dt dW_t^i = dW_t^i dt = dW_t^i dW_t^j = 0 \quad (i \neq j), \quad (dW_t^i)^2 = dt.$$

Using Taylor expansion, we have

$$(7.22) \qquad dY_t = \nabla f(\boldsymbol{X}_t) \cdot d\boldsymbol{X}_t + \frac{1}{2}(d\boldsymbol{X}_t)^T \cdot \nabla^2 f(\boldsymbol{X}_t) \cdot (d\boldsymbol{X}_t).$$

With (7.21), we get

$$(7.23) \qquad \begin{aligned}(d\boldsymbol{X}_t)^T \cdot \nabla^2 f(\boldsymbol{X}_t) \cdot (d\boldsymbol{X}_t) &= \sum_{l,k,i,j} dW_t^l \sigma_{il} \partial_{ij}^2 f \sigma_{jk} dW_t^k \\ &= \sum_{k,i,j} \sigma_{ik}\sigma_{jk}\partial_{ij}^2 f dt = \boldsymbol{\sigma}\boldsymbol{\sigma}^T : \nabla^2 f dt,\end{aligned}$$

where $\boldsymbol{A} : \boldsymbol{B} = \sum_{ij} a_{ij} b_{ji}$ is the contraction for second-order tensors. Equation (7.20) is obtained by substituting (7.23) into (7.22).

Example 7.11. An example of integration by parts is

$$(7.24) \qquad \int_0^t s\, dW_s = tW_t - \int_0^t W_s\, ds.$$

Proof. Define $f(x, y) = xy$, $X_t = t$, $Y_t = W_t$. Then from the multidimensional Itô formula

$$df(X_t, Y_t) = X_t dY_t + Y_t dX_t + dX_t dY_t.$$

Since $dt dW_t = 0$, we obtain $d(tW_t) = tdW_t + W_t dt$ and the result follows. $\square$

Example 7.12. Iterated Itô integrals

$$(7.25) \qquad \int_0^t dW_{t_1} \int_0^{t_1} dW_{t_2} \dots \int_0^{t_{n-1}} dW_{t_n} = \frac{1}{n!}t^{\frac{n}{2}} H_n\left(\frac{W_t}{\sqrt{t}}\right),$$

where $H_n(x)$ is the nth-order Hermite polynomial

$$H_n(x) = (-1)^n e^{\frac{1}{2}x^2} \frac{d^n}{dx^n}\left(e^{-\frac{1}{2}x^2}\right).$$

Proof. It is easy to verify that

$$\int_0^t W_s dW_s = \frac{t}{2!} H_2 \left(\frac{W_t}{\sqrt{t}} \right),$$

where $H_2(x) = x^2 - 1$ is the second-order Hermite polynomial. In the same fashion, we have

$$\int_0^t \left(\int_0^s W_u dW_u \right) dW_s = \frac{1}{2} \int_0^t (W_s^2 - s) dW_s.$$

Using Itô's formula, we have

$$\int_0^t W_s^2 dW_s = \frac{1}{3} W_t^3 - \int_0^t W_s ds.$$

Hence, using (7.24) we obtain

$$\int_0^t \left(\int_0^s W_u dW_u \right) dW_s = \frac{1}{6} W_t^3 - \frac{1}{2} t W_t = \frac{1}{3!} t^{\frac{3}{2}} H_3 \left(\frac{W_t}{\sqrt{t}} \right),$$

where $H_3(x) = x^3 - 3x$ is the third-order Hermite polynomial. The general case is left as an exercise. $\qquad\square$

Finally let us mention a very useful inequality about the Itô integral. Define the martingale (see Section D of the appendix for the definition)[**KS91**]

$$\boldsymbol{M}_t = \int_0^t \boldsymbol{\sigma}(\omega, s) d\boldsymbol{W}_s, \quad t \in [0, T],$$

where $\boldsymbol{\sigma}$ is $\mathcal{F}_t$-adapted and belongs to $L_\omega^2 L_t^2$. Denote

$$Q_t = \int_0^t |\boldsymbol{\sigma}(\omega, s)|^2 ds = \int_0^t \sum_{ij} |\sigma_{ij}(\omega, s)|^2 ds.$$

Theorem 7.13 (Burkholder-Davis-Gundy inequality)**.** *For any $m > 0$, there exist constants $k_m, K_m > 0$ such that*

$$(7.26) \qquad k_m \mathbb{E}\big(Q_T^m\big) \leq \mathbb{E}\big(\sup_{0 \leq t \leq T} |\boldsymbol{M}_t|^{2m} \big) \leq K_m \mathbb{E}\big(Q_T^m\big).$$

See [**KS91**] for detailed proof.

7.3. Stochastic Differential Equations

We are now ready to discuss stochastic differential equations of the type introduced at the beginning of this chapter:

$$(7.27) \qquad d\boldsymbol{X}_t = \boldsymbol{b}(\boldsymbol{X}_t, t) dt + \boldsymbol{\sigma}(\boldsymbol{X}_t, t) d\boldsymbol{W}_t.$$

Theorem 7.14. *Assume that the coefficients $\boldsymbol{b} \in \mathbb{R}^n, \boldsymbol{\sigma} \in \mathbb{R}^{n \times m}$ satisfy the global Lipschitz and linear growth conditions:*

$$(7.28) \qquad |\boldsymbol{b}(\boldsymbol{x},t) - \boldsymbol{b}(\boldsymbol{y},t)| + |\boldsymbol{\sigma}(\boldsymbol{x},t) - \boldsymbol{\sigma}(\boldsymbol{y},t)| \leq K|\boldsymbol{x} - \boldsymbol{y}|,$$

$$(7.29) \qquad |\boldsymbol{b}(\boldsymbol{x},t)|^2 + |\boldsymbol{\sigma}(\boldsymbol{x},t)|^2 \leq K^2(1 + |\boldsymbol{x}|^2)$$

for any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n, t \in [0,T]$, where K is a positive constant and $|\cdot|$ is the Frobenius norm; i.e.,

$$|\boldsymbol{b}|^2 := \sum_i b_i^2, \quad |\boldsymbol{\sigma}|^2 := \sum_{i,j} \sigma_{ij}^2.$$

Assume the initial value $\boldsymbol{X}_0 = \boldsymbol{\xi}$ is a random variable which is independent of $\mathcal{F}_\infty^{\boldsymbol{W}} = \sigma\left(\bigcup_{t \geq 0} \mathcal{F}_t^{\boldsymbol{W}}\right)$ and $\mathbb{E}|\boldsymbol{\xi}|^2 < \infty$. Then (7.27) has a unique solution that satisfies $\boldsymbol{X}_t \in \mathcal{V}[0,T]$ for each component. Furthermore, $\boldsymbol{X}_t$ is continuous in t almost surely.

Proof. We will only consider the one-dimensional case. The high-dimensional case is similar. First we prove uniqueness. Let $X_t, \hat{X}_t \in \mathcal{V}[0,T]$ be solutions of the SDEs (7.27) with the same initial value X_0. Then

$$X_t - \hat{X}_t = \int_0^t (b(X_s,s) - b(\hat{X}_s,s))ds + \int_0^t (\sigma(X_s,s) - \sigma(\hat{X}_s,s))dW_s.$$

Squaring both sides, taking expectation, and using the Lipschitz condition, we obtain

$$\mathbb{E}|X_t - \hat{X}_t|^2 \leq 2\mathbb{E}\left(\int_0^t (b(X_s,s) - b(\hat{X}_s,s))ds\right)^2$$

$$+ 2\mathbb{E}\left(\int_0^t (\sigma(X_s,s) - \sigma(\hat{X}_s,s))dW_s\right)^2$$

$$\leq 2K^2 t \int_0^t \mathbb{E}|X_s - \hat{X}_s|^2 ds + 2K^2 \int_0^t \mathbb{E}|X_s - \hat{X}_s|^2 ds$$

$$= 2K^2(t+1)\int_0^t \mathbb{E}|X_s - \hat{X}_s|^2 ds$$

Using Gronwall's inequality (see Theorem B.1 in the appendix), we get

$$\mathbb{E}|X_t - \hat{X}_t|^2 = 0$$

for any $t > 0$. Thus $X_t = \hat{X}_t$ a.s. for any rational t. From the continuity of the trajectories of X and $\hat{X}$, we see that there is a set $\tilde{\Omega}$ of full measure in Ω, such that for $\omega \in \tilde{\Omega}$, $X_t(\omega) = \hat{X}_t(\omega)$ for all t.

Existence can be proved using Picard iteration. Define
$$(7.30)$$
$$X_t^{(k+1)} = X_0 + \int_0^t b(X_s^{(k)},s)ds + \int_0^t \sigma(X_s^{(k)},s)dW_s, \ k \geq 0, \ \ X_t^{(0)} := \xi.$$

Similar to the proof of uniqueness, we have

$$\mathbb{E}|X_t^{(k+1)} - X_t^{(k)}|^2 \leq 2K^2(t+1)\int_0^t \mathbb{E}|X_s^{(k)} - X_s^{(k-1)}|^2 ds, \quad k \geq 1.$$

In particular, we have

$$\mathbb{E}|X_t^{(1)} - X_t^{(0)}|^2 \leq 2K^2(t^2 + t)(1 + \mathbb{E}\xi^2) \leq Lt$$

where $L = 2K^2(T+1)(1 + \mathbb{E}\xi^2)$, which depends on K, T, and $\mathbb{E}\xi^2$.

By induction we obtain

$$(7.31) \qquad \mathbb{E}|X_t^{(k+1)} - X_t^{(k)}|^2 \leq \frac{(Lt)^{k+1}}{(k+1)!}, \quad k \geq 0, \ t \in [0, T].$$

Similar arguments can be applied to (7.30) to get

$$(7.32) \qquad \mathbb{E}|X_t^{(k)}|^2 \leq \tilde{L}(1 + \mathbb{E}\xi^2)\exp(\tilde{L}t), \quad \text{for all } k,$$

where $\tilde{L} = 3K^2(T+1)^2 + 3$, which only depends on K and T.

Taking the difference between the equations for $X_t^{(k+1)}$ and $X_t^{(k)}$, we have

$$\sup_{t \in [0,T]} |X_t^{(k+1)} - X_t^{(k)}| \leq \int_0^T |b(X_t^{(k)}, t) - b(X_t^{(k-1)}, t)| dt$$

$$+ \sup_{t \in [0,T]} \left|\int_0^t (\sigma(X_s^{(k)}, s) - \sigma(X_s^{(k-1)}, s)) dW_s\right|.$$

Thus

$$\mathbb{P}\left(\sup_{t \in [0,T]} |X_t^{(k+1)} - X_t^{(k)}| > 2^{-k}\right)$$

$$\leq \mathbb{P}\left[\left(\int_0^T |b(X_t^{(k)}, t) - b(X_t^{(k-1)}, t)| dt\right)^2 > 2^{-2k-2}\right]$$

$$+ \mathbb{P}\left[\sup_{t \in [0,T]} \left|\int_0^t (\sigma(X_s^{(k)}, s) - \sigma(X_s^{(k-1)}, s)) dW_s\right| > 2^{-k-1}\right] := P_1 + P_2.$$

From Chebyshev inequality we have

$$P_1 \leq 2^{2k+2}\mathbb{E}\left(\int_0^T |b(X_t^{(k)}, t) - b(X_t^{(k-1)}, t)| dt\right)^2$$

$$\leq 2^{2k+2}T \int_0^T \mathbb{E}|b(X_t^{(k)}, t) - b(X_t^{(k-1)}, t)|^2 dt$$

$$(7.33) \qquad \leq 2^{2k+2}K^2T \int_0^T \frac{(Lt)^k}{k!} dt \leq 2^{2k+2}K^2 \frac{L^k T^{k+2}}{(k+1)!}.$$

To estimate P_2, we need Doob's martingale inequality for martingales in Section D of the appendix which states that

$$(7.34) \qquad \mathbb{P}\left(\sup_{t\in[0,T]}|M_t| \geq \lambda\right) \leq \frac{1}{\lambda^p}\mathbb{E}|M_T|^p, \quad p \geq 1,$$

for $T > 0, \lambda > 0$, where $\{M_t\}_{t\geq 0}$ is a martingale. Using (7.34) for $p = 2$ and $\lambda = 2^{-k-1}$, we obtain

$$P_2 \leq 2^{2k+2}\mathbb{E}\left(\int_0^T (\sigma(X_s^{(k)}, s) - \sigma(X_s^{(k-1)}, s))dW_s\right)^2$$

$$\leq 2^{2k+2}\int_0^T \mathbb{E}|\sigma(X_s^{(k)}, s) - \sigma(X_s^{(k-1)}, s)|^2 ds$$

$$(7.35) \qquad \leq 2^{2k+2}K^2\int_0^T \frac{(Lt)^k}{k!}dt \leq 2^{2k+2}K^2\frac{L^k T^{k+1}}{(k+1)!}.$$

By the Borel-Cantelli lemma, we have

$$\mathbb{P}\left(\sup_{t\in[0,T]}|X_t^{(k+1)} - X_t^{(k)}| > 2^{-k} \text{ infinitely often}\right) = 0.$$

Thus for almost every ω, there exists $k_0(\omega)$ such that

$$\sup_{t\in[0,T]}|X_t^{(k+1)} - X_t^{(k)}| \leq 2^{-k} \quad \text{for } k \geq k_0(\omega).$$

This leads to the uniform convergence of the series

$$X_t^{(n)} = X_t^{(0)} + \sum_{k=0}^{n-1}(X_t^{(k+1)} - X_t^{(k)})$$

in the almost sure sense. Denote its limit by $X_t(\omega)$. Then X_t is t-continuous and $\mathcal{F}_t$-adapted since $X_t^{(k)}$ is t-continuous and $\mathcal{F}_t$-adapted. Using Fatou's lemma (see Theorem C.12) and the bound (7.32), we get

$$\mathbb{E}|X_t|^2 \leq \tilde{L}(1 + \mathbb{E}\xi^2)\exp(\tilde{L}t).$$

Now let us show that X_t satisfies the SDE. It is enough to take the limit $k \to \infty$ on both sides of (7.30). For the integral term with respect to t, we have

$$\left|\int_0^t (b(X_s^{(k)}, s) - b(X_s, s))ds\right| \leq \int_0^t |b(X_s^{(k)}, s) - b(X_s, s)|ds$$

$$\leq K\int_0^T |X_s^{(k)} - X_s|ds \to 0 \text{ as } k \to \infty \quad \text{a.s.}$$

Thus

$$(7.36) \qquad \int_0^t b(X_s^{(k)}, s)ds \to \int_0^t b(X_s, s)ds \quad \text{a.s. for } t \in [0, T].$$

For the stochastic integral, we note that $X_t^{(k)}$ is a Cauchy sequence in L_ω^2 for any fixed t. Based on the fact that $X_t^{(k)} \to X_t$ a.s., we obtain $X_t^{(k)} \to X_t$ in L_ω^2. This gives

$$\mathbb{E}\left(\int_0^t (\sigma(X_s^{(k)}, s) - \sigma(X_s, s))dW_s\right)^2 = \int_0^t \mathbb{E}(\sigma(X_s^{(k)}, s) - \sigma(X_s, s))^2 ds$$

$$\leq K^2 \int_0^t \mathbb{E}|X_s^{(k)} - X_s|^2 ds \to 0 \quad \text{as } k \to \infty.$$

By taking $t \in \mathbb{Q}^+$, the set of positive rational numbers, and using the t-continuity of both stochastic integrals, we get

$$(7.37) \qquad \int_0^t \sigma(X_s^{(k)}, s)dW_s \to \int_0^t \sigma(X_s, s)dW_s \quad \text{a.s. for } t \in [0, T].$$

Combining (7.36), (7.37), and the fact that $X_t^{(k)} \to X_t$ almost surely, we conclude that X_t is the solution of the SDE (7.27). $\qquad\square$

Simple SDEs.

Example 7.15 (Ornstein-Uhlenbeck process)**.** The Ornstein-Uhlenbeck (OU) process is the solution of the following linear SDE with the additive noise:

$$(7.38) \qquad dX_t = -\gamma X_t dt + \sigma dW_t, \quad X_t|_{t=0} = X_0.$$

Here we assume $\gamma, \sigma > 0$.

If we use this to model the dynamics of a particle, then the drift term represents a restoring force that prevents the particle from getting too far away from the origin. We will see that the distribution of the particle position has a limit as time goes to infinity. This is a very different behavior from that of the Brownian motion.

Solution. Multiplying both sides of (7.38) by $e^{\gamma t}$ and integrating, we get

$$e^{\gamma t} X_t - X_0 = \int_0^t \sigma e^{\gamma s} dW_s.$$

Thus

$$X_t = e^{-\gamma t} X_0 + \sigma \int_0^t e^{-\gamma(t-s)} dW_s$$

is the solution. Let $Q_t := \int_0^t e^{-\gamma(t-s)} dW_s$. Here Q_t is a Gaussion process with

$$\mathbb{E}Q_t = 0, \qquad \mathbb{E}Q_t^2 = \int_0^t \mathbb{E}e^{-2\gamma(t-s)} ds = \frac{1}{2\gamma}(1 - e^{-2\gamma t}).$$

Hence X_t is also a Gaussian process if X_0 is Gaussian, and

$$(7.39) \qquad X_t \to N\left(0, \frac{\sigma^2}{2\gamma}\right), \qquad \text{as} \quad t \to +\infty.$$

It can also be shown that if $X_0 \sim N(0, \sigma^2/(2\gamma))$, then X_t is a stationary Gaussian process. $\qquad\square$

This stationary Ornstein-Uhlenbeck process has an important property that, up to a constant mean, it is the unique stationary Gaussian and Markovian process with continuous trajectories [**Doo42**].

Example 7.16 (Geometric Brownian motion)**.** The geometric Brownian motion is the solution of a linear SDE with multiplicative noise

$$(7.40) \qquad dN_t = rN_t dt + \alpha N_t dW_t, \quad N_t|_{t=0} = N_0.$$

We assume $r, \alpha > 0$. Equation (7.40) is also called the Black-Scholes-Merton model in mathematical finance, in which N_t represents the price of an asset, r is the interest rate, and α is the volatility.

Solution. Dividing both sides by N_t, we have $dN_t/N_t = rdt + \alpha dW_t$. Applying Itô's formula to $\log N_t$, we get

$$\begin{aligned}
d(\log N_t) &= \frac{1}{N_t} dN_t - \frac{1}{2N_t^2}(dN_t)^2 \\
&= \frac{1}{N_t} dN_t - \frac{1}{2N_t^2}\alpha^2 N_t^2 dt \\
&= \frac{1}{N_t} dN_t - \frac{\alpha^2}{2} dt.
\end{aligned}$$

Therefore, we have

$$d(\log N_t) = \left(r - \frac{\alpha^2}{2}\right) dt + \alpha dW_t.$$

Integrating from 0 to t, we get

$$N_t = N_0 \exp\left\{ \left(r - \frac{\alpha^2}{2}\right) t + \alpha W_t \right\}.$$

$\qquad\square$

Example 7.17 (Langevin equation)**.** The simplest model for an inertial particle in a force field subject to friction and noise is given by

$$(7.41) \qquad \begin{cases} d\boldsymbol{X}_t &= \boldsymbol{V}_t dt, \\ m d\boldsymbol{V}_t &= \left(-\gamma \boldsymbol{V}_t - \nabla U(\boldsymbol{X}_t)\right) dt + \sigma d\boldsymbol{W}_t, \end{cases}$$

where γ is the frictional coefficient, $U(\boldsymbol{X})$ is the potential for the force field, $\boldsymbol{W}_t$ is the standard Wiener process, and σ is the strength of the noise force. We will show $\sigma = \sqrt{2k_B T\gamma}$ in Chapter 11 to ensure the correct physics.

Diffusion Process. Diffusion processes are the Markov process with continuous paths. From what we have just established, Itô processes defined as the solutions of stochastic differential equations are diffusion processes if the coefficients satisfy the conditions presented above. It is interesting to note that the converse is also true, namely that diffusion processes are nothing but solutions of stochastic differential equations.

We will not prove this last statement. Instead, we will see formally how a diffusion process can give rise to a stochastic differential equation. Let $p(\boldsymbol{x}, t | \boldsymbol{y}, s)$ $(t \geq s)$ be the transition probability density of the diffusion process, and let

$$(7.42) \qquad \lim_{t \to s} \frac{1}{t-s} \int_{|\boldsymbol{x}-\boldsymbol{y}|<\epsilon} (\boldsymbol{x}-\boldsymbol{y}) p(\boldsymbol{x}, t | \boldsymbol{y}, s) d\boldsymbol{x} = \boldsymbol{b}(\boldsymbol{y}, s) + O(\epsilon),$$

$$(7.43) \quad \lim_{t \to s} \frac{1}{t-s} \int_{|\boldsymbol{x}-\boldsymbol{y}|<\epsilon} (\boldsymbol{x}-\boldsymbol{y})(\boldsymbol{x}-\boldsymbol{y})^T p(\boldsymbol{x}, t | \boldsymbol{y}, s) d\boldsymbol{x} = \boldsymbol{A}(\boldsymbol{y}, s) + O(\epsilon).$$

Here $\boldsymbol{b}(\boldsymbol{y}, s)$ is called the drift of the diffusion process and $\boldsymbol{A}(\boldsymbol{y}, s)$ is called the diffusion matrix at time s and position $\boldsymbol{y}$. The conditions (7.42) and (7.43) can also be represented as

$$(7.44) \qquad\qquad \lim_{t \to s} \frac{1}{t-s} \mathbb{E}^{\boldsymbol{y}, s}(\boldsymbol{X}_t - \boldsymbol{y}) = \boldsymbol{b}(\boldsymbol{y}, s),$$

$$(7.45) \qquad\qquad \lim_{t \to s} \frac{1}{t-s} \mathbb{E}^{\boldsymbol{y}, s}(\boldsymbol{X}_t - \boldsymbol{y})(\boldsymbol{X}_t - \boldsymbol{y}) = \boldsymbol{A}(\boldsymbol{y}, s).$$

For solutions of stochastic differential equations, it is easy to see that $\boldsymbol{A} = \boldsymbol{\sigma}\boldsymbol{\sigma}^T$ in (7.27).

7.4. Stratonovich Integral

Among alternative treatments of the stochastic integral, we discuss briefly the Stratonovich (or Fisk-Stratonovich) integral, which is defined as the limit of the following approximation:

$$\int_0^T f(\omega, t) \circ dW_t \approx \sum_j \frac{f(t_j) + f(t_{j+1})}{2} (W_{t_{j+1}} - W_{t_j}).$$

We use the special notation $\circ$ for the Stratonovich integral. One can show that for a large class of the integrand, this limit is well-defined. Based on this, one can also give a treatment of the stochastic differential equation:

$$(7.46) \qquad\qquad dX_t = b(X_t, t)dt + \sigma(X_t, t) \circ dW_t$$

in the Stratonovich sense. However, Itô isometry is lost, and the integral is no longer a martingale.

The connection between the Itô and Stratonovich solutions to SDEs is as follows. If X_t is the solution to (7.46), then X_t is also the solution to the following Itô SDE:

$$(7.47) \qquad dX_t = \left(b(X_t, t) + \frac{1}{2}\partial_x\sigma\sigma(X_t, t)\right)dt + \sigma(X_t, t)dW_t.$$

To see this, assume that X_t satisfies an Itô SDE of the form

$$(7.48) \qquad dX_t = \alpha(X_t, t)dt + \beta(X_t, t)dW_t.$$

By the definition of the Stratonovich integral

$$\int_0^t \sigma(X_s, s) \circ dW_s \approx \sum_j \frac{1}{2}(\sigma(X_{t_j}, t_j) + \sigma(X_{t_{j+1}}, t_{j+1}))(W_{t_{j+1}} - W_{t_j}).$$

From (7.48) we have

$$X_{t_{j+1}} = X_{t_j} + \alpha(X_{t_j}, t_j)\delta t_j + \beta(X_{t_j}, t_j)\delta W_{t_j} + \text{h.o.t.},$$

where h.o.t. stands for *higher-order terms*. Thus

$$\sum_j \sigma(X_{t_{j+1}}, t_{j+1})\delta W_{t_j}$$

$$= \sum_j \left(\sigma(X_{t_j}, t_j)\delta W_{t_j} + \partial_t\sigma(X_{t_j}, t_j)\delta t_j\delta W_{t_j}\right.$$

$$\left. + \partial_x\sigma\alpha(X_{t_j}, t_j)\delta t_j\delta W_{t_j} + \partial_x\sigma\beta(X_{t_j}, t_j)\delta W_{t_j}^2 + \text{h.o.t.}\right)$$

$$\to \int_0^t \sigma(X_s, s)dW_s + \int_0^t \partial_x\sigma\beta(X_s, s)ds.$$

Hence X_t satisfies

$$(7.49) \qquad dX_t = \left(b(X_t, t) + \frac{1}{2}\partial_x\sigma\beta(X_t, t)\right)dt + \sigma(X_t, t)dW_t.$$

For consistency between (7.48) and (7.49), we must take

$$\beta(x, t) = \sigma(x, t), \quad \alpha(x, t) = b(x, t) + \frac{1}{2}\partial_x\sigma\sigma(x, t).$$

There is a similar version of this result in high dimension. If $\boldsymbol{X}$ satisfies

$$(7.50) \qquad d\boldsymbol{X}_t = \boldsymbol{b}(\boldsymbol{X}_t, t)dt + \boldsymbol{\sigma}(\boldsymbol{X}_t, t) \circ d\boldsymbol{W}_t,$$

then $\boldsymbol{X}_t$ also satisfies

$$(7.51) \qquad d\boldsymbol{X}_t = \left(\boldsymbol{b}(\boldsymbol{X}_t, t) + \frac{1}{2}\nabla_x\boldsymbol{\sigma} : \boldsymbol{\sigma}(\boldsymbol{X}_t, t)\right)dt + \boldsymbol{\sigma}(\boldsymbol{X}_t, t) \cdot d\boldsymbol{W}_t$$

where $(\nabla_x\boldsymbol{\sigma} : \boldsymbol{\sigma})_i := \sum_{jk} \partial_k\sigma_{ij}\sigma_{kj}$.

One advantage of the Stratonovich integral is that the usual Newton-Leibnitz chain rule holds:

$$df(X_t) = f'(X_t) \circ dX_t = f'(X_t)b(X_t, t)dt + f'(X_t)\sigma(X_t, t) \circ dW_t.$$

The multidimensional form is

$$df(\boldsymbol{X}_t) = \nabla f(\boldsymbol{X}_t) \circ d\boldsymbol{X}_t = \nabla f(\boldsymbol{X}_t) \cdot \boldsymbol{b}(\boldsymbol{X}_t, t)dt + \nabla f(\boldsymbol{X}_t) \cdot \boldsymbol{\sigma}(\boldsymbol{X}_t, t) \circ d\boldsymbol{W}_t.$$

One reason why the Stratonovich interpretation of SDEs can be of interest is that it is the limit of smoothing the noise. One main difficulty for dealing with SDEs is that white noise is not smooth enough. A natural idea is to smooth the noise and then take the limit as the smoothing parameter goes to 0. Such an approach is physically appealing. The noise that we encounter in practice cannot be real white noise since it has to come with some ultraviolet cutoff. Such an ultraviolet cutoff can be seen as a way of smoothing the white noise. With smoothing, the SDEs can be treated pathwise as an ordinary differential equation (ODE). We can show that in the limit as one takes away the smoothing, the solution to the SDEs with smoothed noise converges to the solution of the original SDEs with the Stratonovich interpretation. See [**Sus78**, **WZ65**] for more details.

7.5. Numerical Schemes and Analysis

In this section, we discuss numerical algorithms for solving the scalar SDE

$$(7.52) \qquad\qquad dX_t = b(X_t)dt + \sigma(X_t)dW_t.$$

Most of the ideas can be extended to more general situations.

To begin with, let us note that there are two different ways of thinking about approximating the solutions of the SDE (7.52): pathwise approximation and approximation in an averaged sense, i.e., approximating expectation values. These correspond to two different forms of convergence that we will discuss later: strong convergence and weak convergence.

Itô-Taylor expansion. Let us assume that the time axis is partitioned into small intervals separated by the grid points $\{t_n\}$. One starting point for developing numerical schemes for solving ordinary differential equations is the Taylor expansion. It is useful to first consider the application of the Taylor expansion to SDEs.

From Itô's formula, we get

(7.53)
$$df(X_t) = f'(X_t)dX_t + \frac{1}{2}f''(X_t)(dX_t)^2 = (\mathcal{L}_1 f)(X_t)dt + (\mathcal{L}_2 f)(X_t)dW_t,$$

where

$$(\mathcal{L}_1 f)(x) = b(x)f'(x) + \frac{1}{2}\sigma^2(x)f''(x), \quad (\mathcal{L}_2 f)(x) = \sigma(x)f'(x).$$

Integrating from t_n to t_{n+1} and taking $f(x) = b(x)$ and $\sigma(x)$, we have

$$
X_{t_{n+1}} = X_{t_n} + \int_{t_n}^{t_{n+1}} b(X_s)ds + \int_{t_n}^{t_{n+1}} \sigma(X_s)dW_s
$$

$$
(7.54) \quad = X_{t_n} + b(X_{t_n})\delta t_n + \sigma(X_{t_n})(W_{t_{n+1}} - W_{t_n})
$$

$$
(7.55) \qquad + \int_{t_n}^{t_{n+1}} dW_s \int_{t_n}^{s} (\mathcal{L}_2\sigma)(X_\tau)dW_\tau
$$

$$
(7.56) \qquad + \int_{t_n}^{t_{n+1}} dW_s \int_{t_n}^{s} (\mathcal{L}_1\sigma)(X_\tau)d\tau + \int_{t_n}^{t_{n+1}} ds \int_{t_n}^{s} (\mathcal{L}_2 b)(X_\tau)dW_\tau
$$

$$
(7.57) \qquad + \int_{t_n}^{t_{n+1}} ds \int_{t_n}^{s} (\mathcal{L}_1 b)(X_\tau)d\tau,
$$

where $\delta t_n = t_{n+1} - t_n$ is the step size. The above procedure can be iterated. One just has to replace $\mathcal{L}_i b(X_\tau)$, $\mathcal{L}_i\sigma(X_\tau)$ by $\mathcal{L}_i b(X_t)$, $\mathcal{L}_i\sigma(X_t)$. This gives us the so-called Itô-Taylor expansion for SDEs. It is easy to see that the terms in the Ito-Taylor expansion have the form

$$
I_{\boldsymbol{i}}(g) = \int_{t_n}^{t_{n+1}} dW_{s_1}^{i_1} \int_{t_n}^{s_1} dW_{s_2}^{i_2} \cdots \int_{t_n}^{s_{k-1}} dW_{s_k}^{i_k} g(X_{s_k})
$$

for some $k \in \{1, 2, \ldots\}$. Here the index $\boldsymbol{i} = (i_1, i_2, \ldots, i_k)$ and $i_j \in \{0, 1\}$ for $j = 1, 2, \ldots, k$. The integrand g is the action of some compositions of operators $\mathcal{L}_1$ and $\mathcal{L}_2$ on the function b or σ. We use the convention that $W_t^0 := t$ and $W_t^1 := W_t$.

By truncating the Itô-Taylor series at different order, we obtain different schemes. For example, if we only keep terms in (7.54), we get

(1) Euler-Maruyama scheme.

$$
(7.58) \qquad X_{n+1} = X_n + b(X_n)\delta t_n + \sigma(X_n)\delta W_n,
$$

where $\delta W_n \sim N(0, \delta t_n)$. Due to its simplicity, the Euler-Maruyama scheme is the most commonly used numerical scheme.

From the basic intuition $dW_t \sim \sqrt{dt}$, we have (7.55)$\sim O(\delta t)$, (7.56)$\sim O(\delta t^{3/2})$, and (7.57)$\sim O(\delta t^2)$. By extracting the leading order term (7.55), we obtain

$$
\int_{t_n}^{t_{n+1}} dW_s \int_{t_n}^{s} (\mathcal{L}_2\sigma)(X_\tau)dW_\tau \approx (\mathcal{L}_2\sigma)(X_{t_n}) \int_{t_n}^{t_{n+1}} dW_s \int_{t_n}^{s} dW_\tau
$$

$$
= \frac{1}{2}(\mathcal{L}_2\sigma)(X_{t_n})[(\delta W_n)^2 - \delta t_n].
$$

Substituting this into the Ito-Taylor expansion, we obtain the well-known Milstein scheme.

(2) Milstein scheme.

(7.59) $X_{n+1} = X_n + b(X_n)\delta t_n + \sigma(X_n)\delta W_n + \dfrac{1}{2}(\sigma\sigma')(X_n)[(\delta W_n)^2 - \delta t_n].$

We should remark that the Milstein scheme is only practical for the SDEs driven by a single Wiener process. This is because the explicit characterization

$$\int_{t_n}^{t_{n+1}} \int_{t_n}^{s} dW_s dW_\tau = \frac{1}{2}\big((\delta W_n)^2 - \delta t_n\big)$$

is only valid in the one-dimensional case. In multidimensions, when $i \neq j$, one encounters terms of the form

$$\int_{t_n}^{t_{n+1}} \int_{t_n}^{s} dW_s^i dW_\tau^j,$$

where W_t^i, W_t^j are independent Wiener processes. Terms of this kind are difficult to sample[**KP92**].

Another problem for the Milstein scheme is that it can be hard to compute $\sigma'(X_t)$ even in the one-dimensional case. To overcome this difficulty, one can borrow ideas from the Runge-Kutta method for solving ODEs.

(3) Runge-Kutta scheme.

$$\hat{X}_n = X_n + b(X_n)\delta t_n + \sigma(X_n)\sqrt{\delta t_n},$$
$$X_{n+1} = X_n + b(X_n)\delta t_n + \sigma(X_n)\delta W_n$$

(7.60)
$$+ \frac{1}{2}\frac{1}{\sqrt{\delta t_n}}[\sigma(\hat{X}_n) - \sigma(X_n)][(\delta W_n)^2 - \delta t_n].$$

If we formally take a higher-order Itô-Taylor expansion, say applying (7.53) to

$$(\mathcal{L}_1 b)(X_\tau), \ (\mathcal{L}_2 b)(X_\tau), \ (\mathcal{L}_1 \sigma)(X_\tau), \ (\mathcal{L}_2 \sigma)(X_\tau)$$

and dropping higher-order terms, we get the following higher-order scheme.

(4) Higher-order scheme.

$$X_{n+1} = X_n + b\delta t_n + \sigma\delta W_{t_n} + \frac{1}{2}\sigma\sigma'\{(\delta W_n)^2 - \delta t_n\}$$
$$+ \sigma b'\delta Z_n + \frac{1}{2}\Big(bb' + \frac{1}{2}\sigma^2 b''\Big)\delta t_n^2$$
$$+ \Big(b\sigma' + \frac{1}{2}\sigma^2\sigma''\Big)(\delta W_n\delta t_n - \delta Z_n)$$

(7.61)
$$+ \frac{1}{2}\sigma\Big[\sigma\sigma'' + (\sigma')^2\Big]\Big[\frac{1}{3}(\delta W_n)^2 - \delta t_n\Big]\delta W_n,$$

where

$$\delta Z_n := \int_{t_n}^{t_{n+1}} \int_{t_n}^{s} dW_\tau ds$$

is a Gaussian random variable satisfying $\mathbb{E}(\delta Z_n) = 0$, $\mathbb{E}((\delta Z_n)^2) = \delta t_n^3/3$, $\mathbb{E}(\delta Z_n \delta W_n) = \delta t_n^2/2$.

To understand the difference in the performance of these schemes, we need to introduce the notion of the order of accuracy. Let $\{X_t^{\delta t}\}$ be the numerical solution of the SDE with (maximal) stepsize δt and let X_t be the exact solution.

Definition 7.18. (1) Strong convergence (mean square convergence). If

$$\max_{0 \leq t \leq T} \mathbb{E}|X_t^{\delta t} - X_t|^2 \leq C(\delta t)^{2\alpha},$$

where C is a constant independent of δt, then we say $\{X_t^{\delta t}\}$ strongly converges, or converges in the mean square sense, to X_t with order α.

(2) Weak convergence (convergence w.r.t. expectation). If

$$\max_{0 \leq t \leq T} |\mathbb{E}f(X_t^{\delta t}) - \mathbb{E}f(X_t)| \leq C_f(\delta t)^{\beta},$$

for any $f \in C_b^\infty(\mathbb{R}^n)$, the space of bounded, infinitely differentiable functions (with bounded derivatives), where C_f is a constant independent of δt but may depend on f, then we say $\{X_t^{\delta t}\}$ weakly converges to X_t with order β.

Proposition 7.19. $\beta \geq \alpha$.

Proof. Let K be a constant such that $|f'| \leq K$. By the mean value theorem, we have

$$|\mathbb{E}f(X_t^{\delta t}) - \mathbb{E}f(X_t)| \leq \mathbb{E}|f(X_t^{\delta t}) - f(X_t)| \leq K\mathbb{E}|X_t^{\delta t} - X_t|$$
$$\leq K(\mathbb{E}|X_t^{\delta t} - X_t|^2)^{\frac{1}{2}}. \qquad \square$$

Strong Convergence.

Theorem 7.20 (Convergence order)**.** *Define the length of the multi-index* $\boldsymbol{i} = (i_1, i_2, \ldots, i_k)$ *as*

$$l(\boldsymbol{i}) := k, \quad n(\boldsymbol{i}) := \{\text{the number of zeros in } \boldsymbol{i}\}$$

and the set of indices

$$\mathcal{S}_\alpha = \left\{ \boldsymbol{i} \mid l(\boldsymbol{i}) + n(\boldsymbol{i}) \leq 2\alpha \text{ or } l(\boldsymbol{i}) = n(\boldsymbol{i}) = \alpha + \frac{1}{2} \right\} \text{ for } \alpha \in \left\{ \frac{1}{2}, 1, \frac{3}{2}, \ldots \right\},$$

$$\mathcal{W}_\beta = \{\boldsymbol{i} \mid l(\boldsymbol{i}) \leq \beta\} \qquad \text{for } \beta \in \{1, 2, 3, \ldots\}.$$

Then with mild smoothness conditions on b, σ, and the function f in weak approximation, the scheme derived by truncating the Ito-Taylor expansion up to all indices with $\boldsymbol{i} \in \mathcal{S}_\alpha$, have strong order α; the scheme derived by truncating the Ito-Taylor expansion up to terms with $\boldsymbol{i} \in \mathcal{W}_\beta$ has weak order β.

The proof and detailed requirements about the smoothness conditions on b, σ, and f may be found in [**KP92**, Theorems 10.6.3 and 14.5.1]. Applying this theorem to the schemes discussed above, we obtain Table 7.1.

Table 7.1. The convergence order of some numerical schemes for the SDE.

	Strong order	Weak order
Euler-Maruyama	$1/2$	1
Milstein	1	1
Scheme (7.60)	1	1
Scheme (7.61)	2	2

To get some concrete feeling about the convergence process, we will analyze the mean square convergence of the Euler-Maruyama scheme under the assumption that b satisfies the global Lipschitz condition with Lipschitz constant L and the linear grow condition. We also assume that $\sigma = 1$.

The SDE takes the form

$$(7.62) \qquad\qquad dX_t = b(X_t)dt + dW_t.$$

The Euler-Maruyama scheme is

$$(7.63) \qquad\qquad X_{n+1} = X_n + b(X_n)\delta t_n + \delta W_n.$$

Introduce the "linear stochastic" interpolation of X_n as

$$d\bar{X}_t = b(X_n)dt + dW_t, \quad t \in [t_n, t_{n+1}),$$

where the driving force W_t is the same as that in (7.62). Then $\bar{X}_{t_n} = X_n$ and we have the so-called "discrete Itô formula" for $f \in C^2(\mathbb{R})$

$$df(\bar{X}_t) = f'(\bar{X}_t)d\bar{X}_t + \frac{1}{2}f''(\bar{X}_t)(d\bar{X}_t)^2;$$

i.e.,

$$f(\bar{X}_t) = f(X_n) + \int_{t_n}^t \left[f'(\bar{X}_s)b(X_n) + \frac{1}{2}f''(\bar{X}_s) \right]ds + \int_{t_n}^t f'(\bar{X}_s)dW_s$$

for $t \in [t_n, t_{n+1})$.

Lemma 7.21. *Let $\delta t = \max_n \delta t_n$. We have the following bounds for X_t:*

$$\sup_{t \leq T} \mathbb{E}|X_t|^2 \leq K_1(T), \qquad \sup_{t \in [t_n, t_{n+1})} \mathbb{E}|X_t - X_{t_n}|^2 \leq K_2(T)\delta t,$$

where the constant $K_1(T)$ depends on T, L, and $\mathbb{E}|X_0|^2$ and $K_2(T)$ depends on $L, \delta t$, and $K_1(T)$.

Proof. Applying Itô's formula to $|X_t|^2$, we have

$$d|X_t|^2 = 2X_t \cdot (b(X_t) + dW_t) + dt.$$

Integrating from 0 to t and taking the expectation, we have

$$\mathbb{E}|X_t|^2 = \mathbb{E}|X_0|^2 + 2\mathbb{E}\int_0^t X_s \cdot b(X_s)ds + 2\mathbb{E}\int_0^t X_s dW_s + t.$$

We also have

$$\mathbb{E}|X_t|^2 \leq \mathbb{E}|X_0|^2 + T + \int_0^t \mathbb{E}|X_s|^2 ds + L\int_0^t (1 + \mathbb{E}|X_s|^2)ds.$$

Using the Gronwall inequality, we get

$$\sup_{t \leq T} \mathbb{E}|X_t|^2 \leq (\mathbb{E}|X_0|^2 + T + LT)\exp((L+1)T).$$

Since

$$X_t - X_{t_n} = \int_{t_n}^t b(X_s)ds + (W_t - W_{t_n}),$$

squaring both sides and taking the expectation, we get

$$\mathbb{E}|X_t - X_{t_n}|^2 \leq 2\mathbb{E}\left(\int_{t_n}^t b(X_s)ds\right)^2 + 2\delta t.$$

Hence, we have

$$\mathbb{E}|X_t - X_{t_n}|^2 \leq 2L\delta t \int_{t_n}^t (1 + \mathbb{E}|X_s|^2)ds + 2\delta t$$
$$\leq 2L\delta t^2(1 + K_1(T)) + 2\delta t, \quad t \in [t_n, t_{n+1}).$$

This completes the proof. $\qquad\square$

Proposition 7.22. *The Euler-Maruyama scheme is of strong order 1/2.*

Proof. From (7.62) we have

$$X_{t_{n+1}} = X_{t_n} + \int_{t_n}^{t_{n+1}} b(X_t)dt + \delta W_n.$$

Note that (7.63) can be rewritten as

$$X_{n+1} = X_n + \int_{t_n}^{t_{n+1}} b(X_n)dt + \delta W_n.$$

Define $e_{n+1} = X_{t_{n+1}} - X_{n+1}$. Then

$$e_{n+1} = e_n + \int_{t_n}^{t_{n+1}} (b(X_t) - b(X_n))dt.$$

Squaring both sides and using $2ab \leq a^2 \delta t + b^2/\delta t$, we obtain

$$(7.64) \qquad |e_{n+1}|^2 = |e_n|^2 + \Big[\int_{t_n}^{t_{n+1}} (b(X_t) - b(X_n)) dt \Big]^2$$

$$+ 2e_n \cdot \Big[\int_{t_n}^{t_{n+1}} (b(X_t) - b(X_n)) dt \Big]$$

$$\leq |e_n|^2 (1 + \delta t) + \Big(1 + \frac{1}{\delta t} \Big) \Big[\int_{t_n}^{t_{n+1}} (b(X_t) - b(X_n)) dt \Big]^2$$

$$\leq |e_n|^2 (1 + \delta t) + L^2 (1 + \delta t) \int_{t_n}^{t_{n+1}} |X_t - X_n|^2 dt.$$

Since $|X_t - X_n|^2 \leq 2|X_t - X_{t_n}|^2 + 2|X_{t_n} - X_n|^2$, we have

$$\mathbb{E}|e_{n+1}|^2 \leq \mathbb{E}|e_n|^2 (1 + L_1 \delta t) + L_2 \delta t^2,$$

where $L_1 = 1 + 2L^2(1 + \delta t)$ and $L_2 = 2L^2(1 + \delta t)K_2(T)$ can be bounded by positive constants independent of δt if δt is small.

The direct induction then gives

$$\mathbb{E}|e_n|^2 \leq \mathbb{E}|e_0|^2 (1 + L_1 \delta t)^n + L_2 \delta t^2 \frac{(1 + L_1 \delta t)^n - 1}{L_1 \delta t} \leq \frac{L_2}{L_1}(e^{L_1 T} - 1)\delta t$$

if we assume $e_0 = 0$.   □

In the additive noise case, the Euler-Maruyama scheme is exactly the same as the Milstein scheme since $\sigma'\sigma = 0$ and thus the last term in (7.55) vanishes! From Theorem 7.20, we should be able to prove that it is of strong order 1. This is indeed true but the proof is a bit more tedious. We leave this as an exercise for the reader.

7.6. Multilevel Monte Carlo Method

We know that the Euler-Maruyama scheme is of weak order 1 in computing $Y_E = \mathbb{E}f(X_T)$ for the SDE (7.52) on $[0, T]$. In real computations, we take the weak approximator

$$(7.65) \qquad Y_{h,N} = \frac{1}{N} \sum_{k=1}^{N} f(X_n^{(k)}), \qquad n = T/h \in \mathbb{N},$$

with stepsize h and N independent samples, where X_n is obtained by the Euler-Maruyama scheme. The mean square error (MSE) has the bias-variance decomposition

$$\text{MSE} = \mathbb{E}(Y_E - Y_{h,N})^2 \leq 2|Y_E - \mathbb{E}f(X_n)|^2 + 2\mathbb{E}|\mathbb{E}f(X_n) - Y_{h,N}|^2$$

$$(7.66) \qquad\qquad\qquad \leq C_1 h^2 + C_2 N^{-1}.$$

The total cost is $C_3 N h^{-1}$. The cost-accuracy tradeoff

$$\min_{h,N} \text{MSE} \qquad \text{subject to a given cost } K = C_3 N h^{-1} \gg 1$$

gives the optimal choice

(7.67) $\qquad N \sim O(Kh), \quad h \sim O(K^{-\frac{1}{3}}), \quad \text{and} \quad \text{MSE} \sim O(K^{-\frac{2}{3}}).$

This means that if we require the accuracy $\text{MSE} \sim O(\varepsilon^2)$, we must have $h \sim O(\varepsilon)$, $N \sim O(\varepsilon^{-2})$ and thus the total cost is $K \sim O(\varepsilon^{-3})$.

Multilevel Monte Carlo, proposed by Giles in recent years [**Gil08**, **Gil14**], achieves the same accuracy at the cost of $K \sim O(\varepsilon^{-2}(\log \varepsilon)^2)$.

The construction of the multilevel Monte Carlo method is as follows. Define the L-level grids with time stepsize $h_l = M^{-l}T$ for $l = 0, 1, \ldots, L$. Denote by $F_l = f(X_{l,M^l})$ the approximation of $f(X_T)$ at the level l, where X_{l,M^l} is the approximation of X_T with stepsize h_l. We have

(7.68) $\qquad \mathbb{E}F_L = \sum_{l=0}^{L} \mathbb{E}(F_l - F_{l-1}) \qquad \text{where } F_{-1} := 0.$

Take N_l realizations for each summand in (7.68), and define

$$Y_l = \frac{1}{N_l} \sum_{k=1}^{N_l} \left(F_l^{(k)} - F_{l-1}^{(k)} \right), \qquad l = 0, 1, \ldots, L.$$

Correspondingly, define the final estimator

(7.69) $\qquad \hat{Y}_L = \sum_{l=0}^{L} Y_l.$

Note that $\text{Var}(Y_l) = V_l/N_l$, where $V_l := \text{Var}(F_l - F_{l-1})$ for $l = 0, 1, \ldots, L$. With independent sampling in (7.69), we get

(7.70) $\qquad \text{Var}(\hat{Y}_L) = \sum_{l=0}^{L} \text{Var}(Y_l) = \sum_{l=0}^{L} \frac{V_l}{N_l}.$

The total computational cost is

$$K \sim O\left(\sum_{l=0}^{L} N_l h_l^{-1} \right).$$

The key point of multilevel Monte Carlo is that with the decomposition (7.68), the term $F_l - F_{l-1}$ has smaller variance at higher levels provided that the realizations of $F_l - F_{l-1}$ come from two discrete approximations with different time stepsizes but the same Brownian paths. This property suggests that we can use fewer Monte Carlo samples at higher levels, i.e.,

finer grids, but more samples for lower levels, i.e., coarser grids. This cost-accuracy tradeoff is the origin of the improved efficiency of the multilevel Monte Carlo method.

Now let us consider the minimization

$$\min_{N_l} \text{Var}(\hat{Y}_L) = \sum_{l=0}^{L} \frac{V_l}{N_l} \qquad \text{subject to the cost } K = \sum_{l=0}^{L} N_l h_l^{-1} \gg 1.$$

This is generally a very difficult problem so we relax it and make N_l to be continuous. Upon introducing the Lagrange multiplier, we obtain the minimizer

$$(7.71) \qquad N_l = \lambda \sqrt{V_l h_l}, \qquad \text{where} \quad \lambda = K \left(\sum_{l=0}^{L} \sqrt{V_l h_l^{-1}} \right)^{-1}.$$

From the strong and weak convergence result of the Euler-Maruyama scheme, we have

$$|\mathbb{E}(F_l) - Y_E| = O(h_l), \quad \mathbb{E}|X_T - X_{l,M^l}|^2 = O(h_l).$$

By assuming the Lipschitz continuity of f, we obtain

$$\text{Var}(F_l - f(X_T)) \le \mathbb{E}|f(X_{l,M^l}) - f(X_T)|^2 \le C\mathbb{E}|X_T - X_{l,M^l}|^2 = O(h_l)$$

and thus

$$V_l = \text{Var}(F_l - F_{l-1}) \le 2\,\text{Var}(F_l - f(X_T)) + 2\,\text{Var}(F_{l-1} - f(X_T)) = O(h_l)$$

since $h_{l-1} = Mh_l$ and $M \sim O(1)$. We remark that the terms $F_l(\omega)$ and $F_{l-1}(\omega)$ should be driven by the same Brownian path $W(\omega)$; otherwise $F_l - F_{l-1}$ would not be a small quantity. This point should be strictly realized in the numerical computations.

For a given tolerance $\varepsilon \ll 1$, take

$$(7.72) \qquad\qquad\qquad N_l = O(\varepsilon^{-2} L h_l);$$

according to the optimal choice (7.71), we get the variance estimate

$$(7.73) \qquad\qquad\qquad \text{Var}(\hat{Y}_L) = O(\varepsilon^2)$$

from (7.70). Further taking $L = \log \varepsilon^{-1} / \log M$, we have

$$h_L = M^{-L} = O(\varepsilon).$$

So the bias error

$$(7.74) \qquad\qquad\qquad |\mathbb{E}F_L - Y_E| = O(h_L) = O(\varepsilon).$$

Combining (7.73) and (7.74), we obtain the overall mean square error

$$\text{MSE} = \mathbb{E}(Y_E - \hat{Y}_L)^2 = O(\varepsilon^2)$$

and the computational complexity

$$K = \sum_{l=0}^{L} N_l h_l^{-1} = O(\varepsilon^{-2} L^2) = O\left(\varepsilon^{-2}(\log \varepsilon)^2\right).$$

The optimal choice of M can be found by minimizing the prefactor in the estimate of the computational cost [**Gil08**].

Exercises

7.1. Prove that the definition given in (7.10) is independent of the choice of the approximating sequence $\{\phi_n\}$.

7.2. Prove Proposition 7.3.

7.3. Prove that with the midpoint approximation

$$\int_0^t W_s dW_s \approx \sum_j W_{t_{j+\frac{1}{2}}}(W_{t_{j+1}} - W_{t_j}) \to \frac{W_t^2}{2}$$

and with the rightmost approximation

$$\int_0^t W_s dW_s \approx \sum_j W_{t_{j+1}}(W_{t_{j+1}} - W_{t_j}) \to \frac{W_t^2}{2} + \frac{t}{2}$$

in L_ω^2 as the subdivision $|\Delta| \to 0$.

7.4. Prove the relation (7.25) by following these steps:
(a) Prove that the Hermite polynomials satisfy

$$\sum_{n=0}^{\infty} \frac{u^n}{n!} h_n(x) = \exp\left(ux - \frac{u^2}{2}\right)$$

and

$$\sum_{n=0}^{\infty} \frac{u^n}{n!} H_n(x, a) = \exp\left(ux - \frac{au^2}{2}\right),$$

where $H_n(x, a) = a^{n/2} h_n(x/\sqrt{a})$ $(a > 0)$ and $H_n(x, 0) = x^n$.
(b) Prove that

$$\left(\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial a}\right) H_n(x, a) = 0 \quad \text{and} \quad \frac{\partial}{\partial x} H_n(x, a) = n H_{n-1}(x, a).$$

(c) Prove that (7.25) holds using Itô's formula.

