Lecture notes for mini-course on numerical methods for SDEs

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Umea University, 30 August – 2 September 2016

August 24, 2016

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1 Preface

These lecture notes give a brief introduction to the main ideas of numerical integration of stochastic differential equations (SDEs) together with a basic