7.5. Solve the SDE:
(a) $dX_t = -X_t/(1+t)dt + 1/(1+t)dW_t, \quad X_0 = 0, \ t \in \mathbb{R}_+.$
(b) $dX_t = -X_t dt + e^{-t} dW_t, \quad X_0 = 1, \ t \in \mathbb{R}_+.$
(c) $dX_t = -X_t/(1-t)dt + dW_t, \quad X_0 = 0, \ t \in (0, 1).$
(d) $dX_t = X_t W_t dt + dW_t, \quad X_t|_{t=0} = X_0, \ t \in \mathbb{R}_+.$

7.6. Assume that $\{\boldsymbol{W}_t\}$ is a d-dimensional Wiener process. Here $\boldsymbol{U}(\cdot) \in \mathbb{R}^{d \times d}$ is an $\mathcal{F}_t$-adapted orthogonal matrix, $\boldsymbol{U}\boldsymbol{U}^T = \boldsymbol{I}$. Define the SDEs

$$d\boldsymbol{Y}_t = \boldsymbol{U}(t) \cdot d\boldsymbol{W}_t, \quad \boldsymbol{Y}_0 = \boldsymbol{0}.$$

Prove that $\boldsymbol{Y}_t$ is also a d-dimensional Wiener process.

7.7. Consider the two-dimensional OU process

$$d\boldsymbol{X}_t = -\gamma \boldsymbol{X}_t dt + d\boldsymbol{W}_t,$$

where $\boldsymbol{X}_t = (X_t, Y_t)$. Define the polar coordinates (R_t, Θ_t) through $(X_t, Y_t) = (R_t \cos \Theta_t, \ R_t \sin \Theta_t)$. Derive the corresponding SDEs for (R_t, Θ_t).

7.8. For the multidimensional OU process

$$d\boldsymbol{X}_t = \boldsymbol{B}\boldsymbol{X}_t dt + \boldsymbol{\sigma} d\boldsymbol{W}_t,$$

derive the relations that the stationary mean and covariance matrix should satisfy.

7.9. Derive the autocorrelation function

$$C(t, s) = \mathbb{E}X_t X_s, \quad t > s,$$

for the stationary OU process with distribution $N(0, \sigma^2/(2\gamma))$. Generalize this result to the multidimensional case.

7.10. Prove that for the diffusion process the higher-order moments have the following estimates:

$$\lim_{t \to s} \frac{1}{t - s} \int_{|\boldsymbol{x}-\boldsymbol{y}|<\epsilon} (x_{i_1} - y_{i_1}) \cdots (x_{i_k} - y_{i_k}) p(\boldsymbol{x}, t | \boldsymbol{y}, s) d\boldsymbol{x} = O(\epsilon), \ k > 2.$$

7.11. Prove that if one takes the rightmost endpoint to define the stochastic integral (backward stochastic integral)

$$\int_0^T f(\omega, t) * dW_t \approx \sum_j f(t_{j+1})(W_{t_{j+1}} - W_{t_j}),$$

then the SDE defined by

(7.75) $$dX_t = b(X_t, t)dt + \sigma(X_t, t) * dW_t$$

is equivalent to the following Itô SDE:

$$dX_t = \Big(b(X_t, t) + \partial_x \sigma \sigma(X_t, t)\Big)dt + \sigma(X_t, t)dW_t.$$

7.12. Verify that the Newton-Leibnitz chain rule $df(\boldsymbol{X}_t) = \nabla f \cdot d\boldsymbol{X}_t$ holds for the Stratonovich SDEs (7.50).

7.13. Prove the estimate (7.32) by induction.

7.14. Assume that $\{L_t\}$ is a compound Poisson process (defined in Exercise 3.13) and $f \in C[0, T]$. Define the stochastic integral

$$X := \int_0^T f(t) dL_t = \lim_{|\Delta| \to 0} \sum_{i=1}^n f(t_i) \delta L_i$$

where Δ is a subdivision of $[0, T]$ and $\delta L_i = L_{t_{i+1}} - L_{t_i}$. Compute $\mathbb{E}X$ and $\text{Var}(X)$.

7.15. Prove that if the drift function $\boldsymbol{b}$ is sufficiently smooth, the Euler-Maruyama scheme for the SDEs

$$d\boldsymbol{X}_t = \boldsymbol{b}(\boldsymbol{X}_t) dt + d\boldsymbol{W}_t, \quad t \in [0, T],$$

is of strong order 1.

Notes

Since Itô's groundbreaking work on the stochastic integral, the theory of SDEs has been developed into a mature subject in stochastic analysis [**Oks98**, **IW81**, **KS91**, **RY05**, **RW94a**, **RW94b**]. For people interested in applications, we recommend the references [**Gar09**, **Pav14**, **VK04**].

The numerical solution of SDEs is still a developing field. Among the topics that we did not cover, we mention strong and weak approximation of multiple Itô integrals [**KP92**], implicit methods for overcoming the stiffness, stability analysis, and explicit methods for stiff SDEs [**AC08**, **AL08**], high-order Runge-Kutta methods [**Rö3**], extrapolation methods [**TT90**], structure-preserving methods and applications in molecular dynamics [**LM15**], etc. Interested readers can refer to [**KP92**, **MT04**] for more details.

Fokker-Planck Equation

There are three different but related ways of studying diffusion processes. The first is to take a pathwise viewpoint and represent the paths by solutions of SDEs. This was done in the last chapter. The second approach is to study the dynamics of the probability distribution and expectation values using partial differential equations. This is the approach that we will take in this chapter. The third is to study the probability distribution on path space induced by the diffusion process. This is the approach of path integrals, which will be taken up in the next chapter.

Let us first consider the situation of ordinary differential equations. Imagine a point particle in $\mathbb{R}^d$ whose dynamics is described by

$$(8.1) \qquad \frac{d\boldsymbol{x}}{dt} = \boldsymbol{b}(\boldsymbol{x}), \quad \boldsymbol{x}|_{t=0} = \boldsymbol{x}_0.$$

Assuming that the initial distribution density of the particle is $p_0(\boldsymbol{x})$, at later times the distribution density of the particle $p(\boldsymbol{x}, t)$ then satisfies the Liouville equation:

$$(8.2) \qquad \partial_t p + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{b}p) = 0.$$

Alternatively, one can also think of the solutions of the ODE (8.1) as being the characteristics of this first-order PDE (8.2).

We will see that if (8.1) is replaced by an SDE, then the first-order PDE above is replaced by a second-order parabolic equation, the so-called Fokker-Planck equation. Alternatively, one can also think of the solutions of the SDE as the characteristics of the corresponding Fokker-Planck equation.

This connection allows us to use PDE methods to study SDEs. For example, one can use the asymptotic methods developed for PDEs to study SDEs, as we will illustrate later.

8.1. Fokker-Planck Equation

Consider the SDE

$$(8.3) \qquad d\boldsymbol{X}_t = \boldsymbol{b}(\boldsymbol{X}_t, t)dt + \boldsymbol{\sigma}(\boldsymbol{X}_t, t)d\boldsymbol{W}_t.$$

Assume that the transition probability density exists and is defined as

$$p(\boldsymbol{x}, t|\boldsymbol{y}, s)d\boldsymbol{x} = \mathbb{P}\big(\boldsymbol{X}_t \in [\boldsymbol{x}, \boldsymbol{x} + d\boldsymbol{x})|\boldsymbol{X}_s = \boldsymbol{y}\big) \quad \text{for } t \geq s.$$

For any function $f \in C_c^\infty(\mathbb{R}^d)$, the Itô formula gives

$$\begin{aligned}
df(\boldsymbol{X}_t) &= \nabla f(\boldsymbol{X}_t) \cdot d\boldsymbol{X}_t + \frac{1}{2}(d\boldsymbol{X}_t)^T \cdot \nabla^2 f(\boldsymbol{X}_t) \cdot (d\boldsymbol{X}_t) \\
&= \Big(\boldsymbol{b} \cdot \nabla f + \frac{1}{2}\boldsymbol{\sigma}\boldsymbol{\sigma}^T : \nabla^2 f\Big)dt + \nabla f \cdot \boldsymbol{\sigma} \cdot d\boldsymbol{W}_t.
\end{aligned}$$

Integrating both sides from s to t, we get

$$\begin{aligned}
f(\boldsymbol{X}_t) - f(\boldsymbol{X}_s) &= \int_s^t \nabla f(\boldsymbol{X}_\tau) \cdot \{\boldsymbol{b}(\boldsymbol{X}_\tau, \tau)d\tau + \boldsymbol{\sigma}(\boldsymbol{X}_\tau, \tau)d\boldsymbol{W}_\tau\} \\
&\quad + \frac{1}{2}\int_s^t \sum_{i,j} \partial_{ij}^2 f(\boldsymbol{X}_\tau)a_{ij}(\boldsymbol{X}_\tau, \tau)d\tau,
\end{aligned}$$

where the diffusion matrix $\boldsymbol{A}(\boldsymbol{x}, t) = \boldsymbol{\sigma}(\boldsymbol{x}, t)\boldsymbol{\sigma}^T(\boldsymbol{x}, t) = (a_{ij}(\boldsymbol{x}, t))$. Taking the expectation on both sides conditioned on $\boldsymbol{X}_s = \boldsymbol{y}$, we have

$$(8.4) \qquad \mathbb{E}^{\boldsymbol{y}, s}f(\boldsymbol{X}_t) - f(\boldsymbol{y}) = \mathbb{E}^{\boldsymbol{y}, s}\int_s^t (\mathcal{L}f)(\boldsymbol{X}_\tau, \tau)d\tau,$$

where the operator $\mathcal{L}$ is defined by

$$(8.5) \qquad (\mathcal{L}f)(\boldsymbol{x}, t) = \boldsymbol{b}(\boldsymbol{x}, t) \cdot \nabla f(\boldsymbol{x}) + \frac{1}{2}\sum_{i,j} a_{ij}(\boldsymbol{x}, t)\partial_{ij}^2 f(\boldsymbol{x}).$$

$\mathcal{L}$ is in fact the generator of the diffusion process defined by the SDE.

In terms of transition probability density $p(\boldsymbol{x}, t|\boldsymbol{y}, s)$, we have

$$\int_{\mathbb{R}^d} f(\boldsymbol{x})p(\boldsymbol{x}, t|\boldsymbol{y}, s)d\boldsymbol{x} - f(\boldsymbol{y}) = \int_s^t \int_{\mathbb{R}^d} (\mathcal{L}f)(\boldsymbol{x}, \tau)p(\boldsymbol{x}, \tau|\boldsymbol{y}, s)d\boldsymbol{x}d\tau.$$

This is exactly the definition of the weak solution of the following PDE:

$$(8.6) \quad \partial_t p(\boldsymbol{x}, t|\boldsymbol{y}, s) = (\mathcal{L}^* p)(\boldsymbol{x}, t|\boldsymbol{y}, s), \quad p(\boldsymbol{x}, t|\boldsymbol{y}, s)|_{t=s} = \delta(\boldsymbol{x} - \boldsymbol{y}), \quad t > s,$$

where the operator $\mathcal{L}^*$ is the formal adjoint of $\mathcal{L}$ defined through

$$(\mathcal{L}f, g) = (f, \mathcal{L}^* g).$$

Here $(\cdot, \cdot)$ denotes the standard inner product in $L^2(\mathbb{R}^d)$. An easy calculation gives

$$(8.7) \qquad (\mathcal{L}^* f)(\boldsymbol{x}, t) = -\nabla_{\boldsymbol{x}} \cdot (\boldsymbol{b}(\boldsymbol{x}, t) f(\boldsymbol{x})) + \frac{1}{2} \nabla_{\boldsymbol{x}}^2 : (\boldsymbol{A}(\boldsymbol{x}, t) f(\boldsymbol{x})),$$

where $\nabla_{\boldsymbol{x}}^2 : (\boldsymbol{A} f) = \sum_{ij} \partial_{ij}(a_{ij} f)$.

Equation (8.6) is called the *Kolmogorov forward equation*, or the *Fokker-Planck equation* in the physics literature. The term "forward" means that it describes a situation which is forward in time; i.e., $t \geq s$ and t is the independent variable. The backward equation, which describes a situation which is backward in time, will be derived in Section 8.3. There the natural time variable is s and $s \leq t$.

If the probability density of $\boldsymbol{X}_s$ is ρ_0 and if we denote the probability density of $\boldsymbol{X}_t$ by $\rho(\cdot, t)$, then ρ also satisfies the forward Kolmogorov equation. This is true since

$$\rho(\boldsymbol{x}, t) = \int p(\boldsymbol{x}, t | \boldsymbol{y}, s) \rho_0(\boldsymbol{y}) d\boldsymbol{y}$$

and one can integrate both sides of the forward Kolmogorov equation against ρ_0.

Example 8.1 (Brownian motion)**.** The SDE reads

$$d\boldsymbol{X}_t = d\boldsymbol{W}_t, \quad \boldsymbol{X}_0 = 0.$$

Thus the Fokker-Planck equation is

$$(8.8) \qquad \partial_t p = \frac{1}{2} \Delta p, \quad p(\boldsymbol{x}, 0) = \delta(\boldsymbol{x}).$$

It is well known that

$$p(\boldsymbol{x}, t) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{\boldsymbol{x}^2}{2t}\right),$$

which is the probability distribution density of $N(0, t\boldsymbol{I})$.

Example 8.2 (Brownian dynamics)**.** Consider the over-damped dynamics of a stochastic particle described by

$$(8.9) \qquad d\boldsymbol{X}_t = -\frac{1}{\gamma} \nabla U(\boldsymbol{X}_t) dt + \sqrt{\frac{2k_B T}{\gamma}} d\boldsymbol{W}_t.$$

The Fokker-Planck equation is

$$(8.10) \qquad \partial_t p - \nabla \cdot \left(\frac{1}{\gamma} \nabla U(\boldsymbol{x}) p\right) = \frac{k_B T}{\gamma} \Delta p = D \Delta p,$$

where $D = k_B T / \gamma$ is the diffusion coefficient.

Equation (8.10) is called the Smoluchowski equation in physics [**DE86**]. It can also be derived from the following recipe. Define the free energy associated with the probability density p by

$$(8.11) \quad F[p] = U[p] - TS[p] = \int_{\mathbb{R}^d} \Big(U(\boldsymbol{x})p(\boldsymbol{x}) + k_B T p(\boldsymbol{x}) \log p(\boldsymbol{x}) \Big) d\boldsymbol{x},$$

where the first term $\int_{\mathbb{R}^d} U(\boldsymbol{x})p(\boldsymbol{x})d\boldsymbol{x}$ is the internal energy U and the second term $k_B \int_{\mathbb{R}^d} p(\boldsymbol{x}) \log p(\boldsymbol{x})d\boldsymbol{x}$ is the negative entropy $-S$ in thermodynamics. The chemical potential μ, defined as the change of free energy with respect to the change of probability density, is then given by

$$\mu = \frac{\delta F}{\delta p} = k_B T(1 + \log p(\boldsymbol{x})) + U(\boldsymbol{x}).$$

In the over-damped regime, the velocity field $\boldsymbol{u}$ is given by Fick's law

$$\boldsymbol{u}(\boldsymbol{x}) = -\frac{1}{\gamma}\nabla\mu,$$

where γ is the friction coefficient. The current density is then given by

$$(8.12) \qquad\qquad \boldsymbol{j}(\boldsymbol{x}) = p(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x}).$$

Then the Smoluchowski equation (8.10) is just the continuity equation

$$\partial_t p + \nabla \cdot \boldsymbol{j} = 0.$$

This is the same as the Fokker-Planck equation derived earlier.

If the underlying stochastic dynamics is a Stratonovich SDE (7.50), then its transition probability density satisfies

$$(8.13) \qquad\qquad \partial_t p + \nabla \cdot (\boldsymbol{b}p) = \frac{1}{2}\nabla \cdot (\boldsymbol{\sigma} \cdot \nabla \cdot (\boldsymbol{\sigma}p)),$$

where $\nabla \cdot (\boldsymbol{\sigma} \cdot \nabla \cdot (\boldsymbol{\sigma}p)) = \sum_{ijk} \partial_i(\sigma_{ik}\partial_j(\sigma_{jk}p))$.

Example 8.3 (Langevin dynamics)**.** We have already defined the Langevin dynamics (7.41) for an inertial particle in a force field subject to friction and noise. It is straightforward to write down its Fokker-Planck equation

$$(8.14) \qquad \partial_t p + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} p - \nabla_{\boldsymbol{v}} \cdot \Big((\gamma\boldsymbol{v} + \nabla U(\boldsymbol{x}))p \Big) = \frac{k_B T}{\gamma}\Delta_{\boldsymbol{v}} p.$$

Note that the diffusion is degenerate since we only have the term $\Delta_{\boldsymbol{v}} p$.

Example 8.4 (Brownian motion on $\mathbb{S}^{n-1}$)**.** The SDE for the Brownian motion on the unit sphere $\mathbb{S}^{n-1}$ has the Stratonovich form

$$(8.15) \qquad d\boldsymbol{X}_t = (\boldsymbol{I} - \boldsymbol{X}_t \otimes \boldsymbol{X}_t) \circ d\boldsymbol{W}_t, \quad \boldsymbol{X}_t|_{t=0} = \boldsymbol{X}_0 \in \mathbb{S}^{n-1}.$$

The Itô form of this SDE is given by

$$d\boldsymbol{X}_t = -\frac{n-1}{2}\boldsymbol{X}_t dt + (\boldsymbol{I} - \boldsymbol{X}_t \otimes \boldsymbol{X}_t)d\boldsymbol{W}_t.$$

The operator $\mathcal{L}$ associated with this process is then

$$\mathcal{L}f(\boldsymbol{x}) = -\frac{n-1}{2}\boldsymbol{x} \cdot \nabla f(\boldsymbol{x}) + \frac{1}{2}\Delta f(\boldsymbol{x}) + \frac{1}{2}\boldsymbol{x} \otimes \boldsymbol{x} : \nabla^2 f(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{S}^{n-1}.$$

When $n = 3$, the Fokker-Planck equation can be written as

$$(8.16) \qquad \partial_t p = \frac{1}{2}\mathcal{R}_{\boldsymbol{x}}^2 p, \quad \boldsymbol{x} \in \mathbb{S}^2,$$

where $\mathcal{R}_{\boldsymbol{x}} = \boldsymbol{x} \times \nabla_{\boldsymbol{x}}$ and $\mathcal{R}_{\boldsymbol{x}}^2 = \mathcal{R}_{\boldsymbol{x}} \cdot \mathcal{R}_{\boldsymbol{x}}$. Using spherical coordinates

$$x_1 = r\sin\theta\cos\varphi, \ x_2 = r\sin\theta\sin\varphi, \ x_3 = r\cos\theta, \quad (\theta, \varphi) \in [0, \pi] \times [0, 2\pi), \ r \geq 0,$$

for $\mathcal{R}_{\boldsymbol{x}}^2$, we get the Laplace-Bertrami operator on $\mathbb{S}^2$

$$(8.17) \qquad \mathcal{R}_{\boldsymbol{x}}^2 = \Delta_{\mathbb{S}^2} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}.$$

8.2. Boundary Condition

Many stochastic problems occur in a bounded domain U, in which case the boundary conditions are needed. To pose suitable boundary conditions in different situations, we need to understand the probability current

$$(8.18) \qquad \boldsymbol{j}(\boldsymbol{x}, t) = \boldsymbol{b}(\boldsymbol{x}, t)p(\boldsymbol{x}, t) - \frac{1}{2}\nabla \cdot (\boldsymbol{A}(\boldsymbol{x}, t)p(\boldsymbol{x}, t))$$

in the continuity form of the Fokker-Planck equation

$$(8.19) \qquad \partial_t p(\boldsymbol{x}, t) + \nabla \cdot \boldsymbol{j}(\boldsymbol{x}, t) = 0.$$

To do this, let us investigate the role of probability flux between regions R_1 and R_2 separated by a boundary S_{12} (see Figure 8.1).
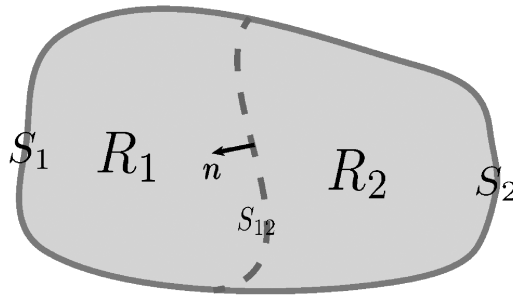
Figure 8.1. Probability flux across a boundary S_{12} between regions R_1 and R_2. Here $\boldsymbol{n}$ is the unit outer normal of the region R_2 on S_{12}, and S_1 and S_2 are the boundary parts of R_1 and R_2 except S_{12}.

Consider the probability transfer from region R_1 to R_2 during the time t to $t + \delta t$. we have

$$P_{1 \to 2} = \int_{R_2} d\boldsymbol{x} \int_{R_1} d\boldsymbol{y} p(\boldsymbol{x}, t + \delta t; \boldsymbol{y}, t),$$

and with similar reasoning the probability transfer from region R_2 to R_1 has the form

$$P_{2 \to 1} = \int_{R_1} d\boldsymbol{x} \int_{R_2} d\boldsymbol{y} p(\boldsymbol{x}, t + \delta t; \boldsymbol{y}, t).$$

Thus the net probability flow rate from R_2 to R_1 is

$$J_{2 \to 1} = \lim_{\delta t \to 0} (P_{2 \to 1} - P_{1 \to 2}) / \delta t.$$

With the equality

$$\int_{R_2} d\boldsymbol{x} \int_{R_1} d\boldsymbol{y} p(\boldsymbol{x}, t; \boldsymbol{y}, t) = 0,$$

we obtain

$$J_{2 \to 1} = \int_{R_1} d\boldsymbol{x} \int_{R_2} d\boldsymbol{y} \partial_t p(\boldsymbol{x}, t; \boldsymbol{y}, s = t) - \int_{R_2} d\boldsymbol{x} \int_{R_1} d\boldsymbol{y} \partial_t p(\boldsymbol{x}, t; \boldsymbol{y}, s = t)$$

$$= \int_{R_2} d\boldsymbol{x} \nabla_{\boldsymbol{x}} \cdot \boldsymbol{j}(\boldsymbol{x}, t; R_1, t) - \int_{R_1} d\boldsymbol{x} \nabla_{\boldsymbol{x}} \cdot \boldsymbol{j}(\boldsymbol{x}, t; R_2, t)$$

$$= \int_{S_{12}} dS \boldsymbol{n} \cdot (\boldsymbol{j}(\boldsymbol{x}, t; R_1, t) + \boldsymbol{j}(\boldsymbol{x}, t; R_2, t)),$$

where $\boldsymbol{j}(\boldsymbol{x}, t; R_1, t) := \int_{R_1} d\boldsymbol{y} \boldsymbol{j}(\boldsymbol{x}, t; \boldsymbol{y}, t)$ and $\boldsymbol{n}$ is the normal pointing from R_2 to R_1. The last equality is obtained by the divergence theorem and the fact that $\boldsymbol{j}(\boldsymbol{x}, t; R_2, t) = 0$ when $\boldsymbol{x} \in S_1$ and $\boldsymbol{j}(\boldsymbol{x}, t; R_1, t) = 0$ when $\boldsymbol{x} \in S_2$. From the fact that $\boldsymbol{x} \in R_1 \cup R_2$ we have $\boldsymbol{j}(\boldsymbol{x}, t) = \int_{\mathbb{R}^d} d\boldsymbol{y} \boldsymbol{j}(\boldsymbol{x}, t; \boldsymbol{y}, t) = \boldsymbol{j}(\boldsymbol{x}, t; R_1, t) + \boldsymbol{j}(\boldsymbol{x}, t; R_2, t)$ and thus

$$J_{2 \to 1} = \int_{S_{12}} dS \boldsymbol{n} \cdot \boldsymbol{j}(\boldsymbol{x}, t).$$

Recall that in a discrete time Markov chain, the probability flux is defined as

$$J_{ij}^n = \mu_{n,i} p_{ij} - \mu_{n,j} p_{ji}$$

from state i to state j at time n and for a continuous time Markov chain

$$J_{ij}(t) = \mu_i(t) p_{ij} - \mu_j(t) p_{ji},$$

we see that $\boldsymbol{n} \cdot \boldsymbol{j}(\boldsymbol{x}, t)$ is exactly the continuous space version of $J_{ij}(t)$ along a specific direction $\boldsymbol{n}$.

The two most commonly used boundary conditions are as follows. It will be instructive for the readers to compare them with the boundary conditions for the Wiener process in Chapter 6.

The reflecting boundary condition. Particles are reflected at the boundary ∂U. Thus there will be no probability flux across ∂U. Therefore we have

$$(8.20) \qquad \boldsymbol{n} \cdot \boldsymbol{j}(\boldsymbol{x}, t) = 0, \quad \boldsymbol{x} \in \partial U.$$

In this case the total probability is conserved since

$$\frac{d}{dt} \int_U p(\boldsymbol{x}, t) d\boldsymbol{x} = -\int_U \nabla_{\boldsymbol{x}} \cdot \boldsymbol{j}(\boldsymbol{x}, t) d\boldsymbol{x}$$
$$= -\int_{\partial U} \boldsymbol{n} \cdot \boldsymbol{j}(\boldsymbol{x}, t) dS = 0.$$

Absorbing boundary condition. Particles are absorbed (or removed) once they hit the boundary ∂U. Thus the probability on the boundary ∂U is zero. The absorbing boundary condition is then

$$(8.21) \qquad p(\boldsymbol{x}, t) = 0, \quad \boldsymbol{x} \in \partial U.$$

The total probability is no longer conserved in this case.

8.3. The Backward Equation

We now derive the equation for the transition probability density $p(\boldsymbol{x}, t | \boldsymbol{y}, s)$ with respect to the variables $\boldsymbol{y}$ and s. Assume that $\boldsymbol{X}_t$ satisfies (8.3). Let f be a smooth function with compact support, and let

$$u(\boldsymbol{y}, s) = \mathbb{E}^{\boldsymbol{y}, s} f(\boldsymbol{X}_t) = \int_{\mathbb{R}^d} f(\boldsymbol{x}) p(\boldsymbol{x}, t | \boldsymbol{y}, s) d\boldsymbol{x}, \quad s \le t.$$

Under smoothness assumption on $u(\boldsymbol{y}, s)$, we have the formal calculation

$$du(\boldsymbol{X}_\tau, \tau) = (\partial_\tau u + \mathcal{L}u)(\boldsymbol{X}_\tau, \tau) d\tau + \nabla u \cdot \boldsymbol{\sigma} \cdot d\boldsymbol{W}_\tau$$

by Itô formula. Taking the expectation, we obtain

$$\lim_{t \to s} \frac{1}{t-s} (\mathbb{E}^{\boldsymbol{y}, s} u(\boldsymbol{X}_t, t) - u(\boldsymbol{y}, s)) = \lim_{t \to s} \mathbb{E}^{\boldsymbol{y}, s} \frac{1}{t-s} \int_s^t (\partial_\tau u + \mathcal{L}u)(\boldsymbol{X}_\tau, \tau) d\tau$$
$$= \partial_s u(\boldsymbol{y}, s) + (\mathcal{L}u)(\boldsymbol{y}, s).$$

On the other hand it is obvious that

$$\mathbb{E}^{\boldsymbol{y}, s} u(\boldsymbol{X}_t, t) = \mathbb{E}^{\boldsymbol{y}, s} f(\boldsymbol{X}_t) = u(\boldsymbol{y}, s).$$

Therefore, we get

$$(8.22) \qquad \partial_s u(\boldsymbol{y}, s) + (\mathcal{L}u)(\boldsymbol{y}, s) = 0.$$

From the arbitrariness of f, we obtain

(8.23) $\partial_s p(\boldsymbol{x}, t | \boldsymbol{y}, s) + (\mathcal{L}_{\boldsymbol{y}} p)(\boldsymbol{x}, t | \boldsymbol{y}, s) = 0, \quad p(\boldsymbol{x}, t | \boldsymbol{y}, t) = \delta(\boldsymbol{x} - \boldsymbol{y}), \quad s < t.$

This is the *Kolmogorov backward equation*. For a rigorous derivation of (8.23), readers are referred to [**Fri75a**].

Regarding the boundary conditions for the backward equation (8.23) (cf. [**Gar09**]), we have:

Absorbing boundary condition: $p(\boldsymbol{x}, t | \boldsymbol{y}, s) = 0$ for $\boldsymbol{y} \in \partial U.$

Reflecting boundary condition: $\boldsymbol{n} \cdot \boldsymbol{A}(\boldsymbol{y}, s) \cdot \nabla_{\boldsymbol{y}} p(\boldsymbol{x}, t | \boldsymbol{y}, s) = 0$ for $\boldsymbol{y} \in \partial U,$

where $\boldsymbol{n}$ is the unit normal of ∂U. In one dimension, the reflecting boundary condition becomes $\partial_y p = 0$.

8.4. Invariant Distribution

Assume that the drift and the diffusion tensor of the diffusion process are independent of t. We can ask whether the process has a stationary or invariant distribution and whether such distributions are unique. Using the Fokker-Planck equation, this question is turned into asking whether the PDE

(8.24) $$\nabla_{\boldsymbol{x}} \cdot (\boldsymbol{b}(\boldsymbol{x}) p_s(\boldsymbol{x})) = \frac{1}{2} \nabla_{\boldsymbol{x}}^2 : (\boldsymbol{A}(\boldsymbol{x}) \, p_s(\boldsymbol{x}))$$

together with some suitable boundary condition and normalization condition has a unique solution. In general, if the tensor $\boldsymbol{A}(\boldsymbol{x})$ is uniformly bounded and nondegenerate in the sense that there exist positive constants c_1 and c_2 such that

(8.25) $$|\boldsymbol{\xi}^T \boldsymbol{A}(\boldsymbol{x}) \boldsymbol{\zeta}| \leq c_2 |\boldsymbol{\xi}| |\boldsymbol{\zeta}| \quad \text{and} \quad \boldsymbol{\xi}^T \boldsymbol{A}(\boldsymbol{x}) \boldsymbol{\xi} \geq c_1 |\boldsymbol{\xi}|^2$$

for all $\boldsymbol{x}$ and $\boldsymbol{\xi}, \boldsymbol{\zeta} \in \mathbb{R}^d$, then with suitable boundary condition, one expects (8.24) to have a unique normalized solution.

Consider a Brownian particle that obeys (8.9). Its invariant distribution satisfies $\nabla \cdot \boldsymbol{j}_s(\boldsymbol{x}) = 0$, where the stationary flux $\boldsymbol{j}_s$ is defined in (8.18). In this case, we can look for the *equilibrium solution* that satisfies the stronger condition

(8.26) $$\boldsymbol{j}_s(\boldsymbol{x}) = 0.$$

This is the *detailed balance condition* in the continuous case, which implies that the chemical potential μ is constant. The solution is the well-known Gibbs distribution

(8.27) $$p_s(\boldsymbol{x}) = \frac{1}{Z} \exp\left(-\frac{U(\boldsymbol{x})}{k_B T}\right)$$

where Z is the normalization constant

(8.28) $$Z = \int_{\mathbb{R}^d} e^{-\frac{U(\boldsymbol{x})}{k_B T}} d\boldsymbol{x}.$$

As another example, consider the Ornstein-Uhlenbeck process (7.38). From the detailed balance condition $\boldsymbol{j}_s(\boldsymbol{x}) = 0$ we have

$$-\gamma x p_s(x) - \frac{1}{2}\sigma^2 \nabla p_s(x) = 0.$$

Thus the invariant PDF $p_s(x)$ has the form

$$p_s(x) = \frac{1}{Z}\exp\left(-\frac{\gamma x^2}{\sigma^2}\right) \sim N\left(0, \frac{\sigma^2}{2\gamma}\right),$$

which is exactly the result we obtained in (7.39).

Going back to the detailed balance condition, recall that detailed balance for the discrete time Markov chain takes the form $\mu_{s,i}p_{ij} = \mu_{s,j}p_{ji}$ where $\boldsymbol{\mu}_s$ is the invariant distribution. This is equivalent to the condition $J_{ij} = 0$, i.e., the net current on each edge vanishes. This is obviously stronger than the condition for invariance which requires only that the net current in and out of each node vanishes. Similarly in the continuous case, the equilibrium condition that the current $\boldsymbol{j}_s$ vanishes is stronger than the invariance condition which requires only that the divergence of the current vanishes. Obviously there are systems for which the equilibrium condition is never satisfied.

Indeed, the detailed balance condition above is a specific form in a much more general setup [**Gar09**, **Ris89**]. First let us define a variable x to be odd or even if it should change the sign or not under the time reversal transformation. For example, the variable $\boldsymbol{x}$ is even for the dynamics $\dot{\boldsymbol{x}} = -\nabla U(\boldsymbol{x})$ since $\tilde{\boldsymbol{x}}(t) = \boldsymbol{x}(-t)$ simply preserves the time reversal symmetry. The variables $\boldsymbol{x}, \boldsymbol{v}$ are even and odd, respectively, for the dynamics

$$\dot{\boldsymbol{x}} = \boldsymbol{v}, \quad \dot{\boldsymbol{v}} = -\nabla U(\boldsymbol{x})$$

since $(\tilde{\boldsymbol{x}}(t), \tilde{\boldsymbol{v}}(t)) = (\boldsymbol{x}(-t), -\boldsymbol{v}(-t))$ preserves the time reversal symmetry.

With the corresponding diagonal sign matrix $\boldsymbol{s}$, where $s_{ii} = 1$ or -1 according to whether x_i is an even or odd variable, the detailed balance condition requires that the stationary joint PDF $p_s(\boldsymbol{z}, t + s; \boldsymbol{x}, s)$ satisfies

(8.29) $p_s(\boldsymbol{z}, t + s; \boldsymbol{x}, s) = p_s(\boldsymbol{s}\boldsymbol{x}, t + s; \boldsymbol{s}\boldsymbol{z}, s)$ for all $s, t \geq 0$,

which is equivalent to

(8.30) $p_s(\boldsymbol{x}) = p_s(\boldsymbol{s}\boldsymbol{x}), \quad p(\boldsymbol{z}, t|\boldsymbol{x}, 0)p_s(\boldsymbol{x}) = p(\boldsymbol{s}\boldsymbol{x}, t|\boldsymbol{s}\boldsymbol{z}, 0)p_s(\boldsymbol{z}).$

Specifically for the SDEs

(8.31) $d\boldsymbol{Y}_t = \boldsymbol{b}(\boldsymbol{Y}_t)dt + \boldsymbol{\sigma}(\boldsymbol{Y}_t)d\boldsymbol{W}_t,$

it can be shown (Exercise 8.6) that the condition (8.30) is equivalent to

(8.32)
        (i) $\boldsymbol{s} \cdot \boldsymbol{b}(\boldsymbol{s}\boldsymbol{y})p_s(\boldsymbol{y}) = -\boldsymbol{b}(\boldsymbol{y})p_s(\boldsymbol{y}) + \nabla \cdot (\boldsymbol{A}(\boldsymbol{y})p_s(\boldsymbol{y})),$
        (ii) $\boldsymbol{s} \cdot \boldsymbol{A}(\boldsymbol{s}\boldsymbol{y}) = \boldsymbol{A}(\boldsymbol{y}) \cdot \boldsymbol{s}.$

When all the variables are of even type, i.e., $\boldsymbol{s} = \boldsymbol{I}$, the condition (ii) is trivial and (i) gives exactly the detailed balance condition (8.26). This general detailed balance condition is useful when we consider the invariant distribution of the Langevin process (7.41). We have

(8.33)
$$\boldsymbol{y} = \left(\begin{array}{c} \boldsymbol{x} \\ \boldsymbol{v} \end{array} \right), \quad \boldsymbol{b} = \left(\begin{array}{c} \boldsymbol{v} \\ -\frac{\gamma}{m}\boldsymbol{v} - \frac{1}{m}\nabla U \end{array} \right), \quad \boldsymbol{A}(\boldsymbol{y}) = \left(\begin{array}{cc} 0 & 0 \\ 0 & \frac{2k_B T\gamma}{m^2}\boldsymbol{I} \end{array} \right).$$

In this case $\boldsymbol{x}$ is even and $\boldsymbol{v}$ is odd, so we set

$$\boldsymbol{s} = \left(\begin{array}{cc} \boldsymbol{I} & 0 \\ 0 & -\boldsymbol{I} \end{array} \right).$$

With this setup, the condition (ii) is trivial again and (i) gives

$$\frac{1}{p_s(\boldsymbol{y})}\nabla_{\boldsymbol{v}} p_s(\boldsymbol{y}) = -\frac{m\boldsymbol{v}}{k_B T}.$$

Thus

(8.34)
$$p_s(\boldsymbol{y}) = \frac{1}{Z_v}\exp\left(-\frac{m\boldsymbol{v}^2}{2k_B T}\right)f(\boldsymbol{x}).$$

Substituting (8.34) into the steady state equation $\nabla \cdot \boldsymbol{j}_s = 0$, we obtain

$$f(\boldsymbol{x}) = \frac{1}{Z_x}\exp\left(-\frac{U(\boldsymbol{x})}{k_B T}\right).$$

To summarize, the invariant distribution of the Langevin equation (7.41) satisfying the detailed balance condition has the nice form

$$p_s(\boldsymbol{y}) = \frac{1}{Z}\exp\left(-\frac{H(\boldsymbol{x}, \boldsymbol{v})}{k_B T}\right),$$

where $H(\boldsymbol{x}, \boldsymbol{v}) = m|\boldsymbol{v}|^2/2 + U(\boldsymbol{x})$.

Readers are referred to [**Gar09**, **Ris89**] for more discussions on the detailed balance condition.

8.5. The Markov Semigroup

The fact that we can use PDE methods to study the diffusion process originated from its Markovianity, which we will explore a bit further.

For simplicity, we will limit ourselves in this section to time-homogeneous SDEs

(8.35)
$$d\boldsymbol{X}_t = \boldsymbol{b}(\boldsymbol{X}_t)dt + \boldsymbol{\sigma}(\boldsymbol{X}_t)d\boldsymbol{W}_t,$$

where $\boldsymbol{b}$ and $\boldsymbol{\sigma}$ are independent of time t. In this case the transition kernel $p(\cdot, t | \boldsymbol{y}, s)$ is homogeneous in time; i.e.,

$$p(B, t+s | \boldsymbol{y}, s) = p(B, t | \boldsymbol{y}, 0) = p(t, \boldsymbol{y}, B), \quad s, t \geq 0,$$

for $\boldsymbol{y} \in \mathbb{R}^d$ and $B \in \mathcal{R}^d$, where we employ the notation (5.3). Correspondingly we have

$$\mathbb{E}^{\boldsymbol{x}}\mathbb{E}^{\boldsymbol{X}_s}f(\boldsymbol{X}_t) = \mathbb{E}^{\boldsymbol{x}}\Big(\mathbb{E}^{\boldsymbol{x}}\left(f(\boldsymbol{X}_{t+s})|\mathcal{F}_s\right)\Big) = \mathbb{E}^{\boldsymbol{x}}f(\boldsymbol{X}_{t+s})$$

for any bounded measurable function f [**Oks98**, **Fri75a**].

Under the condition that $\boldsymbol{b}$ and $\boldsymbol{\sigma}$ are bounded and Lipschitz, one can further show that the associated Markov semigroup $T_t : C_0(\mathbb{R}^d) \to C_0(\mathbb{R}^d)$ is strongly continuous (Theorem 18.11 in [**Kal97**]) in the sense that

$$\lim_{t \to 0+} \|T_t f - f\|_\infty = 0 \quad \text{for any } f \in C_0(\mathbb{R}^d).$$

Here T_t is called the *Feller semigroup*. With this setup, we can use tools from semigroup theory to study T_t [**Yos95**]. We thus define the infinitesimal generator $\mathcal{A}$ of T_t by

$$\mathcal{A}f(\boldsymbol{x}) = \lim_{t \to 0+} \frac{\mathbb{E}^{\boldsymbol{x}}f(\boldsymbol{X}_t) - f(\boldsymbol{x})}{t},$$

where $f \in D(\mathcal{A}) := \{f \in C_0(\mathbb{R}^d) \text{ such that the limit exists}\}$. For $f \in C_c^2(\mathbb{R}^d) \subset D(\mathcal{A})$ we have

$$\mathcal{A}f(\boldsymbol{x}) = \mathcal{L}f(\boldsymbol{x}) = \boldsymbol{b}(\boldsymbol{x}) \cdot \nabla f(\boldsymbol{x}) + \frac{1}{2}(\boldsymbol{\sigma}\boldsymbol{\sigma}^T) : \nabla^2 f(\boldsymbol{x})$$

from Itô's formula (8.4).

Theorem 8.5. *The function $u(\boldsymbol{x}, t) = \mathbb{E}^{\boldsymbol{x}}f(\boldsymbol{X}_t)$ satisfies the Kolmogorov backward equation for $f \in C_c^2(\mathbb{R}^d)$; i.e.,*

(8.36)
$$\partial_t u = \mathcal{A}u(\boldsymbol{x}), \quad u|_{t=0} = f(\boldsymbol{x}).$$

Proof. Observe that $u(\boldsymbol{x}, t)$ is differentiable with respect to t, as a result of Ito's formula and the condition $f \in C_c^2(\mathbb{R}^d)$. For any fixed $t > 0$, define $g(\boldsymbol{x}) = u(\boldsymbol{x}, t)$. Then we have

$$
\begin{aligned}
\mathcal{A}g(\boldsymbol{x}) &= \lim_{s \to 0+} \frac{1}{s}\Big(\mathbb{E}^{\boldsymbol{x}}g(\boldsymbol{X}_s) - g(\boldsymbol{x})\Big) \\
&= \lim_{s \to 0+} \frac{1}{s}\Big(\mathbb{E}^{\boldsymbol{x}}\mathbb{E}^{\boldsymbol{X}_s}f(\boldsymbol{X}_t) - \mathbb{E}^{\boldsymbol{x}}f(\boldsymbol{X}_t)\Big) \\
&= \lim_{s \to 0+} \frac{1}{s}\Big(\mathbb{E}^{\boldsymbol{x}}f(\boldsymbol{X}_{t+s}) - \mathbb{E}^{\boldsymbol{x}}f(\boldsymbol{X}_t)\Big) \\
&= \lim_{s \to 0+} \frac{1}{s}(u(\boldsymbol{x}, t + s) - u(\boldsymbol{x}, t)) = \partial_t u(\boldsymbol{x}, t).
\end{aligned}
$$

This means $u(\cdot, t) \in D(\mathcal{A})$ and the proof is complete. $\qquad\square$

8.6. Feynman-Kac Formula

So far our viewpoint has been to use PDE methods to study the diffusion
process. The opposite is also true: One can study PDEs using probablistic
methods. The reason is that for some PDEs, their solutions can be rep-
resented explicitly using stochastic processes. A very nice example is the
Feynman-Kac formula.

Consider

$$(8.37) \qquad \partial_t v = \mathcal{L}v + qv, \quad v|_{t=0} = f(\boldsymbol{x}),$$

where $\mathcal{L}$ is the generator of a diffusion process $\{\boldsymbol{X}_t\}$ and q is some given
function, assumed to be smooth. Physically it may represent some potential
function. In the absence of the last term, we have

$$(8.38) \qquad v(\boldsymbol{x}, t) = \mathbb{E}^x(f(\boldsymbol{X}_t)).$$

This means that the solution of the problem (8.37) in the case when $q = 0$
can be represented as averages over diffusion processes. The Feynman-Kac
formula handles the situation when $q \neq 0$.

To motivate the formula, note that in the absence of the diffusion term,
the solution of the PDE

$$(8.39) \qquad \partial_t v = \boldsymbol{b} \cdot \nabla v + qv, \quad v|_{t=0} = f(\boldsymbol{x})$$

can be represented by the solution of the ODE

$$\frac{d\boldsymbol{X}_t}{dt} = \boldsymbol{b}(\boldsymbol{X}_t), \quad \boldsymbol{X}_0 = \boldsymbol{x},$$

using the method of characteristics [**Eva10**]:

$$(8.40) \qquad v(\boldsymbol{x}, t) = \exp\left(\int_0^t q(\boldsymbol{X}_s)ds\right) f(\boldsymbol{X}_t).$$

Theorem 8.6 (Feynman-Kac formula). *Let $f \in C_c^2(\mathbb{R}^d)$ and $q \in C(\mathbb{R}^d)$.
Assume that q is continuous and bounded. Then the solution of (8.37) is
given by*

$$(8.41) \qquad v(\boldsymbol{x}, t) = \mathbb{E}^x\left(\exp\left(\int_0^t q(\boldsymbol{X}_s)ds\right) f(\boldsymbol{X}_t)\right).$$

The proof goes as follows. Let $Y_t = f(\boldsymbol{X}_t)$, $Z_t = \exp(\int_0^t q(\boldsymbol{X}_s)ds)$ and define $v(\boldsymbol{x}, t) = \mathbb{E}^{\boldsymbol{x}}(Y_t Z_t)$. Here $v(\boldsymbol{x}, t)$ is differentiable with respect to t and

$$\frac{1}{s}\Big(\mathbb{E}^{\boldsymbol{x}}v(\boldsymbol{X}_s, t) - v(\boldsymbol{x}, t)\Big)$$

$$= \frac{1}{s}\Big(\mathbb{E}^{\boldsymbol{x}}\mathbb{E}^{\boldsymbol{X}_s}Z_t f(\boldsymbol{X}_t) - \mathbb{E}^{\boldsymbol{x}}Z_t f(\boldsymbol{X}_t)\Big)$$

$$= \frac{1}{s}\Big(\mathbb{E}^{\boldsymbol{x}}\exp\Big(\int_0^t q(\boldsymbol{X}_{r+s})dr\Big)f(\boldsymbol{X}_{t+s}) - \mathbb{E}^{\boldsymbol{x}}Z_t f(\boldsymbol{X}_t)\Big)$$

$$= \frac{1}{s}\mathbb{E}^{\boldsymbol{x}}\Big(\exp\Big(-\int_0^s q(\boldsymbol{X}_r)dr\Big)Z_{t+s}f(\boldsymbol{X}_{t+s}) - Z_t f(\boldsymbol{X}_t)\Big)$$

$$= \frac{1}{s}\mathbb{E}^{\boldsymbol{x}}\Big(Z_{t+s}f(\boldsymbol{X}_{t+s}) - Z_t f(\boldsymbol{X}_t)\Big)$$

$$+ \frac{1}{s}\mathbb{E}^{\boldsymbol{x}}\Big(Z_{t+s}f(\boldsymbol{X}_{t+s})\Big(\exp\Big(-\int_0^s q(\boldsymbol{X}_r)dr\Big) - 1\Big)\Big)$$

$$\to \partial_t v - q(\boldsymbol{x})v(\boldsymbol{x}, t) \quad \text{as } s \to 0.$$

The left-hand side is $\mathcal{A}v(\boldsymbol{x}, t)$ by definition.
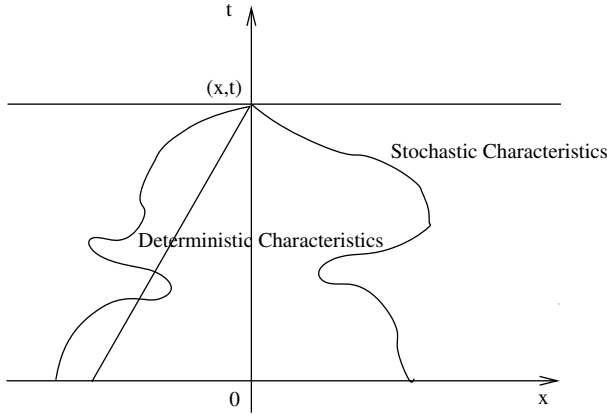
Figure 8.2. Schematics of the Feynman-Kac formula.

8.7. Boundary Value Problems

Next, we consider the boundary value problem for elliptic equations. We start with

$$(8.42) \qquad \mathcal{L}u = -g(\boldsymbol{x}) \text{ in } U, \quad u = f(\boldsymbol{x}) \text{ on } \partial U.$$

Here U is a smooth domain in $\mathbb{R}^d$. We will assume that the diffusion tensor $\boldsymbol{A}$ is nondegenerate in the sense of (8.25). Standard PDE theory tells us that under suitable conditions on U, this problem has a unique solution.

We need the following improved version of (7.12) in order to give a probabilistic interpretation of the solution of (8.42). In this version the fixed time T is replaced by a stopping time τ which satisfies some integrability condition.

Lemma 8.7 (Dynkin's formula). *Let $f \in C_c^2(\mathbb{R}^d)$. Suppose τ is a stopping time with $\mathbb{E}^{\boldsymbol{x}} \tau < \infty$. Then*

$$(8.43) \qquad \mathbb{E}^{\boldsymbol{x}} f(\boldsymbol{X}_\tau) = f(\boldsymbol{x}) + \mathbb{E}^{\boldsymbol{x}} \int_0^\tau \mathcal{A} u(\boldsymbol{X}_t) dt.$$

Theorem 8.8. *Assume that $U \subset \mathbb{R}^d$ is a bounded domain and the boundary ∂U is C^2. Assume also that $\boldsymbol{b}$ and $\boldsymbol{\sigma}$ satisfy the Lipschitz condition on $\bar{U}$. Then for $g \in C(\bar{U}), f \in C(\partial U)$, the solution of (8.42) can be represented as*

$$(8.44) \qquad u(\boldsymbol{x}) = \mathbb{E}^{\boldsymbol{x}} \Big(f(\boldsymbol{X}_{\tau_U}) + \int_0^{\tau_U} g(\boldsymbol{X}_t) dt \Big),$$

where τ_U is the first exit time from domain U:

$$(8.45) \qquad \tau_U := \inf_t \{ t \geq 0, \boldsymbol{X}_t \notin U \}.$$

$\boldsymbol{X}_{\tau_U}$ *is the first exit point.*

Proof. The proof of the fact that τ_U is a stopping time and that $\mathbb{E}^{\boldsymbol{x}} \tau_U < \infty$ is quite technical and can be found in [**KS91**, **Fri75a**].

Standard PDE theory tells us that $u \in C^2(U) \cap C(\bar{U})$. Applying Dynkin's formula, we get to $u(\boldsymbol{X}_t)$:

$$(8.46) \qquad \mathbb{E}^{\boldsymbol{x}} u(\boldsymbol{X}_{\tau_U}) - u(\boldsymbol{x}) = \mathbb{E}^{\boldsymbol{x}} \int_0^{\tau_U} \mathcal{A} u(\boldsymbol{X}_t) dt.$$

Thus

$$u(\boldsymbol{x}) = \mathbb{E}^{\boldsymbol{x}} \Big(u(\boldsymbol{X}_{\tau_U}) - \int_0^{\tau_U} \mathcal{A} u(\boldsymbol{X}_t) dt \Big) = \mathbb{E}^{\boldsymbol{x}} \Big(f(\boldsymbol{X}_{\tau_U}) + \int_0^{\tau_U} g(\boldsymbol{X}_t) dt \Big).$$

This gives the desired result. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \square$

A special case is when $\mathcal{L} u = \Delta u$ and $g = 0$, which gives $u(\boldsymbol{x}) = \mathbb{E}^{\boldsymbol{x}}(f(\boldsymbol{W}_{\tau_U}))$. This stochastic interpretation opens the door for Monte Carlo simulation of the solutions of PDEs. Moreover, in this special case, the spherical symmetry of the distribution of $\boldsymbol{W}$ implies an elegant simplification of the Monte Carlo implementations, the walk on sphere (WOS) algorithm, which was first proposed in [**Mul56**]. One interesting aspect of the stochastic methods is that it allows us to evaluate the solution at a single point $\boldsymbol{x}$ of interest without having to obtain the solution elsewhere.

Mean First Passage Time. As an application of the PDE approach, we study the mean first passage time problem in one dimension. Consider a diffusion process $\{X_t\}$ in the domain $U = (a, b)$ with reflecting and absorbing boundary conditions at a and b, respectively. Denote the first passage time to b by

$$\tau_b := \inf\{t \geq 0 : X_t = b\}$$

and the mean first passage time starting from x by

$$\tau(x) = \mathbb{E}^x \tau_b.$$

Assume that $x \in [a, b]$. The probability of remaining in $[a, b]$ at time t is given by

$$R(x, t) = \mathbb{P}^x(X_t \in [a, b)) = \int_a^b p(y, t|x, 0) dy = \mathbb{P}^x(\tau_b \geq t).$$

We have

$$(8.47) \qquad \tau(x) = \mathbb{E}^x \tau_b = -\int_0^\infty t \partial_t R(x, t) dt = \int_0^\infty R(x, t) dt$$

under the assumption that $tR(x, t) \to 0$ as $t \to \infty$. Applying $\mathcal{L}$ to both sides of (8.47) we get

$$\mathcal{L}\tau(x) = \int_0^\infty \mathcal{L}R(x, t) dt = \int_0^\infty \int_a^b \partial_t p(y, t|x, 0) dy dt$$

$$(8.48) \qquad = \int_a^b p|_{t=\infty} - p|_{t=0} dy = -\int_a^b \delta(x - y) dy = -1.$$

From the boundary conditions for the backward equation, we have $R(x, t)|_{x=b} = 0$ and $\partial_x R(x, t)|_{x=a} = 0$, which implies the boundary conditions for $\tau(x)$:

$$(8.49) \qquad \partial_x \tau(x)|_{x=a} = 0, \quad \tau(x)|_{x=b} = 0.$$

The study of the first passage time problem is then turned into a simple PDE problem.

8.8. Spectral Theory

When the condition of detailed balance is satisfied, the spectral theory for the operators $\mathcal{L}$ and $\mathcal{L}^*$ takes a very elegant form very similar to the case of discrete time Markov chains. To illustrate this, we consider the example of Brownian dynamics with periodic boundary condition on $[0, 1]^d$, i.e., the PDF $p(\boldsymbol{x} + L\boldsymbol{e}_i, t) = p(\boldsymbol{x}, t)$ for any $\boldsymbol{x} \in [0, 1]^d$ and $i \in \{1, 2, \ldots, d\}$. We will take $\gamma = D = 1$ for simplicity. The operators are then given by
$$(8.50)$$
$$\mathcal{L}f(\boldsymbol{x}) = -\nabla U(\boldsymbol{x}) \cdot \nabla f(\boldsymbol{x}) + \Delta f(\boldsymbol{x}), \quad \mathcal{L}^* f(\boldsymbol{x}) = \nabla \cdot (\nabla U(\boldsymbol{x}) f(\boldsymbol{x})) + \Delta f(\boldsymbol{x}).$$

In analogy with Section 3.10, we define a Hilbert space L^2_μ with the invariant distribution $\mu = Z^{-1} \exp(-U(\boldsymbol{x}))$ as the weight function. The inner product and the norm are defined by

$$(f,g)_\mu = \int_{[0,1]^d} f(\boldsymbol{x}) g(\boldsymbol{x}) \mu(\boldsymbol{x}) d\boldsymbol{x} \quad \text{and} \quad \|f\|^2_\mu = (f,f)_\mu.$$

The operator $\mathcal{L}$ is selfadjoint in L^2_μ. This can be seen as follows. First note that

$$(8.51) \quad \mathcal{L}^*(g\mu) = \nabla \cdot (\nabla U \mu) g + \nabla U \cdot \nabla g \mu + \Big[\Delta g \mu + \Delta \mu g + 2 \nabla g \cdot \nabla \mu \Big] = \mu \mathcal{L} g,$$

$$(8.52) \quad (\mathcal{L}f, g)_\mu = \int \mathcal{L}f(\boldsymbol{x}) g(\boldsymbol{x}) \mu(\boldsymbol{x}) d\boldsymbol{x} = \int f(\boldsymbol{x}) \mathcal{L}^*(g\mu) d\boldsymbol{x} = (f, \mathcal{L}g)_\mu.$$

In addition, $-\mathcal{L}$ is positive definite:

$$\begin{aligned} (-\mathcal{L}f, f)_\mu &= -\int \Big(-\nabla U \cdot \nabla f f \mu - \nabla f \cdot \nabla f \mu - \nabla f \cdot \nabla \mu f \Big) d\boldsymbol{x} \\ &= \|\nabla f\|^2_\mu \ge 0. \end{aligned}$$

Hence we conclude that the eigenvalues of $\mathcal{L}$ and $\mathcal{L}^*$ are real and nonpositive. Denote by ϕ_λ the eigenfunctions of $\mathcal{L}$ with eigenvalue λ, with the normalization

$$(\phi_\lambda(\boldsymbol{x}), \phi_{\lambda'}(\boldsymbol{x}))_\mu = \delta_{\lambda\lambda'}.$$

We immediately see that the eigenfunctions of $\mathcal{L}^*$ can be chosen as

$$(8.53) \qquad\qquad \psi_\lambda(\boldsymbol{x}) = \mu(\boldsymbol{x}) \phi_\lambda(\boldsymbol{x})$$

because of (8.51). We also have as a consequence that $(\phi_\lambda, \psi_{\lambda'}) = \delta_{\lambda\lambda'}$.

In the case of the discrete Markov chain with detailed balance, there is a simple way to symmetrize the generator. Let $\boldsymbol{P}$ be the transition probability matrix, let $\boldsymbol{\mu} = (\mu_1, \mu_2, \cdots, \mu_n)$ be the invariant distribution, and let $\boldsymbol{D} = \text{diag}(\mu_1, \mu_2, \ldots, \mu_n)$. Then

$$(8.54) \qquad\qquad\qquad \boldsymbol{D}\boldsymbol{P} = \boldsymbol{P}^T \boldsymbol{D}.$$

Thus we can define the symmetrization of $\boldsymbol{P}$ by

$$(8.55) \qquad\qquad \boldsymbol{D}^{\frac{1}{2}} \boldsymbol{P} \boldsymbol{D}^{-\frac{1}{2}} = \boldsymbol{D}^{-\frac{1}{2}} \boldsymbol{P}^T \boldsymbol{D}^{\frac{1}{2}}.$$

In the same way, let

$$(8.56) \qquad\qquad\qquad \Delta_U = e^{-U/2} \mathcal{L} e^{U/2}.$$

A direction calculation gives

$$(8.57) \qquad\qquad \Delta_U = e^{U/2} \mathcal{L}^* e^{-U/2} = \Delta - \frac{1}{4} |\nabla U|^2 + \frac{1}{2} \Delta U.$$

This operator is sometimes called the *Witten Laplacian*. It is formally self-adjoint under the usual L^2 inner product. In physics, it is the Hamiltonian operator of a quantum particle with the potential

$$(8.58) \qquad V = \frac{1}{4}|\nabla U|^2 - \frac{1}{2}\Delta U.$$

This establishes a connection between diffusion and quantum mechanics. This connection can be exploited to study, for example, thermal activation and quantum tunneling.

8.9. Asymptotic Analysis of SDEs

As an example of the application of PDE methods to the study of diffusion processes, we discuss briefly some results on asymptotic analysis. For SDEs or ODEs, the presence of a small parameter usually means that the system has some disparate time scales. One interesting issue is to eliminate the fast time scales in the system and derive effective equations that govern the dynamics on the slow time scale.

We start with a simple example, the *random telegraph process*. Let $Y_t = y(t)$ be a stationary two-state Markov jump process taking values $\pm\alpha$ with jump rate β between these two states. With matrix notation, the infinitesimal generator for Y has the form

$$\mathcal{A} = \begin{pmatrix} -\beta & \beta \\ \beta & -\beta \end{pmatrix}.$$

Let $y^\epsilon(t) = y(t/\epsilon^2)$ where ϵ is a small parameter. Consider the SDE

$$(8.59) \qquad \frac{dx^\epsilon(t)}{dt} = \frac{1}{\epsilon}y^\epsilon(t), \quad x^\epsilon(0) = x.$$

Let

$$u^\epsilon(x, y, t) = \mathbb{E}^{(x,y)}(f(x^\epsilon(t), y^\epsilon(t))),$$

where f is any given smooth function. Then u^ϵ satisfies the backward Kolmoogorov equation:

$$(8.60) \qquad \frac{\partial u^\epsilon}{\partial t} = \frac{1}{\epsilon}y\frac{\partial u^\epsilon}{\partial x} + \frac{1}{\epsilon^2}\mathcal{A}u^\epsilon, \quad u^\epsilon(x, y, 0) = f(x, y).$$

Since y can only take two values, by defining

$$u_\pm(x, t) = u^\epsilon(x, \pm\alpha, t), \quad f_\pm(x, t) = f(x, \pm\alpha),$$

we can rewrite (8.60) as

$$\frac{\partial}{\partial t}\begin{pmatrix} u_+ \\ u_- \end{pmatrix} = \frac{1}{\epsilon}\begin{pmatrix} +\alpha & 0 \\ 0 & -\alpha \end{pmatrix}\frac{\partial}{\partial x}\begin{pmatrix} u_+ \\ u_- \end{pmatrix} + \frac{1}{\epsilon^2}\begin{pmatrix} -\beta & \beta \\ \beta & -\beta \end{pmatrix}\begin{pmatrix} u_+ \\ u_- \end{pmatrix}$$

with initial condition $u_\pm(x, 0) = f_\pm(x)$.

Let $w = u_+ + u_-$. We have

$$\epsilon^2 \frac{\partial^2 w}{\partial t^2} = \alpha^2 \frac{\partial^2 w}{\partial x^2} - 2\beta \frac{\partial w}{\partial t}, \quad w|_{t=0} = f_+ + f_-, \ \partial_t w|_{t=0} = \frac{\alpha}{\epsilon} \partial_x (f_+ - f_-).$$

Consider the case when $f_+ = f_- = f$. In this case the time derivative of w vanishes at $t = 0$; hence we avoid the extra complication coming from the initial layer. Following the standard approach in asymptotic analysis, we make the ansatz

$$w = w_0 + \epsilon w_1 + \epsilon^2 w_2 + \cdots.$$

To leading order, this gives

(8.61) $$\frac{\partial w_0}{\partial t} = \frac{\alpha^2}{2\beta} \frac{\partial^2 w_0}{\partial x^2}, \quad w_0|_{t=0} = 2f.$$

This means that to leading order, x^ϵ behaves like Brownian motion with diffusion constant $D = \alpha/\sqrt{\beta}$. This is not surprising since it is what the central limit theorem tells us for the process

$$\tilde{x}^\epsilon(t) = \frac{1}{\epsilon} \int_0^t y^\epsilon(s) ds \quad \text{as } \epsilon \to 0.$$

We turn now to the general case. Suppose that the backward equation for the stochastic process $\{\boldsymbol{X}_t^\epsilon\}$ has the form

(8.62) $$\frac{\partial u^\epsilon}{\partial t} = \frac{1}{\epsilon^2} \mathcal{L}_1 u^\epsilon + \frac{1}{\epsilon} \mathcal{L}_2 u^\epsilon + \mathcal{L}_3 u^\epsilon, \quad u^\epsilon(0) = f,$$

where $\mathcal{L}_1, \mathcal{L}_2,$ and $\mathcal{L}_3$ are differential operators defined on some Banach space $\mathscr{B}$, whose properties will be specified below. We would like to study the asymptotic behavior of u^ϵ when $\epsilon \to 0$ for $0 \le t \le T, T < \infty$. This discussion follows the work of Khasminski, Kurtz, Papanicolaou, etc. [**Pap77**].

As a general framework we assume that the following conditions hold.

(a) $\mathcal{L}_1$ is an infinitesimal generator of a stationary Markov process, and the semigroup $\exp(\mathcal{L}_1 t)$ generated by $\mathcal{L}_1$ converges to a projection operator to the null space of $\mathcal{L}_1$, which we will denote as $\mathcal{P}$:

$$\exp(\mathcal{L}_1 t) \to \mathcal{P}, \quad t \to \infty.$$

The reason and meaning for this will become clear later.

(b) Solvability condition: $\mathcal{P}\mathcal{L}_2\mathcal{P} = 0$.

(c) Consistency condition for the initial value: $\mathcal{P}f = f$. This allows us to avoid the initial layer problem.

Note that the following holds:

(8.63) $$\text{Range}(\mathcal{P}) = \text{Null}(\mathcal{L}_1), \quad \text{Null}(\mathcal{P}) = \overline{\text{Range}(\mathcal{L}_1)}.$$

But $\mathcal{P}$ does not need to be an orthogonal projection since generally $\mathcal{P}^* \ne \mathcal{P}$ (see Exercise 8.13 for more details).

Assume that u^ϵ can be expressed in the following form:

$$u^\epsilon = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \cdots .$$

Substituting it into (8.62) and collecting terms of the same order in ϵ, we get

(8.64) $\qquad O(\epsilon^{-2}): \quad \mathcal{L}_1 u_0 = 0,$

(8.65) $\qquad O(\epsilon^{-1}): \quad \mathcal{L}_1 u_1 = -\mathcal{L}_2 u_0,$

(8.66) $\qquad O(\epsilon^0): \quad \mathcal{L}_1 u_2 = -\mathcal{L}_2 u_1 - \mathcal{L}_3 u_0 + \dfrac{\partial u_0}{\partial t},$

$$\ldots$$

and $u_0(0) = f$ from the initial condition.

From (8.64) and (8.63), we obtain that u_0 is in the null space of $\mathcal{L}_1$, which is the same as the range of $\mathcal{P}$; i.e.,

(8.67) $$\mathcal{P} u_0 = u_0.$$

Note that at $t = 0$, we have $\mathcal{P} f = f$.

To solve u_1 from (8.65), we assume that the *Fredholm alternative* holds for the operator $\mathcal{L}_1$. This should be examined for each concrete problem [**Eva10**]. The Fredholm alternative states that (8.65) has a solution if $\langle g, \mathcal{L}_2 u_0 \rangle = 0$ for any $g \in \mathrm{Null}(\mathcal{L}_1^*) \subset \mathscr{B}^*$. This is true since $g \in \mathrm{Null}(\mathcal{L}_1^*)$ implies that

$$g \in {}^\perp\overline{\mathrm{Range}(\mathcal{L}_1)} = {}^\perp\mathrm{Null}(\mathcal{P});$$

thus $\langle g, \mathcal{L}_2 u_0 \rangle = 0$ by (8.67) and the solvability condition (b). Here $g \in {}^\perp\overline{\mathrm{Range}(\mathcal{L}_1)}$ or ${}^\perp\mathrm{Null}(\mathcal{P})$ means that for any $h \in \overline{\mathrm{Range}(\mathcal{L}_1)}$ or $\mathrm{Null}(\mathcal{P})$, we have $\langle g, h \rangle = 0$.

Let

(8.68) $$u_1 = -\mathcal{L}_1^{-1} \mathcal{L}_2 \mathcal{P} u_0$$

be a solution of (8.65). Substituting this into (8.66) and applying $\mathcal{P}$ on both sides, we obtain

(8.69) $$\frac{\partial u_0}{\partial t} = (\mathcal{P}\mathcal{L}_3\mathcal{P} - \mathcal{P}\mathcal{L}_2\mathcal{L}_1^{-1}\mathcal{L}_2\mathcal{P}) u_0 := \bar{\mathcal{L}} u_0, \quad u_0(0) = f.$$

This is the effective equation for the leading order u_0 in the range of $\mathcal{P}$. It is important to note that although (8.65) might have multiple solutions, the solvability condition ensures that the choice of the solution of (8.68) does not affect the final reduced system (8.69). One can also derive effective equations for the higher-order terms u_1, u_2, etc. But it is more complicated and usually not very useful.

To see how this abstract framework actually works, we use it for the simple model introduced at the beginning of this section. We have

$$\mathcal{L}_1 = \mathcal{A}, \quad \mathcal{L}_2 = \begin{pmatrix} +\alpha & 0 \\ 0 & -\alpha \end{pmatrix} \frac{\partial}{\partial x}, \quad \mathcal{L}_3 = 0.$$

Thus the projection operator $\mathcal{P}$ is given by

$$\mathcal{P} = \lim_{t \to \infty} \exp(\mathcal{L}_1 t) = \lim_{t \to \infty} \frac{1}{2} \begin{pmatrix} 1 + e^{-2\beta t} & 1 - e^{-2\beta t} \\ 1 - e^{-2\beta t} & 1 + e^{-2\beta t} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

In the current example, we can simply pick a version of $\mathcal{L}_1^{-1}$ as

$$\mathcal{L}_1^{-1} = -\int_0^\infty (\exp(\mathcal{L}_1 t) - \mathcal{P}) dt = -\frac{1}{4\beta} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

It is easy to verify that the solvability condition $\mathcal{P}\mathcal{L}_2\mathcal{P} = 0$ is satisfied. The consistency condition $\mathcal{P}f = f$ gives $f_+ = f_-$, which we still denote as f. Finally the effective operator is given by

$$-\mathcal{P}\mathcal{L}_2\mathcal{L}_1^{-1}\mathcal{L}_2\mathcal{P} = \frac{\alpha^2}{4\beta} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \frac{\partial^2}{\partial x^2}.$$

Combining these, we obtain the effective equation

$$\frac{\partial}{\partial t}(u_0^+ + u_0^-) = \frac{\alpha^2}{2\beta} \frac{\partial^2}{\partial x^2}(u_0^+ + u_0^-), \quad (u_0^+ + u_0^-)|_{t=0} = f_+ + f_- = 2f,$$

where $u_0 = (u_0^+, u_0^-)$. Set $w_0 = u_0^+ + u_0^-$; we recover (8.61).

Other interesting applications can be found in [**ELVE05a**, **ELVE07**, **Pap77**] and the references therein.

8.10. Weak Convergence

As another application of PDE methods to the study of the diffusion process, we analyze the weak convergence properties of the numerical schemes for SDEs presented in the last chapter. We will focus on the Euler-Maruyama scheme and consider only scalar equations. We will also assume $\sigma = 1$ for simplicity. The argument that we will present applies to much more general situations.

Given some smooth function f, let

$$(8.70) \qquad\qquad e_n = \mathbb{E}f(X_n) - \mathbb{E}f(X_{t_n}).$$

Theorem 7.20 tells us that the Euler-Maruyama scheme is of weak order 1. We will give an elementary proof of this statement. Before doing so, let us try to see this intuitively.

Let $X_0 = x$. Consider the weak form of the Itô-Taylor expansion

$$(8.71) \qquad \mathbb{E}^x f(X_h) = f(x) + \int_0^h \mathcal{L}f(X_t)dt = \sum_{n=0} \frac{\mathcal{L}^n f(x)}{n!} h^n,$$

where $\mathcal{L}$ is the infinitesimal generator of $\{X_t\}$ and $h = \delta t$ is the time stepsize. For the numerical solution X_t^N, we have

$$(8.72) \qquad \mathbb{E}^x f(X_h^N) = f(x) + \int_0^h \mathcal{L}_N f(X_t^N)dt = \sum_{n=0} \frac{\mathcal{L}_N^n f(x)}{n!} h^n,$$

where $\mathcal{L}_N$ is the infinitesimal generator of the discretized process $\{X_t^N\}$ (see below construction). Here the Taylor series is a formal expansion, which does not mean it is convergent.

To analyze the global error, one needs to estimate first the local truncation error. Consider

$$(8.73) \qquad dX_t = b(X_t)dt + dW_t.$$

The Euler-Maruyama scheme reads

$$(8.74) \qquad X_{n+1} = X_n + b(X_n)\Delta t + \Delta W_n.$$

Define a continuous extension of the numerical solution by

$$dX_t^N = b(X_n)dt + dW_t, \quad t \in [t_n, t_{n+1}).$$

We have

$$\mathcal{L}f(y) = b(y)f'(y) + \frac{1}{2}f''(y)$$

$$\mathcal{L}^2 f(y) = b(y)\left(b(y)f'(y) + \frac{1}{2}f''(y)\right) + \frac{1}{2}\left(b(y)f'(y) + \frac{1}{2}f''(y)\right)''.$$

$$\mathcal{L}_N f(y) = b(x)f'(y) + \frac{1}{2}f''(y)$$

and

$$\mathcal{L}_N^2 f(y) = b(x)\left(b(x)f'(y) + \frac{1}{2}f''(y)\right) + \frac{1}{2}\left(b(x)f'(y) + \frac{1}{2}f''(y)\right)'',$$

where x is the initial value. Now it is obvious that

$$(8.75) \qquad \mathbb{E}^x f(X_h^N) - \mathbb{E}^x f(X_h) = O(h^2).$$

Since the local truncation error is of second order, we expect the global error to be of weak order 1. In fact if one can bound the expansions in (8.71) and (8.72) up to a suitable order, the above formal derivations based on the local error analysis can be made rigorous.

It will become clear soon that the weak convergence analysis boils down to some estimates about the solution of the backward equation. Let us first consider the PDE

$$(8.76) \qquad \partial_t u(x,t) = \mathcal{L}u(x,t) = b(x)\partial_x u + \frac{1}{2}\partial_x^2 u, \quad u(x,0) = f(x).$$

Let $C_P^m(\mathbb{R}^d, \mathbb{R})$ be the space of functions $w \in C^m(\mathbb{R}^d, \mathbb{R})$ for which all partial derivatives up to order m have polynomial growth. More precisely, there exist a constant $K > 0$ and $m, p \in \mathbb{N}$ such that

$$|\partial_{\boldsymbol{x}}^{\boldsymbol{j}} w(\boldsymbol{x})| \leq K(1 + |\boldsymbol{x}|^{2p}), \quad \forall \, |\boldsymbol{j}| < m$$

for any $\boldsymbol{x} \in \mathbb{R}^d$, where $\boldsymbol{j}$ is a d-multi-index. Here we have $d = 1$ and we will simply denote $C_P^m(\mathbb{R}^d, \mathbb{R})$ as C_P^m.

The following important lemma can be found in [**KP92**, Theorem 4.8.6, p. 153].

Lemma 8.9. *Suppose that $f \in C_P^{2\beta}$ for some $\beta \in \{2, 3, \ldots\}$, $\boldsymbol{X}_t$ is time-homogeneous, and $b \in C_P^{2\beta}$ with uniformly bounded derivatives. Then $\partial u / \partial t$ is continuous and*

$$u(\cdot, t) \in C_P^{2\beta}, \quad t \leq T,$$

for any fixed $T < \infty$.

Theorem 8.10 (Weak convergence)**.** *Assume that b is Lipschitz and the conditions in Lemma* 8.9 *hold for b and f. Then the Euler-Maruyama scheme for* (8.73) *is of weak order* 1.

Proof. Define the backward operator

$$\tilde{\mathcal{L}} = \partial_t + b(x)\partial_x + \frac{1}{2}\partial_{xx},$$

and denote by v the solution of

$$(8.77) \qquad\qquad\qquad \tilde{\mathcal{L}}v = 0, \quad t \in (0, t_n)$$

with the final condition $v(x, t_n) = f(x)$. It is obvious that $v(x, t) = u(x, t_n - t)$, where u is the solution of (8.76).

Let $e_n = \mathbb{E}f(X_n) - \mathbb{E}f(X_{t_n})$. By Itô's formula we have

$$\mathbb{E}v(X_0, 0) = \mathbb{E}v(X_{t_n}, t_n) = \mathbb{E}f(X_{t_n}).$$

Hence

$$|e_n| = |\mathbb{E}f(X_n) - \mathbb{E}f(X_{t_n})| = |\mathbb{E}v(X_n, t_n) - \mathbb{E}v(X_0, 0)|$$

$$= \Big|\mathbb{E}\Big(\int_0^{t_n} \Big(\partial_t v(\bar{X}_s, s) + b(X_{n_s})\partial_x v(\bar{X}_s, s) + \frac{1}{2}\partial_{xx}v(\bar{X}_s, s) - \tilde{\mathcal{L}}v(\bar{X}_s, s)\Big)ds\Big)\Big|,$$

where $n_s := \{m|t_m \leq s < t_{m+1}\}$ and $\{\bar{X}_s\}$ is the continuous extension of $\{X_n\}$ defined by

(8.78) $$d\bar{X}_s = b(X_{n_s})ds + dW_s, \quad x \in [t_m, t_{m+1}).$$

With this definition, we obtain

$$|e_n| = \Big|\mathbb{E}\Big(\int_0^{t_n} \big(b(X_{n_s})\partial_x v(\bar{X}_s, s) - b(\bar{X}_s)\partial_x v(s, \bar{X}_s)\big)ds\Big)\Big|$$

$$\leq \Big|\mathbb{E}\Big(\int_0^{t_n} \big(b(X_{n_s})\partial_x v(X_{n_s}, t_{n_s}) - b(\bar{X}_s)\partial_x v(\bar{X}_s, s)\big)ds\Big)\Big|$$

$$+ \Big|\mathbb{E}\Big(\int_0^{t_n} b(X_{n_s})\big(\partial_x v(\bar{X}_s, s) - \partial_x v(X_{n_s}, t_{n_s})\big)ds\Big)\Big|$$

$$= \Big|\mathbb{E}\sum_m \int_{t_m}^{t_{m+1}} \Big(b(X_m)\partial_x v(X_m, t_m) - b(\bar{X}_s)\partial_x v(\bar{X}_s, s)\Big)ds\Big|$$

(8.79) $$+ \Big|\mathbb{E}\sum_m \int_{t_m}^{t_{m+1}} b(X_m)\big(\partial_x v(\bar{X}_s, s) - \partial_x v(X_m, t_m)\big)ds\Big|.$$

Using Itô's formula again, we have for any function $g(x, t)$

$$g(\bar{X}_t, t) - g(X_m, t_m) = \int_{t_m}^t \Big[\partial_t g(\bar{X}_s, s) + b(X_m)\partial_x g(\bar{X}_s, s) + \frac{1}{2}\partial_{xx}g(\bar{X}_s, s)\Big]ds$$

$$+ \int_{t_m}^t \partial_x g(\bar{X}_s, s)dW_s, \quad t \in [t_m, t_{m+1}).$$

Using this with $g = b\partial_x v$ and $g = \partial_x v$ in (8.79), we have the highest derivatives $\partial_{xxx}v, \partial_{xx}b \in C_P^{2\beta}$ as long as $\beta \geq 2$. Notice that, conditional on X_m, $b(X_m)$ is independent of $\int_{t_m}^t \partial_x g(\bar{X}_s, s)dW_s$. Together with the fact that $\mathbb{E}|X_m|^{2r}$ and $\mathbb{E}|\bar{X}_t|^{2r} \leq C$ for any $r \in \mathbb{N}$ (Exercise 8.14), we get

$$|e_n| \leq C\sum_m \Delta t^2 \leq C\Delta t,$$

which is the desired estimate. $\qquad\square$

Example 8.11 (Weak approximation). For the SDE

$$dX_t = -\frac{1}{2}X_t dt + dW_t, \quad X_0 = 0,$$

we will compute $u = \mathbb{E}X_t^2|_{t=1}$ using the Euler-Maruyama scheme.

The exact solution of u is

$$u = \mathbb{E}X_t^2|_{t=1} = 1 - e^{-1} \approx 0.632.$$

In order to compute the expectation numerically, we take the Euler-Maruyama scheme with stepsize $\Delta t = 1/M$; i.e.,

$$X_{n+1,k} = \left(1 - \frac{\Delta t}{2}\right)X_{n,k} + \sqrt{\Delta t} \cdot R_{n,k}, \; X_{0,k} = 0, \quad n = 0, 1, \ldots, M-1$$

for N independent realizations, where $k = 1, 2, \ldots, N$ and $R_{n,k}$ are i.i.d. $N(0,1)$ random variables. The approximate solution is given by

$$u_{N,\Delta t} = \frac{1}{N}\sum_{k=1}^{N}(X_{M,k})^2.$$

In the numerical experiment we take $\Delta t = 1/M = 0.1, 0.09, \ldots, 0.01$. We note that the final error

$$|u_{N,\Delta t} - u| \sim O\left(\Delta t + \frac{\sigma}{\sqrt{N}}\right),$$

where σ is the standard deviation of the random variable X_t^2 at $t = 1$. In our case, $\sigma = 1$. We take $N = 10^6$. Our smallest time stepsize is chosen as $\Delta t = 0.01$. The result is shown in Figure 8.3. We see that $|u_{N,\Delta t} - u| \approx 0.26\Delta t$. This is a numerical confirmation that the Euler-Maruyama scheme is of weak order 1 within the range of sampling error.
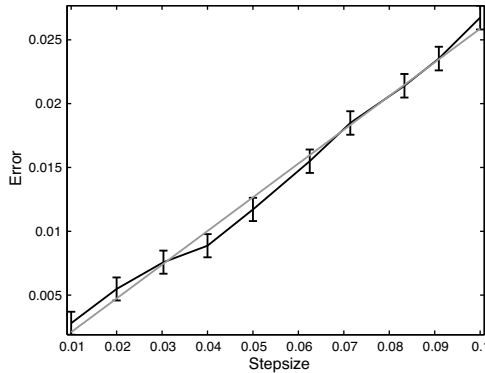
Figure 8.3. The weak approximation of SDEs by the Euler-Maruyama scheme. The thick solid line is a linear fitting according to the obtained error-stepsize data. The fitted slope is 0.26 and the intercept on the error-axis is 5×10^{-3}. The error bar is obtained from 10^6 samples for each timestep.

Exercises

8.1. Prove that $\boldsymbol{X}_t \in \mathbb{S}^{n-1}$ if $\boldsymbol{X}_0 \in \mathbb{S}^{n-1}$ for the process defined by (8.15).

8.2. Prove that the Fokker-Planck equation for the Brownian motion on $\mathbb{S}^2$ is given by (8.16). Prove that for Brownian motion on $\mathbb{S}^1$, the Fokker-Planck operator reduces to $d^2/d\theta^2$ if we use the parameterization: $(x, y) = (\cos\theta, \sin\theta)$, $\theta \in [0, 2\pi)$.

8.3. Derive the Fokker-Planck equation (8.13) for the Stratonovich SDEs.

8.4. Let X be the solution of the SDE

$$dX_t = a(t)X_t dt + \sigma(t) dW_t.$$

Find the PDF of X_t.

8.5. Prove that for the multidimensional OU process

$$d\boldsymbol{X}_t = \boldsymbol{B}\boldsymbol{X}_t dt + \boldsymbol{\sigma} d\boldsymbol{W}_t,$$

if the invariant distribution is a nondegenerate Gaussian with density $Z^{-1}\exp(-\boldsymbol{x}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{x}/2)$, then the detailed balance condition $\boldsymbol{j}_s(\boldsymbol{x}) = 0$ implies

$$\boldsymbol{B}\boldsymbol{\Sigma} = (\boldsymbol{B}\boldsymbol{\Sigma})^T.$$

8.6. Prove that the detailed balance condition (8.30) is equivalent to (8.32) when the diffusion process has the form (8.31).

8.7. Consider the one-dimensional OU process (7.38).
   (a) Find the eigenvalues and eigenfunctions of the Fokker-Planck operator.
   (b) Find the transition probability density.

8.8. Find the transition PDF of the linear Langevin equation

$$dX_t = V_t dt, \ dV_t = -X_t dt - \gamma V_t dt + \sqrt{2\gamma} dW_t$$

starting from the initial state $(X_t, V_t)|_{t=0} = (x_0, v_0)$.

8.9. Suppose that X_t satisfies the SDE

$$dX_t = b(X_t)dt + \sigma(X_t)dW_t,$$

where $b(x) = -a_0 - a_1 x$, $\sigma(x) = b_0 + b_1 x$, and $a_i, b_i \geq 0$ $(i = 0, 1)$.
   (a) Write down the partial differential equations for the PDF $p(x, t)$ of X_t when $X_0 = x_0$ and $u(x, t) = \mathbb{E}^x f(X_t)$. Specify their initial conditions.
   (b) Assume that X_0 is a random variable with PDF $p_0(x)$ that has finite moments. Derive a system of differential equations for the moments of X_t (i.e., the equations for $M_n(t) = \mathbb{E}X_t^n$).

8.10. Let X_t satisfy the SDE with drift $b(x) = 0$ and diffusion coefficient $\sigma(x) = 1$. Assume $X_t \in [0, 1]$ with reflecting boundary conditions and the initial state $X_t|_{t=0} = x_0 \in [0, 1]$.

  (a) Solve the initial-boundary value problem for the Fokker-Planck equation to calculate the transition PDF $p(x, t|x_0, 0)$.

  (b) Find the stationary distribution of the process X_t.

8.11. Derive the Fokker-Planck equation for the SDEs defined using the backward stochastic integral (see Exercise 7.11 for definition)

$$d\boldsymbol{X}_t = \boldsymbol{b}(\boldsymbol{X}, t)dt + \boldsymbol{\sigma}(\boldsymbol{X}_t, t) * d\boldsymbol{W}_t.$$

8.12. Prove that the operator $\mathcal{L}^*$ defined in (8.50) is selfadjoint and non-positive in the space $L^2_{\mu^{-1}}$ with inner product

$$(f, g)_{\mu^{-1}} = \int_{[0,1]^d} f(\boldsymbol{x})g(\boldsymbol{x})\mu^{-1}(\boldsymbol{x})d\boldsymbol{x}.$$

Its eigenfunctions $Q_\lambda(\boldsymbol{x})$ with normalization $(Q_\lambda, Q_{\lambda'})_{\mu^{-1}} = \delta_{\lambda\lambda'}$ satisfy the relation (8.53).

8.13. Consider a semigroup $\mathcal{S}(t)$ generated by $\mathcal{L}$ on a Banach space $\mathscr{B}$ that satisfies $\|\mathcal{S}(t)\| \leq 1$ and

$$\|\mathcal{S}(t)f - f\| \to 0 \text{ as } t \to 0, \text{ for all } f \in \mathscr{B}.$$

Assume $\mathcal{S}(t) \to \mathcal{P}$ as $t \to \infty$. Then we have:

  (a) $\mathcal{P}$ is a linear contraction on B and $\mathcal{P}^2 = \mathcal{P}$, a projection operator.

  (b) $\mathcal{S}(t)\mathcal{P} = \mathcal{P}\mathcal{S}(t) = \mathcal{P}$ for any $t \geq 0$.

  (c) Range$(\mathcal{P}) = \text{Null}(\mathcal{L})$.

  (d) Null$(\mathcal{P}) = \overline{\text{Range}(\mathcal{L})}$.

8.14. Prove that under the conditions in Theorem 8.10, for any $T > 0, r \in \mathbb{N}$, there exists a constant C such that the solution of the SDE (8.73) X_t, the numerical solution X_n, and the continuous extension $\bar{X}_t$ defined by (8.78) obey the estimates

$$\mathbb{E}|X_n|^{2r}, \ \mathbb{E}|X_t|^{2r}, \ \mathbb{E}|\bar{X}_t|^{2r} \leq C$$

for $t \leq T, \ n \leq T/\Delta T$.

Notes

The connection between PDE and SDE is one of the most exciting areas in stochastic analysis, with connections to potential theory [**Doo84**, **Szn98**], semigroup theory [**Fri75a**, **Fri75b**, **Tai04**], among other topics. Historically, the study of the distributions of diffusion processes was even earlier, and this motivated the study of stochastic differential equations [**Shi92**].

More on asymptotic analysis of SDEs can be found in [**Pap77**]. Other applications to multiscale problems, such as the averaging principle for SDEs or chemical reaction kinetics, the large volume limit, high frictional limit of Langevin equations, homogenizations, etc., can be found in [**E11**, **EK86**].

Part 2

Advanced Topics

Path Integral

One can think of diffusion processes as random variables. As such, their probability distributions are measures on some space of paths. Computing expectations is like performing integration on path space, i.e., the evaluation of path integrals. One can then use tools for integals, such as change of variables, the Laplace method for the asymptotic evaluation of integrals that involve small parameters, and integration by parts. This perspective is not only intuitive but has also motivated an important part of stochastic process theory including the Girsanov transformation, large deviation theory, the Feynman-Kac formula, etc. It is particularly popular in the physics community, due to the connection to Feynman's interpretation of quantum mechanics.

The difficulty, however, is that the integration has to be carried out in an infinite-dimensional space, the space of paths. There are essential obstacles for extending the results of integration in finite-dimensional space to infinite dimension. For one thing, there is no analog of Lebesgue measure on path spaces. Another problem that we often encounter is that many natural functionals are not integrable.

Another major advantage of the path integral approach is that it can be extended to random fields, i.e., random functions of more than one variable. One just has to consider measures on spaces of functions of more than one variable. As one can expect, the difficulties mentioned above become much more severe in higher dimensions. The subject of constructive quantum field theory is heavily concerned with overcoming these difficulties.

9.1. Formal Wiener Measure

Let us go back to the definition of the Wiener process, say on $[0,1]$. Let Ω be the space of continuous functions on $[0,1]$ that vanish at $t = 0$. We know that the joint distribution of $(W_{t_1}, W_{t_2}, \ldots, W_{t_n})$ is given by

$$(9.1) \qquad p_n(w_1, w_2, \ldots, w_n) = \frac{1}{Z_n} \exp(-I_n(w)),$$

where $0 < t_1 < t_2 < \cdots < t_n \leq 1$,

$$Z_n = (2\pi)^{\frac{n}{2}} \left[t_1(t_2 - t_1) \cdots (t_n - t_{n-1}) \right]^{\frac{1}{2}},$$

$$I_n(w) = \frac{1}{2} \sum_{j=1}^{n} \left(\frac{w_j - w_{j-1}}{t_j - t_{j-1}} \right)^2 (t_j - t_{j-1}), \quad t_0 := 0, w_0 := 0.$$

Formally, if we take the limit as $n \to \infty$, we obtain

$$(9.2) \qquad p_n dw_1 dw_2 \cdots dw_n \to \delta(w_0) Z^{-1} \exp(-I[w]) \mathcal{D}w,$$

where $\delta(w_0)$ means the initial state $W_0 = 0$. Here $\mathcal{D}w$ is shorthand notation for $\prod_{0 \leq t \leq 1} dw_t$, which is the formal analog of the Lebesgue measure on the path space $C[0,1]$. Here Z is the normalization factor. Also, $I[w]$, the *action functional* of the Wiener process, is defined as

$$I[w] = \frac{1}{2} \int_0^1 \dot{w}_t^2 dt.$$

For notation, we use the lowercase w_t to denote the dummy variable for the integration, keeping the uppercase W_t for the stochastic process.

The right-hand side of (9.2) is formally the product of a term that equals 0 and another that equals infinity. To see this, let us examine the situation when $t_j - t_{j-1} = 1/n, j = 1, 2, \ldots, n$. In this case

$$Z_n = (2\pi/n)^{\frac{n}{2}} \to 0.$$

At the same time we also have $\int_0^1 \dot{w}_t^2 dt = +\infty$ almost surely for Brownian paths. Hence the weight $\exp(-\int_0^1 \dot{w}_t^2 dt) = 0$. In addition, it is known from functional analysis that the infinite-dimensional analog of the Lebesgue measure $\mathcal{D}w$ does not really exist. This can be seen as follows. Assume to the contrary that there is such a measure $\mu(\cdot)$. As a Lebesgue measure, it should be translation invariant and finite for bounded sets. Let

$$B_n = B_{\frac{1}{2}}(e_n) = \{x | \|x - e_n\| \leq 1/2\}, \quad B = B_2(0) = \{x | \|x\| \leq 2\}.$$

We have

$$0 < \mu(B_1) = \mu(B_2) = \cdots = \mu(B_n) = \cdots < \infty, \quad 0 < \mu(B) < \infty.$$

However from the disjointness of $\{B_n\}$ and $B_n \subset B$ for any n, we obtain

$$\mu(B) \geq \sum_n \mu(B_n) = \infty,$$

which is a contradiction!

These facts explain why the path integral is often used as a formal tool. Nevertheless, the path integral is a very useful approach and in many important cases, things can be made rigorous.

Example 9.1. Compute the expectation

$$\mathbb{E} \exp\Big(-\frac{1}{2}\int_0^1 W_t^2 dt\Big).$$

We have seen in Chapter 6 that the answer is $\sqrt{2e/(1+e^2)}$ using the Karhunen-Loève expansion. Here we will use the path integral approach.

Step 1. Finite-dimensional approximation.

Assume that, as before, $\{t_j\}$ defines a subdivision of $[0,1]$:

$$\exp\left(-\frac{1}{2}\int_0^1 W_t^2 dt\right) \approx \exp\Big(-\frac{1}{2}\sum_{j=1}^n W_{t_j}^2 \delta t\Big) = \exp\Big(-\frac{1}{2}\delta t \boldsymbol{X}^T \boldsymbol{A} \boldsymbol{X}\Big),$$

where $\delta t = t_j - t_{j-1}$ for $j = 1, 2, \ldots, n$, $\boldsymbol{A} = \boldsymbol{I}$, and $\boldsymbol{X} = (W_{t_1}, W_{t_2}, \cdots, W_{t_n})^T$. Thus
(9.3)
$$\mathbb{E}\exp\Big(-\frac{1}{2}\int_0^1 W_t^2 dt\Big) \approx \int_{\mathbb{R}^n} \exp\Big(-\frac{1}{2}\delta t \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x}\Big) \cdot \frac{1}{Z_n} \exp\Big(-\frac{1}{2}\delta t \boldsymbol{x}^T \boldsymbol{B} \boldsymbol{x}\Big) d\boldsymbol{x},$$

where $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$, $Z_n = (2\pi)^{\frac{n}{2}}(\det(\delta t \boldsymbol{B})^{-1})^{\frac{1}{2}}$, and

(9.4)
$$\boldsymbol{B} = \frac{1}{\delta t^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -1 \end{pmatrix}.$$

From (9.3), we have

$$\mathbb{E}\exp\Big(-\frac{1}{2}\int_0^1 W_t^2 dt\Big) \approx \frac{(2\pi)^{\frac{n}{2}}(\det(\delta t(\boldsymbol{A}+\boldsymbol{B}))^{-1})^{\frac{1}{2}}}{(2\pi)^{\frac{n}{2}}(\det(\delta t \boldsymbol{B})^{-1})^{\frac{1}{2}}}$$

$$= \Big(\frac{\det(B)}{\det(\boldsymbol{A}+\boldsymbol{B})}\Big)^{\frac{1}{2}} = \Big(\frac{\prod_i \lambda_i^{\boldsymbol{B}}}{\prod_i \lambda_i^{\boldsymbol{A}+\boldsymbol{B}}}\Big)^{\frac{1}{2}},$$

where $\{\lambda_i^{\boldsymbol{B}}\}, \{\lambda_i^{\boldsymbol{A}+\boldsymbol{B}}\}$ are eigenvalues of $\boldsymbol{B}$ and $\boldsymbol{A}+\boldsymbol{B}$, respectively.

Step 2. Infinite-dimensional analog.

Formally, as we take the limit as $n \to +\infty$, the matrix $\boldsymbol{B}$ will converge to the differential operator $\mathcal{B} = d^2/dt^2$ with $u(0) = 1, u'(1) = 0$. In fact, the eigenvalue problem for the operator $\mathcal{B}$ can be expressed as

$$\frac{1}{\delta t^2}(u_{i+1} - 2u_i + u_{i-1}) = \lambda u_i, \quad i = 1, \ldots, n$$

with with the boundary conditions

$$u_0 = 0, \quad \frac{1}{\delta t}(u_{n+1} - u_n) = 0.$$

Define $\mathcal{A}$ to be the identity operator $\mathcal{I}$, which can also be regarded as the limit of the operators A. Then we have

$$\int_0^1 W_t^2 dt = (\mathcal{A}W_t, W_t).$$

We have formally

$$\mathbb{E}\exp\Big(-\frac{1}{2}\int_0^1 W_t^2 dt\Big)$$
$$= \int \exp\Big(-\frac{1}{2}(\mathcal{A}w_t, w_t)\Big) \cdot \frac{1}{Z}\exp\Big(-\frac{1}{2}(\mathcal{B}w_t, w_t)\Big)\delta(w_0)\mathcal{D}w$$

where the operator $\mathcal{B}u(t) := d^2u/dt^2$ and

$$Z = \int \exp\Big(-\frac{1}{2}(\mathcal{B}w_t, w_t)\Big)\delta(w_0)\mathcal{D}w.$$

Now compute formally the infinite-dimensional Gaussian integrals. We obtain

$$\mathbb{E}\exp\Big(-\frac{1}{2}\int_0^1 W_t^2 dt\Big) = \Big(\frac{\det \mathcal{B}}{\det(\mathcal{A} + \mathcal{B})}\Big)^{\frac{1}{2}},$$

where $\det \mathcal{B}$, $\det(\mathcal{A} + \mathcal{B})$ mean the products of all eigenvalues for the following boundary value problems:

$$\begin{cases} \mathcal{B}u = \lambda u, & \text{or} \quad (\mathcal{A} + \mathcal{B})u = \lambda u, \\ u(0) = 0, & u'(1) = 0. \end{cases}$$

Both determinants are infinite. But their ratio is well-defined. It is easy to check that by discretizing and taking the limit, one obtains the same result as before. In fact the eigenvalue problem for the operator $\mathcal{B}$ is the same as the eigenvalue problem considered in the Karhunen-Loève expansion (6.11).

Although it seems to be more complicated than before, this example illustrates the main steps involved in computing expectation values using the path integral approach.

9.2. Girsanov Transformation

We have seen that the Wiener measure over $C[0,1]$ can be formally expressed as

$$d\mu_W = \delta(w_0)Z^{-1}\exp\left(-\frac{1}{2}\int_0^1 \dot{w}_t^2 dt\right)\mathcal{D}w.$$

The solution of the SDE

$$dX_t = b(X_t, t) + \sigma(X_t, t)dW_t, \quad X_0 = 0,$$

can be viewed as a mapping between the Wiener path $\{W_t\}$ and $\{X_t\}$:

$$\{W_t\} \xrightarrow{\Phi} \{X_t\}.$$

Consequently, Φ induces another measures on $C[0,1]$, the distribution of $\{X_t\}$. One naturally asks:

  (1) Is the new measure absolutely continuous with respect to the Wiener measure?

  (2) If it is, what is the Radon-Nykodym derivative?

Note that in the finite-dimensional situation, the measure induced by a smooth mapping is always absolutely continuous with respect to the original measure and the Radon-Nykodym derivative is simply the Jacobian. Part of what we will do here can be regarded as a step towards establishing an infinite-dimensional analog of such a calculus.

We first address these questions for the situation when $\sigma = 1$. As before, we proceed in a two-step fashion.

Step 1. Finite-dimensional approximation.

Discretize the SDE using the Euler-Maruyama scheme,

(9.5) $$X_{t_{j+1}} = X_{t_j} + b(X_{t_j}, t_j)\delta t_j + \delta W_j,$$

where $\delta t_j = t_{j+1} - t_j, \delta W_j = W_{t_{j+1}} - W_{t_j}$. In matrix form we have

$$\boldsymbol{B} \cdot \begin{pmatrix} X_{t_1} \\ X_{t_2} \\ \vdots \\ X_{t_n} \end{pmatrix} - \begin{pmatrix} b(X_{t_0}, t_0)\delta t_0 \\ b(X_{t_1}, t_1)\delta t_1 \\ \vdots \\ b(X_{t_{n-1}}, t_{n-1})\delta t_{n-1} \end{pmatrix} = \boldsymbol{B} \cdot \begin{pmatrix} W_{t_1} \\ W_{t_2} \\ \vdots \\ W_{t_n} \end{pmatrix},$$

where $t_0 = 0$, $X_{t_0} = 0$, and the matrix $\boldsymbol{B}$ has the form

$$\boldsymbol{B} = \begin{pmatrix} 1 & & & & \\ -1 & 1 & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{pmatrix}_{n \times n}.$$

Equation (9.5) induces a finite-dimensional mapping Φ_n defined by

$$\{W_{t_1}, W_{t_2}, \ldots, W_{t_n}\} \xrightarrow{\Phi_n} \{X_{t_1}, X_{t_2}, \ldots, X_{t_n}\}.$$

With the notation defined earlier, one can write this mapping as

$$(9.6) \qquad x_{j+1} = x_j + b(x_j, t_j)\delta t_j + \delta w_j, \quad j = 0, \ldots, n-1$$

where $\delta w_j = w_{j+1} - w_j$, $w_0 = x_0 = 0$. The Jacobian of this mapping is

$$(9.7) \qquad \frac{\partial(w_1, \ldots, w_n)}{\partial(x_1, \ldots, x_n)} = 1.$$

Suppose we want to compute the average $\langle F[X_t] \rangle$. Then

$$\langle F[X_t] \rangle \approx \langle F(X_{t_1}, X_{t_2}, \ldots, X_{t_n}) \rangle = \langle G(W_{t_1}, W_{t_2}, \ldots, W_{t_n}) \rangle,$$

where $G = F \circ \Phi_n$. With the change of variables, we get

$$\langle F[X_t] \rangle \approx \int G(w_1, w_2, \ldots, w_n) \frac{1}{Z_n} \exp(-I_n(\boldsymbol{w})) dw_1 dw_2 \cdots dw_n$$

$$(9.8) \qquad = \int F(x_1, x_2, \ldots, x_n) \frac{1}{Z_n} \exp(-\tilde{I}_n(\boldsymbol{x})) dx_1 dx_2 \cdots dx_n,$$

where $\tilde{I}_n(\boldsymbol{x}) = I_n \circ \Phi_n^{-1}(\boldsymbol{x})$. From (9.6), we get

$$\tilde{I}_n(\boldsymbol{x}) = \frac{1}{2} \sum_{j=1}^{n} \left(\frac{x_j - x_{j-1}}{t_j - t_{j-1}} \right)^2 \delta t_{j-1} + \frac{1}{2} \sum_{j=1}^{n} b^2(x_{j-1}, t_{j-1}) \delta t_{j-1}$$

$$- \sum_{j=1}^{n} b(x_{j-1}, t_{j-1}) \cdot (x_j - x_{j-1}).$$

Changing the dummy variables from x_i to w_i, we obtain

$$\langle F[X_t] \rangle \approx \int F(w_1, w_2, \ldots, w_n) \frac{1}{Z_n} \exp(-I_n(\boldsymbol{w})) \exp\Big(-\frac{1}{2}\sum_{j=1}^{n} b_{j-1}^2 \delta t_{j-1}\Big)$$

$$\cdot \exp\Big(\sum_{j=1}^{n} b_{j-1}(w_j - w_{j-1})\Big) dw_1 dw_2 \cdots dw_n$$

$$(9.9) \quad = \Big\langle F(W_{t_1}, W_{t_2}, \ldots, W_{t_n}) \exp\Big(-\frac{1}{2}\sum_{j=1}^{n} b^2(W_{t_{j-1}}, t_{j-1})\delta t_{j-1}\Big)$$

$$\cdot \exp\Big(\sum_{j=1}^{n} b(W_{t_{j-1}}, t_{j-1}) \cdot \delta W_{t_{j-1}}\Big)\Big\rangle.$$

where $b_{j-1} = b(w_{j-1}, t_{j-1})$.

Step 2. Take the formal limit as $n \to \infty$.

Taking the limit, we get formally

$$(9.10) \quad \langle F[X_t] \rangle = \Big\langle F[W_t] \exp\Big(-\frac{1}{2}\int_0^1 b^2(W_t, t)dt + \int_0^1 b(W_t, t)dW_t\Big)\Big\rangle.$$

Note that from (9.9) the stochastic integral is in the Itô sense. Since (9.10) is valid for arbitrary F, we conclude that the distribution of $\{X_t\}$, μ_X, is absolutely continuous with respect to the Wiener measure μ_W and

$$\frac{d\mu_X}{d\mu_W} = \exp\Big(-\frac{1}{2}\int_0^1 b^2(W_t, t)dt + \int_0^1 b(W_t, t)dW_t\Big).$$

We can also derive this formula directly in continuous form:

$$\langle F[X_t] \rangle = \langle G[W_t] \rangle \quad \text{(where } G = F \circ \Phi)$$

$$= \int G[w_t] \cdot \delta(w_0) \frac{1}{Z} \exp\big(-I[w]\big) \mathcal{D}w$$

$$= \int F[x_t] \cdot \delta(x_0) \frac{1}{Z} \exp\Big(-I[x] - \frac{1}{2}\int_0^1 b^2(x_t, t)dt + \int_0^1 b(x_t, t)\dot{x}_t dt\Big) \mathcal{D}x$$

$$= \int F[w_t] \cdot \delta(w_0) \frac{1}{Z} \exp\Big(-I[w] - \frac{1}{2}\int_0^1 b^2(w_t, t)dt + \int_0^1 b(w_t, t)\dot{w}_t dt\Big) \mathcal{D}w$$

$$= \Big\langle F[W_t] \exp\Big(-\frac{1}{2}\int_0^1 b^2(W_t, t)dt + \int_0^1 b(W_t, t)dW_t\Big)\Big\rangle.$$

A special case is the *Cameron-Martin formula*, for the transformation

$$(9.11) \qquad\qquad\qquad \boldsymbol{X}_t = \boldsymbol{W}_t + \boldsymbol{\phi}(t)$$

where ϕ is a deterministic smooth function. In this case, one has $\boldsymbol{b}(\boldsymbol{X}_t, t) = \dot{\phi}(t)$ and

$$(9.12) \qquad \frac{d\mu_X}{d\mu_W} = \exp\left(-\frac{1}{2}\int_0^1 \dot{\phi}^2(t)dt + \int_0^1 \dot{\phi}(t)d\boldsymbol{W}_t\right).$$

One can also see from the derivation that if the condition that $\sigma = 1$ is violated, the measure induced by X_t fails to be absolutely continuous with respect to the Wiener measure.

The following theorems are the rigorous statements of the formal derivations above.

Theorem 9.2 (Girsanov Theorem I). *Consider the Itô process*

$$(9.13) \qquad d\tilde{\boldsymbol{W}}_t = \boldsymbol{\phi}(t, \omega)dt + d\boldsymbol{W}_t, \quad \tilde{\boldsymbol{W}}_0 = 0,$$

where $\boldsymbol{W} \in \mathbb{R}^d$ is a d-dimensional standard Wiener process on $(\Omega, \mathcal{F}, \mathbb{P})$. Assume that $\boldsymbol{\phi}$ satisfies the Novikov condition

$$(9.14) \qquad \mathbb{E}\exp\left(\frac{1}{2}\int_0^T |\boldsymbol{\phi}|^2(s, \omega)ds\right) < \infty,$$

where $T \leq \infty$ is a fixed constant. Let

$$(9.15) \qquad Z_t(\omega) = \exp\left(-\int_0^t \boldsymbol{\phi}(s, \omega)d\boldsymbol{W}_s - \frac{1}{2}\int_0^t \phi^2(s, \omega)ds\right)$$

and

$$(9.16) \qquad \tilde{\mathbb{P}}(d\omega) = Z_T(\omega)\mathbb{P}(d\omega).$$

Then $\tilde{\boldsymbol{W}}$ is a d-dimensional Wiener process on $[0, T]$ with respect to $(\Omega, \mathcal{F}_T, \tilde{\mathbb{P}})$.

To see how (9.15) and (9.12) are related to each other, we note that for any functional F

$$\begin{aligned}
\left\langle F[\tilde{\boldsymbol{W}}_t]\right\rangle_{\tilde{\mathbb{P}}} &= \left\langle F[\tilde{\boldsymbol{W}}_t]Z_T\right\rangle_{\mathbb{P}} \\
&= \left\langle F[\tilde{\boldsymbol{W}}_t]\exp\left(-\int_0^T \boldsymbol{\phi}(s, \omega)d\tilde{\boldsymbol{W}}_s + \frac{1}{2}\int_0^T \phi^2(s, \omega)ds\right)\right\rangle_{\mathbb{P}} \\
&= \left\langle F[\boldsymbol{W}_t]\exp\left(-\int_0^T \boldsymbol{\phi}(s, \omega)d\boldsymbol{W}_s + \frac{1}{2}\int_0^T \phi^2(s, \omega)ds\right)\frac{d\mu_{\tilde{\boldsymbol{W}}}}{d\mu_{\boldsymbol{W}}}\right\rangle_{\mathbb{P}} \\
&= \left\langle F[\boldsymbol{W}_t]\right\rangle_{\mathbb{P}}.
\end{aligned}$$

Next we consider the situation when σ is more general. Consider the two SDEs

$$\begin{cases}
d\boldsymbol{X}_t = \boldsymbol{b}(\boldsymbol{X}_t, t)dt + \boldsymbol{\sigma}(\boldsymbol{X}_t, t)d\boldsymbol{W}_t, \\
d\boldsymbol{Y}_t = (\boldsymbol{b}(\boldsymbol{Y}_t, t) + \boldsymbol{\gamma}(t, \omega))dt + \boldsymbol{\sigma}(\boldsymbol{Y}_t, t)d\boldsymbol{W}_t,
\end{cases}$$

where $\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{b}, \boldsymbol{\gamma} \in \mathbb{R}^n$, $\boldsymbol{W} \in \mathbb{R}^n$, and $\boldsymbol{\sigma} \in \mathbb{R}^{n \times n}$. Assume that $\boldsymbol{X}_0 = \boldsymbol{Y}_0 = \boldsymbol{x}$. The Girsanov theorem asserts that under suitable conditions, the distributions of $\boldsymbol{X}$ and $\boldsymbol{Y}$ over $[0,1]$ are absolutely continuous with respect to each other. The Radon-Nikodym derivative is given by

$$(9.17) \qquad \frac{d\mu_Y}{d\mu_X}[\boldsymbol{X}.] = \exp\left(-\frac{1}{2}\int_0^1 |\boldsymbol{\phi}(t,\omega)|^2 dt + \int_0^1 \boldsymbol{\phi}(t,\omega) d\boldsymbol{W}_t\right),$$

where $\boldsymbol{\phi}$ is defined by

$$\boldsymbol{\phi}(t,\omega) = (\boldsymbol{\sigma}(\boldsymbol{X}_t,t))^{-1} \cdot \boldsymbol{\gamma}(t,\omega).$$

Theorem 9.3 (Girsanov Theorem II). *Let $\boldsymbol{X}_t, \boldsymbol{Y}_t$, and $\boldsymbol{\phi}$ be defined as above. Assume that $\boldsymbol{b}$ and $\boldsymbol{\sigma}$ satisfy the same conditions as in Theorem 7.14, $\boldsymbol{\sigma}$ is nonsingular, $\boldsymbol{\gamma}$ is an $\mathcal{F}_t$-adapted process, and the Novikov condition holds for $\boldsymbol{\phi}$:*

$$(9.18) \qquad \mathbb{E}\exp\left(\frac{1}{2}\int_0^T |\boldsymbol{\phi}|^2(s,\omega) ds\right) < \infty.$$

Define $\tilde{\boldsymbol{W}}_t$, Z_t, and $\tilde{\mathbb{P}}$ as in Theorem 9.2. Then $\tilde{\boldsymbol{W}}$ is a standard Wiener process with respect to $(\Omega, \mathcal{F}_T, \tilde{\mathbb{P}})$ and $\boldsymbol{Y}$ satisfies

$$d\boldsymbol{Y}_t = \boldsymbol{b}(\boldsymbol{Y}_t,t)dt + \boldsymbol{\sigma}(\boldsymbol{Y}_t,t)d\tilde{\boldsymbol{W}}_t, \quad \boldsymbol{Y}_0 = \boldsymbol{x}, \quad t \le T.$$

Thus the law of $\boldsymbol{Y}_t$ under $\tilde{\mathbb{P}}$ is the same as that of $\boldsymbol{X}_t$ under $\mathbb{P}$ for $t \le T$.

Details of the proof can be found in [**Fri75a, Oks98**].

9.3. Feynman-Kac Formula Revisited

The Feynman-Kac formula tells us that the solution of the PDE

$$\partial_t v = \frac{1}{2}\Delta v + q(\boldsymbol{x})v, \quad v|_{t=0} = f(\boldsymbol{x})$$

can be represented as

$$v(x,t) = \mathbb{E}^{\boldsymbol{x}}\left(\exp\left(\int_0^t q(\boldsymbol{W}_s)ds\right)f(\boldsymbol{W}_t)\right).$$

In path integral form, this can be written as

$$v(\boldsymbol{x},t) = \int \delta(\boldsymbol{w}_0 - \boldsymbol{x})\frac{1}{Z}\exp\left(-\int_0^t \left(\frac{1}{2}\dot{\boldsymbol{w}}_s^2 - q(\boldsymbol{w}_s)\right)ds\right)f(\boldsymbol{w}_t)\mathcal{D}\boldsymbol{w},$$

where the Delta function $\delta(\boldsymbol{w}_0 - \boldsymbol{x})$ is to ensure that the Wiener process is initiated from $\boldsymbol{x}$.

The Feynmann-Kac formula originated from Feynmann's interpretation of quantum mechanics. Feynman noted that the solution of the Schrödinger

equation

(9.19) $$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi + V(\boldsymbol{x})\psi, \quad \psi|_{t=0} = \psi_0(\boldsymbol{x})$$

can be expressed formally as

(9.20) $$\psi(\boldsymbol{x},t) = \int \delta(\boldsymbol{w}_0 - \boldsymbol{x})\frac{1}{Z}\exp\Big(\frac{i}{\hbar}I[\boldsymbol{w}]\Big)\psi_0(\boldsymbol{w}_t)\mathcal{D}\boldsymbol{w},$$

where $I[\cdot]$ is the action functional defined in classical mechanics

$$I[\boldsymbol{w}] = \int_0^t \Big(\frac{m}{2}\dot{\boldsymbol{w}}_s^2 - V(\boldsymbol{w}_s)\Big)ds$$

and $\hbar$ is the reduced Planck constant. Formally, if we take

$$m = 1, \quad \hbar = -i$$

in (9.19) and (9.20), we obtain the Feynman-Kac formula. This was what motivated Kac to propose the Feynman-Kac formula for the parabolic problem.

Feynman's formal expression is yet to be made rigorous, even though Kac's reinterpretation for the parabolic equation is a rigorous mathematical tool widely used in mathematical physics.

Exercises

9.1. Derive (9.17) via the path integral approach.

9.2. Derive the infinite-dimensional characteristic function for Wiener process W_t

$$\Big\langle \exp\Big(i\int_0^1 \varphi(t)dW_t\Big)\Big\rangle = \exp\Big(-\frac{1}{2}\int_0^1 |\varphi|^2 dt\Big)$$

using the path integral approach.

Notes

The idea of path integral originated from Feynman's thesis in which solutions to the Schrödinger equation were expressed formally as averages over measures on the space of classical paths. Feynman's formal expressions have not yet been put on a firm mathematical basis. Kac had the insight that Feynman's work can be made rigorous if instead one considers the parabolic analog of the Schrödinger equation. This can be understood as taking the time variable to be imaginary in the Schrödinger equation.

One example of the application of the path integral approach is the asymptotic analysis of Wiener processes (see Chapter 12 and Freidlin's book [**Fre85**]). For application of path integrals to physics, we refer to [**Kle06**].

Random Fields

Stochastic processes can be regarded as random functions of one variable. We now turn to random fields which are random functions, or generalized functions, of more than one variable or on graphs.

Random fields arise in many important contexts, including:

(1) *Statistical mechanics.* The most well-known example is the Ising model. Here random fields are used to model the spin configurations on a lattice [**Rei98**].

(2) *Quantum field theory.* Quantum fields are random fields [**GJ87**]. There are many different ways to think about quantum field theory, but the functional integral approach is appealing both to physicists and mathematicians. From a mathematical viewpoint, the basic problem is to show that the (formal) functional integrals do make sense.

(3) *Vision and image processing.* Natural images can be regarded as random fields. Different images are different realizations of the random field. The Markov random field model has been used to make inferences [**Win03**].

(4) *Risk analysis of structures.* Structures such as buildings, dams, bridges inevitably fail due to material heterogeneities. To assess the risk of failure, it is useful to model the material using random fields [**Van83**].

(5) *Turbulence.* Turbulent velocity fields are often modeled using random fields [**MY71**].

Our study of the random processes focused on two large classes: the Gaussian processes and the Markov processes, and we devoted a large part of this book to the study of diffusion processes, a particular class of Markov processes with continuous paths. We will proceed similarly for random fields: We will study Gaussian random fields and Markov random fields. However, there are two important differences. The first is that for Markov processes, a very powerful tool is the Fokker-Planck equation. This allowed us to use differential equation methods. This has not been the case so far for Markov random fields. The second is that constructing nontrivial continuous random fields, a subject in constructive quantum field theory, is among the hardest problems in mathematics. For this reason, there has not been much work on continuous random fields, and for non-Gaussian random fields, we are forced to limit ourselves to discrete fields.

10.1. Examples of Random Fields

Let us start by discussing some concrete examples of random fields.

Example 10.1 (The percolation model)**.** Imagine that we have an $N \times N$ square lattice. Let $p \in [0, 1]$. For each edge on the lattice, we keep the edge with probability p and delete it with probability $1 - p$. This operation is done independently for all the edges. We are interested in the connectivity of the structure left after such an operation. This is the bond percolation problem. Figure 10.1 shows an example of a percolation network. This kind of network is used to model the microscopic structure of a porous medium, among other things.

A typical question of interest is the size of the connected clusters in such a structure as $N \to \infty$. It was proven by H. Kesten that if $p < 1/2$, then the probability of having infinite clusters is 0; if $p > 1/2$, then the probability of having infinite clusters is 1 [**Kes80**]. In other words, the critical value for the bond percolation model on a two-dimensional square lattice is $1/2$.

There is another version of the percolation problem, the site percolation model. In that case, each little square is independently kept or removed with probability p and $1 - p$, respectively.

Example 10.2 (Noisy images)**.** An image can be viewed as a function on a two-dimensional $N \times M$ lattice, i.e., the pixels. One can also think of an image as a random sample from some random field model, particularly so for noisy images. As a toy model for the noise degradation of an image $\boldsymbol{x} = (x_{ij})$ for $i = 1, \ldots, N$, $j = 1, \ldots, M$, one can specify the conditional distribution

$$p_{\boldsymbol{x}}(\boldsymbol{y}) = \sum_{i,j} \frac{1}{2\sigma_{ij}^2} (y_{ij} - x_{ij})^2.$$
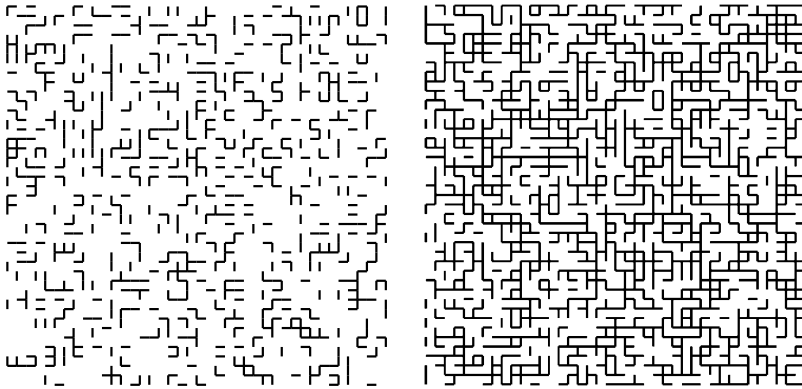
Figure 10.1. A bond percolation model, $N = 40$. Left panel: $p = 0.25$. Right panel: $p = 0.52$.

Figure 10.2 shows an image degraded by adding Gaussian noise.
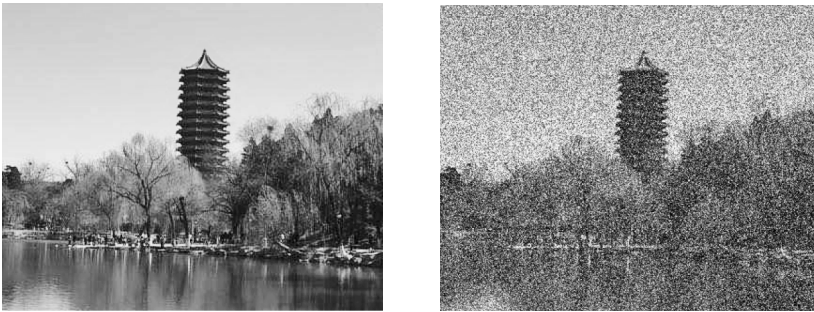
Figure 10.2. The original PKU (Peking University) tower image and the degraded image by adding Gaussian random noise.

Example 10.3 (Point processes). Point processes are a random distribution of points in $\mathbb{R}^d$ with the following property: For any two given non-intersecting domains D_1 and D_2, the number of points that fall in D_1 and D_2 are independent Poisson random variables with parameters λ_1 and λ_2. If there is a nonnegative function ρ on $\mathbb{R}^d$ such that $\lambda_1 = \int_{D_1} \rho(\boldsymbol{x})d\boldsymbol{x}$ and $\lambda_2 = \int_{D_2} \rho(\boldsymbol{x})d\boldsymbol{x}$, then we say that the density of the point process is ρ.

Other examples include the realizations of the high-dimensional Ising model, solutions of stochastic partial differential equations, the wind velocity distribution in a storm, the stress distribution of a random composite material, etc.

In the case of random processes, we were able to identify large classes of such processes, for example the Markov processes, for which we developed

some powerful tools. For random fields, perhaps the most general tool one can think of is the functional integral representation, which is a generalization of the path integrals.

We will skip the details of defining random fields, except for one terminolgy: We say that a random field is homogeneous if its statistics are translation invariant. For example, the point process is homogeneous if and only if the density ρ is a constant.

10.2. Gaussian Random Fields

A mathematically rigorous introduction of the Gaussian random fields will require introducing terminologies in functional analysis and the theory of distributions, neither of which are we willing to launch into. Therefore, we will limit ourselves to a more heuristic presentation.

The most important points concerning Gaussian random fields are:

(1) Like most other continuous random fields, Gaussian random fields are often probability measures on the space of generalized functions Ω. In other words, more often than not, its realizations $\omega \in \Omega$ are random distributions rather than random functions. As such, one has to think of everything in terms of test functions. For example, to define cylinder sets, one has to introduce smooth test functions $(\psi_1, \psi_2, \ldots, \psi_n)$ and study the distribution of the random vector $\boldsymbol{\psi} = ((\psi_1, \omega), (\psi_2, \omega), \ldots, (\psi_n, \omega))$, where (ψ_k, ω) is the duality pairing between the distribution and the test function.

(2) A random field is Gaussian if the distributions of the random vectors of the form $\boldsymbol{\psi} = ((\psi_1, \omega), (\psi_2, \omega), \ldots, (\psi_n, \omega))$ are Gaussian for all choices of the test functions.

(3) A Gaussian random field is completely determined by its mean and covariance functions. To define these objects, let ψ and ϕ be smooth test functions. The mean of a Gaussian random field is a linear functional m defined by

$$(10.1) \qquad m(\psi) = (\psi, m) := \mathbb{E}(\psi, \omega).$$

The covariance is an operator $\mathcal{K}$, defined by the bilinear form

$$(10.2) \qquad (\psi, \mathcal{K}\phi) = \mathbb{E}(\psi, \omega - m)(\phi, \omega - m).$$

(4) Another important object that completely determines the random field is its characteristic functional or the generating functional defined by

$$(10.3) \qquad S(\psi) = \mathbb{E}e^{i(\psi, \omega)}.$$

Next, let us discuss some of the most well-known examples of Gaussian random fields. We will limit ourselves to fields on $\mathbb{R}^d$.

Example 10.4 (Gaussian white noise)**.** Roughly speaking, Gaussian white noise is the Gaussian random field with mean 0 and covariance operator being defined by the δ-function. In rigorous terms, the Gaussian white noise random field is a probability measure on the space of tempered distributions $\Omega = \mathcal{S}'(\mathbb{R}^d)$ such that for any given rapidly decreasing smooth test functions $\phi, \psi \in \mathcal{S}(\mathbb{R}^d)$, we have

$$m(\psi) = 0, \quad (\psi, \mathcal{K}\phi) = \int_{\mathbb{R}^d} \psi(\boldsymbol{x})\phi(\boldsymbol{x})d\boldsymbol{x} = \int_{\mathbb{R}^d} \psi(\boldsymbol{x}) \int_{\mathbb{R}^d} \delta(\boldsymbol{x} - \boldsymbol{y})\phi(\boldsymbol{y})d\boldsymbol{y}d\boldsymbol{x}.$$

The latter equation means that the covariance operator $\mathcal{K} = \mathcal{I}$. This fact implies that the restrictions of the field to disjoint domains in $\mathbb{R}^d$ are independent.

The definition (10.2) obviously implies that the random variable (ψ, ω) is Gaussian with mean 0 and variance $\|\psi\|^2 = \int_{\mathbb{R}^d} \psi^2 d\boldsymbol{x}$ for any ψ. This immediately gives the characteristic functional of the white noise

$$(10.4) \qquad S(\psi) = \mathbb{E}e^{i(\psi,\omega)} = e^{-\frac{1}{2}\|\psi\|^2}.$$

It is easy to see that in one dimension, white noise is formally the derivative of the Wiener process.

Example 10.5 (The Ornstein-Uhlenbeck measure)**.** This is the Gaussian random field with mean 0 and covariance operator

$$(10.5) \qquad \mathcal{K} = (-\Delta + \mathcal{I})^{-1}.$$

In one dimension, it corresponds to the stationary Ornstein-Uhlenbeck process

$$dX_t = -X_t dt + dW_t.$$

To see this, note that

$$(\psi, \mathcal{K}\phi) = \mathbb{E}(\psi, X)(\phi, X) = \int_{\mathbb{R}} \psi(t) \int_{\mathbb{R}} \frac{1}{2} e^{-|t-s|} \phi(s) ds dt$$

for arbitrary ψ and ϕ, which implies $\mathcal{K} = (-d^2/dt^2 + \mathcal{I})^{-1}$. This is an example of a random field which can be defined in the space of usual functions.

Example 10.6 (The Brownian sheet)**.** This is the analog of Brownian motion in higher dimension. In two dimension, $B(s, t)$ satisfies

$$(10.6) \qquad \mathbb{E}B(s,t) = 0, \quad \mathbb{E}B(s,t)B(\tilde{s}, \tilde{t}) = (s \wedge \tilde{s}) \cdot (t \wedge \tilde{t}).$$

$B(s, t)$ can be constructed by the invariance principle as was done for the Wiener process. Let $\xi_{i,j}$ $(i, j = 1, 2, \ldots)$ be a two-parameter sequence of

i.i.d. random variables with mean 0 and variance 1. Let

$$(10.7) \qquad S_{m,n} = \sum_{1 \leq i \leq m} \sum_{1 \leq j \leq n} \xi_{i,j}.$$

Then for any $s, t \geq 0$, one can show that

$$(10.8) \qquad \frac{1}{N} S_{[Ns],[Nt]} \Rightarrow B(s,t), \quad N \to \infty,$$

where $[x]$ denotes the integer part of x. The Brownian sheet is a random field defined in the space of usual functions. However it is not a homogeneous field.

More on Gaussian random fields can be found in [**GJ87**, **HS08**, **Roz82**].

10.3. Gibbs Distribution and Markov Random Fields

Now we restrict ourselves to discrete random fields, defined on lattices or networks.

Let (V, E) be a finite graph. The random fields we will consider are functions defined on V with values in a state space Λ. Therefore the probability space is $\Omega = \Lambda^V$. We will denote the elements in Ω by $\boldsymbol{x}, \boldsymbol{y}$, etc., and the random variables as $\boldsymbol{X} = (\ldots, X_\alpha, \ldots)_{\alpha \in V}$.

Definition 10.7. We say that the random variable $\boldsymbol{X}$ is a Markov random field if for any partition of V, $V = V_1 \cup V_2 \cup V_3$ with no edges between the vertices in V_1 and V_3,

$$(10.9) \qquad \mathbb{P}(\boldsymbol{X}_1 = \boldsymbol{x}_1 | \boldsymbol{X}_2 = \boldsymbol{x}_2, \boldsymbol{X}_3 = \boldsymbol{x}_3) = \mathbb{P}(\boldsymbol{X}_1 = \boldsymbol{x}_1 | \boldsymbol{X}_2 = \boldsymbol{x}_2)$$

where $\boldsymbol{X}_j = \boldsymbol{X}|_{V_j}$, $j = 1, 2, 3$.

Equation (10.9) says that $\boldsymbol{X}_1$ and $\boldsymbol{X}_3$ are conditionally independent, given $\boldsymbol{X}_2$. In other words,

$$(10.10) \qquad \begin{aligned} &\mathbb{P}(\boldsymbol{X}_1 = \boldsymbol{x}_1, \boldsymbol{X}_3 = \boldsymbol{x}_3 | \boldsymbol{X}_2 = \boldsymbol{x}_2) \\ &\qquad = \mathbb{P}(\boldsymbol{X}_1 = \boldsymbol{x}_1 | \boldsymbol{X}_2 = \boldsymbol{x}_2) \mathbb{P}(\boldsymbol{X}_3 = \boldsymbol{x}_3 | \boldsymbol{X}_2 = \boldsymbol{x}_2). \end{aligned}$$

Another important concept is the Gibbs distribution. Let $\mathcal{C}$ denote the set of all cliques of V, i.e., the set of subsets $C \subset V$ such that there is an edge between any two distinct vertices in C. A family of functions $\{U_C\}_{C \in \mathcal{C}}$ is said to be a family of potentials on cliques if for any $C \in \mathcal{C}$, U_C depends only on the values at vertices in C. Define

$$(10.11) \qquad U(\boldsymbol{x}) = \sum_{C \in \mathcal{C}} U_C(\boldsymbol{x}), \quad P(\boldsymbol{x}) = \frac{1}{Z} \exp\left(-U(\boldsymbol{x})\right)$$

where $Z = \sum_{\boldsymbol{x}} e^{-U(\boldsymbol{x})}$ is the normalization constant. We say that P is a Gibbs distribution on Ω.

A fundamental result is the Hammersley-Clifford theorem, which states that these two notions are actually equivalent.

Theorem 10.8 (Hammersley-Clifford)**.** *The existence of the Gibbs distribution and the Markovianity of a random field are equivalent; i.e.,*

(1) *If P is a Gibbs distribution, then it defines a Markov random field; i.e., it satisfies (10.9).*

(2) *If P is the distribution of a Markov random field such that $P(\boldsymbol{x}) > 0$ for any $\boldsymbol{x} \in \Omega$, then there exists a family of potentials $\{U_C\}_{C \in \mathcal{C}}$, such that*

$$(10.12) \qquad P(\boldsymbol{x}) = \frac{1}{Z} \exp\left(-U(\boldsymbol{x})\right), \quad U(\boldsymbol{x}) = \sum_{C \in \mathcal{C}} U_C(\boldsymbol{x}).$$

For the proof of this result, see [**MD10**].

Example 10.9 (The generalized Ising model)**.** Consider a two-dimensional $N \times N$ regular lattice with label $\boldsymbol{i} = (i_1, i_2)$ for each site. Let V be the set of the lattice sites. Nearest neighbors are those sites $\boldsymbol{i} = (i_1, i_2)$ and $\boldsymbol{j} = (j_1, j_2)$ with label difference $|i_1 - j_1| \vee |i_2 - j_2| = 1$. Some examples of cliques and noncliques are shown in Figure 10.3 [**Bou95**].
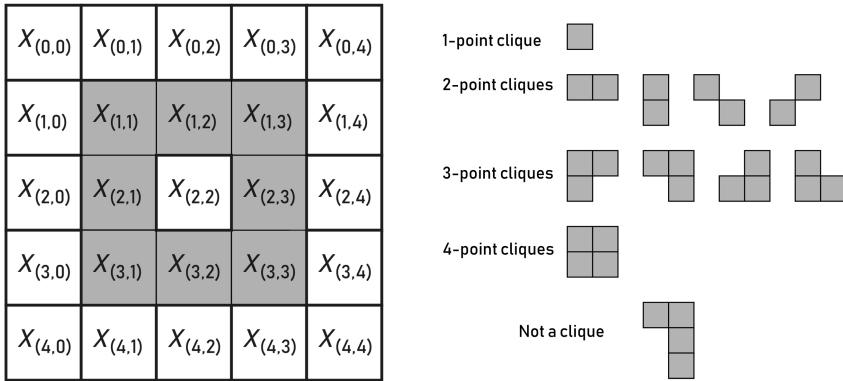
Figure 10.3. Examples of cliques and noncliques for the neighborhood system defined by nearest neighbors. Left panel: The shaded points indicate the nearest neighbors of the site $(2,2)$. Right panel: Cliques and noncliques.

Let $\boldsymbol{u}$ be a function defined on V. Let $\Lambda = \{0, 1\}$. For $\boldsymbol{x} = \{x_j\} \in \Omega$, consider the energy function U defined on $\Omega = \Lambda^V$

$$(10.13) \qquad U(\boldsymbol{x}) = \sum_{\langle \boldsymbol{i}, \boldsymbol{j} \rangle} (x_{\boldsymbol{i}} - x_{\boldsymbol{j}})^2 + \lambda \sum_j (x_{\boldsymbol{j}} - u_{\boldsymbol{j}})^2,$$

where $\langle \boldsymbol{i}, \boldsymbol{j} \rangle$ means that the sites $\boldsymbol{i}$ and $\boldsymbol{j}$ are nearest neighbors and $\lambda > 0$ is a penalty parameter. Define the probability measure

(10.14) $$P(\boldsymbol{x}) = \frac{1}{Z} \exp\left(-\beta U(\boldsymbol{x})\right).$$

Here β^{-1} is the parameter that plays the role of temperature. As $\beta \to 0$, this converges to the uniform distribution on Ω, i.e., equal weights for all configurations. As $\beta \to \infty$, then P converges to the point mass centered at the global minimum of U.

This has been used as a model for image segmentation with $\boldsymbol{u}$ being the image [**MD10**].

Exercise

10.1. Find the covariance operator $\mathcal{K}$ of the two-dimensional Brownian sheet.

Notes

For a mathematical introduction to random fields, we refer to the classical book by Gelfand and Shilov [**GS66**]. Practical issues are discussed in the well-known book by Vanmarcke [**Van83**]. For an interesting perspective on the application of random fields to pattern recognition, we refer to [**MD10**].

Introduction to Statistical Mechanics

As an integral part of physics, statistical mechanics establishes the connection between macro- and microscopic physics. As such, it is also of fundamental importance for multiscale multiphysics modeling, a subject that is now at the center stage of applied mathematics. For mathematicians, it should be appreciated that statistical mechanics, particularly equilibrium statistical mechanics, is a rather rigorous subject. The basic premise of statistical mechanics is that *any accessible quantum state of the system is equally likely to happen in nature*, and the observed macrostate is the one that corresponds to the largest number of microstates. Much of equilibrium statistical mechanics can be derived from this premise. For this reason, the most important calculation in statistical mechanics is to compute the number of microstates. This is embodied in the notion of entropy, which in thermodynamics is regarded as a measure of disorder of the system, but in statistical physics it is simply the number of microstates that give rise to a particular macrostate. We should remark that even though quantum mechanics should in principle enter into the definition of microstates, we can discuss most of the key notions of statistical mechanics without thinking about quantum mechanics.

At this point, deriving the basic premise stated above from dynamic first principles is still a widely open question. Nevertheless, it allows us to treat statistical mechanics by studying microscopic interacting particle systems using probabilistic methods. As we will see below, the starting point of statistical mechanics is a probability space, with the postulated probability distribution, namely the microcanonical ensemble, that is derived directly

from the premise stated above. The fact that the observed macrostates are quite deterministic even though the microstates are very much random is a consequence of the law of large numbers and large deviation theory.

In equilibrium statistical mechanics, we assume that the macrostate is stationary. Our aim is to understand the connection between the micro- and macrostates. Among other things, this will provide a foundation for thermodynamics. For simplicity, we assume that the total volume V is fixed. According to how the system exchanges particles and energy with its environment, one can consider three kinds of situations:

(1) Isolated system: The system under consideration does not exchange mass or energy with its environment. In this case, the particle number N and total energy E are both fixed. We call this an (N, V, E) ensemble, or microcanonical ensemble.

(2) Closed system: The system does not exchange mass with the environment but it does exchange energy with the environment. We further assume that the system is at thermal equilibrium with the environment; i.e., its temperature T is the same as the environment. We call this an (N, V, T) ensemble, or canonical ensemble.

(3) Open system: The system exchanges both mass and energy. We further assume that it is at both thermal and chemical equilibrium with the environment. The latter is equivalent to saying that the chemical potential μ is the same as that of the environment. Physically one can imagine particles in a box but the boundary of the box is both permeable and perfectly conducting for heat. We call this a (μ, V, T) ensemble, or grand canonical ensemble.

One can also consider the situation in which the volume is allowed to change. For example, one can imagine that the position of the boundary of the box, such as the piston inside a cylinder, is maintained at a constant pressure. In this case, the system under consideration is at mechanical equilibrium with the environment. This is saying that the pressure P is the same as that of the environment. One can then speak about, for example, the (N, P, T) ensemble, or isothermal-isobaric ensemble.

In nonequilibrium statistical mechanics, the systems are time-dependent and generally driven by frictional force and random fluctuations. Since the frictional and random forces are both induced from the same microscopic origin, that is, the random impacts of surrounding particles, they must be related to each other. A cornerstone in nonequilibrium statistical mechanics is the fluctuation-dissipation theorem. It connects the response functions,

which are related to the frictional component of the system, with the corresponding correlation functions, which are related to the fluctuation component. When the applied force is weak, the linear response theory is adequate for describing the relaxation of the system. From the reductionist viewpoint, one can derive the nonequilibrium dynamical model for a system interacting with a heat bath using the Mori-Zwanzig formalism. We will demonstrate this reduction for the simplest case, the Kac-Zwanzig model, which gives rise to a generalized Langevin equation for a distinguished particle coupled with many small particles via harmonic springs.

We should remark that the theory of nonequilibrium statistical mechanics is still an evolving field. For example, establishing thermodynamic laws and using them to understand experiments for biological systems is an active research field in biophysics. It is even less known for quantum open systems.

11.1. Thermodynamic Heuristics

Here we briefly review the heuristic arguments that are often used in thermodynamics. This helps us to define the macroscopic state variables.

The Boltzmann and Gibbs Entropy. For an isolated system, we know from classical mechanics that the Hamiltonian, i.e., the total energy, H, is conserved. Let $g(E)$ be the number of microstates corresponding to a particular energy $H = E$. The Boltzmann entropy of the system is defined to be

$$(11.1) \qquad S = k_B \log g(E),$$

where k_B is the Boltzmann constant.

In more general ensembles, the energy of the system may fluctuate and the Boltzmann entropy has to be generalized to Gibbs's form:

$$(11.2) \qquad S = -k_B \sum_x p(x) \log p(x),$$

where the summation is with respect to all possible states x and $p(x)$ is the probability of finding the system at state x. For an isolated system, we have, as a consequence of the basic premise stated earlier,

$$(11.3) \qquad p(x) = \begin{cases} 1/g(E), & H(x) = E, \\ 0, & \text{otherwise.} \end{cases}$$

In this case, the Gibbs entropy reduces to the Boltzmann entropy (11.1).

The Thermal Equilibrium States. Consider two systems A_1 and A_2 that are in thermal contact, i.e., they may exchange energy but not particles, and other than that the combined system is isolated from the rest of the world. The energy of both systems fluctuates in time and we are interested in its probability distribution. Denote by E_1 the value of the instantaneous energy of system A_1 at a particular time and by $g_1(E_1)$ the number of microstates at energy E_1. Similarly we define E_2 and $g_2(E_2)$. Let $g(E)$ be the number of microstates at energy E of the combined system. Then

$$(11.4) \qquad g(E) = \sum_{E_1 \leq E} g_1(E_1) g_2(E - E_1).$$

Let E_1^* be the value of E_1 such that the summand attains its largest value. Then

$$(11.5) \qquad \frac{d}{dE_1} \left(g_1(E_1) g_2(E - E_1) \right) = 0 \quad \text{at } E_1 = E_1^*.$$

Let $\sigma_1(E_1) = \log g_1(E_1)$, $\sigma_2(E_2) = \log g_2(E_2)$, $E_2^* = E - E_1^*$. Then the corresponding entropy

$$S_1(E_1) = k_B \sigma_1(E_1), \quad S_2(E_2) = k_B \sigma_2(E_2)$$

by (11.1). Then the condition (11.5) becomes

$$(11.6) \qquad \frac{\partial S_1}{\partial E_1}(E_1^*) = \frac{\partial S_2}{\partial E_2}(E_2^*).$$

Define the temperatures

$$(11.7) \qquad T_1 = \left(\frac{\partial S_1}{\partial E_1}(E_1^*) \right)^{-1}, \quad T_2 = \left(\frac{\partial S_2}{\partial E_2}(E_2^*) \right)^{-1}.$$

Then (11.6) says that

$$(11.8) \qquad T_1 = T_2.$$

This means that if two systems are at thermal equilibrium, then their temperatures must be the same.

We postulate that the main contribution to the summation in the definition of $g(E)$ above comes from the maximum term of the summand at E_1^*. As we see later, this is supported by large deviation theory.

Assume that the initial energy of the two systems when they are brought into contact are E_1^0 and E_2^0, respectively. Then

$$(11.9) \qquad g_1(E_1^0) g_2(E_2^0) \leq g_1(E_1^*) g_2(E_2^*);$$

i.e., the number of states of the combined system can only increase. We will see later that the number of states of a system is related to its entropy. So this says that entropy can only increase. This gives an interpretation of the second law of thermodynamics from the microscopic point of view.

Now we ask the question: At a given temperature, what can we say about the state of a system A that we are interested in? In the canonical ensemble, one can imagine that the constant temperature of the system A is maintained by putting it in contact with a large heat reservoir R. The total energy E of the combined system $R \cup A$ is fixed. But the energy of the system A can fluctuate. Denote by $p(x)$ the probability that the system is at state x and with energy $\varepsilon(x)$. Let $E_R = E - \varepsilon(x)$. According to the equal probability hypothesis, we have

$$(11.10) \qquad p(x) \propto g_R(E - \varepsilon(x)) = \exp\left(\sigma_R(E - \varepsilon(x))\right).$$

Since the energy of system $\varepsilon(x)$ is extremely small compared with E, we have

$$\sigma_R(E - \varepsilon) = \sigma_R(E) - \varepsilon \frac{\partial \sigma_R}{\partial E_R}(E) + O(\varepsilon^2)$$

$$= \sigma_R(E) - \frac{\varepsilon}{k_B T} + O(\varepsilon^2).$$

Keeping the leading order terms, we get the well-known Boltzmann distribution (or Gibbs distribution)

$$(11.11) \qquad p(x) = \frac{1}{Z(T)} \exp\left(-\frac{1}{k_B T} \varepsilon(x)\right),$$

introduced in (1.25), where $Z(T)$ is the partition function:

$$(11.12) \qquad Z(T) = \sum_x \exp\left(-\beta \varepsilon(x)\right).$$

The partition function has another equivalent form:

$$Z(T) = \sum_\varepsilon g(\varepsilon) \exp\left(-\beta \varepsilon\right),$$

where $g(\varepsilon)$ is number of microstates of the system having energy ε. In the continuous formulation,

$$(11.13) \qquad Z(T) = \int_0^\infty g(\varepsilon) \exp\left(-\beta \varepsilon\right) d\varepsilon.$$

We call $g(\varepsilon)$ the *density of states*. It is related to the partition function by the Laplace transform.

The internal energy is defined as the average energy of the system:

$$(11.14) \qquad U = \langle \varepsilon \rangle = \frac{1}{Z(T)} \sum_x \varepsilon(x) e^{-\beta \varepsilon(x)} = -\frac{\partial \log Z(T)}{\partial \beta}.$$

The Helmholtz free energy is defined as

$$(11.15) \qquad F = -k_B T \log Z(T).$$

The readers can easily check that the thermodynamic relation

(11.16) $$F = U - TS$$

holds, where S is the Gibbs entropy of the Boltzmann distribution (11.11). A basic principle of thermodynamics is that in the canonical (N, V, T) ensemble the Helmholtz free energy attains its minimum at the equilibrium state. The proof is left as an exercise.

Now let us consider the magnitude of the energy fluctuation in the canonical ensemble. We have

$$\langle (\delta \varepsilon)^2 \rangle = \langle (\varepsilon - \langle \varepsilon \rangle)^2 \rangle = \langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2$$

$$= \sum_x \varepsilon^2(x)p(x) - \left(\sum_x \varepsilon(x)p(x) \right)^2$$

(11.17) $$= \frac{\partial^2 \log Z(T)}{\partial \beta^2} = -\frac{\partial U}{\partial \beta}.$$

From the definition of heat capacity $C_V = (\partial U / \partial T)_{N,V}$, where the subscript means that the variables are held fixed when taking the partial derivative, we get

(11.18) $$\langle (\delta \varepsilon)^2 \rangle = k_B T^2 C_V.$$

For an N-particle system, the internal energy $\langle \varepsilon \rangle$ and heat capacity C_V are both of order N since they are extensive variables. We have that relative fluctuation satisfies

(11.19) $$\frac{\sqrt{\langle (\delta \varepsilon)^2 \rangle}}{\langle \varepsilon \rangle} \sim O\left(\frac{1}{\sqrt{N}} \right).$$

This suggests the equivalence of microcanonical and canonical ensembles in the thermodynamic limit as $N \to \infty$; i.e., most microstates of the system have approximately the energy $U = \langle \varepsilon \rangle$.

The Chemical Equilibrium States. Consider two systems, A_1 and A_2, that are in diffusive contact at a fixed temperature T. One can imagine that A_1 and A_2 are in thermal contact with a heat reservoir R, which maintains their temperature at T; at the same time A_1 and A_2 can exchange particles. The total particle number $N_1 + N_2$ is fixed at N. The total Helmholtz free energy of the system is

(11.20) $$F = F_1(N_1, V_1, T) + F_2(N_2, V_2, T).$$

At equilibrium (with fixed V_1, V_2, and T) the particle number distribution (N_1, N_2) is such that F attains its minimum value, which requires

(11.21) $$dF = \frac{\partial F_1}{\partial N_1} dN_1 + \frac{\partial F_2}{\partial N_2} dN_2 = 0.$$

Since $dN_1 + dN_2 = 0$, we have

$$(11.22) \qquad \frac{\partial F_1}{\partial N_1} = \frac{\partial F_2}{\partial N_2}.$$

Define the chemical potential as

$$(11.23) \qquad \mu = \left(\frac{\partial F}{\partial N} \right)_{V,T}.$$

Equation (11.22) says that at chemical (or diffusive) equilibrium, the chemical potential of the two subsystems must be the same.

If the particle number n is allowed to change, then similar derivations as those in previous subsection by putting the system in contact with a large heat and particle reservoir yield the Gibbs distribution in the (μ, V, T) ensemble:

$$(11.24) \qquad p(x) = \frac{1}{Z(\mu, T)} \exp\left(\beta(\mu n(x) - \varepsilon(x)) \right),$$

where

$$(11.25) \qquad Z(\mu, T) = \sum_x \exp\left(\beta(\mu n(x) - \varepsilon(x)) \right)$$

is the grand partition function in the (μ, V, T) ensemble.

Correspondingly, define the mean particle number of the system by

$$(11.26) \qquad N = \langle n \rangle = \frac{1}{Z(\mu, T)} \sum_x n(x) e^{\beta(\mu n(x) - \varepsilon(x))}.$$

The Landau free energy in this case, or commonly called grand potential, is defined as

$$(11.27) \qquad \Phi = -k_B T \log Z(\mu, T).$$

We recover the well-known thermodynamic relation

$$(11.28) \qquad \Phi = U - TS - \mu N.$$

Similarly we have that in the grand canonical ensemble the grand potential attains its minimum at the equilibrium state.

The Mechanical Equilibrium States. In the same way, one can show that if the two systems can only exchange volume, i.e., their temperature and particle numbers remain fixed, then at equilibrium we must have

$$(11.29) \qquad \left(\frac{\partial F_1}{\partial V_1} \right)_{N_1, T} = \left(\frac{\partial F_2}{\partial V_2} \right)_{N_2, T}.$$

This is the mechanical equilibrium. This defines the pressure:

$$(11.30) \qquad P = - \left(\frac{\partial F}{\partial V} \right)_{N, T}.$$

The negative sign is simply a convention so that pressure is normally positive.

One can similarly derive the Gibbs distribution, partition function, and corresponding free energy in the (N, P, T) ensemble. We call this the Gibbs free energy G. We have the thermodynamic relation

$$(11.31) \qquad G = F + PV = U - TS + PV.$$

It is useful to note that the Gibbs free energy can also be obtained through

$$(11.32) \qquad G(P, T) = \inf_V \big\{ F(V, T) + PV \big\},$$

which is the Legendre-Fenchel transform of the Helmholtz free energy F with respect to V. Here we take the infimum since the transformed functions are indeed $-F$ and $-G$ [**Ell85**]. This is a general observation for other thermodynamic potentials. In the (N, P, T) ensemble, the Gibbs free energy also attains its minimum at the equilibrium state.

11.2. Equilibrium Statistical Mechanics

In this section, we establish the microscopic foundation for the thermodynamic considerations introduced in the last section. This is done by studying the different ensembles, i.e., the probability space, that characterize the microscopic states of the system.

Macroscopic and Microscopic States. Consider an N-particle system. We will assume that the particles are identical. The microscopic state of the system is simply the position and momentum of all the particles

$$\boldsymbol{X} = (\boldsymbol{x}, \boldsymbol{p}) = (\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N, \boldsymbol{p}_1, \boldsymbol{p}_2, \ldots, \boldsymbol{p}_N) \in \mathbb{R}^{6N}.$$

In other words, the microscopic state space is the $6N$-dimensional phase space of the system. Since the probability measures that we will work with are parametrized by the macroscopic variables of the system, we must first establish a connection between the microscopic and macroscopic state variables.

The simplest macroscopic variable is the density:

$$(11.33) \qquad \rho = \frac{mN}{V},$$

where m is the mass of each particle.

Assuming that the average velocity of the system is 0, temperature is simply the average kinetic energy per degree of freedom of the particles; i.e.,

$$(11.34) \qquad T = \frac{1}{3k_B N} \sum_{j=1}^{N} \frac{|\boldsymbol{p}_j|^2}{2m}.$$

This is the translational part of the temperature. If the particle has a shape, say it shapes like a rod, and it can undergo other kinds of motion such as rotation, then one can speak about the corresponding temperature such as rotational temperature. The definition would be similar.

To get an expression for the pressure, assuming that the force between the ith and jth particle is $\boldsymbol{f}_{ij}$, then the pressure of the system is given by [**E11**]:

$$(11.35) \qquad P = \frac{1}{V} \sum_{i \neq j} (\boldsymbol{x}_i - \boldsymbol{x}_j) \cdot \boldsymbol{f}_{ij}.$$

The most interesting quantity is the entropy $S = k_B \log g$, which is defined as the number of microscopic states that give rise to the particular value of the macroscopic variable. Taking the logarithm makes it an extensive variable.

Example 11.1 (The entropy of mixing)**.** On a one-dimensional lattice of size N, put down k particles based on a single occupance rule. The number of ways of putting down these particles is equal to

$$(11.36) \qquad g(N, k) = \frac{N!}{(N - k)! k!}.$$

For $N \gg 1$, using the Stirling formula $\log N! \approx N \log N - N$, the entropy per site is then given by (ignoring k_B)

$$(11.37) \qquad \frac{1}{N} \log g(N, k) \approx -(1 - x) \log(1 - x) - x \log x,$$

where $x = k/N$ is the number density of the particles. Equation (11.37) gives the entropy of mixing. This result is reminiscent of the large deviation rate function considered in Example 2.10 and the related equation (2.12).

Construction of the Ensembles. Now let us define our probability space. An important quantity is the Hamiltonian $H = H(\boldsymbol{x}, \boldsymbol{p})$ defined on the phase space, which is usually the sum of the kinetic and potential energy of the system

$$H(\boldsymbol{x}, \boldsymbol{p}) = \sum_j \frac{|\boldsymbol{p}_j|^2}{2m} + U(\boldsymbol{x}).$$

This is the total energy of the system.

For the microcanonical ensemble representing an isolated system, the space Ω is

$$(11.38) \qquad \Omega = \big\{ (\boldsymbol{x}, \boldsymbol{p}) : \ H(\boldsymbol{x}, \boldsymbol{p}) = E \big\}.$$

It is assumed that this space is compact. Then the microcanonical probability distribution is simply

$$(11.39) \qquad p(\boldsymbol{x}, \boldsymbol{p}) = \frac{1}{Z} \delta \left(H(\boldsymbol{x}, \boldsymbol{p}) - E \right), \quad (\boldsymbol{x}, \boldsymbol{p}) \in \mathbb{R}^{6N},$$

or expressed as the probability measure on Ω by $Z^{-1}|\nabla H(\boldsymbol{x}, \boldsymbol{p})|^{-1}d\sigma$ for $(\boldsymbol{x}, \boldsymbol{p}) \in \Omega$, where $d\sigma$ is the surface measure on Ω and Z is the normalization constant

$$(11.40) \qquad Z = \int_{\Omega} |\nabla H(\boldsymbol{x}, \boldsymbol{p})|^{-1}d\sigma = \int_{\mathbb{R}^{6N}} \delta \left(H(\boldsymbol{x}, \boldsymbol{p}) - E \right) d\boldsymbol{x} d\boldsymbol{p}.$$

For the canonical ensemble representing a closed system, the space Ω is the whole phase space $\Omega = \mathbb{R}^{6N}$. The probability density is given by

$$(11.41) \qquad p(\boldsymbol{x}, \boldsymbol{p}) = \frac{1}{Z} \exp \left(-\beta H(\boldsymbol{x}, \boldsymbol{p}) \right)$$

and Z is the partition function

$$(11.42) \qquad Z = \int_{\mathbb{R}^{6N}} e^{-\beta H(\boldsymbol{x}, \boldsymbol{p})} d\boldsymbol{x} d\boldsymbol{p}.$$

These are the fundamental postulates of statistical mechanics. For the most part, we will focus on the canonical ensemble.

Ideal Gas. The microscopic ideal gas model consists of N noninteracting particles in a box of volume V. The partition function of a single particle can be computed using the classical approximation via quantum mechanics [**Cha87**]. It gives

$$(11.43) \qquad Z_1 = \frac{V}{h^3} \int d\boldsymbol{p} \exp \left(-\sum_j \frac{\beta |\boldsymbol{p}_j|^2}{2m} \right) = n_Q V,$$

where $n_Q = (2\pi m k_B T/h^2)^{\frac{3}{2}}$ and h is the Planck constant. The partition function of the N-particle system is then

$$(11.44) \qquad Z_N = \frac{1}{N!} Z_1^N = \frac{1}{N!} (n_Q V)^N.$$

Here the factorial in the denominator takes into account the indistinguishability of classical particles.

From this result, one can compute the other thermodynamic quantities:

$$F = -k_B T \log Z_N = -k_B T \log Z_1^N + k_B T \log N!$$

$$\approx -k_B T N \log \left(\left(\frac{2\pi m k_B T}{h^2} \right)^{\frac{3}{2}} V \right) + k_B T (N \log N - N),$$

$$P = -\left(\frac{\partial F}{\partial V} \right)_{N,T} = \frac{k_B T N}{V}.$$

This gives the equation of state for ideal gas

$$(11.45) \qquad\qquad PV = Nk_BT = nRT,$$

where $n = N/N_0$ is the mole number and $N_0 \approx 6.023 \times 10^{23}$ is the Avogadro constant. Here $R = k_BN_0$ is the ideal gas constant. The entropy is given by

$$S = -\left(\frac{\partial F}{\partial T}\right)_{N,V} = k_BN\left(\log\frac{n_Q}{n_V} + \frac{5}{2}\right),$$

where $n_V = N/V$ is the number density. In the isentropic case, S, N are both constants. This implies that

$$(11.46) \qquad\qquad \log T^{\frac{3}{2}} + \log V = \text{constant};$$

i.e., $T^{\frac{3}{2}}V = \text{constant}$. Combined with (11.45), we get the well-known relation

$$(11.47) \qquad\qquad P = C_0\rho^{5/3},$$

where ρ is the mass density of the gas. The chemical potential is given by

$$(11.48) \qquad \mu = \left(\frac{\partial F}{\partial N}\right)_{V,T} = -k_BT\left(\log Z_1 - \frac{d}{dN}\log N!\right).$$

With the leading order approximation $d\log N!/dN \approx \log N$, we get

$$\mu = k_BT\log\frac{N}{Z_1} = k_BT\log\frac{n_V}{n_Q} = k_BT\log\frac{P}{k_BTn_Q}.$$

Example 11.2 (Discrete ideal gas). Let D be a finite interval on $\mathbb{R}$ with nonempty interior. Consider the dynamics of N noninteracting unit-mass particles in D with velocity uniformly picked from a finite set L, with the property that if $v \in L$, then $-v \in L$. The velocity of the particle does not change unless it hits the boundary. At the boundary of D the particles are elastically reflected; i.e., their velocities change sign.

Let x_j and v_j be the instantaneous position and velocity of the jth particle. The phase space of this system is the space of the positions and velocities of the particles

$$\Omega_N = \{\omega = (x_1, \ldots, x_N, v_1, \ldots, v_N) : x_j \in D, v_j \in L \text{ for } j = 1, \ldots, N\}.$$

Denote by λ the normalized Lebesgue measure on D and by ρ the uniform distribution on L

$$\rho(y) = \frac{1}{|L|}\sum_{j=1}^{|L|}\delta(y - y_j),$$

where $|L|$ is the cardinality of the set L and y_j is the jth element in L. Given $\beta > 0$, define the discrete probability

(11.49) $$\rho_{\beta,j} = \frac{e^{-\beta y_j^2/2}}{\sum_k e^{-\beta y_k^2/2}}, \quad j = 1, \ldots, |L|,$$

and the single-particle canonical measure

(11.50) $$\rho_\beta(y) = \sum_j \rho_{\beta,j} \delta(y - y_j).$$

Then the canonical distribution on the N-particle state space Ω_N has the form

(11.51) $$\mathbb{P}_{N,eq}(d\omega) = \lambda(dx_1) \cdots \lambda(dx_N) \rho_\beta(dv_1) \cdots \rho_\beta(dv_N).$$

For this problem, one can simply integrate out the degrees of freedom for the position and consider the reduced canonical ensemble for the velocities $\omega = (v_1, \ldots, v_N)$. The probability distribution is then defined on $\Omega_N = \{\omega = (v_1, \ldots, v_N)\}$:

(11.52) $$\mathbb{P}_{N,eq}(d\omega) = \frac{1}{Z_N(\beta)} e^{-\beta U_N(\omega)} \rho(dv_1) \cdots \rho(dv_N)$$

where $U_N(\omega) = \sum_{j=1}^N |v_j|^2/2$ and

(11.53) $$Z_N(\beta) = \int_{\Omega_N} e^{-\beta U_N(\omega)} \rho(dv_1) \cdots \rho(dv_N)$$

is the partition function.

It is straightforward to obtain the specific free energy (by skipping the factor $-k_B T$),

(11.54) $$\frac{1}{N} \log Z_N(\beta) \to \log \int e^{-\beta y^2/2} \rho(dy).$$

The limit as $N \to \infty$ is referred to as the thermodynamic limit. It is in this limit that one recovers rigorously the thermodynamic states and thermodynamic relations. The connection between thermodynamic limit and large deviation theory is discussed in [**Ell85**].

Ising Model. In the following example, we consider the nearest neighbor Ising model in one dimension, which is the simplest model of ferromagnets with finite-range interactions. A ferromagnet in one dimension can be thought of as a set of N spins sitting on a subset of the integer lattice. On each site, the spin points either up or down. We identify this configuration space with $\mathcal{S}^N = \{-1, 1\}^N$, so that each configuration

$\boldsymbol{x} = (x_1, x_2, \ldots, x_N) \in \mathcal{S}^N$ is a sequence of $+1$ (spin up) or -1 (spin down). The Hamiltonian of the system is given by

$$(11.55) \qquad H^N(\boldsymbol{x}; \beta, h) = -\beta J_0 \sum_{i=1}^{N-1} x_i x_{i+1} - \beta h \sum_{i=1}^{N} x_i,$$

where $J_0 > 0$ and the first part of H^N indicates that only nearest neighbor interactions are taken into account.

For such thermodynamic systems, we naturally define the Gibbs distribution

$$(11.56) \qquad \mathbb{P}_{N,eq}(d\boldsymbol{x}) = \frac{1}{Z_N(\beta, h)} \exp\left(-H^N(\boldsymbol{x}; \beta, h)\right) \mathbb{P}_N(d\boldsymbol{x})$$

in the canonical ensemble, where $\mathbb{P}_N$ is the product measure on $\mathcal{B}(\mathcal{S}^N)$ with identical one-dimensional marginals equal to $\frac{1}{2}\delta_1 + \frac{1}{2}\delta_{-1}$ and the partition function

$$(11.57) \qquad Z_N(\beta, h) = \int_{\mathcal{S}^N} \exp\left[-H^N(\boldsymbol{x}; \beta, h)\right] \mathbb{P}_N(d\boldsymbol{x}).$$

Macroscopically, suppose that we are interested in a particular observable, the average magnetization

$$Y = O^N(\boldsymbol{X}) = \frac{1}{N} \sum_{i=1}^{N} X_i, \quad \boldsymbol{X} \in \mathcal{S}^N,$$

which is an *order parameter* reduced from microscopic states. The corresponding reduced distribution for the order parameter Y has the form

$$(11.58) \qquad \mathbb{P}_{N,eq}^Y(dy) = \left(\int_{\{\boldsymbol{x} \in \mathcal{S}^N, O^N(\boldsymbol{x}) = y\}} \mathbb{P}_{N,eq}(d\boldsymbol{x}) \right) \mathbb{P}_N^Y(dy),$$

where $\mathbb{P}_N^Y(dy)$ is simply the Lebesgue measure in the current setup. The free energy per site $F_N(y; \beta, h)$ for Y has the form

(11.59)
$F_N(y; \beta, h)$

$$= -\frac{1}{N} \log \left\{ \frac{1}{Z_N(\beta, h)} \int_{\{\boldsymbol{x} \in \mathcal{S}^N, O^N(\boldsymbol{x}) = y\}} \exp\left[-H^N(\boldsymbol{x}; \beta, h)\right] \mathbb{P}_N(d\boldsymbol{x}) \right\}.$$

The purpose of this example is to study the thermodynamic limit of F_N as $N \to \infty$; i.e.,

$$F(y; \beta, h) = \lim_{N \to \infty} F_N(y; \beta, h).$$

We will calculate the analytical expression of the free energy F by using transfer matrices and Legendre-Fenchel transforms.

Evaluating the Partition Function via Transfer Matrices. First we will calculate the log-asymptotics of the partition function $Z_N(\beta, h)$ using a powerful technique known as *transfer matrices*. We write

$$Z_N(\beta, h) = 2^{-N} \sum_{\boldsymbol{x} \in \mathcal{S}^N} \exp \left[\beta J_0 \sum_{i=1}^{N-1} x_i x_j + \beta h \sum_{i=1}^{N} x_i \right]$$

(11.60)

$$= \frac{1}{2} \sum_{x_1 = \pm 1} \sum_{x_2 = \pm 1} \cdots \sum_{x_N = \pm 1} \left\{ a(x_1) B(x_1, x_2) \ldots B(x_{N-1}, x_N) a(x_N) \right\}.$$

We have defined $a(x_i) = \exp(\beta h x_i)$ and

$$B(x_i, x_j) = \frac{1}{2} \exp \left[\beta J_0 x_i x_j + \frac{1}{2} \beta h (x_i + x_j) \right].$$

By considering the 2×2 *transfer matrix* $\boldsymbol{B}$ defined by

(11.61) $$\boldsymbol{B} = \begin{pmatrix} B(1,1) & B(1,-1) \\ B(-1,1) & B(-1,-1) \end{pmatrix},$$

we can simply represent (11.60) using a matrix product

(11.62) $$Z_N(\beta, h) = \frac{1}{2} \sum_{x_1 = \pm 1} \cdots \sum_{x_N = \pm 1} a(x_1) B^{N-1}(x_1, x_N) a(x_N).$$

By the Perron-Frobenius theorem, the log-asymptotics of (11.62) is determined by the leading eigenvalue $\lambda_{\boldsymbol{B}}$ of the transfer matrix $\boldsymbol{B}$; i.e.,

(11.63) $$\frac{1}{N} \log Z_N(\beta, h) \sim \log \lambda_{\boldsymbol{B}}.$$

A straightforward calculation shows that

(11.64) $$\lambda_{\boldsymbol{B}} = e^{\beta J_0} \left[\cosh \beta h + \left(\sinh^2 \beta h + e^{-4\beta J_0} \right)^{1/2} \right].$$

Free Energy Function via Legendre-Fenchel Transform. For $\theta \in \mathbb{R}$, we define the *cumulant generating function* $H(\theta; \beta, h)$ for the Ising system as

(11.65) $$H(\theta; \beta, h) = \lim_{N \to \infty} \frac{1}{N} \log \int_{-1}^{1} e^{N\theta y} \mathbb{P}_{N,eq}^{Y}(dy).$$

Recall from (11.59) that the free energy function $F(y; \beta, h)$ can be thought of as a rate function for a large deviation principle for the sequence of measures of $\left\{ \mathbb{P}_{N,eq}^{Y} \right\}$ as $N \to \infty$. Hence, an application of Laplace's asymptotics gives

(11.66) $$H(\theta; \beta, h) = \sup_{y \in [-1,1]} \left\{ \theta y - F(y; \beta, h) \right\}.$$

Equation (11.66) says that H is the Legendre-Fenchel transform of F. If H is a continuous convex function of $\theta \in \mathbb{R}$, then it can be shown that we can recover F by the duality of Legendre-Fenchel transform [**Ell85**, **RW09**]

$$(11.67) \qquad F(y; \beta, h) = \sup_{\theta \in \mathbb{R}} \{\theta y - H(\theta; \beta, h)\}.$$

This is also known as the *Gärtner-Ellis theorem*. We will carry out this program for the nearest neighbor Ising model.

First note that $H(\theta; \beta, h)$ can be expressed in terms of the partition function calculated previously:

$$H(\theta; \beta, h) = \lim_{N \to \infty} \frac{1}{N} \log \int_{-1}^{1} e^{N\theta y} \mathbb{P}_{N,eq}^{Y}(dy)$$

$$= \lim_{N \to \infty} \frac{1}{N} \log \frac{\int_{\mathcal{S}^N} \exp\left[-H^N(\boldsymbol{x}; \beta, h) + \theta \sum_{i=1}^{N} x_i\right] \mathbb{P}_{N,eq}(d\boldsymbol{x})}{\int_{\mathcal{S}^N} \exp\left[-H^N(\boldsymbol{x}; \beta, h)\right] \mathbb{P}_{N,eq}(d\boldsymbol{x})}$$

$$(11.68) \qquad = \lim_{N \to \infty} \frac{1}{N} \log \frac{Z_N\left(\beta, h + \frac{\theta}{\beta}\right)}{Z_N(\beta, h)}.$$

Using (11.63) and (11.64) we have

$$(11.69) \quad H(\theta; \beta, h) = \log\left[\frac{\cosh(\beta h + \theta) + \left(\sinh^2(\beta h + \theta) + e^{-4\beta J_0}\right)^{1/2}}{\cosh \beta h + \left(\sinh^2 \beta h + e^{-4\beta J_0}\right)^{1/2}}\right].$$

One can easily check that H is a smooth convex function of $\theta \in \mathbb{R}$. By the Gärtner-Ellis theorem, we can obtain F by a Legendre-Fenchel transform

$$
\begin{aligned}
F(y; \beta, h) &= \sup_{\theta \in \mathbb{R}} \{\theta y - H(\theta; \beta, h)\} \\
&= -h\beta y + y \sinh^{-1}\left[y\left(\frac{e^{-4\beta J_0}}{1 - y^2}\right)^{1/2}\right] \\
(11.70) &\qquad - \log \frac{e^{2\beta J_0} + \left(1 - \left(1 - e^{-4\beta J_0}\right) y^2\right)^{1/2}}{(1 - y^2)^{1/2}\left[\cosh \beta h + \left(\sinh^2 \beta h + e^{-4\beta J_0}\right)^{1/2}\right]}.
\end{aligned}
$$

Figure 11.1 shows F for several values of β and h.

Phase Transition. We see that F always has a unique minimum. Indeed by differentiating (11.70) we can see that F is strictly convex and has a unique minimum at $y = y_0(\beta, h)$ which satisfies $\partial F/\partial y(y_0; \beta, h) = 0$. Hence, the net magnetization must be given by this minimum point; i.e., $\bar{Y} = y_0(\beta, h)$. We thus have the exact expression

$$(11.71) \qquad \bar{Y} = \frac{\sinh \beta h}{\left(e^{-4\beta J_0} + \sinh^2 \beta h\right)^{1/2}}.$$
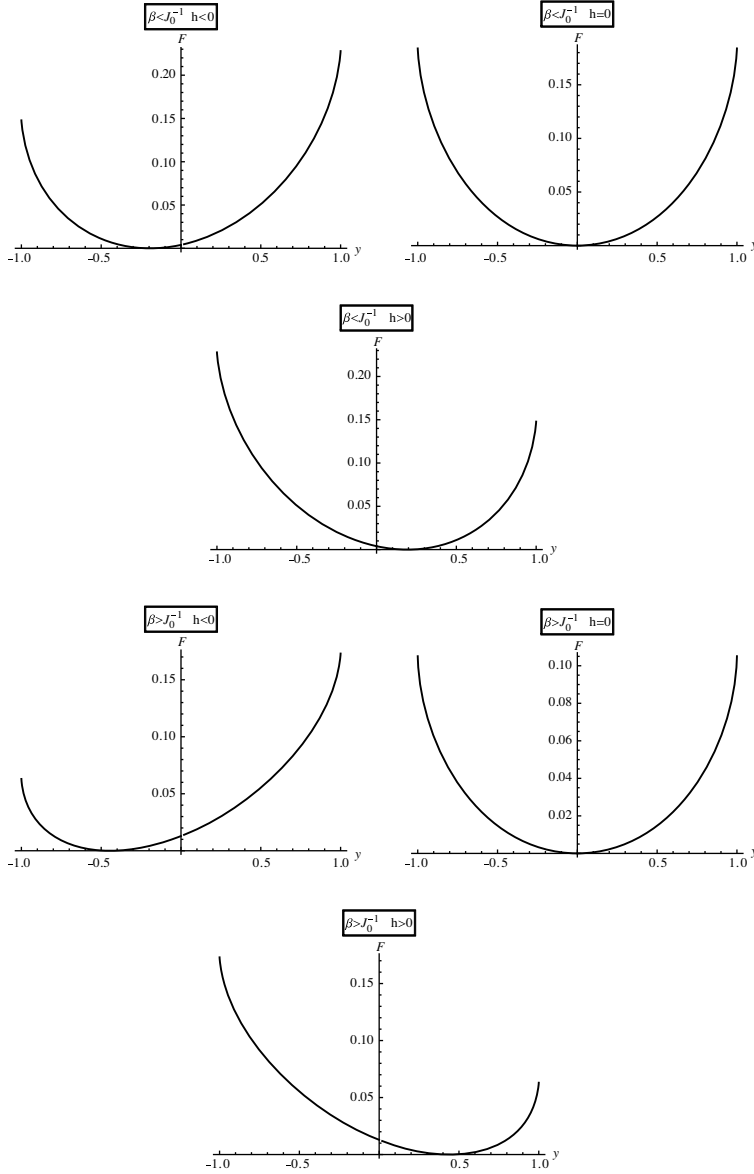
Figure 11.1. Free energy function $F(y; \beta, h)$ for various β and h. We see that for the nearest neighbor case, there is no qualitative change in the shape of F as the thermodynamic parameters are varied. This suggests that there is no phase transition for the net magnetization.

A typical plot of $\bar{Y}$ against β and h is given in Figure 11.2. It is clear from (11.71) that $\bar{Y}$ is a smooth function of its arguments. Hence, we arrive at the well-known result that there is no *phase transition*, intuitively no discontinuity or divergence in β or h, in the one-dimensional nearest neighbor
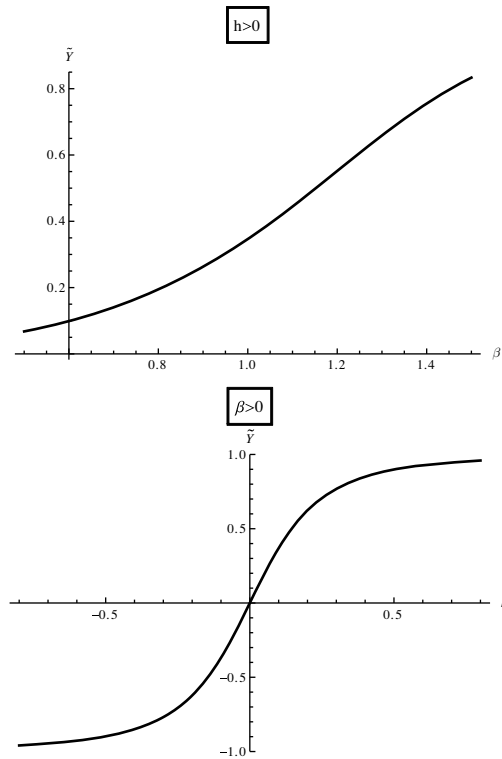
Figure 11.2. Plot of $\bar{Y}$ versus β (top) and h (bottom). In both cases $\bar{Y}$ is smooth so that there is no phase transition in the net magnetization.

Ising model. Indeed, the nearest neighbor Ising model only exhibits phase transitions in more than one dimension [**Gol92**, **Ell85**].

11.3. Generalized Langevin Equation

When the system under consideration is away from equilibrium, its time evolution is then of interest. Langevin and generalized Langevin equations are commonly used to model the dynamics of such systems. We will see later that the Mori-Zwanzig formalism naturally leads to generalized Langevin equations.

Langevin and Brownian Dynamics.

Example 11.3 (Langevin equation). Consider the dynamics of an inertial particle moving in a potential U, subject to friction and random noise:

$$(11.72) \qquad \begin{cases} \dot{\boldsymbol{X}}_t &= \boldsymbol{V}_t, \\ m\dot{\boldsymbol{V}}_t &= -\gamma\boldsymbol{V}_t - \nabla U(\boldsymbol{X}_t) + \sqrt{2\sigma}\dot{\boldsymbol{W}}_t. \end{cases}$$

In this chapter we will adopt the notation commonly used in the physics literature for SDEs.

In the absence of the external potential, we have

$$m\dot{\boldsymbol{V}}_t = -\gamma\boldsymbol{V}_t + \sqrt{2\sigma}\dot{\boldsymbol{W}}_t.$$

This is the Ornstein-Uhlenbeck process for $\boldsymbol{V}_t$. In the limit $t \to \infty$, we have

$$\left\langle \frac{1}{2}m\boldsymbol{V}^2 \right\rangle_{eq} = \frac{3\sigma}{2\gamma}.$$

From thermodynamics, the average kinetic energy is related to the temperature T by

$$\left\langle \frac{1}{2}m\boldsymbol{V}^2 \right\rangle_{eq} = \frac{3k_BT}{2}.$$

Thus we obtain the simplest version of the *fluctuation-dissipation relation*:

$$(11.73) \qquad\qquad\qquad \sigma = k_BT\gamma,$$

which connects the strength of the fluctuation σ and the friction coefficient γ. It can be proved that in this case the diffusion coefficient

$$(11.74) \qquad\qquad D := \lim_{t\to\infty} \frac{\left\langle (\boldsymbol{X}_t - \boldsymbol{X}_0)^2 \right\rangle}{6t} = \frac{k_BT}{\gamma}.$$

This is called the *Einstein relation.*

Equation (11.73) can also be proved by requiring that the probability measure with density $\rho = Z^{-1}e^{-\beta H}$, $H(\boldsymbol{x},\boldsymbol{v}) = m\boldsymbol{v}^2/2 + U(\boldsymbol{x})$, is invariant under the dynamics (11.72).

In the regime when $t \gg m/\gamma$, one can formally eliminate the velocity $\boldsymbol{V}_t$ in (11.72) as a fast variable and get the well-know over-damped Brownian dynamics:

$$(11.75) \qquad\qquad \gamma\dot{\boldsymbol{X}}_t = -\nabla U(\boldsymbol{X}_t) + \sqrt{2k_BT\gamma}\dot{\boldsymbol{W}}_t.$$

One can make this derivation rigorous by using the asymptotic analysis framework introduced in Section 8.9. This is left as an exercise.

Generalized Langevin Equation. In nonequilibrium statistical mechanics, one also encounters colored noise with finite correlation length, and the frictional coefficient is not necessarily a constant. The following is an example:

$$(11.76) \qquad \dot{\boldsymbol{X}}_t = \boldsymbol{V}_t, \quad m\dot{\boldsymbol{V}}_t = -\int_{-\infty}^{t} \gamma(t-s)\boldsymbol{V}_s ds - \nabla U(\boldsymbol{X}_t) + \boldsymbol{\xi}_t,$$

where the friction kernel $\gamma(t) \geq 0$ and $\boldsymbol{\xi}_t = (\xi_{t,1}, \xi_{t,2}, \xi_{t,3})$ is assumed to be a stationary Gaussian noise with

$$(11.77) \quad \langle\boldsymbol{\xi}_t\rangle = 0, \quad \langle\xi_{t,i}\xi_{s,j}\rangle = k_BT\gamma(|t-s|)\delta_{ij}, \quad t,s \in \mathbb{R}, \ i,j \in \{1,2,3\}.$$

The relation (11.77) is the well-known fluctuation-dissipation relation for the generalized Langevin equation. Later we will derive it for the Kac-Zwanzig model. We note that when the kernel $\gamma(t) = 2\gamma\delta(t)$, (11.76) reduces to the Langevin equation (11.72).

We will show that in the absence of the potential U, the velocity $\{\boldsymbol{V}_t\}$ is indeed a stationary Gaussian process with

(11.78) $\langle \boldsymbol{V}_t \rangle = 0, \quad \langle V_{t,i}V_{s,j} \rangle = k_B T G(|t-s|)\delta_{ij}, \quad t, s \in \mathbb{R}, \ i, j \in \{1, 2, 3\},$

where $G(t)$ is the correlation function of $\{\boldsymbol{V}_t\}$ with $G(-t) = G(t)$ and its Fourier transform

(11.79) $$\hat{G}(\omega) = \frac{2\mathrm{Re}(\hat{\gamma}_+(\omega))}{|i\omega m + \hat{\gamma}_+(\omega)|^2}.$$

Here $\hat{\gamma}_+(\omega)$ is the Fourier transform of the function

$$\gamma_+(t) = \begin{cases} \gamma(t), & t \geq 0, \\ 0, & t < 0, \end{cases}$$

and we assume $\gamma \in L^1(\mathbb{R}^+)$; i.e.,

(11.80) $$\int_0^\infty \gamma(t)dt < \infty.$$

It is enough to consider only the one-dimensional case since the components of $\boldsymbol{V}_t$ are mutually independent. We first note that the velocity V_t can be obtained via Fourier transform as $\hat{V}(\omega) = \hat{\mu}(\omega)\hat{\xi}(\omega)$, where

$$\hat{\mu}(\omega) = \left(i\omega m + \hat{\gamma}_+(\omega)\right)^{-1}.$$

Consequently, we have

(11.81) $$V_t = \int_{-\infty}^\infty \mu(t - s)\xi_s ds,$$

where $\mu(t)$ is the inverse Fourier transform of $\hat{\mu}(\omega)$. This gives

(11.82) $$\langle V_t \rangle = 0, \quad \langle V_t V_s \rangle = k_B T C(t, s)$$

where

$$C(t, s) = \int_{-\infty}^\infty \int_{-\infty}^\infty \mu(t - t')\mu(s - s')\gamma(|t' - s'|)dt'ds'.$$

The Fourier transform of $C(t, s)$ can be computed and it is

$$\hat{C}(\omega, \omega') = |\hat{\mu}(\omega)|^2 \cdot 2\mathrm{Re}\hat{\gamma}_+(\omega) \cdot 2\pi\delta(\omega + \omega') = \hat{G}(\omega) \cdot 2\pi\delta(\omega + \omega').$$

This is exactly the Fourier transform of $G(|t - s|)$. This proves (11.78).

11.4. Linear Response Theory

Consider a system at equilibrium. At $t = 0$ switch on a small time-dependent external field $F(t)$. Let $\langle \delta A \rangle$ be the perturbation of some physical quantity of interest $\langle A \rangle$. If the field is weak, then one can use perturbation theory to derive a linear relation between $\langle \delta A \rangle$ and the applied field $F(t)$. This is the major concern of the linear response theory. Below we will illustrate this theory for the case of Brownian dynamics. Our discussion will be formal but the rigorous justification can be carried out using semigroup theory.

Consider

$$\dot{\boldsymbol{X}}_t = -\zeta \nabla U_F(\boldsymbol{X}_t) + \sqrt{2\beta^{-1}\zeta}\,\dot{\boldsymbol{W}}_t, \quad t \in \mathbb{R},$$

where $\boldsymbol{W}_t$ is the standard Wiener process, $\zeta = 1/\gamma$ is the mobility constant, and the perturbed potential $U_F(\boldsymbol{x}) = U(\boldsymbol{x}) + U_{ext}(\boldsymbol{x})$. The external potential is assumed to be of the form $U_{ext}(x) = -F(t)B(\boldsymbol{x})$ and $B(x)$ is the conjugate variable with respect to the field $F(t)$, in the sense that $F(t)B(x)$ has the unit of energy. An example is the force and displacement pair. We assume $|F| \ll 1$ and $\boldsymbol{X}_t$ is at equilibrium initially; i.e., $\boldsymbol{X}_0$ has the PDF

$$p_{eq}(\boldsymbol{x}) = \frac{1}{Z}\exp\left(-\beta U(\boldsymbol{x})\right).$$

The Fokker-Planck equation has the form

$$\partial_t p(\boldsymbol{x}, t) = \left(\mathcal{L}_0^* + \mathcal{L}_{ext}(t)\right)p(\boldsymbol{x}, t),$$

where $\mathcal{L}_0^*$ is the unperturbed Fokker-Planck operator

$$\mathcal{L}_0^* p = \zeta\left(\nabla \cdot \left(\nabla U(\boldsymbol{x})p(\boldsymbol{x}, t)\right) + \beta^{-1}\Delta p(\boldsymbol{x}, t)\right)$$

and the stationary Gibbs distribution satisfies $\mathcal{L}_0^* p_{eq}(\boldsymbol{x}) = 0$. The external perturbation has the form

$$\mathcal{L}_{ext}(t)p(\boldsymbol{x}, t) = -\zeta F(t)\nabla \cdot \left(\nabla B(\boldsymbol{x})p(\boldsymbol{x}, t)\right).$$

The Duhamel's principle implies that

$$p(\boldsymbol{x}, t) = p_{eq}(\boldsymbol{x}) + \int_0^t ds\,\exp\left((t-s)\mathcal{L}_0^*\right)\left(\mathcal{L}_{ext}(s)p(\boldsymbol{x}, s)\right)$$

(11.83) $$\approx p_{eq}(\boldsymbol{x}) + \int_0^t ds\,\exp\left((t-s)\mathcal{L}_0^*\right)\left(\mathcal{L}_{ext}(s)p_{eq}(\boldsymbol{x})\right).$$

Therefore we have

$$\langle \delta A(t) \rangle = \langle A(t) \rangle - \langle A \rangle_{eq} = \int d\boldsymbol{x}\,A(\boldsymbol{x})p(\boldsymbol{x}, t) - \int d\boldsymbol{x}\,A(x)p_{eq}(\boldsymbol{x})$$

$$\approx \int_0^t ds \int d\boldsymbol{x}\,A(\boldsymbol{x})\exp\left((t-s)\mathcal{L}_0^*\right)\left(\mathcal{L}_{ext}(s)p_{eq}(\boldsymbol{x})\right).$$

Denote

(11.84) $$\langle \delta A(t) \rangle = \int_0^t \chi_{AB}(t-s)F(s)ds,$$

where we take the definition of the so-called response function

(11.85) $$\chi_{AB}(t) = -\zeta\Big(A(\boldsymbol{x}), \exp(t\mathcal{L}_0^*)\big(\nabla \cdot (\nabla B(\boldsymbol{x})p_{eq}(\boldsymbol{x}))\big)\Big), \quad t \geq 0,$$

and $(\cdot, \cdot)$ is the standard L^2 inner-product. Direct calculation shows

$$\zeta\nabla \cdot \big(\nabla B(\boldsymbol{x})p_{eq}(\boldsymbol{x})\big) = \beta p_{eq}(\boldsymbol{x})\mathcal{L}_0 B(\boldsymbol{x}),$$

where $\mathcal{L}_0$ is the adjoint operator of $\mathcal{L}_0^*$. We have

$$\chi_{AB}(t) = -\beta\Big(A(\boldsymbol{x}), \exp(t\mathcal{L}_0^*)\big(p_{eq}(\boldsymbol{x})\mathcal{L}_0 B(\boldsymbol{x})\big)\Big)$$
$$= -\beta\big(\exp(t\mathcal{L}_0)A(\boldsymbol{x}), p_{eq}(\boldsymbol{x})\mathcal{L}_0 B(\boldsymbol{x})\big)$$
(11.86) $$= -\beta\big(A(\boldsymbol{x}), \exp(t\mathcal{L}_0)\mathcal{L}_0 B(\boldsymbol{x})\big)_{eq},$$

where we used the weighted inner product $(\cdot, \cdot)_{eq}$ with respect to the Gibbs distribution $p_{eq}(\boldsymbol{x})$ and the selfadjoint property (8.52) of $\mathcal{L}_0$ with respect to $(\cdot, \cdot)_{eq}$.

On the other hand, the cross correlation satisfies

$$\langle A(t)B(0) \rangle_{eq} = \int d\boldsymbol{x}d\boldsymbol{y} A(\boldsymbol{x})B(\boldsymbol{y})p_{eq}(\boldsymbol{y}) \exp(t\mathcal{L}_{0,\boldsymbol{x}}^*)\delta(\boldsymbol{x}-\boldsymbol{y})$$
$$= \big(\exp(t\mathcal{L}_0)A(\boldsymbol{x}), B(\boldsymbol{x})\big)_{eq}$$
(11.87) $$= \big(A(\boldsymbol{x}), \exp(t\mathcal{L}_0)B(\boldsymbol{x})\big)_{eq},$$

where $\mathcal{L}_{0,\boldsymbol{x}}^*$ means the differential operator w.r.t. the variable $\boldsymbol{x}$.

From (11.87) and (11.86), we immediately get

(11.88) $$\chi_{AB}(t) = -\beta\frac{d}{dt}\langle A(t)B(0) \rangle_{eq} = -\beta\frac{d}{dt}C_{AB}(t), \quad t \geq 0,$$

where $C_{AB}(t) = \langle(A(t)-\langle A \rangle_{eq})(B(0)-\langle B \rangle_{eq})\rangle_{eq}$ is the cross-correlation function. Equations (11.84) and (11.88) form a cornerstone in nonequilibrium statistical mechanics. The left-hand side is the quantity that characterizes the response in the nonequilibrium setting when the system is driven by external force. The right-hand side is the cross-correlations of the spontaneous fluctuations in equilibrium. Note that if we understand (11.84) from a more general response relation

$$\int_0^\infty \chi_{AB}(t-s)F(s)ds,$$

then we have $\chi_{AB}(t) = 0$ when $t < 0$. This is causality.

The relation (11.88) has another useful form in the frequency domain. Define the so-called complex admittance $\hat{\mu}(\omega)$, the Fourier transform of the response function

$$(11.89) \qquad \hat{\mu}(\omega) = \int_0^\infty \chi_{AB}(t)e^{-i\omega t}dt.$$

Due to the stationarity of the equilibrium process, we formally have

$$\frac{d}{dt}C_{AB}(t) = \langle \dot{A}(t)B(0)\rangle_{eq} = -\langle A(t)\dot{B}(0)\rangle_{eq}.$$

Thus we obtain the general form of the *Green-Kubo relation*

$$(11.90) \qquad \hat{\mu}(\omega) = \beta \int_0^\infty \langle A(t)\dot{B}(0)\rangle_{eq}e^{-i\omega t}dt.$$

If we take $B(\boldsymbol{x}) = x$ and $A(\boldsymbol{x}) = u$ for the Langevin dynamics (11.72) in one dimension, we obtain

$$(11.91) \qquad \hat{\mu}(0) = \beta \int_0^\infty \langle u(t)u(0)\rangle_{eq}dt.$$

Under the ergodicity and stationarity condition

$$\lim_{t\to\infty} \langle u(t)u(t+\tau)\rangle = \langle u(0)u(\tau)\rangle_{eq},$$

we have

$$D = \lim_{t\to\infty} \frac{\langle x^2(t)\rangle}{2t} = \lim_{t\to\infty} \frac{1}{2t}\int_0^t dt_1 \int_0^t dt_2 \langle u(t_1)u(t_2)\rangle$$

$$(11.92) \qquad = \int_0^\infty \langle u(t)u(0)\rangle_{eq}dt.$$

This gives

$$(11.93) \qquad D = \hat{\mu}(0)k_BT,$$

which is exactly the Einstein relation.

Linear response theory (11.84) is not limited to the Brownian dynamics considered here. It is quite universal for the classical, Langevin dynamics or even quantum systems. Readers are referred to [**Cha87**, **Kub66**, **KTH95**, **MPRV08**] for further details.

11.5. The Mori-Zwanzig Reduction

In modeling we often encounter the situation that we are only interested in some (coarse-grained) variables of the system and we would like to obtain a model for these variables only, eliminating the other ones from the model. The Mori-Zwanzig formalism gives a general framework to do this reduction. Abstractly speaking, it states that this reduction is generally possible and it gives rise to generalized Langevin equations with memory and noise.

Consider a general nonlinear system

(11.94) $$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{b}(x), \quad \boldsymbol{x}(0) = \boldsymbol{x}_0,$$

with the infinitesimal generator $\mathcal{L}\psi(\boldsymbol{x}) = \boldsymbol{b}(\boldsymbol{x}) \cdot \nabla\psi(\boldsymbol{x})$. We will assume $\boldsymbol{x} = (\hat{\boldsymbol{x}}, \tilde{\boldsymbol{x}})$, where the $\hat{\boldsymbol{x}} = (\hat{x}_1, \ldots, \hat{x}_m)$ represent the resolved variables (i.e., the variables we are interested in) and the $\tilde{\boldsymbol{x}}$ are the unsolved ones. We assume also that the initial value $\boldsymbol{x}_0$ follows a probability distribution ρ. For Hamiltonian systems, a natural choice of ρ is the Gibbs distribution; i.e., $\rho(\boldsymbol{x}) = \exp(-\beta H(\boldsymbol{x}))/Z$.

Denote

$$\varphi(t) = \varphi(\boldsymbol{x}, t) = e^{\mathcal{L}t}\varphi_0(\boldsymbol{x}),$$

which is the solution of the equation $d\varphi/dt = \mathcal{L}\varphi$ with initial value $\varphi(0) = \varphi_0(\boldsymbol{x})$. Define the projection operator $\mathcal{P}$ as the conditional expectation given $\hat{\boldsymbol{x}}$:

(11.95) $$\mathcal{P}f(\hat{\boldsymbol{x}}) = \mathbb{E}(f(\boldsymbol{x})|\hat{\boldsymbol{x}}) = \frac{\int f(\boldsymbol{x})\rho(\boldsymbol{x})d\tilde{\boldsymbol{x}}}{\int \rho(\boldsymbol{x})d\tilde{\boldsymbol{x}}}.$$

Other choices of projections are also possible [**CHK02**]. We assume all these projections are on the space spanned by the functions of $\hat{\boldsymbol{x}}$.

Let $\mathcal{Q} = \mathcal{I} - \mathcal{P}$ and let φ_0 be a function of $\hat{\boldsymbol{x}}$ only. The simplest situation is that $\varphi_0(\boldsymbol{x}) = \hat{x}_j$ for $j = 1, \ldots, m$. Then we have $\varphi(t) = \hat{x}_j(t)$. More generally we get

(11.96) $$\frac{d\varphi}{dt} = e^{t\mathcal{L}}\mathcal{L}\varphi_0 = e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\varphi_0 + e^{t\mathcal{L}}\mathcal{Q}\mathcal{L}\varphi_0.$$

Using Dyson's formula

(11.97) $$e^{t\mathcal{L}} = e^{t\mathcal{Q}\mathcal{L}} + \int_0^t e^{(t-s)\mathcal{L}}\mathcal{P}\mathcal{L}e^{s\mathcal{Q}\mathcal{L}}ds$$

we obtain

(11.98) $$\frac{d\varphi}{dt} = e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\varphi_0 + \int_0^t e^{(t-s)\mathcal{L}}K(s)ds + R(t),$$

where

(11.99) $$R(t) = e^{t\mathcal{Q}\mathcal{L}}\mathcal{Q}\mathcal{L}\varphi_0, \quad K(t) = \mathcal{P}\mathcal{L}R(t).$$

Equation (11.98) is a generalized Langevin equation; see (11.76). The first term on the right-hand side of (11.98) is a Markovian term. The second term is a memory-dependent term. The third term depends on the full knowledge of the initial condition $\boldsymbol{x}_0$. One can regard this term as a noise term by treating the initial data for unresolved variable as being noise. The

fact that the memory depends on the noise corresponds to the fluctuation-dissipation relation, as will be exemplified in next section. To eliminate the noise, one can simply apply $\mathcal{P}$ to both sides and obtain

$$\frac{d}{dt}\mathcal{P}\varphi = \mathcal{P}e^{t\mathcal{L}}\mathcal{P}\mathcal{L}\varphi_0 + \int_0^t \mathcal{P}e^{(t-s)\mathcal{L}}K(s)ds$$

from the orthogonality condition $\mathcal{P}\mathcal{Q} = \mathcal{P} - \mathcal{P}^2 = 0$.

11.6. Kac-Zwanzig Model

We will illustrate the procedure of Mori-Zwanzig reduction for the well-known Kac-Zwanzig model. The Kac-Zwanzig model is a Hamiltonian system for $N+1$ particles with the total energy

$$(11.100) \qquad H(\boldsymbol{x}, \boldsymbol{v}) = \frac{1}{2}v^2 + U(x) + \sum_{i=1}^N \frac{1}{2}m_i v_i^2 + \frac{k}{2N}\sum_{i=1}^N (x_i - x)^2,$$

where $\boldsymbol{x} = (x, x_1, \ldots, x_N)$, $\boldsymbol{v} = (v, v_1, \ldots, v_N) \in \mathbb{R}^{N+1}$ are the coordinates and velocities of the system. One of the particle is a distinguished particle with a unit mass. We are only interested in this particle. This particle is placed in an external potential $U(\cdot)$ and coupled to N additional particles via harmonic springs. These additional particles provide the heat bath for the distinguished particle. The interaction between each heat bath particle and the distinguished particle is weak, as is revealed from the scaling of the spring constant k/N. The governing equations for this Hamiltonian system are

$$(11.101) \quad \ddot{X}^N = -U'(X^N) - \frac{k}{N}\sum_{i=1}^N (X^N - X_i^N), \quad X^N(0) = x_0, \dot{X}^N(0) = v_0,$$

$$(11.102) \qquad \ddot{X}_i^N = \omega_i^2(X^N - X_i^N), \quad X_i^N(0) = x_i, \dot{X}_i^N(0) = v_i,$$

where $\omega_i^2 = k/Nm_i$ and X^N and X_i^N are the coordinates of the distinguished particle and bath particles, respectively.

Solving the equations for the bath particles, we get
(11.103)

$$X_i^N(t) = X^N(t) - \int_0^t \dot{X}^N(s)\cos\omega_i(t-s)ds + (x_i - x_0)\cos\omega_i t + \frac{v_i}{\omega_i}\sin\omega_i t.$$

Substituting this expression into (11.101), we have

$$(11.104) \qquad \ddot{X}^N = -U'(X^N) - \int_0^t \gamma_N(t-s)\dot{X}^N(s)ds + \frac{1}{\sqrt{\beta}}\xi_N(t),$$

where the memory kernel

$$\gamma_N(t) = \frac{k}{N} \sum_{i=1}^{N} \cos \omega_i t \tag{11.105}$$

and

$$\xi_N(t) = \sqrt{\beta} \frac{k}{N} \sum_{i=1}^{N} \left((x_i - x_0) \cos \omega_i t + \frac{v_i}{\omega_i} \sin \omega_i t \right). \tag{11.106}$$

The initial condition for the bath variables is random, and its distribution can be obtained as the marginal distribution of the Gibbs distribution associated with $H(\boldsymbol{x}, \boldsymbol{v})$. This gives the density

$$\rho(x_1, \ldots, x_N, v_1, \ldots, v_N) = \frac{1}{Z} \exp(-\beta \hat{H}(\boldsymbol{x}, \boldsymbol{v})), \tag{11.107}$$

where Z is a normalization constant and $\hat{H}$ is the reduced Hamiltonian

$$\hat{H}(\boldsymbol{x}, \boldsymbol{v}) = \frac{k}{N} \sum_{i=1}^{N} \left(\frac{v_i^2}{\omega_i^2} + (x_i - x_0)^2 \right)$$

given (x_0, v_0) for the distinguished particle and fixed ω_i for $i = 1, \ldots, N$.

Define

$$a_i = \sqrt{\frac{\beta k}{N}}(x_i - x_0), \quad b_i = \sqrt{\frac{\beta k}{N\omega_i^2}} v_i.$$

Then a_i, b_i are normally distributed with mean 0 and variance 1 according to (11.107). We have

$$\xi_N(t) = \sqrt{\frac{k}{N}} \sum_{i=1}^{N} \left(a_i \cos \omega_i t + b_i \sin \omega_i t \right). \tag{11.108}$$

With this definition, we have the fluctuation-dissipation relation; i.e.,

$$\mathbb{E}\xi_N(t)\xi_N(s) = \frac{k}{N} \sum_{i=1}^{N} \cos \omega_i(t - s) = \gamma_N(t - s). \tag{11.109}$$

Furthermore, we assume that the frequencies $\{\omega_i\}_{i=1}^{N}$ are independent and identically distributed random variables with probability density $\rho(\omega)$. This assumption suggests that the mass $m_i \sim \mathcal{O}(N^{-1})$ when $N \to \infty$. We then have by the law of large numbers

$$\gamma_N(t) \to \gamma(t) = k \int_{\mathbb{R}} \cos(\omega t)\rho(\omega)d\omega, \quad N \to \infty. \tag{11.110}$$

The noise term $\xi_N(t)$ then converges to a Gaussian process $\xi(t)$ with $\mathbb{E}\xi(t) = 0$ and covariance function

$$\mathbb{E}\xi(t)\xi(s) = \lim_{N\to\infty} \frac{k}{N} \sum_{i=1}^{N} \cos\omega_i(t-s) = k \int_{\mathbb{R}} \cos\omega(t-s)\rho(\omega)d\omega$$

$$(11.111) \qquad = \gamma(t-s).$$

In summary, we obtain a reduced model for the distinguished particle:

$$(11.112) \qquad \ddot{X} = -U'(X) - \int_0^t \gamma(t-s)\dot{X}(s)ds + \sqrt{\beta^{-1}}\xi(t).$$

This final result embodies many essential aspects in the reduction of general dynamical systems, particularly the memory and the noise terms, as well as the fluctuation-dissipation relation (11.111).

Exercises

11.1. By putting the system in contact with a heat reservoir, prove that the Helmholtz free energy F achieves minimum at equilibrium using the fact that the entropy $S = k_B \log g(E)$ achieves maximum at equilibrium in the canonical ensemble. Generalize this argument to other ensembles.

11.2. Derive the Gibbs distribution $p(x)$ by the maximum entropy principle in the canonical ensemble: Maximize the Gibbs entropy

$$S = -k_B \sum_x p(x) \log p(x)$$

subject to the constraints

$$0 \leq p(x) \leq 1, \quad \sum_x p(x) = 1, \quad U = \sum_x p(x)E(x).$$

Generalize the result to the other ensembles.

11.3. Consider the Langevin dynamics

$$d\boldsymbol{X}_t = \boldsymbol{V}_t dt,$$

$$md\boldsymbol{V}_t = -\nabla U(\boldsymbol{X}_t)dt - \gamma\boldsymbol{K}(\boldsymbol{X}_t)\cdot\boldsymbol{V}_t dt + \sqrt{2\gamma}\boldsymbol{K}^{\frac{1}{2}}(\boldsymbol{X}_t)\cdot d\boldsymbol{W}_t,$$

where γ is the frictional coefficient, $\boldsymbol{W}_t \in \mathbb{R}^d$ is the standard Brownian motion, and $\boldsymbol{K}(\boldsymbol{x}) \in \mathbb{R}^{d\times d}$ is a uniformly symmetric positive definite matrix. Set $m = 1$. Using asymptotic analysis for SDEs, derive the reduced Brownian dynamics for $\boldsymbol{X}$ in the high frictional limit $\gamma = \varepsilon^{-1} \to +\infty$ in the timescale t/ε through the following steps.

(a) The invariant distribution $p_{eq}(\boldsymbol{v})$ of the SDEs

$$d\boldsymbol{V}_t = -\boldsymbol{K}(\boldsymbol{X}_t) \cdot \boldsymbol{V}_t dt + \sqrt{2}\boldsymbol{K}^{\frac{1}{2}}(\boldsymbol{X}_t) \cdot d\boldsymbol{W}_t$$

is simply the Maxwellian distribution $\boldsymbol{V}_t \sim N(\boldsymbol{0}, \boldsymbol{I})$.

(b) The projection operator is simply the expectation with respect to the invariant distribution.

(c) The infinitesimal generator of $\boldsymbol{V}_t$ has representation

$$\begin{aligned}
\mathcal{A}f &= -(\boldsymbol{K}(\boldsymbol{x}) \cdot \boldsymbol{v}) \cdot \nabla_{\boldsymbol{v}} f + \boldsymbol{K}(\boldsymbol{x}) : \nabla_{\boldsymbol{v}}^2 f \\
&= p_{eq}^{-1}(\boldsymbol{v})\nabla_{\boldsymbol{v}} \cdot (\boldsymbol{A}(\boldsymbol{x}) \cdot \nabla_{\boldsymbol{v}} f p_{eq}(\boldsymbol{v})).
\end{aligned}$$

11.4. Derive the zero mass limit of the Langevin equation in Exercise 11.3, i.e., the limit as $m = \varepsilon \to 0$ when γ is a constant.

11.5. Prove the positivity of the energy spectrum of a stationary stochastic process X_t; i.e.,

$$\hat{C}_X(\omega) \geq 0$$

where $C_X(|t - s|) = \langle X_t X_s \rangle$ is the autocorrelation function and $\hat{C}_X(\omega) = \int_{-\infty}^{\infty} C_X(|t|)e^{-i\omega t} dt$.

11.6. Suppose that X_t is a stationary process and $A(t) = A(X_t)$, $B(t) = B(X_t)$ are two observables. Prove that the cross-correlation functions $\langle A(t)B(s) \rangle$ satisfies the relation $\langle \dot{A}(t)B(0) \rangle = -\langle A(t)\dot{B}(0) \rangle$ if $A(t)$, $B(t)$ are differentiable.

11.7. Prove that under the ergodicity and stationarity condition

$$\lim_{t \to \infty} \langle u(t)u(t + \tau) \rangle = \langle u(0)u(\tau) \rangle_{eq},$$

we have

$$\lim_{t \to \infty} \frac{1}{2t} \int_0^t dt_1 \int_0^t dt_2 \langle u(t_1)u(t_2) \rangle = \int_0^{\infty} \langle u(t)u(0) \rangle_{eq} dt.$$

11.8. Consider both the Hamiltonian and Langevin dynamics. Derive the linear response model

$$\langle \delta A(t) \rangle = \int_0^t \chi_{AB}(t - s)F(s)ds,$$

when the total energy is perturbed by a small external force; i.e., $H_F(\boldsymbol{x}) = H(\boldsymbol{x}) - F(t)B(\boldsymbol{x})$. Give the explicit formula of the response function χ_{AB}.

11.9. Apply the Metropolis algorithm to the two-dimensional Ising model on the $M \times M$ lattice with $J = 1, k_B = 1, h = 0$ and periodic boundary condition; i.e., $x_{i+M,j+M} = x_{i,j}$ for any (i, j). Plot the

temperature versus internal energy (β-u) and temperature versus specific heat (β-c) curves, where

$$u = \frac{1}{M}\langle H \rangle = -\frac{1}{M}\frac{\partial \log Z_M}{\partial \beta},$$

$$c = \frac{\beta^2}{M}\big(\langle H^2 \rangle - \langle H \rangle^2\big) = \frac{\beta^2}{M}\frac{\partial^2 \log Z_M}{\partial \beta^2}.$$

Identify the phase transition temperature.

11.10. Apply the BKL algorithm to the problem described above. Compare its efficiency with the Metropolis algorithm.

Notes

There are many good textbooks and monographs on the introduction of the foundation of statistical mechanics. On the physics side we have chosen to rely mainly on [**Cha87**, **KK80**, **KTH95**, **Rei98**]. On the mathematics side, our main reference is [**Ell85**], a classic text on the mathematical foundation of equilibrium statistical mechanics. It has been widely recognized that the mathematical language behind statistical mechanics is ergodic theory and large deviation theory. We discussed these topics from the viewpoint of thermodynamic limit and phase transition. The interested readers are referred to [**Gal99**, **Sin89**, **Tou09**] for further material.

The linear response theory is a general approach for studying different kinds of dynamics ranging from the Hamiltonian dynamics, Langevin dynamics, Brownian dynamics to quantum dynamics. It provides the basis for deriving response functions and sometimes equilibrium correlation functions. We only considered Brownian dynamics as a simple illustration. See [**KTH95**, **MPRV08**] for more details.

The fluctuation-dissipation theorem is a cornerstone in nonequilibrium statistical mechanics. In recent years, interest on small systems in biology and chemistry has given rise to further impetus to pursue this topic and this resulted in the birth of a new field called stochastic thermodynamics. Representative results include Jarzynski's equality and Crooks's fluctuation theorem. See [**JQQ04**, **Sei12**, **Sek10**] for the latest developments.

Model reduction is an important topic in applied mathematics. The Mori-Zwanzig formalism gives a general framework for eliminating uninteresting variables from a given system. However, approximations have to be made in practical applications. How to effectively perform such approximation is still an unresolved problem in many real applications. Some interesting attempts can be found in [**DSK09**, **HEnVEDB10**, **LBL16**].

Rare Events

Many phenomena in nature are associated with the occurence of some rare events. A typical example is chemical reaction. The vibration of chemical bonds occurs on the time scale of pico- to femto-seconds (i.e., 10^{-15} to 10^{-12} seconds). But a typical reaction may take seconds or longer to accomplish. This means that it takes on the order of 10^{12} to 10^{15} or more trials in order to succeed in one reaction. Such an event is obviously a rare event. Other examples of rare events include conformational changes of biomolecules, the nucleation process, etc.

Rare events are caused by large deviations or large fluctuations. Chemical reactions succeed when the chemical bonds of the participating molecules manage to get into some particular configurations so that a sufficient amount of kinetic energy is converted to potential energy in order to bring the system over some potential energy barrier. These particular configurations are usually quite far from typical configurations for the molecules and are only visited very rarely. Although these events are driven by noise and consequently are stochastic in nature, some of their most important features, such as the transition mechanism, are often deterministic and can be predicted using a combination of theory and numerical algorithms.

The analysis of such rare events seems to have proceeded in separate routes in the mathematics and science literature. Mathematicians have over the years built a rigorous *large deviation theory*, starting from the work of Cramérs and Schilder and ultimately leading to the work of Donsker and Varadhan and of Freidlin and Wentzell [**FW98**, **Var84**]. This theory gives a rigorous way of computing the leading order behavior of the probability of large deviations. It has now found applications in many branches of mathematics and statistics.

Physicists and chemists, on the other hand, proceeded with a different route. In 1931, Onsager laid down the foundation for a macroscopic theory of chemical kinetics and made connections with the microscopic properties of the system. The chemical physics community proposed various versions of the reaction-rate theory in the 1930s (see the work of Wigner, Eyring, et al. [**HPM90**]). In 1940, Kramers wrote the landmark paper [**Kra40**] which became the basis of later developments in computing rates of rare events and in particular reaction rates. These form the basis of the *transition state theory*, which is part of the folklore of physical chemistry. A modern account of the transition state theory can be found in [**Cha78**, **HPM90**].

These developments were mostly analytical and are suitable for simple systems for which the transition mechanism can be guessed beforehand. For more complex systems, for which the transition mechanism itself is very much of an issue, numerical methods have been developed recently to find the transition pathways and transition rates. This is an exciting area of ongoing research.

12.1. Metastability and Transition Events

Consider the diffusion process defined by

$$(12.1) \qquad\qquad d\boldsymbol{X}_t^\varepsilon = -\nabla U(\boldsymbol{X}_t^\varepsilon)dt + \sqrt{\varepsilon}d\boldsymbol{W}_t$$

where $\boldsymbol{W}_t$ is the standard multidimensional Wiener process and $U(\boldsymbol{x})$ is assumed to be a smooth Morse function; i.e., the critical points of U are nondegenerate in the sense that the Hessian matrices at the critical points are nondegenerate. When $\varepsilon = 0$, for generic initial conditions, the solution of this ODEs converges to a local minimum of the potential function U. For each local minimum, the set of initial conditions from which the solutions of the ODEs converge to that local minimum is the *basin of attraction* of that local minimum. The whole configuration space is then divided into the union of the different basins of attraction. The boundaries of the basins of the attraction are the *separatrices*, which are themselves invariant sets of the deterministic dynamics. In particular, each local minimum is stable under the dynamics.

When ε is positive but small, on the $O(1)$ time scale, the picture just described still pretty much holds. In particular, with overwhelming probability, the solution to the SDEs will stay within the basin of attraction of a local minimum. However, as we discuss below, on exponentially large time scales in $O(1/\varepsilon)$, the solution will hop over from one basin of attraction to another, giving rise to a noise-induced instability. Such hopping events are the rare events we are interested in.

The above can be best illustrated in the following one-dimensional example (see Figure 12.1) with the double-well potential

$$(12.2) \qquad\qquad U(x) = \frac{1}{4}(x^2 - 1)^2.$$

U has two local minima at $x_+ = 1$ and $x_- = -1$ and one saddle at $x_s = 0$. Here x_s is also called the transition state between x_+ and x_-. Thus we have two basins of attraction,

$$B_- = \{x|\ x \le 0\} \quad \text{and} \quad B_+ = \{x|\ x \ge 0\}.$$

Most of the time, X_t wanders around x_+ or x_-. But at exponentially long time scales in $O(1/\varepsilon)$, X_t^ε hops between the regions B_+ and B_-. This is the typical manifestation of rare events (see Figure 12.1).

Potential function $U(x)$ 　　　　　　 A typical trajectory of X_t
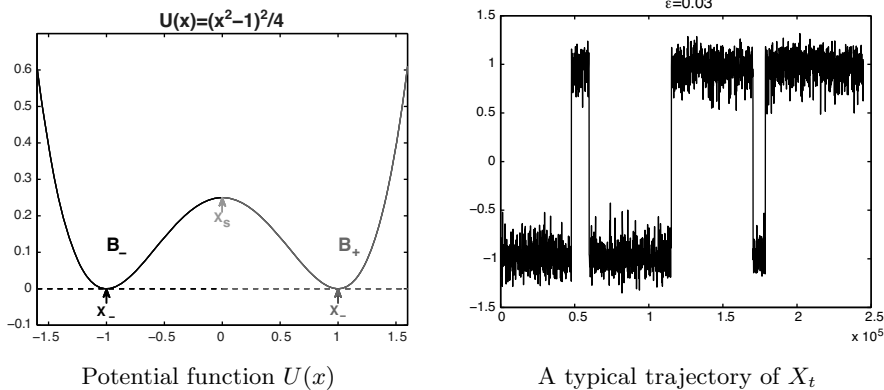
Figure 12.1. Illustration of rare events in the one-dimensional double-well potential. Left panel: The symmetric double-well potential with two metastable states at $x_+ = 1$ and $x_- = -1$. Right panel: A typical trajectory of X_t. One can see that it wanders around x_+ or x_- and hops over after sufficiently long times.

In physical terms, the local minima or the basin of attractions are called *metastable states*. Obviously, when discussing metastability, the key issue is that of the time scale. In rare event studies, one is typically concerned about the following three key questions:

(1) What is the most probable transition path? In high dimension, we should also ask the following question: How should we compute it?

(2) Where is the transition state, i.e., the neighboring saddle point, for a transition event starting from a metastable state? Presumably saddle points can be identified from the eigenvalue analysis of

the Hessian of U. However, when the dimension is high and the landscape of U is complex, this becomes nontrivial.

(3) How long is the typical transition time from a metastable state?

Our current understanding of these issues is not yet complete but we will discuss some of the most important progress that has been made.

12.2. WKB Analysis

Consider the SDEs

$$(12.3) \qquad d\boldsymbol{X}_t^\varepsilon = \boldsymbol{b}(\boldsymbol{X}_t^\varepsilon)dt + \sqrt{\varepsilon}\boldsymbol{\sigma}(\boldsymbol{X}_t^\varepsilon) \cdot d\boldsymbol{W}_t, \qquad \boldsymbol{X}_0^\varepsilon = \boldsymbol{y} \in \mathbb{R}^d.$$

We assume that the standard Lipschitz and uniform ellipticity conditions on $\boldsymbol{b}$ and $\boldsymbol{\sigma}$ hold and denote the transition PDF by $p_\varepsilon(\boldsymbol{x}, t|\boldsymbol{y})$. We are interested in the behavior of its solution for small ε. Let $\boldsymbol{X}_t^0$ be the solution of the ODE

$$\dot{\boldsymbol{X}}_t^0 = \boldsymbol{b}(\boldsymbol{X}_t^0), \qquad \boldsymbol{X}_0^0 = \boldsymbol{y}.$$

It can be shown using the law of large numbers that (cf. [**FW98**] for reference) for any fixed $T > 0$ and $\delta > 0$,

$$\lim_{\varepsilon \to 0} \mathbb{P}\left(\max_{t \in [0,T]} |\boldsymbol{X}_t^\varepsilon - \boldsymbol{X}_t^0| > \delta\right) = 0.$$

This implies that for any open set $B \subset \mathbb{R}^d$, we have

$$\lim_{\varepsilon \to 0} \int_B p_\varepsilon(\boldsymbol{x}, t|\boldsymbol{y})d\boldsymbol{x} = \begin{cases} 1, & \text{if } \boldsymbol{X}_t^0 \in B, \\ 0, & \text{otherwise,} \end{cases}$$

or equivalently $\lim_{\varepsilon \to 0} p_\varepsilon(\boldsymbol{x}, t|\boldsymbol{y}) = \delta(\boldsymbol{x} - \boldsymbol{X}_t^0)$.

Inspired by the form of probability distribution function of Brownian dynamics, we insert the Wentzel-Kramers-Brillouin (WKB) ansatz

$$p_\varepsilon(\boldsymbol{x}, t|\boldsymbol{y}) \propto \exp\left(-\varepsilon^{-1}\phi(\boldsymbol{x}, t|\boldsymbol{y})\right)$$

into the forward Kolmogorov equation associated with the SDEs (12.3)

$$(12.4) \qquad \frac{\partial p_\varepsilon}{\partial t} = -\nabla \cdot (\boldsymbol{b}(\boldsymbol{x})p_\varepsilon) + \frac{\varepsilon}{2}\nabla^2 : (\boldsymbol{A}(\boldsymbol{x})p_\varepsilon),$$

where $\boldsymbol{A}(\boldsymbol{x}) = \boldsymbol{\sigma}\boldsymbol{\sigma}^T(\boldsymbol{x}) = (a_{ij}(\boldsymbol{x}))$ is the diffusion matrix. Collecting the leading order terms gives a time-dependent Hamilton-Jacobi equation

$$(12.5) \qquad \frac{\partial \phi}{\partial t} = H(\boldsymbol{x}, \nabla_{\boldsymbol{x}}\phi),$$

where H is the Hamiltonian:

$$(12.6) \qquad H(\boldsymbol{x}, \boldsymbol{p}) = \boldsymbol{b}^T(\boldsymbol{x})\boldsymbol{p} + \frac{1}{2}\boldsymbol{p}^T\boldsymbol{A}(\boldsymbol{x})\boldsymbol{p} = \sum_i b_i p_i + \frac{1}{2}\sum_{ij} a_{ij}p_i p_j.$$

We will call $\boldsymbol{p}$ the momentum variable in analogy with classical mechanics [**Arn89, Gol80**]. The solution of this equation can be characterized by a variational principle:

(12.7) $\phi(\boldsymbol{x}, t | \boldsymbol{y}) = \inf_{\varphi} \big\{ I_t[\boldsymbol{\varphi}] : \boldsymbol{\varphi}$ is absolutely continuous in $[0, t]$

$$\text{and } \boldsymbol{\varphi}(0) = \boldsymbol{y}, \boldsymbol{\varphi}(t) = \boldsymbol{x} \big\},$$

where I_t is the action functional

(12.8) $$I_t[\boldsymbol{\varphi}] = \int_0^t L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) ds.$$

Here L is the Lagrangian:

(12.9) $$L(\boldsymbol{x}, \boldsymbol{z}) = \frac{1}{2} (\boldsymbol{z} - \boldsymbol{b}(\boldsymbol{x}))^T \boldsymbol{A}^{-1}(\boldsymbol{x})(\boldsymbol{z} - \boldsymbol{b}(\boldsymbol{x})).$$

The Lagrangian L is the dual of the Hamiltonian H in the sense of Legendre-Fenchel transform

$$L(\boldsymbol{x}, \boldsymbol{z}) = \sup_{\boldsymbol{p}} \{ \boldsymbol{p} \cdot \boldsymbol{z} - H(\boldsymbol{x}, \boldsymbol{p}) \}.$$

The readers are referred to [**Gol80, Arn89**] for more details about these connections.

12.3. Transition Rates

Transition rates can be studied using the mean first exit times from the metastable state. First let us consider the one-dimensional diffusion process

(12.10) $$dX_t = -\partial_x U(X_t) dt + \sqrt{2\varepsilon} dW_t.$$

We assume that $U(x)$ has two local minima at $x_- = -1$ and $x_+ = 1$ and a local maximum, which in this case is also a saddle point, at $x_s = 0$. We are interested in estimating the mean first passage time from x_- to x_+.

First recall the result in Section 8.7 that for X_t in the domain $[a, b]$ with reflecting boundary at a and absorbing boundary at b, the mean first passage time $\tau(x) = \mathbb{E}^x \tau_b$, where $\tau_b = \inf\{t \geq 0 : X_t = b\}$, satisfies the differential equation

(12.11) $\mathcal{A}\tau(x) = -U'(x)\tau'(x) + \varepsilon\tau''(x) = -1$

$$\text{for } x \in (a, b) \text{ and } \tau|_{x=b} = 0, \ \tau'|_{x=a} = 0.$$

The solution to this problem is given simply by

(12.12) $$\tau(x) = \frac{1}{\epsilon} \int_x^b e^{\frac{U(y)}{\varepsilon}} \int_a^y e^{-\frac{U(z)}{\varepsilon}} dz dy.$$

Now let us take $a \to -\infty$, $b \to x_+$, and $x = x_-$. We obtain

$$(12.13) \qquad \tau(x_-) = \frac{1}{\epsilon} \int_{x_-}^{x_+} \int_{-\infty}^{y} e^{\frac{U(y)-U(z)}{\varepsilon}} \, dz \, dy.$$

Under the condition that $U''(x_-)$ and $|U''(x_s)|$ are positive, using Laplace asymptotics on the (y, z)-plane, we have, to leading order,

$$(12.14) \qquad \tau(x) \approx \tau(x_-) \sim \frac{2\pi}{\sqrt{|U''(x_s)|U''(x_-)}} e^{\frac{\delta U}{\varepsilon}}$$

for any $x \le x_s - \delta_0$, where $\delta U = U(x_s) - U(x_-)$ and δ_0 is a positive constant.

Equation (12.14) tells us that the transition time is exponentially large in $O(\delta U / \varepsilon)$. This is typical for rare events. The transition time is insensitive to where the particle starts from. Even if the particle starts close to x_s, most likely it will first relax to the neighborhood of x_- and then transit to x_+. The choice of the first passage point after x_s does not affect much the final result.

In the case considered above, it is natural to define the transition rate

$$(12.15) \qquad k = \frac{1}{\tau(x_-)} = \frac{\sqrt{|U''(x_s)|U''(x_-)}}{2\pi} \exp\left(-\frac{\delta U}{\varepsilon}\right).$$

This is the celebrated Kramers reaction rate formula, also referred to as the Arrhenius's law of reaction rates. Here δU is called the activation energy. In the multidimensional case when $\boldsymbol{x}_s$ is an index-one saddle point, one can also derive the reaction rate formula using similar ideas:

$$(12.16) \qquad k = \frac{|\lambda_s|}{2\pi} \sqrt{\frac{\det H_-}{|\det H_s|}} \exp\left(-\frac{\delta U}{\varepsilon}\right).$$

Here $\lambda_s < 0$ is the unique negative eigenvalue of the Hessian at $\boldsymbol{x}_s$, $H_s = \nabla^2 U(\boldsymbol{x}_s)$, $H_- = \nabla^2 U(\boldsymbol{x}_-)$. Interested readers are referred to [**Sch80**] for more details.

12.4. Large Deviation Theory and Transition Paths

The WKB analysis in this chapter suggests that the probability

$$\mathbb{P}(\boldsymbol{X}_t^\varepsilon \in B) \asymp \exp(-\varepsilon^{-1} C) \quad \text{as } \varepsilon \to 0,$$

where B is an open set. The constant C is positive if $\boldsymbol{x}(t) \notin B$, and 0 otherwise. Large deviation theory gives a rigorous mathematical foundation for these statements. In particular, for SDEs, large deviation theory gives the following result [**DZ98**, **Var84**]:

Theorem 12.1. *Under the conditions that $\boldsymbol{b}(\boldsymbol{x})$ and $\boldsymbol{\sigma}(\boldsymbol{x})$ are bounded and Lipschitz and that $\boldsymbol{A}(\boldsymbol{x})$ is uniformly elliptic, we have that for any $T > 0$, the following large deviation estimates for $\boldsymbol{X}^\varepsilon$ defined in (12.3) hold.*

(i) *Upper bound. For any closed set $F \subset (C[0,T])^d$,*

$$\limsup_{\varepsilon \to 0} \varepsilon \log \mathbb{P}(\boldsymbol{X}^\epsilon \in F) \leq - \inf_{\boldsymbol{\varphi} \in F} I_T[\boldsymbol{\varphi}].$$

(ii) *Lower bound. For any open set $G \subset (C[0,T])^d$,*

$$\liminf_{\varepsilon \to 0} \varepsilon \log \mathbb{P}(\boldsymbol{X}^\epsilon \in G) \geq - \inf_{\boldsymbol{\varphi} \in G} I_T[\boldsymbol{\varphi}].$$

Here the rate functional $I_T[\boldsymbol{\varphi}]$ is defined in (12.8)–(12.9) if $\boldsymbol{\varphi}$ is absolutely continuous, $\dot{\boldsymbol{\varphi}}$ is square integrable, and $\boldsymbol{\varphi}(0) = \boldsymbol{y}$; otherwise $I_T[\boldsymbol{\varphi}] = \infty$.

The proof of Theorem 12.1 is beyond the scope of this book. We will give a formal derivation using path integrals.

It is obvious that the one-dimensional SDE

$$dX_t^\varepsilon = \sqrt{\varepsilon} dW_t, \qquad X_0 = 0,$$

has the solution $X_t^\varepsilon = \sqrt{\varepsilon} W_t$. Using the path integral representation, we have that the probability distribution induced by $\{X_t^\varepsilon\}$ on $C[0,T]$ can be formally written as

(12.17)
$$dP^\varepsilon[\varphi] = Z^{-1} \exp\left(-\frac{1}{2\varepsilon} \int_0^T |\dot{\varphi}(s)|^2 ds\right) \mathcal{D}\varphi = Z^{-1} \exp\left(-\frac{1}{\varepsilon} I_T[\varphi]\right) \mathcal{D}\varphi.$$

This gives the statement of the theorem for the simple case in (12.4). Now let us consider the general case:

$$dX_t^\varepsilon = b(X_t^\varepsilon) dt + \sqrt{\varepsilon} \sigma(X_t^\varepsilon) dW_t, \qquad X_0 = y.$$

To understand how the action functional I_T has the form (12.8)–(12.9), we can reason formally as follows. From the SDE we have $\dot{W}_t = (\sqrt{\varepsilon})^{-1} \sigma^{-1}(X_t^\varepsilon) \cdot (\dot{X}_t^\varepsilon - b(X_t^\varepsilon))$. Hence

$$\int_0^T \dot{W}_t^2 dt = \varepsilon^{-1} \int_0^T |\sigma^{-1}(X_t^\varepsilon)(\dot{X}_t^\varepsilon - b(X_t^\varepsilon))|^2 dt.$$

Using the formal expression for the distribution (12.17) induced by $\sqrt{\varepsilon} W_t$, we obtain

$$dP^\varepsilon[\varphi] = Z^{-1} \exp\left(-\frac{1}{\varepsilon} I_T[\varphi]\right) \mathcal{D}\varphi.$$

From Theorem 12.1, we have

$$-\varepsilon \log P^\varepsilon(F) \sim \inf_{\varphi \in F} I_T[\varphi], \quad \varepsilon \to 0,$$

for a reasonable set F in $C[0,T]$. This motivates a natural characterization of the most probable transition paths in the limit $\varepsilon \to 0$. Given a set of

paths F in $C[0, T]$ we can define the optimal path in F as the path $\varphi^\star$ that has the maximum probability or minimal action

$$I_T[\varphi^\star] = \inf_{\varphi \in F} I_T[\varphi]$$

if this minimization problem has a solution. Such a path is called a *minimum (or least) action path*.

Consider the special case of Brownian dynamics when $\boldsymbol{b}(\boldsymbol{x}) = -\nabla U(\boldsymbol{x})$ and $\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{I}$. Assume that $\boldsymbol{x}_-$ and $\boldsymbol{x}_+$ are two neighboring local minima of U separated by a saddle point $\boldsymbol{x}_s$. We are interested in the minimum action path among all possible transition times T

(12.18) $$\inf_{T > 0} \inf_{\varphi(0) = \boldsymbol{x}_-, \varphi(T) = \boldsymbol{x}_+} I_T[\boldsymbol{\varphi}].$$

We have the following characterization.

Lemma 12.2. *The minimum action path $\boldsymbol{\varphi}$ of the Brownian dynamics is comprised of two parts defined through functions $\boldsymbol{\varphi}_1$ and $\boldsymbol{\varphi}_2$ by*

(12.19) $$\dot{\boldsymbol{\varphi}}_1(s) = \nabla U(\boldsymbol{\varphi}_1(s)), \quad \boldsymbol{\varphi}_1(-\infty) = \boldsymbol{x}_-, \quad \boldsymbol{\varphi}_1(\infty) = \boldsymbol{x}_s,$$

(12.20) $$\dot{\boldsymbol{\varphi}}_2(s) = -\nabla U(\boldsymbol{\varphi}_2(s)), \quad \boldsymbol{\varphi}_2(-\infty) = \boldsymbol{x}_s, \quad \boldsymbol{\varphi}_2(\infty) = \boldsymbol{x}_+,$$

and the minimum action is given by

(12.21) $$I^* = I_\infty(\boldsymbol{\varphi}_1) + I_\infty(\boldsymbol{\varphi}_2) = I_\infty(\boldsymbol{\varphi}_1) = 2(U(\boldsymbol{x}_s) - U(\boldsymbol{x}_-)) = 2\delta U.$$

Proof. It is easy to see that the minimum in T in (12.18) is attained when $T = \infty$ since $\boldsymbol{x}_-$, $\boldsymbol{x}_+$, and $\boldsymbol{x}_s$ are all critical points (see Exercise 12.2). To see why the minimization problem in (12.18) is solved by the path defined above, we first note that

(12.22) $$I_\infty[\boldsymbol{\varphi}_1] = 2\delta U, \quad I_\infty[\boldsymbol{\varphi}_2] = 0.$$

In addition, for any path $\boldsymbol{\varphi}$ connecting $\boldsymbol{x}_-$ and a point $\tilde{\boldsymbol{x}}_s$ on the separatrix that separates the basins of attraction of $\boldsymbol{x}_-$ and $\boldsymbol{x}_+$, we have

$$I_\infty[\boldsymbol{\varphi}] = \frac{1}{2} \int_{\mathbb{R}} (\dot{\boldsymbol{\varphi}} - \nabla U, \dot{\boldsymbol{\varphi}} - \nabla U) dt + 2 \int_{\mathbb{R}} \dot{\boldsymbol{\varphi}} \cdot \nabla U \, dt$$

$$\geq 2 \int_{\mathbb{R}} \dot{\boldsymbol{\varphi}} \cdot \nabla U \, dt = 2(U(\tilde{\boldsymbol{x}}_s) - U(\boldsymbol{x}_-)) \geq 2\delta U$$

since $\boldsymbol{x}_s$ is the minimum of U on the separatrix. Combining the results above, we obtain $I^* = 2\delta U$. $\qquad\square$

Thus the most probable transition path is the combination of $\boldsymbol{\varphi}_1$ and $\boldsymbol{\varphi}_2$: $\boldsymbol{\varphi}_1$ goes along the steepest *ascent* direction and therefore requires the

action of the noise, and $\boldsymbol{\varphi}_2$ simply follows the steepest *descent* dynamics and therefore does not require help from the noise. Both satisfy

$$(12.23) \qquad \dot{\boldsymbol{\varphi}}(s) = \pm \nabla U(\boldsymbol{\varphi}(s)).$$

Paths that satisfy this equation are called the *minimum energy path* (MEP). One can write (12.23) equivalently as

$$(12.24) \qquad \big(\nabla U(\boldsymbol{\varphi})\big)^{\perp} = 0,$$

where $(\nabla U(\boldsymbol{\varphi}))^{\perp}$ denotes the component of $\nabla U(\boldsymbol{\varphi})$ normal to the curve described by $\boldsymbol{\varphi}$.

An important feature of the minimum energy paths is that they pass through saddle points, more precisely, index one saddle points, i.e., saddle points at which the Hessian of U has one negative eigenvalue. One can imagine the following coarse-grained picture: The configuration space is mapped into a network where the basins of the local minima are the nodes of the network, neighboring basins are connected by edges, each edge is associated with an index one saddle point. At an exponentially long time scale, the dynamics of the diffusion process is effectively described by a Markov chain on this network, with hopping rates computed by a formula similar to (12.15). For a concrete application of this reduction in micromagnetics, the readers are referred to [**ERVE03**].

12.5. Computing the Minimum Energy Paths

The characterization of the MEP (12.24) yields a natural way for computing the optimal transition path connecting two metastable states $\boldsymbol{x}_-$ and $\boldsymbol{x}_+$ for the Brownian dynamics, by a pseuso-steepest descent flow

$$(12.25) \qquad \partial_t \boldsymbol{\varphi}(\alpha, t) = -(\nabla U(\boldsymbol{\varphi}))^{\perp}, \qquad \boldsymbol{\varphi}(0) = \boldsymbol{x}_-, \quad \boldsymbol{\varphi}(1) = \boldsymbol{x}_+,$$

where $\boldsymbol{\varphi}(\alpha, t)$ is a parametric curve, $\alpha \in (0, 1)$ is the parameterization, $\hat{\boldsymbol{\tau}} = \boldsymbol{\varphi}_\alpha / |\boldsymbol{\varphi}_\alpha|$, and

$$(\nabla U(\boldsymbol{\varphi}))^{\perp} = \nabla U(\boldsymbol{\varphi}) - (\hat{\boldsymbol{\tau}} \otimes \hat{\boldsymbol{\tau}}) \cdot \nabla U(\boldsymbol{\varphi}).$$

This can also be expressed as

$$(12.26) \qquad \partial_t \boldsymbol{\varphi}(\alpha, t) = -\nabla U(\boldsymbol{\varphi}) + r\hat{\boldsymbol{\tau}}, \qquad \boldsymbol{\varphi}(0) = \boldsymbol{x}_-, \quad \boldsymbol{\varphi}(1) = \boldsymbol{x}_+.$$

The function r is simply a Lagrange multiplier in order to ensure some particular parameterization for the curve. A common choice is the equal-arclength parametrization. In this case, the following equation holds:

$$(|\boldsymbol{\varphi}_\alpha|)_\alpha = 0.$$

This is called the *string method* [**ERVE02**] in the literature.

To implement (12.26), one can proceed in the following two simple steps:

Step 1. Evolution of the steepest descent dynamics. For example, one can simply apply the forward Euler scheme

$$\tilde{\varphi}_i^{n+1} = \varphi_i^n - \Delta t \nabla U(\varphi_i^n)$$

or Runge-Kutta type schemes for one or several steps.

Step 2. Reparameterization of the string. One can redistribute the points $\{\tilde{\varphi}_i^{n+1}\}$ according to equi-arclength (or other parameterization). The positions of the new points along the string can be obtained by simple interpolation:

   a) Define $s_0 = 0$, $s_i = s_{i-1} + |\tilde{\varphi}_i^n - \tilde{\varphi}_{i-1}^n|$ for $i = 1, \ldots, N$, and $\tilde{\alpha}_i = s_i/s_N$.

   b) Interpolate φ_i^{n+1} at $s_i = i/N$ using the data $\{\tilde{\alpha}_i, \tilde{\varphi}_i^{n+1}\}$. Here $\tilde{\varphi}_i^{n+1}$ is the value of φ^{n+1} at $\tilde{\alpha}_i$.

Here we have assumed that the arclength is normalized so that the total normalized arclength is 1.

A simple illustration of the application of the string method is shown in Figure 12.2.
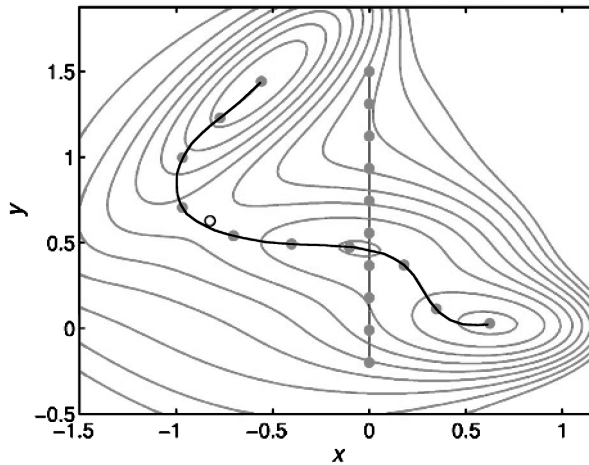
Figure 12.2. Illustration of the performance of the string method for the Mueller potential [**ERVE07**]. The vertical line is the initial string. The other curve is the calculated MEP.

12.6. Quasipotential and Energy Landscape

Quasipotential, introduced by Freidlin and Wentzell, is a very useful notion for general SDEs and is intimately related to rare events. Given a point

$\boldsymbol{y} \in \mathbb{R}^d$, the quasipotential at $\boldsymbol{x}$ with respect to $\boldsymbol{y}$ is given by

(12.27)
$$V(\boldsymbol{x}; \boldsymbol{y}) = \inf_{T>0} \inf_{\boldsymbol{\varphi}(0)=\boldsymbol{y}, \boldsymbol{\varphi}(T)=\boldsymbol{x}} I_T[\boldsymbol{\varphi}].$$

For the so-called gradient systems when

$$\boldsymbol{b}(\boldsymbol{x}) = -\nabla U(\boldsymbol{x}), \quad \boldsymbol{\sigma} = 2\boldsymbol{I},$$

the quasipotential coincides with the usual potential $V(\boldsymbol{x}; \boldsymbol{y}) = U(\boldsymbol{x})$ if $\boldsymbol{x}$ belongs to the basin of attraction of a local minimum $\boldsymbol{y}$ (i.e., following the steepest descent paths from $\boldsymbol{x}$, it will reach $\boldsymbol{y}$ finally). This gives the rationale for calling V the quasipotential: It generalizes the concept of potential to nongradient systems.

Below we will discuss some basic properties of the quasipotential. For simplicity we only consider the case when $\boldsymbol{\sigma} = \boldsymbol{I}$. The stated results hold for the general case.

One fundamental fact about the quasipotential $V(\boldsymbol{x}; \boldsymbol{y})$ is that it is not necessarily smooth but it is locally Lipschitz continuous with respect to $\boldsymbol{x}$ on any bounded domain. To see this, let us define

$$M = \sup_{\boldsymbol{x} \in D} |\boldsymbol{b}(\boldsymbol{x})|$$

for a bounded domain D. Then we have

(12.28) $V(\boldsymbol{x}; \boldsymbol{y}) \leq V(\boldsymbol{z}; \boldsymbol{y}) + K|\boldsymbol{x} - \boldsymbol{z}|$ and $V(\boldsymbol{z}; \boldsymbol{y}) \leq V(\boldsymbol{x}; \boldsymbol{y}) + K|\boldsymbol{x} - \boldsymbol{z}|$

where $K = 2(M^2 + 1)$. This can be proved by constructing paths consisting of two parts which connect $\boldsymbol{y}$ to $\boldsymbol{x}$ and then $\boldsymbol{x}$ to $\boldsymbol{z}$. The part from $\boldsymbol{x}$ to $\boldsymbol{z}$ can be taken as

$$\boldsymbol{\varphi}(t) = \boldsymbol{x} + t\frac{\boldsymbol{z} - \boldsymbol{x}}{|\boldsymbol{z} - \boldsymbol{x}|}, \quad t \in \big[0, |\boldsymbol{z} - \boldsymbol{x}|\big].$$

The part from $\boldsymbol{y}$ to $\boldsymbol{x}$ can be arbitrary. Taking infimum with respect to all paths, we obtain (12.28).

Quasipotential can be studied using the Hamilton-Jacobi theory in calculus of variations. From the definition (12.27), we have

(12.29)
$$V(\boldsymbol{x}; \boldsymbol{y}) = \inf_{t>0} \phi(\boldsymbol{x}, t|\boldsymbol{y})$$

where $\phi(\boldsymbol{x}, t|\boldsymbol{y})$ is defined in (12.7). Since $\phi(\boldsymbol{x}, t|\boldsymbol{y})$ satisfies (12.5) and is a monotonically decreasing function of t and is bounded from below if $\boldsymbol{y}$ is a stable steady state of the dynamics $\dot{\boldsymbol{x}} = \boldsymbol{b}(\boldsymbol{x})$, we obtain a Hamilton-Jacobi equation for $V(\boldsymbol{x}; \boldsymbol{y})$:

(12.30)
$$H(\boldsymbol{x}, \nabla_{\boldsymbol{x}} V) = 0,$$

where H is the Hamiltonian (12.6). Indeed, the infimum of $\phi(\boldsymbol{x}, t | \boldsymbol{y})$ as a function of t is only achieved at $t = \infty$ if $\boldsymbol{y}$ is a metastable state, and we can represent $V(\boldsymbol{x}; \boldsymbol{y})$ by

$$(12.31) \qquad V(\boldsymbol{x}; \boldsymbol{y}) = \inf_{\boldsymbol{\varphi}(-\infty) = \boldsymbol{y}, \boldsymbol{\varphi}(0) = \boldsymbol{x}} \int_{-\infty}^{0} L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) dt$$

upon a suitable shift of time.

The steady Hamilton-Jacobi equation (12.30) motivates an important characterization for the minimum action path. It is well known from the calculus of variations that the minimizer of (12.31) satisfies the Hamiltonian dynamics

$$(12.32) \qquad \frac{d\boldsymbol{\varphi}}{dt} = \nabla_{\boldsymbol{p}} H(\boldsymbol{\varphi}, \boldsymbol{p}), \quad \frac{d\boldsymbol{p}}{dt} = -\nabla_{\boldsymbol{\varphi}} H(\boldsymbol{\varphi}, \boldsymbol{p})$$

and $H(\boldsymbol{\varphi}, \boldsymbol{p})$ is constant along the minimizing path. Here $\boldsymbol{p} = \partial L / \partial \dot{\boldsymbol{\varphi}}$. Take $\rho : (-\infty, 0] \to (0, \infty)$ to be any positive measurable function integrable on finite intervals. Define

$$s(t) = \int_{0}^{t} \rho(u) du, \quad t \in (-\infty, 0]$$

and $\boldsymbol{\psi}(s) = \boldsymbol{\varphi}(t)$. We can extend $\boldsymbol{\psi}$ by setting $\boldsymbol{\psi} \equiv \boldsymbol{y}$ on $(-\infty, s(-\infty)]$ if necessary. By the minimality of $\boldsymbol{\varphi}$, we have

$$\int_{-\infty}^{0} L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) dt \leq \int_{-\infty}^{0} L(\boldsymbol{\psi}, \dot{\boldsymbol{\psi}}) ds = \int_{-\infty}^{0} L(\boldsymbol{\varphi}, \rho^{-1}(t) \dot{\boldsymbol{\varphi}}) \rho(t) dt.$$

The arbitrariness of ρ implies that for any $t \in (-\infty, 0]$

$$L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) = \inf_{\theta > 0} L(\boldsymbol{\varphi}, \theta^{-1} \dot{\boldsymbol{\varphi}}) \theta,$$

which yields

$$0 = \frac{d}{d\theta} \left(L(\boldsymbol{\varphi}, \theta^{-1} \dot{\boldsymbol{\varphi}}) \theta \right) \big|_{\theta = 1} = L(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) - \dot{\boldsymbol{\varphi}} \frac{\partial L}{\partial \dot{\boldsymbol{\varphi}}} = -H(\boldsymbol{\varphi}, \boldsymbol{p}).$$

That is why the minimum action path starting from any critical point of the dynamics $\dot{\boldsymbol{x}} = \boldsymbol{b}(\boldsymbol{x})$ is also called the *zero energy path*.

For gradient systems, the potential energy barrier quantifies the difficulty of transitions. Quasipotential plays a similar role for nongradient systems. We show this by revisiting the exit problem. Let $\boldsymbol{y} = \boldsymbol{0}$ be a stable fixed point of the dynamical system $\dot{\boldsymbol{x}} = \boldsymbol{b}(\boldsymbol{x})$ and let D be a smooth part of the domain of attraction of $\boldsymbol{0}$ which also contains $\boldsymbol{0}$ in its interior. Consider the diffusion process $\boldsymbol{X}^{\varepsilon}$, (12.3), initiated at $\boldsymbol{X}_{0}^{\varepsilon} = \boldsymbol{0}$. It is obvious that $V(\boldsymbol{0}; \boldsymbol{0}) = 0$ by definition. We are interested in the first exit time of $\boldsymbol{X}^{\varepsilon}$ from D, T_{ε} and the most probable point of exit on ∂D, $X_{T_{\varepsilon}}^{\varepsilon}$, as $\varepsilon \to 0$.

Theorem 12.3. *Assume that* $(\boldsymbol{b}(\boldsymbol{x}), \hat{\boldsymbol{n}}(\boldsymbol{x})) < 0$ *for* $\boldsymbol{x} \in \partial D$, *where* $\hat{\boldsymbol{n}}$ *is the outward normal of* ∂D. *Then*

$$\lim_{\varepsilon \to 0} \varepsilon \log \mathbb{E} T_\varepsilon = \min_{\boldsymbol{x} \in \partial D} V(\boldsymbol{x}; \boldsymbol{0})$$

and if there exists a unique minimizer $\boldsymbol{x}_0$ *of* V *at* ∂D, *i.e.,*

$$V(\boldsymbol{x}_0; 0) = \min_{\boldsymbol{x} \in \partial D} V(\boldsymbol{x}; 0),$$

then for any $\delta > 0$,

$$\mathbb{P}\left(|\boldsymbol{X}_{T_\varepsilon}^\varepsilon - \boldsymbol{x}_0| < \delta\right) \to 1 \quad as\ \varepsilon \to 0.$$

The proof can be found in [**FW98**].

So far, the quasipotential $V(\boldsymbol{x}; \boldsymbol{y})$ is defined through the infimum of the action $I_T[\boldsymbol{\varphi}]$ with respect to the paths $\boldsymbol{\varphi}$ and time T. From the Maupertuis principle (the least action principle) in classical mechanics, the optimization with respect to T can be removed by using the formulation

$$(12.33) \qquad V(\boldsymbol{x}; \boldsymbol{y}) = \inf_{H(\boldsymbol{\varphi}, \boldsymbol{p})=0} \int_{\tilde{\gamma}} \boldsymbol{p} \cdot d\boldsymbol{\varphi} = \inf_{H(\boldsymbol{\varphi}, \boldsymbol{p})=0, \boldsymbol{p}=\partial L/\partial \dot{\boldsymbol{\varphi}}} \int_{\gamma} \boldsymbol{p} \cdot d\boldsymbol{\varphi},$$

where the first equality is the minimization with respect to the path $(\boldsymbol{\varphi}(t), \boldsymbol{p}(t))$ in $\mathbb{R}^{2d}$ that connects $\boldsymbol{y}$ and $\boldsymbol{x}$ such that $H(\boldsymbol{\varphi}, \boldsymbol{p}) = 0$, and the second equality is with respect to the path $\boldsymbol{\varphi}(t)$ in $\mathbb{R}^d$ that connects $\boldsymbol{y}$ and $\boldsymbol{x}$ such that $\boldsymbol{p} = \partial L/\partial \dot{\boldsymbol{\varphi}}$ and $H(\boldsymbol{\varphi}, \boldsymbol{p}) = 0$ [**Arn89**].

In this formulation, let us choose a parametrization such that $\alpha \in [0, 1]$ and $\boldsymbol{\varphi} \in (C[0, 1])^d$. From the constraints, we obtain

$$(12.34) \qquad H(\boldsymbol{\varphi}, \boldsymbol{p}) = \boldsymbol{b}(\boldsymbol{\varphi}) \cdot \boldsymbol{p} + \frac{1}{2}|\boldsymbol{p}|^2 = 0, \quad \boldsymbol{p} = \frac{\partial L}{\partial \dot{\boldsymbol{\varphi}}} = \lambda \boldsymbol{\varphi}'(\alpha) - \boldsymbol{b}(\boldsymbol{\varphi}),$$

where $\lambda \geq 0$ is the result of the parameter change from t to α. Solving (12.34) we get

$$(12.35) \qquad \lambda = \frac{|\boldsymbol{b}(\boldsymbol{\varphi})|}{|\boldsymbol{\varphi}'|}, \quad \boldsymbol{p} = \frac{|\boldsymbol{b}(\boldsymbol{\varphi})|}{|\boldsymbol{\varphi}'|}\boldsymbol{\varphi}' - \boldsymbol{b}.$$

Thus

$$(12.36) \qquad V(\boldsymbol{x}; \boldsymbol{y}) = \inf_{\boldsymbol{\varphi}(0)=\boldsymbol{y}, \boldsymbol{\varphi}(1)=\boldsymbol{x}} \hat{I}[\boldsymbol{\varphi}],$$

where

$$(12.37) \qquad \hat{I}[\boldsymbol{\varphi}] = \int_0^1 \left(|\boldsymbol{b}(\boldsymbol{\varphi})||\boldsymbol{\varphi}'| - \boldsymbol{b}(\boldsymbol{\varphi}) \cdot \boldsymbol{\varphi}'\right) d\alpha.$$

The formulation (12.36) and (12.37) is preferable in numerical computations since it removes the additional optimization with respect to time and can be realized in an intrinsic way in the space of curves.

This result can also be obtained from a direct calculation.

Lemma 12.4. *We have*

(12.38) $$V(\boldsymbol{x};\boldsymbol{y}) = \inf_{t>0} \inf_{\boldsymbol{\varphi}(0)=\boldsymbol{y},\boldsymbol{\varphi}(t)=\boldsymbol{x}} I_t[\boldsymbol{\varphi}] = \inf_{\boldsymbol{\psi}(0)=\boldsymbol{y},\boldsymbol{\psi}(1)=\boldsymbol{x}} \hat{I}[\boldsymbol{\psi}].$$

Proof. We have for any fixed $t > 0$

$$I_t[\boldsymbol{\varphi}] = \frac{1}{2}\int_0^t |\dot{\boldsymbol{\varphi}} - \boldsymbol{b}(\boldsymbol{\varphi})|^2 ds = \frac{1}{2}\int_0^t \left(|\dot{\boldsymbol{\varphi}}|^2 + |\boldsymbol{b}(\boldsymbol{\varphi})|^2 - 2\boldsymbol{b}(\boldsymbol{\varphi})\cdot\dot{\boldsymbol{\varphi}}\right) ds$$

(12.39) $$\geq \int_0^t \left(|\boldsymbol{b}(\boldsymbol{\varphi})||\dot{\boldsymbol{\varphi}}| - \boldsymbol{b}(\boldsymbol{\varphi})\cdot\dot{\boldsymbol{\varphi}}\right) ds = \int_0^1 \left(|\boldsymbol{b}(\boldsymbol{\psi})||\boldsymbol{\psi}'| - \boldsymbol{b}(\boldsymbol{\psi})\cdot\boldsymbol{\psi}'\right) d\alpha,$$

where $\boldsymbol{\psi}(\alpha) := \boldsymbol{\varphi}(\tau(\alpha))$ and $\tau : [0,1] \to [0,t]$ is any differentiable and monotonically increasing parameterization. The equality holds if and only if $|\boldsymbol{b}(\boldsymbol{\varphi})| = |\dot{\boldsymbol{\varphi}}|$. This proves

$$\inf_{t>0} \inf_{\boldsymbol{\varphi}(0)=\boldsymbol{y},\boldsymbol{\varphi}(t)=\boldsymbol{x}} I_t[\boldsymbol{\varphi}] \geq \inf_{\boldsymbol{\psi}(0)=\boldsymbol{y},\boldsymbol{\psi}(1)=\boldsymbol{x}} \hat{I}[\boldsymbol{\psi}].$$

On the other hand, if $\boldsymbol{\psi}(\alpha)$ is a global minimizer of (12.39), we can always choose the reparameterization $\tau(\alpha)$ such that

$$\frac{d\tau}{d\alpha} = \frac{|\boldsymbol{\psi}'|}{|\boldsymbol{b}(\boldsymbol{\psi})|}, \quad \alpha \in [0,1], \quad \tau(\alpha_0) = t_0, \ \alpha_0 \in (0,1).$$

We assume that the endpoints τ_1 and τ_2 are finite and $\boldsymbol{\varphi}(\tau_1) = \boldsymbol{y}$, $\boldsymbol{\varphi}(\tau_2) = \boldsymbol{x}$. In this case, we can redefine $\boldsymbol{\varphi}(\tau)$ on $[0, t_2 - t_1]$ by shifting the time coordinate, and this operation does not change the action value. It is not difficult to check that the choice of α_0 and t_0 does not affect the overall optimization. This results in $|\dot{\boldsymbol{\varphi}}| = |\boldsymbol{b}(\boldsymbol{\varphi})|$ and proves the other part. The case when $\tau_1 = -\infty$ or $\tau_2 = \infty$ can be proved with similar idea. $\quad\square$

Consider again the exit problem from the basin of attraction of the metastable state $\boldsymbol{y} = \boldsymbol{0}$. We suppose that the quasipotential is $U(\boldsymbol{x}) = V(\boldsymbol{x};\boldsymbol{y})$, which satisfies the steady Hamilton-Jacobi equation. Define

(12.40) $$\boldsymbol{l}(\boldsymbol{x}) = \boldsymbol{b}(\boldsymbol{x}) + \nabla U(\boldsymbol{x}).$$

We have $\nabla U(\boldsymbol{x}) \cdot \boldsymbol{l}(\boldsymbol{x}) = 0$ from the Hamilton-Jacobi equation (12.30). Assume $U(\boldsymbol{0}) = 0$ and thus $U \geq 0$ elsewhere. Using similar strategies to the proof of Lemma 12.2, we get

$$I_T[\boldsymbol{\varphi}] = \frac{1}{2}\int_0^T |\dot{\boldsymbol{\varphi}} - \nabla U(\boldsymbol{\varphi}) - \boldsymbol{l}(\boldsymbol{\varphi})|^2 dt + 2\int_0^T \dot{\boldsymbol{\varphi}}\cdot\nabla U(\boldsymbol{\varphi}) ds$$
$$\geq 2(U(\boldsymbol{x}) - U(\boldsymbol{0})),$$

where the equality holds only when

$$\dot{\boldsymbol{\varphi}} = \nabla U(\boldsymbol{\varphi}) + \boldsymbol{l}(\boldsymbol{\varphi}).$$

This derivation shows that the quasipotential with respect to $\mathbf{0}$ has the form

$$V(\boldsymbol{x}; \mathbf{0}) = 2(U(\boldsymbol{x}) - U(\mathbf{0}))$$

and the most probable path from $\mathbf{0}$ to $\boldsymbol{x}$ is not of a pure gradient type such as $\dot{\boldsymbol{\varphi}} = \nabla U(\boldsymbol{\varphi})$ but involves the nongradient term $\boldsymbol{l}(\boldsymbol{\varphi})$. The decomposition (12.40) suggests that the quasipotential plays the role of the Lyapunov function for the deterministic ODEs

$$\frac{dU(\boldsymbol{x}(t))}{dt} = \nabla U(\boldsymbol{x}) \cdot \frac{d\boldsymbol{x}}{dt} = -|\nabla U(\boldsymbol{x})|^2 \leq 0.$$

Quasipotential measures the action required to hop from one point to another. It depends on the choice of the starting point $\boldsymbol{y}$, which is usually taken as a stable fixed point of $\boldsymbol{b}$. In this sense, $V(\boldsymbol{x}; \boldsymbol{y})$ should be thought of as *local quasipotentials* of the system if it has more than one stable fixed points. On the other hand, we can introduce another potential by defining

$$(12.41) \qquad U(\boldsymbol{x}) = -\lim_{\varepsilon \to 0} \varepsilon \log p_\infty^\varepsilon(\boldsymbol{x}),$$

where $p_\infty^\varepsilon(\boldsymbol{x})$ is the invariant measure of the diffusion defined by

$$(12.42) \qquad p_\infty^\varepsilon(\boldsymbol{x}) = \lim_{t \to \infty} p_\varepsilon(\boldsymbol{x}, t | \boldsymbol{y}).$$

This definition of U does not depend on the starting point $\boldsymbol{y}$, which is called the *global quasipotential* of the dynamics (12.3). Note that the two limits cannot be exchanged:

$$U(\boldsymbol{x}) = -\lim_{\varepsilon \to 0} \lim_{t \to \infty} \varepsilon \log p_\varepsilon(\boldsymbol{x}, t | \boldsymbol{y}) \neq -\lim_{t \to \infty} \lim_{\varepsilon \to 0} \varepsilon \log p_\varepsilon(\boldsymbol{x}, t | \boldsymbol{y}) = V(\boldsymbol{x}; \boldsymbol{y}).$$

However, it can be shown that the local functions $V(\boldsymbol{x}; \boldsymbol{y})$ can be pruned and stuck together to form the global quasipotential, $U(\boldsymbol{x})$. The readers may refer to [**FW98, ZL16**] for more details.

Exercises

12.1. Assume that $\boldsymbol{x}_s$ is an extremal point of the potential function U and that the Hessian $H_s = \nabla^2 U(\boldsymbol{x}_s)$ has n distinct eigenvalues $\{\lambda_i\}_{i=1,\ldots,n}$ and orthonormal eigenvectors $\{\boldsymbol{v}_i\}_{i=1,\ldots,n}$ such that $H_s \boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$. Prove that the $(\boldsymbol{x}_s, \boldsymbol{v}_i)$ are steady states of the following dynamics:

$$\dot{\boldsymbol{x}} = (I - 2\hat{\boldsymbol{v}} \otimes \hat{\boldsymbol{v}}) \cdot (-\nabla U(\boldsymbol{x})),$$
$$\dot{\boldsymbol{v}} = (I - \hat{\boldsymbol{v}} \otimes \hat{\boldsymbol{v}}) \cdot (-\nabla^2 U(\boldsymbol{x}), \boldsymbol{v}),$$

by imposing the normalization condition $\|\boldsymbol{v}(0)\| = 1$ for the initial value $\boldsymbol{v}(0)$. Prove that $(\boldsymbol{x}_s, \boldsymbol{v}_i)$ is linearly stable if and

only if $\boldsymbol{x}_s$ is an index-1 saddle point of U and $\boldsymbol{v}_i$ is the eigenvector corresponding to the positive eigenvalue of H_s. This is called the gentlest ascent dynamics (GAD), which is used to find saddle points.

12.2. Prove that for absolutely continuous $\boldsymbol{\varphi}$ on $[0, T]$, the variational minimization

$$\inf_{T>0} \inf_{\boldsymbol{\varphi}(0)=\boldsymbol{y}, \boldsymbol{\varphi}(T)=\boldsymbol{x}} I_T[\boldsymbol{\varphi}] = \inf_{\boldsymbol{\varphi}(0)=\boldsymbol{y}, \boldsymbol{\varphi}(\infty)=\boldsymbol{x}} I_\infty[\boldsymbol{\varphi}],$$

where $I_T[\boldsymbol{\varphi}]$ is defined in (12.8)–(12.9) and $\boldsymbol{x}$ is a stationary point; i.e., $\boldsymbol{b}(\boldsymbol{x}) = \boldsymbol{0}$.

Notes

The study of rare events is a classical but still a fast developing field. The classical transition state theory has been a cornerstone in chemical physics [**HPM90**]. The latest developments include the transition path theory [**EVE10**], Markov state models [**BPN14**], and advanced sampling methods in molecular dynamics and Monte Carlo methods.

From a mathematical viewpoint, the large deviation theory is the starting point for analyzing rare transition events. In this regard, the Freidlin-Wentzell theory provides the theoretical basis for understanding optimal transition paths [**FW98**, **SW95**, **Var84**]. In particular, the notion of quasi-potential is useful for extending the concept of energy landscape, very important for gradient systems, to nongradient systems [**Cam12**, **LLLL15**].

From an algorithmic viewpoint, the string method is the most popular path-based algorithm for computing the optimal transition paths. Another closely related approach is the nudged elastic band (NEB) method [**HJ00**], which is the most popular chain-of-state algorithm. The convergence analysis of the string method can be found in [**CKVE11**]. Besides GAD, other ideas for finding saddle points include the dimer method [**HJ99**], shrinking dimer method [**ZD12**], climbing string method [**RVE13**], etc.

Introduction to Chemical Reaction Kinetics

In this chapter, we will study a class of jump processes that are often used to model the dynamics of chemical reactions, particularly biochemical reactions. We will consider only the homogeneous case; i.e., we will assume that the reactants are well mixed in space and will neglect the spatial aspects of the problem.

Chemical reactions can be modeled at several levels. At the most detailed level, we are interested in the mechanism of the reactions and the reaction rates. This is the main theme for the previous chapter, except that to model the system accurately enough, one often has to resort to quantum mechanics. At the crudest level, we are interested in the concentration of the reactants, the products, and the intermediate states. In engineering applications such as combustion where one often has an abundance of participating species, the dynamics of the concentrations is usually modeled by the reaction rate equations, which is a system of ODEs for the concentrations of different species. The rate equations model the result of averaging over many reaction events. However, in situations when the discrete or stochastic effects are important, e.g., when there are only a limited number of some of the crucial species, then one has to model each individual molecule and reaction event. This is often the case in cell biology where there are usually a limited number of relevant proteins or RNAs. In this case, the preferred model is by a Markov jump process. As we will see, in the large volume limit, one recovers the reaction rate equations from the jump process.

13.1. Reaction Rate Equations

We start with the following simple example of decaying-dimerization reaction:

$$S_1 \quad \xrightarrow{\;\;c_1\;\;} \quad \emptyset,$$

$$2S_1 \quad \underset{c_3}{\overset{c_2}{\rightleftharpoons}} \quad S_2,$$

$$S_2 \quad \xrightarrow{\;\;c_4\;\;} \quad S_3,$$
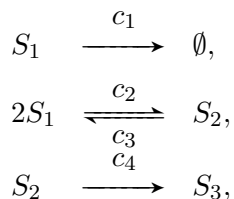
where c_1, c_2, c_3, c_4 are reaction constants and the symbol $\emptyset$ means some type of species which we are not interested in. For example, for the reaction $2S_1 \to S_2$, two S_1-molecules are consumed and one S_2 molecule is generated after each firing of the forward reaction; two S_1-molecules are generated and one S_2 molecule is consumed after each firing of the reverse reaction. This is an example of reversible reaction. The other reactions in this system are irreversible.

Denote by x_j the concentration of the species S_j. The law of mass action states that the rate of reaction is proportional to the reaction constant and the concentration of the participating molecules [**KS09**]. This gives us the following reaction rate equations for the above decaying-dimerization reaction:

$$(13.1) \qquad \frac{dx_1}{dt} \;\; = \;\; -c_1 x_1 - 2c_2 x_1^2 + 2c_3 x_2,$$

$$(13.2) \qquad \frac{dx_2}{dt} \;\; = \;\; c_2 x_1^2 - c_3 x_2 - c_4 x_2,$$

$$(13.3) \qquad \frac{dx_3}{dt} \;\; = \;\; c_4 x_2.$$

The term $-2c_2 x_1^2 + 2c_3 x_2$ in (13.1) and the term $c_2 x_1^2 - c_3 x_2$ in (13.2) are the consequence of the reversible reaction discussed above. Notice that we have, as a consequence of the reversibility for this particular reaction,

$$\frac{dx_2}{dt} + \frac{1}{2}\frac{dx_1}{dt} = 0.$$

This is a popular engineering approach for modeling chemical kinetics and it is adequate for situations when there are a large number of molecules for each species. In this approach, the fact that the reaction events are discrete and stochastic is neglected.

13.2. Chemical Master Equation

When studying chemical reactions inside a single cell, the discrete and stochastic effects usually cannot be neglected. This is very well documented in the pioneering work of Arkin, Ellowitz, et al. [**ARM98, ELSS02**].

Consider a well-stirred system of N molecular species $\{S_1, S_2, \ldots, S_N\}$ interacting through M reaction channels $\{R_1, R_2, \ldots, R_M\}$. The following quantities are used to characterize the discrete reaction dynamics.

(a) *States* $\boldsymbol{X}_t$. The state of the system is described by an N-vector

$$(13.4) \qquad \boldsymbol{X}_t = (X_t^1, X_t^2, \ldots, X_t^N) \in \mathbb{N}^N,$$

where the kth component X_t^k is the number of molecules of species S_k at time t.

(b) *Reactions* $\{R_j\}$. Each reaction channel R_j is characterized by its propensity function $a_j(\boldsymbol{x})$ and its state change vector

$$(13.5) \qquad \boldsymbol{\nu}_j = (\nu_j^1, \nu_j^2, \ldots, \nu_j^N) \in \mathbb{Z}^N,$$

where $a_j(\boldsymbol{x})dt$ gives the probability that the system will experience an R_j reaction in the next infinitesimal amount of time dt when the current state is $\boldsymbol{X}_t = \boldsymbol{x}$. We have $a_j(\boldsymbol{x}) \geq 0$ for physically meaningful states $\boldsymbol{x}$. The component ν_j^k is the change in the number of S_k molecules caused by one R_j reaction.

Sometimes we also introduce the notation

$$\boldsymbol{\nu}_j = \boldsymbol{\nu}_j^+ - \boldsymbol{\nu}_j^-,$$

where $\boldsymbol{\nu}_j^+, \boldsymbol{\nu}_j^- \in \mathbb{N}^N$ are the product (positive) and reactant (negative) part of the state change vector, respectively. The matrix $\boldsymbol{\nu} = (\boldsymbol{\nu}_1^T, \ldots, \boldsymbol{\nu}_M^T) \in \mathbb{Z}^{N \times M}$ is also called the *stoichiometric matrix* in chemistry.

For the decaying-dimerization reaction example, $N = 3$ and $M = 4$. Following the law of mass action, we obtain the propensity functions

$$(13.6) \quad a_1(\boldsymbol{x}) = k_1 x_1, \quad a_2(\boldsymbol{x}) = k_2 \binom{x_1}{2}, \quad a_3(\boldsymbol{x}) = k_3 x_2, \quad a_4(\boldsymbol{x}) = k_4 x_2$$

and the state change vectors

$$\boldsymbol{\nu}_1 = (-1, 0, 0), \quad \boldsymbol{\nu}_2 = (-2, 1, 0), \quad \boldsymbol{\nu}_3 = (2, -1, 0), \quad \boldsymbol{\nu}_4 = (0, -1, 1).$$

Here $\boldsymbol{\nu}_2 = \boldsymbol{\nu}_2^+ - \boldsymbol{\nu}_2^-$, where

$$\boldsymbol{\nu}_2^+ = (0, 1, 0), \quad \boldsymbol{\nu}_2^- = (2, 0, 0).$$

Note that the constants k_j in (13.6) are generally different from c_j in the reaction rate equations. We will come back to this in Section 13.5.

From the molecular theory of chemical reactions [**Gil92**, **Kur72**], the propensity function $a_j(\boldsymbol{x})$ has the form

$$(13.7) \qquad a_j(\boldsymbol{x}) = \frac{\kappa_j}{V^{|\boldsymbol{\nu}_j^-|-1}} \begin{pmatrix} \boldsymbol{x} \\ \boldsymbol{\nu}_j^- \end{pmatrix},$$

where κ_j is the rate of the reaction R_j in transition state theory and V is a scaling parameter usually taken as the volume of the system times the Avogadro constant. In (13.7), we used the multi-index notation:

$$|\boldsymbol{\nu}_j^-| = \sum_{m=1}^N \nu_j^{-,m}, \quad \boldsymbol{\nu}_j^-! = \prod_{m=1}^N \nu_j^{-,m}!, \quad \begin{pmatrix} \boldsymbol{x} \\ \boldsymbol{\nu}_j^- \end{pmatrix} = \prod_{m=1}^N \begin{pmatrix} x_m \\ \nu_j^{-,m} \end{pmatrix}.$$

Compared with (13.6), we get

$$k_j = \frac{\kappa_j}{V^{|\boldsymbol{\nu}_j^-|-1}}.$$

The combinatorial term comes from calculating the probability of molecular collisions.

With this setup, the chemical reaction kinetics is a standard birth-death process, or more generally a jump process. The equation for the transition probability distribution function can be derived through the Chapman-Kolmogorov equation in the time interval $[t, t+dt)$

$$P(\boldsymbol{x}, t+dt|\boldsymbol{x}_0, t_0) = \sum_{j=1}^M P(\boldsymbol{x} - \boldsymbol{\nu}_j, t|\boldsymbol{x}_0, t_0) a_j(\boldsymbol{x} - \boldsymbol{\nu}_j) dt$$

$$+ \left(1 - \sum_{j=1}^M a_j(\boldsymbol{x}) dt\right) P(\boldsymbol{x}, t|\boldsymbol{x}_0, t_0),$$

where dt is an infinitesimal time and we have already omitted the higher-order terms in $o(dt)$. This gives us the well-known *chemical master equation*
(13.8)

$$\partial_t P(\boldsymbol{x}, t|\boldsymbol{x}_0, t_0) = \sum_{j=1}^M a_j(\boldsymbol{x} - \boldsymbol{\nu}_j) P(\boldsymbol{x} - \boldsymbol{\nu}_j, t|\boldsymbol{x}_0, t_0) - a_0(\boldsymbol{x}) P(\boldsymbol{x}, t|\boldsymbol{x}_0, t_0)$$

with initial condition $P(\boldsymbol{x}, t_0|\boldsymbol{x}_0, t_0) = \delta(\boldsymbol{x} - \boldsymbol{x}_0)$, where $a_0(\boldsymbol{x}) := \sum_{j=1}^M a_j(\boldsymbol{x})$ is the total propensity. It is also straightforward to remark that the probability distribution function $P(\boldsymbol{x}, t)$ satisfies the same equation as $P(\boldsymbol{x}, t|\boldsymbol{x}_0, t_0)$.

Equation (13.8) is exactly the Kolmogorov forward equation for chemical reaction kinetics. Because the state space of the system is $\mathbb{N}^N$, it is in fact an infinite-dimensional ODE instead of a PDE.

13.3. Stochastic Differential Equations

The reaction kinetic processes can also be formulated as SDEs via a random time change technique [**EK86**]. It takes an elegant form:

$$(13.9) \qquad \boldsymbol{X}_t = \boldsymbol{X}_0 + \sum_{j=1}^{M} \boldsymbol{\nu}_j \mathcal{P}_j \left(\int_0^t a_j(\boldsymbol{X}_s) ds \right),$$

where the $\mathcal{P}_j(\cdot)$'s are independent, unirate (rate = 1) Poisson processes.

To understand (13.9), we first note that for any $a > 0$, the process $\mathcal{P}_j(at)$ is a Poisson process with rate a. Given $\boldsymbol{X}_t$, we have

$$\boldsymbol{X}_{t+dt} = \boldsymbol{X}_t + \sum_{j=1}^{M} \boldsymbol{\nu}_j \left(\mathcal{P}_j \left(\int_0^{t+dt} a_j(\boldsymbol{X}_s) ds \right) - \mathcal{P}_j \left(\int_0^t a_j(\boldsymbol{X}_s) ds \right) \right).$$

From independence and Markovianity of $\mathcal{P}_j(\cdot)$, we know that the firing probability of the jth reaction channel in $[t, t+dt)$ is exactly $a_j(\boldsymbol{X}_t)dt$ since $\boldsymbol{X}$ continues to be $\boldsymbol{X}_t$ before jumping when dt is an infinitesimal time. This explains why (13.9) makes sense as the SDEs describing the chemical reaction kinetics. The readers are referred to [**EK86**] for rigorous statements.

Another less direct but more general SDE formulation is to use Poisson random measure

$$(13.10) \quad d\boldsymbol{X}_t \quad = \quad \sum_{j=1}^{M} \boldsymbol{\nu}_j \int_0^A c_j(a; \boldsymbol{X}_{t-}) \lambda(dt \times da), \quad \boldsymbol{X}_t|_{t=0} = \boldsymbol{X}_0.$$

Here $A := \max_{\boldsymbol{X}_t} \{a_0(\boldsymbol{X}_t)\}$, which is assumed to be finite for a closed system, and $\lambda(dt \times da)$ is called the reference Poisson random measure associated with a Poisson point process $(q_t, t \geq 0)$ taking values in $(0, A]$. That is,

$$(13.11) \qquad \int_s^t \int_B \lambda(dt \times da) = \big|\{s \leq u < t \text{ and } q_u \in B\}\big|,$$

for any Borel set $B \subset (0, A]$ and $0 \leq s < t$. It is assumed that $\lambda(dt \times da)$ satisfies $\mathbb{E}\lambda(dt \times da) = dt \times da$. The firing rates for M reaction channels are defined through the acceptance-rejection functions

$$(13.12) \quad c_j(a; \boldsymbol{X}_t) = \left\{ \begin{array}{ll} 1, & \text{if } a \in (h_{j-1}(\boldsymbol{X}_t), h_j(\boldsymbol{X}_t)], \\ 0, & \text{otherwise,} \end{array} \right. \quad j = 1, 2, \ldots, M,$$

where $h_j(\boldsymbol{x}) = \sum_{i=1}^{j} a_j(\boldsymbol{x})$ for $j = 0, 1, \ldots, M$. One can see from the above constructions that $\boldsymbol{X}_t$ satisfies the same law for the chemical reaction kinetics. For more on the Poisson random measures and SDEs for jump processes, see [**App04**, **Li07**].

13.4. Stochastic Simulation Algorithm

The most widely used algorithm for simulating chemical reaction kinetics is the *stochastic simulation algorithm* (SSA), or *Gillespie's algorithm*, proposed by Gillespie in 1976 [**Gil76**]. It is essentially the same as the kinetic Monte Carlo (KMC) algorithm introduced in Section 4.5.

Let $p(\tau, j | \boldsymbol{x}, t)$ be the probability density, given $\boldsymbol{X}_t = \boldsymbol{x}$, that the next reaction will occur after waiting time τ and will be an R_j reaction. Then we have

$$p(\tau, j | \boldsymbol{x}, t) = a_j(\boldsymbol{x}) \exp(-a_0(\boldsymbol{x})\tau)$$
$$= \frac{a_j(\boldsymbol{x})}{a_0(\boldsymbol{x})} \cdot a_0(\boldsymbol{x}) \exp(-a_0(\boldsymbol{x})\tau),$$

similar to the derivation of (3.22). This leads to the following algorithm:

Algorithm 10 (Gillespie's algorithm)**.** Suppose that the current state is $\boldsymbol{X}_t$.

> Step 1: Sample the waiting time τ as an exponentially distributed random variable with rate $a_0(\boldsymbol{X}_t)$.
>
> Step 2: Sample a random variable k, where k takes value in the integers from 1 to M, with the probability that $k = j$ is equal to $a_j(\boldsymbol{X}_t)/a_0(\boldsymbol{X}_t)$.
>
> Step 3: Update $\boldsymbol{X}_{t+\tau} = \boldsymbol{X}_t + \boldsymbol{\nu}_k$. Then return to Step 1.

Gillespie's algorithm is considered to be exact since the corresponding forward equation is the same chemical master equation (13.8). Improvements of the SSA can be found in [**CLP04**, **GB00**].

Though the SSA is exact, its efficiency is hindered in several situations. One situation is when the reaction rates are disparate. In this case, the time step size of the simulation is controlled by the fast reaction, but it is often the slow reactions that interest us. Another situation is when some of the molecular numbers are very large. In this case the discrete nature of the algorithm presents a bottleneck. Later in this chapter, we will discuss a few ideas that help to resolve these difficulties.

13.5. The Large Volume Limit

In this section, we study the limit when the number of molecules goes to infinity. We will assume $\boldsymbol{X}_0, \boldsymbol{X}_t \sim O(V)$ and the following *large volume scaling* for the propensity functions

$$(13.13) \qquad a_j(V\boldsymbol{x}) = \frac{\kappa_j}{V^{|\boldsymbol{\nu}_j^-|-1}} \binom{V\boldsymbol{x}}{\boldsymbol{\nu}_j^-} = V a_j^V(\boldsymbol{x}),$$

where

(13.14) $\quad a_j^V(\boldsymbol{x}) = \tilde{a}_j(\boldsymbol{x}) + O(V^{-1}), \ \tilde{a}_j(\boldsymbol{x}) = \dfrac{\kappa_j}{\boldsymbol{\nu}_j^-!}\boldsymbol{x}^{\boldsymbol{\nu}_j^-} = \kappa_j \prod_{m=1}^{N} \dfrac{1}{\nu_j^{-,m}!}x_m^{\nu_j^{-,m}},$

and $a_j^V(\boldsymbol{x})$, $\tilde{a}_j(\boldsymbol{x}) \sim O(1)$ if $\kappa_j, \boldsymbol{x} \sim O(1)$. For simplicity, we will only consider the case when $a_j^V(\boldsymbol{x}) = \tilde{a}_j(\boldsymbol{x})$. The general case can be analyzed similarly.

Consider the rescaled process $\boldsymbol{X}_t^V = \boldsymbol{X}_t/V$, i.e., the concentration variable, with the original jump intensity $a_j(\boldsymbol{X}_t)$. We have

(13.15) $\qquad\qquad \boldsymbol{X}_t^V = \boldsymbol{X}_0^V + \int_0^t \boldsymbol{b}(\boldsymbol{X}_s^V)ds + \boldsymbol{M}_t^V$

where

$$\boldsymbol{b}(\boldsymbol{x}) := \sum_{j=1}^{M} \boldsymbol{\nu}_j \tilde{a}_j(\boldsymbol{x}), \quad \boldsymbol{M}_t^V := \sum_{j=1}^{M} \boldsymbol{\nu}_j V^{-1} \tilde{\mathcal{P}}_j\left(V\int_0^t a_j^V(\boldsymbol{X}_s^V)ds\right),$$

and $\tilde{\mathcal{P}}_j(t) := \mathcal{P}_j(t) - t$ is the centered Poisson process with mean 0. We will assume that $\boldsymbol{b}(\boldsymbol{x})$ satisfies the Lipschitz condition: $|\boldsymbol{b}(\boldsymbol{x}) - \boldsymbol{b}(\boldsymbol{y})| \leq L|\boldsymbol{x} - \boldsymbol{y}|$.

Define the deterministic process $\boldsymbol{x}(t)$:

(13.16) $\qquad\qquad \boldsymbol{x}(t) = \boldsymbol{x}_0 + \int_0^t \boldsymbol{b}(\boldsymbol{x}(s))ds.$

We have

$$|\boldsymbol{X}_t^V - \boldsymbol{x}(t)| \leq |\boldsymbol{X}_0^V - \boldsymbol{x}_0| + \int_0^t L|\boldsymbol{X}_s^V - \boldsymbol{x}(s)|ds + |\boldsymbol{M}_t^V|.$$

Using Gronwall's inequality, we obtain

$$\sup_{s\in[0,t]} |\boldsymbol{X}_s^V - \boldsymbol{x}(s)| \leq \left(|\boldsymbol{X}_0^V - \boldsymbol{x}_0| + \sup_{s\in[0,t]} |\boldsymbol{M}_s^V|\right)e^{Lt}$$

for any $t > 0$. From the law of large numbers for Poisson processes (see Exercise 13.1), we immediately get $\sup_{s\in[0,t]} |\boldsymbol{X}_s^V - \boldsymbol{x}(s)| \to 0$ almost surely as $V \to \infty$ and the initial condition $\boldsymbol{X}_0^V \to \boldsymbol{x}_0$. This is the celebrated large volume limit for chemical reaction kinetics, also known as the *Kurtz limit* in the literature [**Kur72**, **EK86**].

By comparing (13.16) with the reaction rate equations in Section 13.1, we also obtain the relation

(13.17) $\qquad\qquad c_j = \dfrac{\kappa_j}{\boldsymbol{\nu}_j^-!} = \dfrac{k_j}{\boldsymbol{\nu}_j^-!}V^{|\boldsymbol{\nu}_j^-|-1}$

between k_j, κ_j, and c_j. This connects the definition of rate constants at different scales.

The limit from (13.15) to (13.16) can also be derived using asymptotic analysis of the backward operator introduced in Section 8.9. To this end, we first note that the backward operator for the original process $\boldsymbol{X}_t$ has the form

$$\mathcal{A}f(\boldsymbol{x}) = \sum_{j=1}^{M} a_j(\boldsymbol{x})\big(f(\boldsymbol{x} + \boldsymbol{\nu}_j) - f(\boldsymbol{x})\big).$$

For the rescaled process $\boldsymbol{X}_t^V$, define $u(\boldsymbol{x}, t) = \mathbb{E}^{\boldsymbol{x}} f(\boldsymbol{X}_t^V)$ for any bounded continuous function f. We have

$$\partial_t u(\boldsymbol{x}, t) = \mathcal{A}^V u = \sum_{j=1}^{M} V a_j^V(\boldsymbol{x}) \left(u\left(\boldsymbol{x} + \frac{\boldsymbol{\nu}_j}{V}\right) - u(\boldsymbol{x}) \right).$$

Under the same assumption as (13.13) and with the ansatz $u(\boldsymbol{x}, t) = u_0(\boldsymbol{x}, t) + V^{-1} u_1(\boldsymbol{x}, t) + o(V^{-1})$, we get, to leading order,

$$\partial_t u_0(\boldsymbol{x}, t) = \mathcal{A}_0 u_0 = \sum_{j=1}^{M} \tilde{a}_j(\boldsymbol{x}) \boldsymbol{\nu}_j \cdot \nabla u_0(\boldsymbol{x}, t).$$

This is the backward equation for the reaction rate equations (13.16).

13.6. Diffusion Approximation

Having discussed the large volume limit $\boldsymbol{X}_t^V \to \boldsymbol{x}(t)$ as $V \to \infty$, the next natural question is the magnitude of the fluctuations.

To do this, let us first mention the central limit theorem for the rescaled unirate Poisson process

(13.18) $V^{-\frac{1}{2}} \tilde{\mathcal{P}}_j(Vt) \Rightarrow W_j(t) \quad \text{as } V \to \infty,$

where the $\{W_j(t)\}$ are independent standard Brownian motions.

Consider the rescaled process

$$\boldsymbol{Y}_t^V = V^{\frac{1}{2}}(\boldsymbol{X}_t^V - \boldsymbol{x}(t)).$$

By definition, we have

$$\boldsymbol{Y}_t^V = \boldsymbol{Y}_0^V + \sum_{j=1}^{M} \boldsymbol{\nu}_j \left[\int_0^t V^{\frac{1}{2}} \left(a_j^V(\boldsymbol{X}_s^V) - \tilde{a}_j(\boldsymbol{x}(s)) \right) ds \right.$$

$$\left. + V^{-\frac{1}{2}} \tilde{\mathcal{P}}_j \left(V \int_0^t a_j^V(\boldsymbol{X}_s^V) ds \right) \right]$$

$$= \boldsymbol{Y}_0^V + \sum_{j=1}^{M} \boldsymbol{\nu}_j \int_0^t \nabla \tilde{a}_j(\boldsymbol{x}(s)) \cdot \boldsymbol{Y}_s^V ds + \sum_{j=1}^{M} \boldsymbol{\nu}_j W_j \left(\int_0^t \tilde{a}_j(\boldsymbol{x}(s)) ds \right) + \text{h.o.t.}$$

This leads to a central limit theorem for the chemical jump process $\boldsymbol{Y}_t^V \Rightarrow \boldsymbol{Y}(t)$ and $\boldsymbol{Y}$ satisfies the following linear diffusion process:

$$(13.19) \quad \frac{d\boldsymbol{Y}}{dt} = \sum_{j=1}^M \boldsymbol{\nu}_j \nabla \tilde{a}_j(\boldsymbol{x}(t)) \cdot \boldsymbol{Y}(t) + \sum_{j=1}^M \boldsymbol{\nu}_j \sqrt{\tilde{a}_j(\boldsymbol{x}(t))} \dot{W}_j(t), \quad \boldsymbol{Y}_0 = \boldsymbol{0},$$

where we have assumed $\boldsymbol{Y}_0^V \Rightarrow \boldsymbol{0}$ and used the relation

$$(13.20) \quad W_j \left(\int_0^t \tilde{a}_j(\boldsymbol{x}(s)) ds \right) \sim \int_0^t \sqrt{\tilde{a}_j(\boldsymbol{x}(s))} dW_j(s)$$

in stochastic analysis [**KS91**]. Note that we have $\tilde{a}_j(\boldsymbol{x}) \geq 0$ when $\boldsymbol{x} \geq 0$. Interested readers should refer to [**EK86**] for a rigorous treatment. The above results directly lead to the approximation

$$(13.21) \quad \boldsymbol{X}_t^V \approx \boldsymbol{x}(t) + V^{-\frac{1}{2}} \boldsymbol{Y}_t.$$

Another commonly used diffusion approximation for $\boldsymbol{X}_t^V$ is by formally taking (13.18) directly into (13.15), which yields an approximation

$$(13.22) \quad \boldsymbol{Z}_t^V = \boldsymbol{Z}_0^V + \sum_{j=1}^M \boldsymbol{\nu}_j \int_0^t a_j^V(\boldsymbol{Z}_s^V) ds + V^{-\frac{1}{2}} \sum_{j=1}^M \boldsymbol{\nu}_j W_j \left(\int_0^t a_j^V(\boldsymbol{Z}_s^V) ds \right).$$

In the same spirit as (13.20), we obtain the following chemical Langevin equation for the dynamics of the concentrations:

$$(13.23) \quad d\boldsymbol{Z}_t^V = \sum_{j=1}^M \boldsymbol{\nu}_j a_j^V(\boldsymbol{Z}_t^V) dt + V^{-\frac{1}{2}} \sum_{j=1}^M \boldsymbol{\nu}_j \sqrt{a_j^V(\boldsymbol{Z}_t^V)} dW_j(t).$$

In terms of the molecule numbers

$$(13.24) \quad d\boldsymbol{Z}_t = \sum_{j=1}^M \boldsymbol{\nu}_j a_j(\boldsymbol{Z}_t) dt + \sum_{j=1}^M \boldsymbol{\nu}_j \sqrt{a_j(\boldsymbol{Z}_t)} dW_j(t),$$

where we have used the definition $\boldsymbol{Z}^V = \boldsymbol{Z}/V$. This is the chemical Langevin equation in the chemistry literature [**Gil00**]. It can be shown that as $V \to \infty$, $\boldsymbol{Z}_t^V \to \boldsymbol{x}(t)$ and $V^{\frac{1}{2}}(\boldsymbol{Z}_t^V - \boldsymbol{x}(t)) \to \boldsymbol{Y}_t$ in fixed time interval $[0, T]$. In this sense, $\boldsymbol{Z}^V$ approximates $\boldsymbol{X}^V$ at the same order as $\boldsymbol{x}(t) + V^{-\frac{1}{2}} \boldsymbol{Y}_t$.

13.7. The Tau-leaping Algorithm

The SSA keeps track of each reaction event. This is inefficient when the reactions are very frequent. The tau-leaping algorithm, on the other hand, attempts to count only the total number of reactions in each reaction channel in small intervals. The size of the interval is chosen according to the following

interesting *leap condition* [**Gil01**]:

> "*Leap Condition*: Require the leap time τ to be small enough that the change in the state during $[t, t+\tau)$ will be so slight that no propensity function will suffer an appreciable (i.e., macroscopically noninfinitesimal) change in its value."

Of course τ should also be big enough so that some reaction has occurred. With this condition, Gillespie proposed the *tau-leaping algorithm* (or the *Poisson tau-leaping algorithm*): Let τ be a suitably selected time stepsize. The system is advanced by the scheme

$$(13.25) \qquad \boldsymbol{X}_{t+\tau} = \boldsymbol{X}_t + \sum_{j=1}^{M} \boldsymbol{\nu}_j \mathcal{P}_j(a_j(\boldsymbol{X}_t)\tau)$$

where the $\mathcal{P}_j(a_j(\boldsymbol{X}_t)\tau)$ are independent Poisson random variables with parameters $\lambda_j = a_j(\boldsymbol{X}_t)\tau$, respectively. The idea behind the tau-leaping algorithm is that if the reaction rate $a_j(\boldsymbol{X}_t)$ is almost a constant during $[t, t+\tau)$, then the number of fired reactions in the jth reaction channel will be $\mathcal{P}_j(a_j(\boldsymbol{X}_t)\tau)$.

To make the tau-leaping idea a practical scheme, one needs a robust stepsize selection strategy. For this purpose, note that the state after tau-leaping is

$$\boldsymbol{X} \to \boldsymbol{X} + \sum_{j=1}^{M} \boldsymbol{\nu}_j a_j(\boldsymbol{X})\tau := \boldsymbol{X} + \tau\boldsymbol{\xi}.$$

So the leap condition requires

$$|a_j(\boldsymbol{X} + \tau\boldsymbol{\xi}) - a_j(\boldsymbol{X})| \le \epsilon a_0(\boldsymbol{X}),$$

where $0 < \epsilon < 1$ is a specified value. A simple Taylor expansion of the left-hand side gives $\tau|\boldsymbol{\xi} \cdot \nabla a_j| \le \epsilon a_0(\boldsymbol{X})$, which leads to a simple stepsize selection strategy

$$\tau \approx \min_{j=1,\dots,M} \left\{ \frac{\epsilon a_0(\boldsymbol{X})}{|\boldsymbol{\xi} \cdot \nabla a_j|} \right\}.$$

More robust stepsize selection strategies can be found in [**CGP06**] and the references therein.

The convergence of the tau-leaping algorithm is a nontrivial matter. It is proven in [**Li07**] that the explicit tau-leaping scheme is of strong order $1/2$ and weak order 1 in the $\tau \to 0$ scaling, based on the observation that the tau-leaping scheme is essentially an Euler-Maruyama type discretization of the SDEs (13.9) or (13.10). The convergence analysis of the tau-leaping scheme in the large volume scaling is also discussed in [**AGK11**].

13.8. Stationary Distribution

Here we study the stationary distribution for some sample systems. These results will be used in the next section. First let us consider the simplest reversible reaction

(13.26)
$$S_1 \xrightleftharpoons[k_2]{k_1} S_2.$$

If we denote by $\mathcal{L}$ the generator of this process, then the chemical master equation can be written as $\partial_t p(\boldsymbol{x}, t) = \mathcal{L}^* p(\boldsymbol{x}, t)$. The stationary distribution of the process satisfies

(13.27)
$$\mathcal{L}^* p_\infty(\boldsymbol{x}) = 0.$$

Denote the number of molecules of $\{S_1, S_2\}$ by $\boldsymbol{x} = (x, y)$. For the reversible reaction (13.26), we only need to consider the equation for x since we have the conservation law $x + y = n$, where n is the total number of molecules of the system. Equation (13.27) can be written as

$$\Big(k_1(x+1)p(x+1) - k_1 x p(x)\Big) + \Big(k_2(n-x+1)p(x-1) - k_2(n-x)p(x)\Big) = 0.$$

Define $a_2(x) = k_2(n-x)$ and $a_1(x) = k_1 x$ $(0 \leq x \leq n)$. We have

(13.28) $\Big(a_1(x+1)p(x+1) - a_2(x)p(x)\Big) - \Big(a_1(x)p(x) - a_2(x-1)p(x-1)\Big) = 0.$

This is equivalent to stating that the probability flux is a constant:

$$j(x) = a_1(x)p(x) - a_2(x-1)p(x-1) = \text{Const}.$$

The boundary condition for the probability flux at $x = 0$ is

$$j(0) = a_1(0)p(0) = 0$$

since $x - 1 = -1$ is out of the domain, similarly for the boundary at $x = n$.

Equation (13.28) together with the boundary condition lead to the detailed balance relation: $a_1(x)p(x) = a_2(x-1)p(x-1)$. We have

$$\frac{p(x)}{p(x-1)} = \frac{a_2(x-1)}{a_1(x)}, \text{ which implies } \frac{p(x)}{p(0)} = \frac{a_2(x-1)}{a_1(x)} \frac{a_2(x-2)}{a_1(x-1)} \cdots \frac{a_2(0)}{a_1(1)}.$$

Thus the stationary distribution for S_1 is

$$p(x) = p(0)\Big(\frac{k_2}{k_1}\Big)^x \frac{n!}{x!(n-x)!} \propto \frac{n!}{x!(n-x)!}\Big(\frac{k_2}{k_1+k_2}\Big)^x \Big(\frac{k_1}{k_1+k_2}\Big)^{-x}.$$

It follows that the equilibrium distribution of S_1 is binomial:

$$p(x) \sim B(n, q), \quad q = \frac{k_2}{k_1 + k_2}$$

with mean nq and variance $nq(1 - q)$.

The above result can be extended to general irreducible first-order reactions like

$$(13.29) \qquad S_1 \underset{k_{1-}}{\overset{k_{1+}}{\rightleftharpoons}} S_2 \underset{k_{2-}}{\overset{k_{2+}}{\rightleftharpoons}} \cdots \underset{k_{(N-1)-}}{\overset{k_{(N-1)+}}{\rightleftharpoons}} S_N.$$
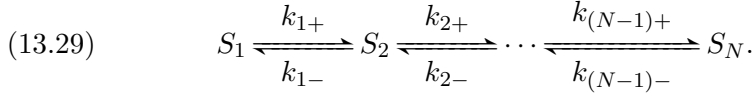
It can be shown that the invariant distribution is unique with the multinomial distribution

$$p(\boldsymbol{x}) = \frac{n!}{x_1! x_2! \cdots x_N!} c_1^{x_1} c_2^{x_2} \cdots c_N^{x_N},$$

where x_i is the number of the molecules for species S_i and n is the total number of molecules for all species; i.e.,

$$n = X_1(0) + X_2(0) + \cdots + X_N(0).$$

The parameter $\boldsymbol{c} = (c_1, \ldots, c_N)$ is a probability vector, which is the unique positive solution of the linear system

$$\boldsymbol{c} \cdot Q = 0$$

with constraint $\sum_{i=1}^N c_i = 1$. Here $Q \in \mathbb{R}^{N \times N}$ is the generator

$$Q = \begin{pmatrix} -k_{1+} & k_{1+} & \cdots & 0 & 0 \\ k_{1-} & -(k_{1-} + k_{2+}) & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -(k_{(N-2)-} + k_{(N-1)+}) & k_{(N-1)+} \\ 0 & 0 & \cdots & k_{(N-1)-} & -k_{(N-1)-} \end{pmatrix}.$$

More examples can be found in [**ACK10, VK04**].

13.9. Multiscale Analysis of a Chemical Kinetic System

Chemical kinetic systems often involve multiple time scales. It is usually the case that we are mostly interested in the dynamics on the slow scale. In this section, we derive the effective dynamical system on slow time scales by averaging over the fast reactions.

Consider a sample chemical kinetic system described by

$$(13.30) \qquad S_1 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} S_2, \qquad S_2 \underset{k_4}{\overset{k_3}{\rightleftharpoons}} S_3, \qquad S_3 \underset{k_6}{\overset{k_5}{\rightleftharpoons}} S_4,$$

with rate constants

$$k_1 = k_2 = 10^5, \quad k_3 = k_4 = 1, \quad k_5 = k_6 = 10^5.$$

Let us partition the reactions into two sets: the slow ones and the fast ones. The fast reactions $R^f = \{(a^f, \boldsymbol{\nu}^f)\}$ are

(13.31)
$$
\begin{aligned}
a_1^f &= 10^5 x_1, & \boldsymbol{\nu}_1^f &= (-1, +1,\ 0,\ 0), \\
a_2^f &= 10^5 x_2, & \boldsymbol{\nu}_2^f &= (+1, -1,\ 0,\ 0), \\
a_5^f &= 10^5 x_3, & \boldsymbol{\nu}_5^f &= (\ 0,\ 0, -1, +1), \\
a_6^f &= 10^5 x_4, & \boldsymbol{\nu}_6^f &= (\ 0,\ 0, +1, -1).
\end{aligned}
$$

The slow reactions $R^s = \{(a^s, \boldsymbol{\nu}^s)\}$ are

(13.32)
$$
\begin{aligned}
a_3^s &= x_2, & \boldsymbol{\nu}_3^s &= (0, -1, +1, 0), \\
a_4^s &= x_3, & \boldsymbol{\nu}_4^s &= (0, +1, -1, 0).
\end{aligned}
$$

Observe that during the fast reactions, the variables

(13.33)
$$
z_1 = x_1 + x_2, \qquad z_2 = x_3 + x_4
$$

do not change. They are the slow variables. Intuitively, one can think of the whole process as follows. In the fast time scale, z_1 and z_2 are almost fixed and there is a fast exchange between x_1 and x_2 and between x_3 and x_4. This process reaches equilibrium during the fast time scale and the equilibrium is given by a Bernoulli distribution with parameter $q = 10^5/(10^5 + 10^5) = 1/2$:
(13.34)
$$
\mu_{z_1,z_2}(x_1, x_2, x_3, x_4) = \frac{z_1!\, z_2!}{x_1!\, x_2!\, x_3!\, x_4!} \left(\frac{1}{2}\right)^{z_1} \left(\frac{1}{2}\right)^{z_2} \delta_{x_1+x_2=z_1} \delta_{x_3+x_4=z_2}.
$$

Here the function $\delta_{x_1+x_2=z_1}$ means that it equals 1 only when $x_1 + x_2 = z_1$ and 0 otherwise, and $\delta_{x_3+x_4=z_2}$ is similar. At the slow time scale, the values of z_1 and z_2 do change. The effective dynamics on this time scale reduces to a dynamics on the space of $\boldsymbol{z} = (z_1, z_2)$ with effective reaction channels given by

(13.35)
$$
\begin{aligned}
\bar{a}_3^s &= \langle x_2 \rangle = \frac{x_1 + x_2}{2} = \frac{z_1}{2}, & \bar{\boldsymbol{\nu}}_3^s &= (-1, +1), \\
\bar{a}_4^s &= \langle x_3 \rangle = \frac{x_3 + x_4}{2} = \frac{z_2}{2}, & \bar{\boldsymbol{\nu}}_4^s &= (+1, -1).
\end{aligned}
$$

These expressions follow from the general theory that we describe below.

For the general case, let us consider the observable $u(\boldsymbol{x}, t) = \mathbb{E}^{\boldsymbol{x}} f(\boldsymbol{X}_t)$. Then $u(\boldsymbol{x}, t)$ satisfies the backward Kolmogorov equation

(13.36)
$$
\partial_t u(\boldsymbol{x}, t) = \sum_{j=1}^{M} a_j(\boldsymbol{x})(u(\boldsymbol{x} + \boldsymbol{\nu}_j, t) - u(\boldsymbol{x}, t)) = \mathcal{L} u(\boldsymbol{x}, t),
$$

where $\mathcal{L}$ is the infinitesimal generator of the chemical kinetic system.

Now assume that the rate functions have the form

$$(13.37) \qquad a(\boldsymbol{x}) = \left(a^s(\boldsymbol{x}), \frac{1}{\varepsilon} a^f(\boldsymbol{x}) \right),$$

where $\varepsilon \ll 1$ represents the ratio of the fast and slow time scales of the system. The corresponding reactions and the associated stoichiometric vectors can be grouped accordingly:

$$(13.38) \qquad R^s = \{(a^s, \boldsymbol{\nu}^s)\}, \qquad R^f = \left\{ \left(\frac{1}{\varepsilon} a^f, \boldsymbol{\nu}^f \right) \right\}.$$

We call R^s the slow reactions and R^f the fast reactions.

Define the *virtual fast processes* by turning off the slow reactions [**ELVE05b**]. Due to the time scale separation, we expect the virtual fast process to describe the dynamics between slow reactions.

Let v be a function of the state variable $\boldsymbol{x}$. We say that $v(\boldsymbol{x})$ is a slow variable if it does not change during the fast reactions, i.e., if for any $\boldsymbol{x}$ and any stoichiometric vector $\boldsymbol{\nu}_j^f$ associated with a fast reaction

$$(13.39) \qquad v(\boldsymbol{x} + \boldsymbol{\nu}_j^f) = v(\boldsymbol{x}).$$

This is equivalent to saying that the slow variables are conserved quantities for the fast reactions. It is easy to see that $v(\boldsymbol{x}) = \boldsymbol{b} \cdot \boldsymbol{x}$ is a slow variable if and only if

$$(13.40) \qquad \boldsymbol{b} \cdot \boldsymbol{\nu}_j^f = 0$$

for all $\boldsymbol{\nu}_j^f$. The set of such vectors form a linear subspace in $\mathbb{R}^N$. Let $\{\boldsymbol{b}_1, \boldsymbol{b}_2, \ldots, \boldsymbol{b}_J\}$ be a set of basis vectors of this subspace, and let

$$(13.41) \qquad z_j = \boldsymbol{b}_j \cdot \boldsymbol{x} \quad \text{for} \quad j = 1, \ldots, J.$$

Let $\boldsymbol{z} = (z_1, \ldots, z_J)$ and denote by $\mathcal{Z}$ the space over which $\boldsymbol{z}$ is defined. The stoichiometric vectors associated with these slow variables are naturally defined as

$$(13.42) \qquad \bar{\boldsymbol{\nu}}_i^s = (\boldsymbol{b}_1 \cdot \boldsymbol{\nu}_i^s, \ldots, \boldsymbol{b}_J \cdot \boldsymbol{\nu}_i^s), \qquad i = 1, \ldots, N_s.$$

We now derive the effective dynamics on the slow time scale using singular perturbation theory. We assume, for the moment, that $\boldsymbol{z}$ is a complete set of slow variables; i.e., for each fixed value of the slow variable $\boldsymbol{z}$, the virtual fast process admits a unique equilibrium distribution $\mu_{\boldsymbol{z}}(\boldsymbol{x})$ on the state space $\boldsymbol{x} \in \mathcal{X}$.

The backward Kolmogorov equation for the multiscale chemical kinetic system reads

$$(13.43) \qquad \partial_t u = \mathcal{L}_0 u + \frac{1}{\varepsilon} \mathcal{L}_1 u,$$

where $\mathcal{L}_0$ and $\mathcal{L}_1$ are the infinitesimal generators associated with the slow and fast reactions, respectively. For any $f : \mathcal{X} \to \mathbb{R}$,

(13.44)
$$(\mathcal{L}_0 f)(\boldsymbol{x}) = \sum_{j=1}^{M_s} a_j^s(\boldsymbol{x})(f(\boldsymbol{x} + \boldsymbol{\nu}_j^s) - f(\boldsymbol{x})),$$

$$(\mathcal{L}_1 f)(\boldsymbol{x}) = \sum_{j=1}^{M_f} a_j^f(\boldsymbol{x})(f(\boldsymbol{x} + \boldsymbol{\nu}_j^f) - f(\boldsymbol{x})),$$

where M_s is the number of slow reactions in R^s and M_f is the number of fast reactions in R^f. We look for a solution of (13.43) in the form of

(13.45)
$$u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + \cdots .$$

Inserting this into (13.43) and equating the coefficients of equal powers of ε, we arrive at the hierarchy of equations

(13.46) $$\mathcal{L}_1 u_0 = 0,$$

(13.47) $$\mathcal{L}_1 u_1 = \partial_t u_0 - \mathcal{L}_0 u_0,$$

(13.48) $$\mathcal{L}_1 u_2 = \cdots .$$

The first equation implies that u_0 belongs to the null-space of $\mathcal{L}_1$, which, by the ergodicity assumption of the fast process, is equivalent to saying that

(13.49) $$u_0(\boldsymbol{x}, t) = \bar{U}(\boldsymbol{b} \cdot \boldsymbol{x}, t) \equiv \bar{U}(\boldsymbol{z}, t),$$

for some $\bar{U}$ yet to be determined. Define the projection operator $\mathcal{P}$

(13.50) $$(\mathcal{P}v)(\boldsymbol{z}) = \sum_{\boldsymbol{x} \in \mathcal{X}} \mu_{\boldsymbol{z}}(\boldsymbol{x})v(\boldsymbol{x}).$$

For any $v : \mathcal{X} \to \mathbb{R}$, $\mathcal{P}v$ depends only on the slow variable $\boldsymbol{z}$; i.e., $\mathcal{P}v : \mathcal{Z} \to \mathbb{R}$. At the same time, we have $\mathcal{P}\mathcal{L}_1 = \mathcal{L}_1\mathcal{P} = 0$.

Inserting (13.49) into (13.47) gives (using the explicit expression for $\mathcal{L}_0$)
(13.51)
$$\mathcal{L}_1 u_1(\boldsymbol{x}, t) = \partial_t \bar{U}(\boldsymbol{b} \cdot \boldsymbol{x}, t) - \sum_{i=1}^{M_s} a_i^s(\boldsymbol{x})\Big(\bar{U}(\boldsymbol{b} \cdot (\boldsymbol{x} + \boldsymbol{\nu}_i^s), t) - \bar{U}(\boldsymbol{b} \cdot \boldsymbol{x}, t)\Big)$$

$$= \partial_t \bar{U}(\boldsymbol{z}, t) - \sum_{i=1}^{M_s} a_i^s(\boldsymbol{x})(\bar{U}(\boldsymbol{z} + \bar{\boldsymbol{\nu}}_i^s, t) - \bar{U}(\boldsymbol{z}, t)).$$

Applying $\mathcal{P}$ to both sides of (13.51), we get

(13.52) $$\partial_t \bar{U}(\boldsymbol{z}, t) = \sum_{i=1}^{M_s} \bar{a}_i^s(\boldsymbol{z})(\bar{U}(\boldsymbol{z} + \bar{\nu}_i^s, t) - \bar{U}(\boldsymbol{z}, t)),$$

where

$$(13.53) \qquad \bar{a}_i^s(\boldsymbol{z}) = (\mathcal{P}a_i^s)(\boldsymbol{z}) = \sum_{\boldsymbol{x}\in\mathcal{X}} a_i^s(\boldsymbol{x})\mu_z(\boldsymbol{x}).$$

Equation (13.53) gives the effective rates on the slow time scale. The effective reaction kinetics on this time scale are given in terms of the slow variables by

$$(13.54) \qquad \bar{R} = (\bar{a}^s(\boldsymbol{z}), \bar{\boldsymbol{\nu}}^s).$$

It is important to note that the limiting dynamics described in (13.52) can be reformulated on the original state space $\mathcal{X}$. Indeed, it is easy to check that (13.52) is equivalent to

$$(13.55) \qquad \partial_t u_0(\boldsymbol{x}, t) = \sum_{i=1}^{M_s} \tilde{a}_i^s(\boldsymbol{x})(u_0(\boldsymbol{x} + \boldsymbol{\nu}_i^s, t) - u_0(\boldsymbol{x}, t)),$$

where $\tilde{a}_i^s(\boldsymbol{x}) = \bar{a}_i^s(\boldsymbol{b}\cdot\boldsymbol{x})$, in the sense that if $u_0(\boldsymbol{x}, t = 0) = f(\boldsymbol{b}\cdot\boldsymbol{x})$, then

$$(13.56) \qquad u_0(\boldsymbol{x}, t) = \bar{U}(\boldsymbol{b}\cdot\boldsymbol{x}, t)$$

where $\bar{U}(\boldsymbol{z}, t)$ solves (13.52) with the initial condition $\bar{U}(\boldsymbol{z}, 0) = f(\boldsymbol{z})$. Note that in (13.55), all of the quantities can be formulated over the original state space using the original variables. This fact is useful for developing numerical algorithms for this kind of problems [**CGP05**, **ELVE05b**, **ELVE07**], which will be introduced in next section.

From a numerical viewpoint, parallel to the discussion in the last section, one would like to have algorithms that automatically capture the slow dynamics of the system, without the need to precompute the effective dynamics or make ad hoc approximations. We will discuss an algorithm proposed in [**ELVE05b**] which is a simple modification of the original SSA, by adding a nested structure according to the time scale of the rates. For simple systems with only two time scales, the nested SSA consists of two SSAs organized with one nested inside the other: an outer SSA for the slow reactions only, but with modified slow rates which are computed in an inner SSA that models the fast reactions only. Averaging is performed automatically "on-the-fly".

Algorithm 11 (Nested SSA for multiscale chemical kinetic systems)**.** Let t_n, $\boldsymbol{X}_n$ be the current time and state of the system, respectively.

- *Inner SSA:* Pick an integer K. Run K independent replicas of the SSA with the fast reactions $R^f = \{(\varepsilon^{-1}a^f, \boldsymbol{\nu}^f)\}$ only, for a time interval of $T_0 + T_f$. During this calculation, compute the modified

slow rates for $j = 1, \ldots, M_s$

(13.57)
$$\tilde{a}_j^s = \frac{1}{K} \sum_{k=1}^{K} \frac{1}{T_f} \int_{T_0}^{T_f+T_0} a_j^s(\boldsymbol{X}_\tau^k) d\tau,$$

where $\boldsymbol{X}_\tau^k$ is the result of the kth replica of the virtual fast process at virtual time τ whose initial value is $\boldsymbol{X}_{t=0}^k = \boldsymbol{X}_n$ and T_0 is a parameter we choose in order to minimize the effect of the transients to the equilibrium in the virtual fast process.

- *Outer SSA:* Run one step of the SSA for the modified slow reactions $\tilde{R}^s = (\tilde{a}^s, \boldsymbol{\nu}^s)$ to generate $(t_{n+1}, \boldsymbol{X}_{n+1})$ from $(t_n, \boldsymbol{X}_n)$.
- Repeat the above nested procedures until the final time T.

Note that the algorithm is formulated in the original state space. Obviously it can be extended to the situation with more time scales. Error and cost analysis can also be performed. See [**ELVE05b**, **ELVE07**].

Exercises

13.1. Prove the strong law of large numbers for the unirate Poisson process $\mathcal{P}(t)$ using Doob's martingale inequality; i.e., for any fixed $T > 0$

$$\lim_{n \to \infty} \sup_{s \leq T} |n^{-1} \tilde{\mathcal{P}}(ns)| = 0, \quad \text{a.s.,}$$

where $\tilde{\mathcal{P}}(t)$ is the centered Poisson process.

13.2. Derive the mean and covariance functions for the process defined in (13.21)
$$\boldsymbol{X}_t^V \approx \boldsymbol{x}(t) + V^{-\frac{1}{2}} \boldsymbol{Y}_t.$$

Notes

Chemical reaction kinetics modeled by jump processes has become a fundamental language in systems biology. See [**ARM98**, **ELSS02**, **GHP13**, **LX11**], etc. In this chapter, we only considered cases with algebraic propensity functions. In more general situations such as the enzymatic reactions, the propensity functions may take the form of rational functions. The most common example is the Michaelis-Menten kinetics. Readers may consult [**KS09**] for more details.

The tau-leaping algorithm was proposed in 2001 [**Gil01**]. Since then, much work has been done to improve its performance and robustness. These efforts included robust stepsize selection [**CGP06**], avoiding negative populations [**CVK05**, **MTV16**, **TB04**], multilevel Monte Carlo methods [**AH12**], etc.

For multiscale problems, we only discussed the situation with disparate time scales. Multiscale problems also arise due to disparate population sizes of the different species. In this case, one typical strategy is to approximate the original system by a discrete-continuous coupled hybrid formulation [**HR02**].

The study of rare events is also an important topic for chemical reaction kinetics [**ARLS11**, **DMRH94**]. In this context, the large deviation theory in the large volume limit has been generalized to systems with multiple time scales [**LL17**, **LLLL14**]. However, the transition rate formula for general chemical kinetic systems is yet to be found. For numerical algorithms for computing the optimal transition paths, we refer to [**HVE08**].

Appendix

A. Laplace Asymptotics and Varadhan's Lemma

Consider the Laplace integral

$$F(t) = \int_{\mathbb{R}} e^{th(x)} dx, \quad t \gg 1,$$

where $h(x) \in C^2(\mathbb{R})$, $h(0)$ is the only global maximum, and $h''(0) \neq 0$. We further assume that for any $c > 0$, there exists $b > 0$ such that

$$h(x) - h(0) \leq -b \quad \text{if } |x| \geq c.$$

Assume also that $h(x) \to -\infty$ fast enough as $x \to \infty$ to ensure the convergence of F for $t = 1$.

Lemma A.1 (Laplace method)**.** *We have the asymptotics*

$$(A.1) \qquad F(t) \sim \sqrt{2\pi}(-th''(0))^{-\frac{1}{2}} \exp(th(0)) \qquad \text{as } t \to \infty,$$

where the equivalence $f(t) \sim g(t)$ means that $\lim_{t\to\infty} f(t)/g(t) = 1$.

The above asymptotic results can be stated as

$$\lim_{t\to\infty} \frac{1}{t} \log F(t) = \sup_{x\in\mathbb{R}} h(x).$$

This formulation is what we will use in the large deviation theory. Its abstract form in the infinite-dimensional setting is embodied in the so-called Varadhan's lemma to be discussed later [**DZ98**, **DS84**, **Var84**].

Proof. Without loss of generality, we can assume $h(0) = 0$ by shifting $h(x)$ correspondingly. With this condition, if $h(x) = h''(0)x^2/2$, $h''(0) < 0$, we

have

$$\int_{\mathbb{R}} e^{th(x)} dx = \sqrt{2\pi}(-th''(0))^{-\frac{1}{2}}.$$

In general, for any $\epsilon > 0$, there exists $\delta > 0$ such that if $|x| \le \delta$,

$$\left| h(x) - \frac{h''(0)}{2} x^2 \right| \le \epsilon x^2.$$

It follows that

$$\int_{[-\delta,\delta]} \exp\left(\frac{tx^2}{2}(h''(0) - 2\epsilon)\right) dx \le \int_{[-\delta,\delta]} \exp\left(th(x)\right) dx$$

$$\le \int_{[-\delta,\delta]} \exp\left(\frac{tx^2}{2}(h''(0) + 2\epsilon)\right) dx.$$

By assumption, for this $\delta > 0$, there exists $\eta > 0$ such that $h(x) \le -\eta$ if $|x| \ge \delta$. Thus

$$\int_{|x|\ge\delta} \exp\left(th(x)\right) dx \le e^{-(t-1)\eta} \int_{\mathbb{R}} e^{h(x)} dx \sim \mathcal{O}(e^{-\alpha t}), \ \alpha > 0, \quad \text{for} \quad t > 1.$$

We first prove the upper bound:

$$\int_{\mathbb{R}} \exp\left(th(x)\right) dx \le \int_{\mathbb{R}} \exp\left(\frac{tx^2}{2}(h''(0) + 2\epsilon)\right) dx$$

$$- \int_{|x|\ge\delta} \exp\left(\frac{tx^2}{2}(h''(0) + 2\epsilon)\right) dx + \mathcal{O}(e^{-\alpha t})$$

$$= \sqrt{2\pi}\left[t(-h''(0) - 2\epsilon)\right]^{-\frac{1}{2}} + \mathcal{O}(e^{-\beta t})$$

where $\beta > 0$. In fact, we ask for $\epsilon < -h''(0)/2$ here.

The proof of the lower bound is similar. By the arbitrary smallness of ϵ, we have

$$\lim_{t\to\infty} F(t)/\sqrt{2\pi}(-th''(0))^{-\frac{1}{2}} = 1,$$

which completes the proof. $\qquad\qquad\square$

Definition A.2 (Large deviation principle). Let $\mathscr{X}$ be a complete separable metric space and let $\{\mathbb{P}^\varepsilon\}_{\varepsilon\ge 0}$ be a family of probability measures on the Borel subsets of $\mathscr{X}$. We say that $\mathbb{P}^\varepsilon$ satisfies the large deviation principle if there exists a rate functional $I : \mathscr{X} \to [0, \infty]$ such that:

    (i) For any $\ell < \infty$,

$$\{x : I(x) \le \ell\} \text{ is compact.}$$

    (ii) Upper bound. For each closed set $F \subset \mathscr{X}$,

$$\varlimsup_{\varepsilon\to 0} \varepsilon \ln \mathbb{P}^\varepsilon(F) \le -\inf_{x\in F} I(x).$$

(iii) Lower bound. For each open set $G \subset \mathscr{X}$,

$$\varliminf_{\varepsilon \to 0} \varepsilon \ln \mathbb{P}^{\varepsilon}(G) \geq - \inf_{x \in G} I(x).$$

Theorem A.3 (Varadhan's lemma). *Suppose that $\mathbb{P}^{\varepsilon}$ satisfies the large deviation principle with rate functional $I(\cdot)$ and $F \in C_b(\mathscr{X})$. Then*

$$(A.2) \qquad \lim_{\varepsilon \to 0} \varepsilon \ln \int_{\mathscr{X}} \exp\left(\frac{1}{\varepsilon} F(x)\right) \mathbb{P}^{\varepsilon}(dx) = \sup_{x \in \mathscr{X}} (F(x) - I(x)).$$

The proof of Varadhan's lemma can be found in [**DZ98**, **Var84**].

B. Gronwall's Inequality

Theorem B.1 (Gronwall's inequality). *Assume that the function $f : [0, \infty) \to \mathbb{R}^+$ satisfies the inequality*

$$f(t) \leq a(t) + \int_0^t b(s)f(s)ds,$$

where $a(t), b(t) \geq 0$. Then we have

$$(B.1) \qquad f(t) \leq a(t) + \int_0^t a(s)b(s) \exp\left(\int_s^t b(u)du\right) ds.$$

Proof. Let $g(t) = \int_0^t b(s)f(s)ds$. We have

$$g'(t) \leq a(t)b(t) + b(t)g(t).$$

Define $h(t) = g(t) \exp(-\int_0^t b(s)ds)$. We obtain

$$h'(t) \leq a(t)b(t) \exp\left(-\int_0^t b(s)ds\right).$$

Integrating both sides from 0 to t, we get

$$g(t) \leq \int_0^t a(s)b(s) \exp\left(\int_s^t b(u)du\right) ds,$$

which yields the desired estimate. $\qquad\qquad\qquad\qquad\qquad\qquad\square$

In the case when $a(t) \equiv a$ and $b(t) \equiv b$, we have

$$f(t) \leq a \exp(bt).$$

Theorem B.2 (Discrete Gronwall's inequality). *Assume that F_n satisfies*

$$(B.2) \qquad\qquad F_{n+1} \leq (1 + b_n \delta t)F_n + a_n, \quad F_0 \geq 0,$$

where $\delta t, a_n, b_n \geq 0$. Then we have

$$(B.3) \qquad F_n \leq \exp\left(\left(\sum_{k=0}^{n-1} b_k\right) \delta t\right) F_0 + \sum_{k=0}^{n-1} \left(a_k \exp\left(\left(\sum_{l=k+1}^{n-1} b_l\right) \delta t\right)\right).$$

Proof. From (B.2), we have

$$F_n \leq \prod_{k=0}^{n-1}(1 + b_k\delta t)F_0 + \sum_{k=0}^{n-1}\left(a_k \sum_{l=k+1}^{n-1} (1 + b_l\delta t)\right).$$

The estimate (B.2) follows by a straightforward application of the inequality $1 + x \leq e^x$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

When $F_0 \leq C\delta t^p$, $b_n \equiv b$, $a_n = K\delta t^{p+1}$, and $n\delta t \leq T$, we have

$$F_n \leq Ce^{bT}\delta t^p + Ke^{bT}\frac{\delta t^{p+1}}{1 - e^{-b\delta t}}.$$

This is the commonly used pth-order error estimate in numerical analysis.

C. Measure and Integration

Let $(\Omega, \mathcal{F})$ be a measurable space.

Definition C.1 (Measure). The measure $\mu : \mathcal{F} \to \bar{\mathbb{R}}_+ = [0, \infty]$ is a set function defined on $\mathcal{F}$ that satisfies

(a) $\mu(\emptyset) = 0$;

(b) the countable additivity; i.e., for pairwise disjoint sets $A_n \in \mathcal{F}$, we have

$$\mu\left(\bigcup_{n=1}^{\infty} A_n \right) = \sum_{n=1}^{\infty}\mu(A_n),$$

where we assume the arithmetic rules (2.7) on the extended reals $\bar{\mathbb{R}}_+$.

When the set function μ takes values in $\bar{\mathbb{R}} = [-\infty, \infty]$ and only the countable additivity condition is assumed, μ is called a *signed measure*.

Definition C.2 (Algebra). An algebra (or field) $\mathcal{F}_0$ is a collection of subsets of Ω that satisfies the following conditions:

(i) $\Omega \in \mathcal{F}_0$;

(ii) if $A \in \mathcal{F}_0$, then $A^c \in \mathcal{F}_0$;

(iii) if $A, B \in \mathcal{F}_0$, then $A \cup B \in \mathcal{F}_0$.

Theorem C.3 (Measure extension). *A finite measure μ on an algebra $\mathcal{F}_0 \subset \mathcal{F}$, i.e., $\mu(\Omega) < \infty$, can be uniquely extended to a measure on $\sigma(\mathcal{F}_0)$.*

Definition C.4 (Measurable function). A function $f : \Omega \to \mathbb{R}$ is called *measurable* or $\mathcal{F}$-*measurable* if $f^{-1}(A) \in \mathcal{F}$ for any $A \in \mathcal{R}$.

Definition C.5 (Simple function). A function $f : \Omega \to \mathbb{R}$ is called a simple function if it has the representation

$$f(\omega) = \sum_{i=1}^{n} a_i \chi_{A_i}(\omega),$$

where $a_i \in \mathbb{R}$ and $A_i \in \mathcal{F}$ for $i = 1, \ldots, n$.

Theorem C.6. *Any nonnegative measurable function f on space $(\Omega, \mathcal{F})$ can be approximated by a sequence of monotonically increasing nonnegative functions $\{f_n\}$; that is, $0 \le f_n(\omega) \le f_{n+1}(\omega)$ for any n and*

$$\lim_{n \to \infty} f_n(\omega) = f(\omega).$$

We will denote such a monotone approximation as $f_n \uparrow f$ for short.

Definition C.7 (Integration of a simple function). The integral of the simple function $f(\omega) = \sum_{i=1}^{n} a_i \chi_{A_i}(\omega)$ is defined as

$$\mu(f) = \int_\Omega f \mu(d\omega) = \sum_{i=1}^{n} a_i \mu(A_i).$$

Theorem C.8 (Properties of the integral of simple functions). *Suppose that f_n, g_n, f, and g are nonnegative simple functions. Then we have:*

(a) *$\mu(\alpha f + \beta g) = \alpha \mu(f) + \beta \mu(g)$ for any $\alpha, \beta \in \mathbb{R}_+$.*

(b) *If $f \le g$, then $\mu(f) \le \mu(g)$.*

(c) *If $f_n \uparrow f$, then $\lim_{n \to \infty} \mu(f_n) = \mu(f)$.*

(d) *If f_n and g_n are monotonically increasing and $\lim_{n \to \infty} f_n \le \lim_{n \to \infty} g_n$, then $\lim_{n \to \infty} \mu(f_n) \le \lim_{n \to \infty} \mu(g_n)$.*

Definition C.9. Let f be a nonnegative measurable function. The integral of f is defined as

$$\mu(f) = \int_\Omega f(\omega) \mu(d\omega) = \lim_{n \to \infty} \mu(f_n),$$

where $f_n \uparrow f$ are nonnegative functions.

It is easy to see that the integral is well-defined, say using Theorem C.8(d).

Definition C.10. Let f be a measurable function. The integral of f is defined as

$$\mu(f) = \int_\Omega f(\omega) \mu(d\omega) = \mu(f^+) - \mu(f^-),$$

where $f^+ = f \vee 0$ and $f^- = (-f) \vee 0$ are both nonnegative measurable functions. If both $\mu(f^+)$ and $\mu(f^-)$ are finite, f is called an integrable function.

Theorem C.11 (Monotone convergence theorem). *Suppose that $\{f_n\}$ are nonnegative integrable functions and $f_n \uparrow f$ almost everywhere. Then*

$$\lim_{n\to\infty} \mu(f_n) = \mu(f).$$

Theorem C.12 (Fatou lemma). *Let $\{f_n\}$ be nonnegative integrable functions. We have*

$$\mu(\liminf_{n\to\infty} f_n) \le \liminf_{n\to\infty} \mu(f_n).$$

Theorem C.13 (Dominated convergence theorem). *Suppose that $\{f_n\}$ are integrable functions and $f_n \to f$ almost everywhere. If $|f_n| \le g$ for any n and $\mu(g) < \infty$, then*

$$\lim_{n\to\infty} \mu(f_n) = \mu(f).$$

Definition C.14 (σ-finite measure). A measure μ on $(\Omega, \mathcal{F})$ is σ-finite if there exists a countable partition of Ω; i.e., $\Omega = \bigcup_{n=1}^{\infty} A_n$ where $\{A_n\}$ are pairwise disjoint, such that $\mu(A_n) < \infty$ for any n.

Definition C.15 (Absolute continuity). Let μ, η be a σ-finite measure and a signed measure, respectively. Here η is called absolutely continuous with respect to μ if $\mu(A) = 0$ implies $\eta(A) = 0$ for any $A \in \mathcal{F}$. It is also denoted as $\eta \ll \mu$ for short.

Theorem C.16 (Radon-Nikodym theorem). *Let μ be a σ-finite measure on $(\Omega, \mathcal{F})$ and let η be a signed measure which is absolutely continuous with respect to μ. Then there exists a measurable function f such that*

$$\eta(A) = \int_A f(\omega)\mu(d\omega)$$

for any $A \in \mathcal{F}$. Here f is unique in the μ-equivalent sense; i.e., $f \overset{\mu}{\sim} g$ if $\mu(f = g) = 1$. It is also called the Radon-Nikodym derivative of η with respect to μ, abbreviated as $f = d\eta/d\mu$.

The readers may refer to [**Bil79**, **Cin11**, **Hal50**] for more details.

D. Martingales

Consider the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and a filtration $\{\mathcal{F}_n\}_{n\in\mathbb{N}}$ or $\{\mathcal{F}_t\}_{t\ge 0}$.

Definition D.1 (Martingale). A continuous time stochastic process X_t is called an $\mathcal{F}_t$-martingale if $X_t \in L^1_\omega$ for any t, X_t is $\mathcal{F}_t$-adapted, and

(D.1) $\mathbb{E}(X_t|\mathcal{F}_s) = X_s$ for all $s \le t$.

X_t is called a submartingale or supermartigale if the above equality is replaced by $\ge$ or $\le$. These concepts can be defined for discrete time stochastic processes if we replace (D.1) by $\mathbb{E}(X_n|\mathcal{F}_m) = X_m$ for any $m \le n$. The discrete submartingale or supermartingale can be defined similarly.

The following theorem is a straightforward application of the conditional Jensen inequality

Theorem D.2. *Assume ϕ is a convex function such that $\phi(X_t) \in L^1_\omega$ for any t. Then $\phi(X_t)$ is a submartingale.*

The simplest choices of ϕ include $\phi(x) = |x|$, $x^+ := x \vee 0$, or x^2 if X_t is a square-integrable martingale.

Theorem D.3 (Martingale inequalities)**.** *Let X_t be a submartingale with continuous paths. Then for any $[s, t] \subset [0, \infty)$ and $\lambda > 0$, we have:*

(i) *Doob's inequality:*

$$\mathbb{P}\left(\sup_{u \in [s,t]} X_u \geq \lambda\right) \leq \frac{\mathbb{E}X_t^+}{\lambda}.$$

(ii) *Doob's L^p-maximal inequality:*

$$\mathbb{E}\left(\sup_{u \in [s,t]} X_u\right)^p \leq \left(\frac{p}{p-1}\right)^p \mathbb{E}X_t^p, \qquad p > 1.$$

Useful results follow immediately if we take $X_t = |Y_t|$ where Y_t is a martingale. Similar inequalities also hold for discrete time martingales. See [**Chu01**, **Dur10**, **KS91**] for more details.

E. Strong Markov Property

Consider a finite Markov chain $\{X_n\}_{n \in \mathbb{N}}$ on S with initial distribution μ and transition probability matrix $\boldsymbol{P}$.

Theorem E.1 (Markov property)**.** *Conditional on $X_m = i$ ($m \in \mathbb{N}$), $\{X_{m+n}\}_{n \in \mathbb{N}}$ is Markovian with initial distribution δ_i and transition probability matrix $\boldsymbol{P}$, and it is independent of $(X_0, X_1, \ldots, X_m)$.*

Theorem E.2 (Strong Markov property)**.** *Let N be a stopping time. Conditional on $\{N < \infty\}$ and $X_N = i$, $\{X_{N+n}\}_{n \in \mathbb{N}}$ is Markovian with initial distribution δ_i and transition probability matrix $\boldsymbol{P}$.*

The above results also hold for the Q-process $\{X_t\}_{t \geq 0}$ with generator $\boldsymbol{Q}$.

Theorem E.3 (Markov property)**.** *Conditional on $X_t = i$ ($t \geq 0$), $\{X_{t+s}\}_{s \geq 0}$ is Markovian with initial distribution δ_i and generator $\boldsymbol{Q}$, and it is independent of $\{X_r, r \leq t\}$.*

Theorem E.4 (Strong Markov property)**.** *Let T be a stopping time. Conditional on $\{T < \infty\}$ and $X_T = i$, $\{X_{T+t}\}_{t \geq 0}$ is Markovian with initial distribution δ_i and generator $\boldsymbol{Q}$.*

See [**Dur10**, **Nor97**] for more details.

F. Semigroup of Operators

Let $\mathscr{B}$ be a Banach space equipped with the norm $\|\cdot\|$.

Definition F.1 (Operator semigroup)**.** A family of bounded linear operators $\{S(t)\}_{t \geq 0} : \mathscr{B} \to \mathscr{B}$ forms a strongly continuous semigroup if for any $f \in \mathscr{B}$:

    (i) $S(0)f = f$; i.e., $S(0) = I$.

    (ii) $S(t)S(s)f = S(s)S(t)f = S(t + s)f$ for any $s, t \geq 0$.

    (iii) $\|S(t)f - f\| \to 0$ for any $f \in \mathscr{B}$ as $t \to 0+$.

We will call $\{S(\cdot)\}$ a contraction semigroup if $\|S(t)\| \leq 1$ for any t, where $\|S(t)\|$ is the operator norm induced by the metric $\|\cdot\|$.

The simplest examples of semigroups include the solution operator for the system

$$\frac{d\boldsymbol{u}(t)}{dt} = \boldsymbol{A}\boldsymbol{u}(t),$$

where $\boldsymbol{u} \in \mathbb{R}^n$, $\boldsymbol{A} \in \mathbb{R}^{n \times n}$, $\mathscr{B} = \mathbb{R}^n$, and $S(t)\boldsymbol{f} := \boldsymbol{u}(t)$ by solving the ODE with initial condition $\boldsymbol{u}(t)|_{t=0} = \boldsymbol{f}$. Similarly, consider the PDE

$$\partial_t u = \Delta u \quad \text{in } U, \qquad u = 0 \ \text{ on } \partial U,$$

where U is a bounded open set with smooth boundary. We can take $\mathscr{B} = L^2(U)$ and $S(t)f := u(t)$, where $u(t)$ is the solution of the above PDE with initial condition $u(x, t = 0) = f$.

Definition F.2 (Infinitesimal generator)**.** Denote

$$D(\mathcal{A}) = \left\{ f \in \mathscr{B} : \lim_{t \to 0+} \frac{S(t)f - f}{t} \text{ exits in } \mathscr{B} \right\}$$

and

$$\mathcal{A}f := \lim_{t \to 0+} \frac{1}{t}(S(t)f - f), \qquad f \in D(\mathcal{A}).$$

The operator $\mathcal{A}$ is called the infinitesimal generator of the semigroup $S(t)$; $D(\mathcal{A})$ is the domain of the operator $\mathcal{A}$.

It can be shown that the infinitesimal generators of the two examples above are $\mathcal{A} = \boldsymbol{A}$ and $\mathcal{A} = \Delta$ and their domains are $\mathbb{R}^n$ and the Sobolev space $H_0^1(U) \cup H^2(U)$, respectively.

Theorem F.3 (Basic properties)**.** *Let $f \in D(\mathcal{A})$. We have:*

    (i) *$S(t)f \in D(\mathcal{A})$ and $S(t)\mathcal{A}f = \mathcal{A}S(t)f$ for any $t \geq 0$.*

    (ii) *$f(t) := S(t)f$ is differentiable on $(0, \infty)$ and*

$$\frac{df(t)}{dt} = \mathcal{A}f(t), \qquad t > 0.$$

Theorem F.4. *The generator $\mathcal{A}$ is a closed operator and $D(\mathcal{A})$ is dense in $\mathscr{B}$.*

In general, the generator $\mathcal{A}$ is unbounded, e.g., $\mathcal{A} = \Delta$ in the previous PDE example, so we only have $D(\mathcal{A}) \subsetneq \mathscr{B}$.

Definition F.5 (Resolvent set and operator)**.** Let $\mathcal{A}$ be a closed linear operator with domain $D(\mathcal{A})$. The resolvent set of $\mathcal{A}$ is defined by

$$\rho(\mathcal{A}) = \{\lambda : \lambda \in \mathbb{R} \text{ and } \lambda I - \mathcal{A} \text{ is bijective from } D(\mathcal{A}) \text{ to } \mathscr{B}\}.$$

If $\lambda \in \rho(\mathcal{A})$, the resolvent operator $R_\lambda : \mathscr{B} \to \mathscr{B}$ is defined by

$$R_\lambda f := (\lambda I - \mathcal{A})^{-1} f.$$

The closed graph theorem ensures that $(\lambda I - \mathcal{A})^{-1}$ is a bounded linear operator if $\lambda \in \rho(\mathcal{A})$.

Theorem F.6 (Hille-Yosida theorem)**.** *Let $\mathcal{A}$ be a closed, densely defined linear operator on $\mathscr{B}$. Then $\mathcal{A}$ generates a contraction semigroup $\{S(t)\}_{t \geq 0}$ if and only if*

$$\lambda \in \rho(\mathcal{A}) \qquad and \qquad \|R_\lambda\| \leq \frac{1}{\lambda} \qquad \text{for all } \lambda > 0.$$

Interested readers are referred to [**Eva10**, **Paz83**, **Yos95**] for more details on semigroup theory.

Bibliography

[AC08]   A. Abdulle and S. Cirilli, *S-ROCK: Chebyshev methods for stiff stochastic differential equations*, SIAM J. Sci. Comput. **30** (2008), no. 2, 997–1014, DOI 10.1137/070679375. MR2385896

[ACK10]   D. F. Anderson, G. Craciun, and T. G. Kurtz, *Product-form stationary distributions for deficiency zero chemical reaction networks*, Bull. Math. Biol. **72** (2010), no. 8, 1947–1970, DOI 10.1007/s11538-010-9517-4. MR2734052

[AGK11]   D. F. Anderson, A. Ganguly, and T. G. Kurtz, *Error analysis of tau-leap simulation methods*, Ann. Appl. Probab. **21** (2011), no. 6, 2226–2262, DOI 10.1214/10-AAP756. MR2895415

[AH12]   D. F. Anderson and D. J. Higham, *Multilevel Monte Carlo for continuous time Markov chains, with applications in biochemical kinetics*, Multiscale Model. Simul. **10** (2012), no. 1, 146–179, DOI 10.1137/110840546. MR2902602

[AL08]   A. Abdulle and T. Li, *S-ROCK methods for stiff Itô SDEs*, Commun. Math. Sci. **6** (2008), no. 4, 845–868. MR2511696

[And86]   H. L. Anderson, *Metropolis, Monte Carlo and the MANIAC*, Los Alamos Science **14** (1986), 96–108.

[App04]   D. Applebaum, *Lévy processes and stochastic calculus*, Cambridge Studies in Advanced Mathematics, vol. 93, Cambridge University Press, Cambridge, 2004. MR2072890

[ARLS11]   M. Assaf, E. Roberts, and Z. Luthey-Schulten, *Determining the stability of genetic switches: Explicitly accounting for mrna noise*, Phys. Rev. Lett. **106** (2011), 248102.

[ARM98]   A. Arkin, J. Ross, and H. H. McAdams, *Stochastic kinetic analysis of developmental pathway bifurcation in phage lambda-infected Escherichia coli cells*, Genetics **149** (1998), 1633–1648.

[Arn89]   V. I. Arnol′d, *Mathematical methods of classical mechanics*, 2nd ed., translated from the Russian by K. Vogtmann and A. Weinstein, Graduate Texts in Mathematics, vol. 60, Springer-Verlag, New York, 1989. MR997295

[BB01]   P. Baldi and S. Brunak, *Bioinformatics*, 2nd ed., The machine learning approach; A Bradford Book, Adaptive Computation and Machine Learning, MIT Press, Cambridge, MA, 2001. MR1849633

[BE67]   L. E. Baum and J. A. Eagon, *An inequality with applications to statistical esti-
            mation for probabilistic functions of Markov processes and to a model for ecology*,
            Bull. Amer. Math. Soc. **73** (1967), 360–363, DOI 10.1090/S0002-9904-1967-11751-
            8. MR0210217

[Bil79]   P. Billingsley, *Probability and measure*, Wiley Series in Probability and Math-
            ematical Statistics, John Wiley & Sons, New York-Chichester-Brisbane, 1979.
            MR534323

[BKL75]   A. B. Bortz, M. H. Kalos, and J. L. Lebowitz, *New algorithm for Monte Carlo
            simulations of Ising spin systems*, J. Comp. Phys. **17** (1975), 10–18.

[Bou95]   C. A. Bouman, *Markov random fields and stochastic image models*, available from
            http://dynamo.ecn.purdue.edu/~bouman, 1995.

[BP98]   S. Brin and L. Page, *The anatomy of a large-scale hypertextual web search engine*,
            Computer Networks and ISDN Systems **30** (1998), 107–117.

[BP06]   Z. P. Bažant and S. Pang, *Mechanics-based statistics of failure risk of quasibrittle
            structures and size effect of safety factors*, Proc. Nat. Acad. Sci. USA **103** (2006),
            9434–9439.

[BPN14]   G. R. Bowman, V. S. Pande, and F. Noé (eds.), *An introduction to Markov
            state models and their application to long timescale molecular simulation*, Ad-
            vances in Experimental Medicine and Biology, vol. 797, Springer, Dordrecht, 2014.
            MR3222039

[Bre92]   L. Breiman, *Probability*, corrected reprint of the 1968 original, Classics in Applied
            Mathematics, vol. 7, Society for Industrial and Applied Mathematics (SIAM),
            Philadelphia, PA, 1992. MR1163370

[Cam12]   M. K. Cameron, *Finding the quasipotential for nongradient SDEs*, Phys. D **241**
            (2012), no. 18, 1532–1550, DOI 10.1016/j.physd.2012.06.005. MR2957825

[CGP05]   Y. Cao, D. Gillespie, and L. Petzold, *Multiscale stochastic simulation algorithm
            with stochastic partial equilibrium assumption for chemically reacting systems*,
            J. Comput. Phys. **206** (2005), no. 2, 395–411, DOI 10.1016/j.jcp.2004.12.014.
            MR2143324

[CGP06]   Y. Cao, D. Gillespie, and L. Petzold, *Efficient stepsize selection for the tau-leaping
            method*, J. Chem. Phys. **124** (2006), 044109.

[CH13]   A. J. Chorin and O. H. Hald, *Stochastic tools in mathematics and science*, 3rd ed.,
            Texts in Applied Mathematics, vol. 58, Springer, New York, 2013. MR3076304

[Cha78]   D. Chandler, *Statistical mechanics of isomerization dynamics in liquids and the
            transition state approximation*, J. Chem. Phys. **68** (1978), 2959–2970.

[Cha87]   D. Chandler, *Introduction to modern statistical mechanics*, The Clarendon Press,
            Oxford University Press, New York, 1987. MR913936

[CHK02]   A. J. Chorin, O. H. Hald, and R. Kupferman, *Optimal prediction with mem-
            ory*, Phys. D **166** (2002), no. 3-4, 239–257, DOI 10.1016/S0167-2789(02)00446-3.
            MR1915310

[Cho03]   A. J. Chorin, *Conditional expectations and renormalization*, Multiscale Model.
            Simul. **1** (2003), no. 1, 105–118, DOI 10.1137/S1540345902405556. MR1960842

[Chu97]   F. R. K. Chung, *Spectral graph theory*, CBMS Regional Conference Series in Math-
            ematics, vol. 92, Published for the Conference Board of the Mathematical Sciences,
            Washington, DC; by the American Mathematical Society, Providence, RI, 1997.
            MR1421568

[Chu01]   K. L. Chung, *A course in probability theory*, 3rd ed., Academic Press, Inc., San
            Diego, CA, 2001. MR1796326

[Cin11]   E. Çınlar, *Probability and stochastics*, Graduate Texts in Mathematics, vol. 261,
            Springer, New York, 2011. MR2767184

[CKVE11]   M. Cameron, R. V. Kohn, and E. Vanden-Eijnden, *The string method as a dynamical system*, J. Nonlinear Sci. **21** (2011), no. 2, 193–230, DOI 10.1007/s00332-010-9081-y. MR2788855

[CLP04]   Y. Cao, H. Li, and L. Petzold, *Efficient formulation of the stochastic simulation algorithm for chemically reacting systems*, J. Chem. Phys. **121** (2004), 4059–4067.

[CM47]   R. H. Cameron and W. T. Martin, *The orthogonal development of non-linear functionals in series of Fourier-Hermite functionals*, Ann. of Math. (2) **48** (1947), 385–392, DOI 10.2307/1969178. MR0020230

[CT06]   T. M. Cover and J. A. Thomas, *Elements of information theory*, 2nd ed., Wiley-Interscience [John Wiley & Sons], Hoboken, NJ, 2006. MR2239987

[CVK05]   A. Chatterjee, D. G. Vlachos, and M. A. Katsoulakis, *Binomial distribution based tau-leap accelerated stochastic simulation*, J. Chem. Phys. **122** (2005), 024112.

[CW05]   K. L. Chung and J. B. Walsh, *Markov processes, Brownian motion, and time symmetry*, 2nd ed., Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences], vol. 249, Springer, New York, 2005. MR2152573

[DE86]   M. Doi and S. F. Edwards, *The theory of polymer dynamics*, Oxford University Press, New York, 1986.

[DLR77]   A. P. Dempster, N. M. Laird, and D. B. Rubin, *Maximum likelihood from incomplete data via the EM algorithm*, J. Roy. Statist. Soc. Ser. B **39** (1977), no. 1, 1–38. With discussion. MR0501537

[DMRH94]   M. I. Dykman, E. Mori, J. Ross, and P. M. Hunt, *Large fluctuations and optimal paths in chemical kinetics*, J. Chem. Phys. **100** (1994), 5735–5750.

[Doo42]   J. L. Doob, *The Brownian movement and stochastic equations*, Ann. of Math. (2) **43** (1942), 351–369, DOI 10.2307/1968873. MR0006634

[Doo84]   J. L. Doob, *Classical potential theory and its probabilistic counterpart*, Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences], vol. 262, Springer-Verlag, New York, 1984. MR731258

[DPZ92]   G. Da Prato and J. Zabczyk, *Stochastic equations in infinite dimensions*, Encyclopedia of Mathematics and its Applications, vol. 44, Cambridge University Press, Cambridge, 1992. MR1207136

[DS84]   J.-D. Deuschel and D. W. Stroock, *Large deviations*, Pure and Applied Mathematics, vol. 137, Academic Press, Inc., Boston, MA, 1989. MR997938

[DSK09]   E. Darve, J. Solomon, and A. Kia, *Computing generalized Langevin equations and generalized Fokker-Planck equations*, Proc. Nat. Acad. Sci. USA **106** (2009), 10884–10889.

[Dur10]   R. Durrett, *Probability: theory and examples*, 4th ed., Cambridge Series in Statistical and Probabilistic Mathematics, vol. 31, Cambridge University Press, Cambridge, 2010. MR2722836

[DZ98]   A. Dembo and O. Zeitouni, *Large deviations techniques and applications*, 2nd ed., Applications of Mathematics (New York), vol. 38, Springer-Verlag, New York, 1998. MR1619036

[E11]   W. E, *Principles of multiscale modeling*, Cambridge University Press, Cambridge, 2011. MR2830582

[EAM95]   R. J. Elliott, L. Aggoun, and J. B. Moore, *Hidden Markov models: Estimation and control*, Applications of Mathematics (New York), vol. 29, Springer-Verlag, New York, 1995. MR1323178

[Eck87]   R. Eckhardt, *Stan Ulam, John von Neumann, and the Monte Carlo method,* with contributions by Tony Warnock, Gary D. Doolen, and John Hendricks; Stanislaw Ulam, 1909–1984, Los Alamos Sci. **15, Special Issue** (1987), 131–137. MR935772

[Ein05]   A. Einstein, *On the movement of small particles suspended in a stationary liquid demanded by the molecular kinetic theory of heat*, Ann. Phys. (in German) **322** (1905), 549–560.

[EK86]   S. N. Ethier and T. G. Kurtz, *Markov processes: Characterization and convergence*, Wiley Series in Probability and Mathematical Statistics: Probability and Mathematical Statistics, John Wiley & Sons, Inc., New York, 1986. MR838085

[Ell85]   R. S. Ellis, *Entropy, large deviations, and statistical mechanics*, Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences], vol. 271, Springer-Verlag, New York, 1985. MR793553

[ELSS02]   M. B. Elowitz, A. J. Levine, E. D. Siggia, and P. S. Swain, *Stochastic gene expression in a single cell*, Science **297** (2002), 1183–1186.

[ELVE05a]   W. E, D. Liu, and E. Vanden-Eijnden, *Analysis of multiscale methods for stochastic differential equations*, Comm. Pure Appl. Math. **58** (2005), no. 11, 1544–1585, DOI 10.1002/cpa.20088. MR2165382

[ELVE05b]   W. E, D. Liu, and E. Vanden-Eijnden, *Nested stochastic simulation algorithm for chemical kinetic systems with disparate rates*, J. Chem. Phys. **123** (2005), 194107.

[ELVE07]   W. E, D. Liu, and E. Vanden-Eijnden, *Nested stochastic simulation algorithms for chemical kinetic systems with multiple time scales*, J. Comput. Phys. **221** (2007), no. 1, 158–180, DOI 10.1016/j.jcp.2006.06.019. MR2290567

[ELVE08]   W. E, T. Li, and E. Vanden-Eijnden, *Optimal partition and effective dynamics of complex networks*, Proc. Natl. Acad. Sci. USA **105** (2008), no. 23, 7907–7912, DOI 10.1073/pnas.0707563105. MR2415575

[ERVE02]   W. E, W. Ren, and E. Vanden-Eijnden, *String method for the study of rare events*, Phys. Rev. B **66** (2002), 052301.

[ERVE03]   W. E, W. Ren, and E. Vanden-Eijnden, *Energy landscape and thermally activated switching of submicron-sized ferromagnetic elements*, J. Appl. Phys. **93** (2003), 2275–2282.

[ERVE07]   W. E, W. Ren, and E. Vanden-Eijnden, *Simplified and improved string method for computing the minimum energy paths in barrier-crossing events*, J. Chem. Phys. **126** (2007), 164103.

[Eva10]   L. C. Evans, *Partial differential equations*, 2nd ed., Graduate Studies in Mathematics, vol. 19, American Mathematical Society, Providence, RI, 2010. MR2597943

[EVE10]   W. E and E. Vanden-Eijnden, *Transition-path theory and path-finding algorithms for the study of rare events*, Ann. Rev. Phys. Chem. **61** (2010), 391–420.

[Fel68]   W. Feller, *An introduction to probability theory and its applications*, Third edition, John Wiley & Sons, Inc., New York-London-Sydney, 1968. MR0228020

[Fre85]   M. Freidlin, *Functional integration and partial differential equations*, Annals of Mathematics Studies, vol. 109, Princeton University Press, Princeton, NJ, 1985. MR833742

[Fri75a]   A. Friedman, *Stochastic differential equations and applications. Vol. 1*, Probability and Mathematical Statistics, Vol. 28, Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1975. MR0494490

[Fri75b]   A. Friedman, *Stochastic differential equations and applications. Vol. 2*, Probability and Mathematical Statistics, Vol. 28, Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1976. MR0494491

[FS02]   D. Frenkel and B. Smit, *Understanding molecular simulations: From algorithms to applications*, 2nd ed., Academic Press, San Diego, 2002.

[FW98]   M. I. Freidlin and A. D. Wentzell, *Random perturbations of dynamical systems*, 2nd ed., translated from the 1979 Russian original by Joseph Szücs, Grundlehren

der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences], vol. 260, Springer-Verlag, New York, 1998. MR1652127

[Gal99]   G. Gallavotti, *Statistical mechanics: A short treatise*, Texts and Monographs in Physics, Springer-Verlag, Berlin, 1999. MR1707309

[Gar09]   C. Gardiner, *Stochastic methods: A handbook for the natural and social sciences*, 4th ed., Springer Series in Synergetics, Springer-Verlag, Berlin, 2009. MR2676235

[GB00]   M. A. Gibson and J. Bruck, *Efficient exact stochastic simulation of chemical systems with many species and channels*, J. Phys. Chem. A **104** (2000), 1876–1889.

[Gey91]   C. Geyer, *Markov chain Monte Carlo maximum likelihood*, Computing Science and Statistics: Proceedings of the 23rd Symposium on the interface (New York) (E. Keramigas, ed.), American Statistical Association, 1991, pp. 156–163.

[GHO17]   R. Ghanem, D. Higdon, and H. Owhadi (eds.), *Handbook of uncertainty quantification*, Springer International Publishing, Switzerland, 2017.

[GHP13]   D. Gillespie, A. Hellander, and L. Petzold, *Perspective: Stochastic algorithms for chemical kinetics*, J. Chem. Phys. **138** (2013), 170901.

[Gil76]   D. T. Gillespie, *A general method for numerically simulating the stochastic time evolution of coupled chemical reactions*, J. Computational Phys. **22** (1976), no. 4, 403–434, DOI 10.1016/0021-9991(76)90041-3. MR0503370

[Gil92]   D. T. Gillespie, *Markov processes: An introduction for physical scientists*, Academic Press, Inc., Boston, MA, 1992. MR1133392

[Gil00]   D. Gillespie, *The chemical Langevin equation*, J. Chem. Phys. **113** (2000), 297.

[Gil01]   D. Gillespie, *Approximate accelerated stochastic simulation of chemically reacting systems*, J. Chem. Phys. **115** (2001), 1716–1733.

[Gil08]   M. B. Giles, *Multilevel Monte Carlo path simulation*, Oper. Res. **56** (2008), no. 3, 607–617, DOI 10.1287/opre.1070.0496. MR2436856

[Gil14]   M. B. Giles, *Multilevel Monte Carlo methods*, Monte Carlo and quasi-Monte Carlo methods 2012, Springer Proc. Math. Stat., vol. 65, Springer, Heidelberg, 2013, pp. 83–103, DOI 10.1007/978-3-642-41095-6_4. MR3145560

[GJ87]   J. Glimm and A. Jaffe, *Quantum physics: A functional integral point of view*, 2nd ed., Springer-Verlag, New York, 1987. MR887102

[Gla04]   P. Glasserman, *Monte Carlo methods in financial engineering: Stochastic modelling and applied probability*, Applications of Mathematics (New York), vol. 53, Springer-Verlag, New York, 2004. MR1999614

[Gol80]   H. Goldstein, *Classical mechanics*, 2nd ed., Addison-Wesley Publishing Co., Reading, Mass., 1980. Addison-Wesley Series in Physics. MR575343

[Gol92]   N. Goldenfeld, *Lectures on phase transitions and the renormalization group*, Perseus Books Publishing, Massachusetts, 1992.

[GS66]   I. M. Gelfand and G. E. Shilov, *Generalized functions*, vols. 1-5, Academic Press, New York and London, 1964–1966.

[GS12]   R. Ghanem and P. Spanos, *Stochastic finite elements: A spectral approach*, revised ed., Dover Publications Inc., Mineola, 2012.

[GT95]   C. Geyer and E. Thompson, *Annealing Markov chain Monte Carlo with applications to ancestral inference*, J. Amer. Stat. Assoc. **90** (1995), 909–920.

[Hal50]   P. R. Halmos, *Measure Theory*, D. Van Nostrand Company, Inc., New York, N. Y., 1950. MR0033869

[HEnVEDB10] C. Hijón, P. Español, E. Vanden-Eijnden, and R. Delgado-Buscalioni, *Mori–Zwanzig formalism as a practical computational tool*, Faraday Disc. **144** (2010), 301–322.

[HJ85]   R. A. Horn and C. R. Johnson, *Matrix analysis*, Cambridge University Press, Cambridge, 1985. MR832183

[HJ99]   G. Henkelman and H. Jónsson, *A dimer method for finding saddle points on high dimensional potential surfaces using only first derivatives*, J. Chem. Phys. **111** (1999), 7010–7022.

[HJ00]   G. Henkelman and H. Jónsson, *Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points*, J. Chem. Phys. **113** (2000), 9978–9985.

[HNW08]   E. Hairer, S. P. Norsett, and G. Wanner, *Solving ordinary differential equations I: Nonstiff problems*, 2nd ed., Springer-Verlag, Berlin and Heidelberg, 2008.

[HPM90]   P. Hanggi, P. Talkner, and M. Borkovec, *Reaction-rate theory: fifty years after Kramers*, Rev. Modern Phys. **62** (1990), no. 2, 251–341, DOI 10.1103/RevModPhys.62.251. MR1056234

[HR02]   E. L. Haseltine and J. B. Rawlings, *Approximate simulation of coupled fast and slow reactions for stochastic kinetics*, J. Chem. Phys. **117** (2002), 6959–6969.

[HS08]   T. Hida and S. Si, *Lectures on white noise functionals*, World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2008. MR2444857

[HVE08]   M. Heymann and E. Vanden-Eijnden, *The geometric minimum action method: a least action principle on the space of curves*, Comm. Pure Appl. Math. **61** (2008), no. 8, 1052–1117, DOI 10.1002/cpa.20238. MR2417888

[IW81]   N. Ikeda and S. Watanabe, *Stochastic differential equations and diffusion processes*, North-Holland Mathematical Library, vol. 24, North-Holland Publishing Co., Amsterdam-New York; Kodansha, Ltd., Tokyo, 1981. MR637061

[Jel97]   F. Jelinek, *Statistical methods for speech recognition*, MIT Press, Cambridge, 1997.

[JM09]   D. Jurafsky and J. H. Martin, *Speech and language processing: An introduction to natural language processing, computational linguistics, and speech recognition*, 2nd ed., Pearson Prentice Hall, Upper Saddle River, 2009.

[JQQ04]   D.-Q. Jiang, M. Qian, and M.-P. Qian, *Mathematical theory of nonequilibrium steady states: On the frontier of probability and dynamical systems*, Lecture Notes in Mathematics, vol. 1833, Springer-Verlag, Berlin, 2004. MR2034774

[Kal97]   O. Kallenberg, *Foundations of modern probability*, Probability and its Applications (New York), Springer-Verlag, New York, 1997. MR1464694

[Kes80]   H. Kesten, *The critical probability of bond percolation on the square lattice equals $\frac{1}{2}$*, Comm. Math. Phys. **74** (1980), no. 1, 41–59. MR575895

[KK80]   C. Kittel and H. Kroemer, *Thermal physics*, 2nd ed., W. H. Freeman and Company, New York, 1980.

[Kle06]   H. Kleinert, *Path integrals in quantum mechanics, statistics, polymer physics, and financial markets*, 4th ed., World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2006. MR2255818

[Knu98]   D. E. Knuth, *The art of computer programming. Vol. 2*, Addison-Wesley, Reading, MA, 1998. Seminumerical algorithms, third edition [of MR0286318]. MR3077153

[Kol56]   A. N. Kolmogorov, *Foundations of the theory of probability*, translation edited by Nathan Morrison, with an added bibliography by A. T. Bharucha-Reid, Chelsea Publishing Co., New York, 1956. MR0079843

[KP92]   P. E. Kloeden and E. Platen, *Numerical solution of stochastic differential equations*, Applications of Mathematics (New York), vol. 23, Springer-Verlag, Berlin, 1992. MR1214374

[Kra40]   H. A. Kramers, *Brownian motion in a field of force and the diffusion model of chemical reactions*, Physica **7** (1940), 284–304. MR0002962

[KS76]   J. G. Kemeny and J. L. Snell, *Finite Markov chains*, reprinting of the 1960 original, Undergraduate Texts in Mathematics, Springer-Verlag, New York-Heidelberg, 1976. MR0410929

[KS91]   I. Karatzas and S. E. Shreve, *Brownian motion and stochastic calculus*, 2nd ed., Graduate Texts in Mathematics, vol. 113, Springer-Verlag, New York, 1991. MR1121940

[KS07]   L. B. Koralov and Y. G. Sinai, *Theory of probability and random processes*, 2nd ed., Universitext, Springer, Berlin, 2007. MR2343262

[KS09]   J. Keener and J. Sneyd, *Mathematical physiology*, 2nd ed., Springer-Verlag, New York, 2009.

[KTH95]   R. Kubo, M. Toda, and N. Hashitsume, *Statistical physics*, vol. 2, Springer-Verlag, Berlin, Heidelberg and New York, 1995.

[Kub66]   R. Kubo, *The fluctuation-dissipation theorem*, Rep. Prog. Phys. **29** (1966), 255.

[Kur72]   T. G. Kurtz, *The relation between stochastic and deterministic models for chemical reactions*, J. Chem. Phys. **57** (1972), 2976–2978.

[KW08]   M. H. Kalos and P. A. Whitlock, *Monte Carlo methods*, 2nd ed., Wiley-Blackwell, Weinheim, 2008. MR2503174

[KZW06]   S. C. Kou, Q. Zhou, and W. H. Wong, *Equi-energy sampler with applications in statistical inference and statistical mechanics,* with discussions and a rejoinder by the authors*, Ann. Statist. **34** (2006), no. 4, 1581–1652, DOI 10.1214/009053606000000515. MR2283711

[Lam77]   J. Lamperti, *Stochastic processes: A survey of the mathematical theory,* Applied Mathematical Sciences, Vol. 23, Springer-Verlag, New York-Heidelberg, 1977. MR0461600

[Lax02]   P. D. Lax, *Functional analysis*, Pure and Applied Mathematics (New York), Wiley-Interscience [John Wiley & Sons], New York, 2002. MR1892228

[LB05]   D. P. Landau and K. Binder, *A guide to Monte Carlo simulations in statistical physics*, 2nd ed., Cambridge University Press, Cambridge, 2005.

[LBL16]   H. Lei, N. A. Baker, and X. Li, *Data-driven parameterization of the generalized Langevin equation*, Proc. Natl. Acad. Sci. USA **113** (2016), no. 50, 14183–14188, DOI 10.1073/pnas.1609587113. MR3600515

[Li07]   T. Li, *Analysis of explicit tau-leaping schemes for simulating chemically reacting systems*, Multiscale Model. Simul. **6** (2007), no. 2, 417–436, DOI 10.1137/06066792X. MR2338489

[Liu04]   J. S. Liu, *Monte Carlo strategies in scientific computing*, Springer-Verlag, New York, 2004.

[LL17]   T. Li and F. Lin, *Large deviations for two-scale chemical kinetic processes*, Commun. Math. Sci. **15** (2017), no. 1, 123–163, DOI 10.4310/CMS.2017.v15.n1.a6. MR3605551

[LLLL14]   C. Lv, X. Li, F. Li, and T. Li, *Constructing the energy landscape for genetic switching system driven by intrinsic noise*, PLoS One **9** (2014), e88167.

[LLLL15]   C. Lv, X. Li, F. Li, and T. Li, *Energy landscape reveals that the budding yeast cell cycle is a robust and adaptive multi-stage process*, PLoS Comp. Biol. **11** (2015), e1004156.

[LM15]   B. Leimkuhler and C. Matthews, *Molecular dynamics: With deterministic and stochastic numerical methods*, Interdisciplinary Applied Mathematics, vol. 39, Springer, Cham, 2015. MR3362507

[Loè77]   M. Loève, *Probability theory. I*, 4th ed., Graduate Texts in Mathematics, Vol. 45, Springer-Verlag, New York-Heidelberg, 1977. MR0651017

[Lov96]   L. Lovász, *Random walks on graphs: a survey*, Combinatorics, Paul Erdős is eighty, Vol. 2 (Keszthely, 1993), Bolyai Soc. Math. Stud., vol. 2, János Bolyai Math. Soc., Budapest, 1996, pp. 353–397. MR1395866

[LX11]   G. Li and X. S. Xie, *Central dogma at the single-molecule level in living cells*, Nature **475** (2011), 308–315.

[Mar68]   G. Marsaglia, *Random numbers fall mainly in the planes*, Proc. Nat. Acad. Sci. U.S.A. **61** (1968), 25–28, DOI 10.1073/pnas.61.1.25. MR0235695

[MD10]   D. Mumford and A. Desolneux, *Pattern theory: The stochastic analysis of real-world signals*, Applying Mathematics, A K Peters, Ltd., Natick, MA, 2010. MR2723182

[Mey66]   P.-A. Meyer, *Probability and potentials*, Blaisdell Publishing Co. Ginn and Co., Waltham, Mass.-Toronto, Ont.-London, 1966. MR0205288

[MN98]   M. Matsumoto and T. Nishimura, *Mersenne twister: A 623-dimensionally equidistributed uniform pseudo-random number generator*, ACM Trans. Mod. Comp. Simul. **8** (1998), 3–30.

[MP92]   E. Marinari and G. Parisi, *Simulated tempering: A new Monte Carlo scheme*, Europhys. Lett. **19** (1992), 451–458.

[MP10]   P. Mörters and Y. Peres, *Brownian motion*, with an appendix by Oded Schramm and Wendelin Werner, Cambridge Series in Statistical and Probabilistic Mathematics, vol. 30, Cambridge University Press, Cambridge, 2010. MR2604525

[MPRV08]   U. M. B. Marconi, A. Puglisi, L. Rondoni, and A. Vulpiani, *Fluctuation-dissipation: Response theory in statistical physics*, Phys. Rep. **461** (2008), 111–195.

[MS99]   C. D. Manning and H. Schütze, *Foundations of statistical natural language processing*, MIT Press, Cambridge, MA, 1999. MR1722790

[MS01]   M. Meila and J. Shi, *A random walks view of spectral segmentation*, Proceedings of the Eighth International Workshop on Artificial Intelligence and Statistics (San Francisco), 2001, pp. 92–97.

[MT93]   S. P. Meyn and R. L. Tweedie, *Markov chains and stochastic stability*, Communications and Control Engineering Series, Springer-Verlag London, Ltd., London, 1993. MR1287609

[MT04]   G. N. Milstein and M. V. Tretyakov, *Stochastic numerics for mathematical physics*, Scientific Computation, Springer-Verlag, Berlin, 2004. MR2069903

[MTV16]   A. Moraes, R. Tempone, and P. Vilanova, *Multilevel hybrid Chernoff tau-leap*, BIT **56** (2016), no. 1, 189–239, DOI 10.1007/s10543-015-0556-y. MR3486459

[Mul56]   M. E. Muller, *Some continuous Monte Carlo methods for the Dirichlet problem*, Ann. Math. Statist. **27** (1956), 569–589, DOI 10.1214/aoms/1177728169. MR0088786

[MY71]   A. S. Monin and A. M. Yaglom, *Statistical fluid mechanics: Mechanics of turbulence*, vol. 1, MIT Press, Cambridge, 1971.

[Nor97]   J. R. Norris, *Markov chains*, Cambridge University Press, Cambridge, 1997.

[Oks98]   B. Øksendal, *Stochastic differential equations: An introduction with applications*, 5th ed., Universitext, Springer-Verlag, Berlin, 1998. MR1619188

[Pap77]   G. C. Papanicolaou, *Introduction to the asymptotic analysis of stochastic equations*, Modern modeling of continuum phenomena (Ninth Summer Sem. Appl. Math., Rensselaer Polytech. Inst., Troy, N.Y., 1975), Lectures in Appl. Math., Vol. 16, Amer. Math. Soc., Providence, R.I., 1977, pp. 109–147. MR0458590

[Pav14]   G. A. Pavliotis, *Stochastic processes and applications: Diffusion processes, the Fokker-Planck and Langevin equations*, Texts in Applied Mathematics, vol. 60, Springer, New York, 2014. MR3288096

[Paz83]   A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, Applied Mathematical Sciences, vol. 44, Springer-Verlag, New York, 1983. MR710486

[PTVF95]   W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical recipes in C*, 2nd ed., Cambridge University Press, Cambridge, New York, Port Chester, Melbourne and Sydney, 1995.

[RÖ3]   A. Rößler, *Runge-Kutta methods for the numerical solution of stochastic differential equation*, Shaker-Verlag, Aachen, 2003.

[Rab89]   L. R. Rabiner, *A tutorial on hidden Markov models and selected applications in speech recognition*, Proceedings of the IEEE **77** (1989), 257–286.

[Ram69]   J. F. Ramaley, *Buffon's noodle problem*, Amer. Math. Monthly **76** (1969), 916–918, DOI 10.2307/2317945. MR0254893

[RC04]   C. P. Robert and G. Casella, *Monte Carlo statistical methods*, 2nd ed., Springer Texts in Statistics, Springer-Verlag, New York, 2004. MR2080278

[Rea10]   A. Rukhin et al., *A statistical test suite for random and pseudorandom number generators for cryptographic applications*, available from https://nvlpubs.nist.gov/nistpubs/legacy/sp/nistspecialpublication800-22r1a.pdf, April 2010.

[Rei98]   L. E. Reichl, *A modern course in statistical physics*, 2nd ed., A Wiley-Interscience Publication, John Wiley & Sons, Inc., New York, 1998. MR1600476

[Ris89]   H. Risken, *The Fokker-Planck equation: Methods of solution and applications*, 2nd ed., Springer Series in Synergetics, vol. 18, Springer-Verlag, Berlin, 1989. MR987631

[Roc70]   R. T. Rockafellar, *Convex analysis*, Princeton Mathematical Series, No. 28, Princeton University Press, Princeton, N.J., 1970. MR0274683

[Roz82]   Yu. A. Rozanov, *Markov random fields*, translated from the Russian by Constance M. Elson, Applications of Mathematics, Springer-Verlag, New York-Berlin, 1982. MR676644

[RSN56]   F. Riesz and B. Sz.-Nagy, *Functional analysis*, Blackie & Son Limited, London and Glasgow, 1956.

[RVE13]   W. Ren and E. Vanden-Eijnden, *A climbing string method for saddle point search*, J. Chem. Phys. **138** (2013), 134105.

[RW94a]   L. C. G. Rogers and D. Williams, *Diffusions, Markov processes, and martingales: Foundations, Vol. 1*, 2nd ed., Wiley Series in Probability and Mathematical Statistics: Probability and Mathematical Statistics, John Wiley & Sons, Ltd., Chichester, 1994. MR1331599

[RW94b]   L. C. G. Rogers and D. Williams, *Diffusions, Markov processes, and martingales: Itô calculus, Vol. 2*, Wiley Series in Probability and Mathematical Statistics: Probability and Mathematical Statistics, John Wiley & Sons, Inc., New York, 1987. MR921238

[RW09]   R. T. Rockafellar and R. J-B. Wets, *Variational analysis*, Springer-Verlag, Berlin and Heidelberg, 2009.

[RY05]   D. Revuz and M. Yor, *Continuous martingales and Brownian motion*, 3rd ed., Springer-Verlag, Berlin and Heidelberg, 2005.

[Sch80]   Z. Schuss, *Singular perturbation methods in stochastic differential equations of mathematical physics*, SIAM Rev. **22** (1980), no. 2, 119–155, DOI 10.1137/1022024. MR564560

[Sei12]   U. Seifert, *Stochastic thermodynamics, fluctuation theorems and molecular machines*, Rep. Prog. Phys. **75** (2012), 126001.

[Sek10]   K. Sekimoto, *Stochastic energetics*, Lecture Notes in Physics, vol. 799, Springer-Verlag, Heidelberg, 2010.

[Shi92]   A. N. Shiryaev (ed.), *Selected works of A.N. Kolmogorov*, vol. II, Kluwer Academic
            Publishers, Dordrecht, 1992.

[Shi96]   A. N. Shiryaev, *Probability*, 2nd ed., translated from the first (1980) Russian
            edition by R. P. Boas, Graduate Texts in Mathematics, vol. 95, Springer-Verlag,
            New York, 1996. MR1368405

[Sin89]   Y. Sinai (ed.), *Dynamical systems II: Ergodic theory with applications to dynam-
            ical systems and statistical mechanics*, Encyclopaedia of Mathematical Sciences,
            vol. 2, Springer-Verlag, Berlin and Heidelberg, 1989.

[SM00]   J. Shi and J. Malik, *Normalized cuts and image segmentation*, IEEE Trans. Pat-
            tern Anal. Mach. Intel. **22** (2000), 888–905.

[Soa94]   P. M. Soardi, *Potential theory on infinite networks*, Lecture Notes in Mathematics,
            vol. 1590, Springer-Verlag, Berlin, 1994. MR1324344

[Sus78]   H. J. Sussmann, *On the gap between deterministic and stochastic ordinary differ-
            ential equations*, Ann. Probability **6** (1978), no. 1, 19–41. MR0461664

[SW95]   A. Shwartz and A. Weiss, *Large deviations for performance analysis*, Queues,
            communications, and computing, with an appendix by Robert J. Vanderbei, Sto-
            chastic Modeling Series, Chapman & Hall, London, 1995. MR1335456

[Szn98]   A.-S. Sznitman, *Brownian motion, obstacles and random media*, Springer Mono-
            graphs in Mathematics, Springer-Verlag, Berlin, 1998. MR1717054

[Tai04]   K. Taira, *Semigroups, boundary value problems and Markov processes*, Springer
            Monographs in Mathematics, Springer-Verlag, Berlin, 2004. MR2019537

[Tan96]   M. A. Tanner, *Tools for statistical inference: Methods for the exploration of pos-
            terior distributions and likelihood functions*, 3rd ed., Springer Series in Statistics,
            Springer-Verlag, New York, 1996. MR1396311

[TB04]   T. Tian and K. Burrage, *Binomial leap methods for simulating stochastic chemical
            kinetics*, J. Chem. Phys. **121** (2004), 10356–10364.

[TKS95]   M. Toda, R. Kubo, and N. Saitô, *Statistical physics*, vol. 1, Springer-Verlag, Berlin,
            Heidelberg and New York, 1995.

[Tou09]   H. Touchette, *The large deviation approach to statistical mechanics*, Phys. Rep.
            478 (2009), no. 1-3, 1–69, DOI 10.1016/j.physrep.2009.05.002. MR2560411

[TT90]   D. Talay and L. Tubaro, *Expansion of the global error for numerical schemes
            solving stochastic differential equations*, Stochastic Anal. Appl. **8** (1990), no. 4,
            483–509 (1991), DOI 10.1080/07362999008809220. MR1091544

[Van83]   E. Vanmarcke, *Random fields: Analysis and synthesis*, MIT Press, Cambridge,
            MA, 1983. MR761904

[Var84]   S. R. S. Varadhan, *Large deviations and applications*, CBMS-NSF Regional Con-
            ference Series in Applied Mathematics, vol. 46, Society for Industrial and Applied
            Mathematics (SIAM), Philadelphia, PA, 1984. MR758258

[VK04]   N. G. Van Kampen, *Stochastic processes in physics and chemistry*, 2nd ed., Else-
            vier, Amsterdam, 2004.

[Wal02]   D. F. Walnut, *An introduction to wavelet analysis*, Applied and Numerical Har-
            monic Analysis, Birkhäuser Boston, Inc., Boston, MA, 2002. MR1854350

[Wel03]   L. R. Welch, *Hidden Markov models and the Baum-Welch algorithm*, IEEE Infor.
            Theory Soc. Newslett. **53** (2003), 10–13.

[Wie23]   N. Wiener, *Differential space*, J. Math. and Phys. **2** (1923), 131–174.

[Win03]   G. Winkler, *Image analysis, random fields and Markov chain Monte Carlo meth-
            ods*, 2nd ed., A mathematical introduction, with 1 CD-ROM (Windows), Stochas-
            tic Modelling and Applied Probability, Applications of Mathematics (New York),
            vol. 27, Springer-Verlag, Berlin, 2003. MR1950762

[WZ65]   E. Wong and M. Zakai, *On the convergence of ordinary integrals to stochastic integrals*, Ann. Math. Statist. **36** (1965), 1560–1564, DOI 10.1214/aoms/1177699916. MR0195142

[XK02]   D. Xiu and G. E. Karniadakis, *The Wiener-Askey polynomial chaos for stochastic differential equations*, SIAM J. Sci. Comput. **24** (2002), no. 2, 619–644, DOI 10.1137/S1064827501387826. MR1951058

[YLAVE16] T. Yu, J. Lu, C. F. Abrams, and E. Vanden-Eijnden, *Multiscale implementation of infinite-swap replica exhange molecular dynamics*, Proc. Nat. Acad. Sci. USA **113** (2016), 11744–11749.

[Yos95]   K. Yosida, *Functional analysis*, reprint of the sixth (1980) edition, Classics in Mathematics, Springer-Verlag, Berlin, 1995. MR1336382

[ZD12]   J. Zhang and Q. Du, *Shrinking dimer dynamics and its applications to saddle point search*, SIAM J. Numer. Anal. **50** (2012), no. 4, 1899–1921, DOI 10.1137/110843149. MR3022203

[ZJ07]   J. Zinn-Justin, *Phase transitions and renormalization group*, Oxford Graduate Texts, Oxford University Press, Oxford, 2007. MR2345069

[ZL16]   P. Zhou and T. Li, *Construction of the landscape for multi-stable systems: Potential landscape, quasi-potential, A-type integral and beyond*, J. Chem. Phys. **144** (2016), 094109.

Index

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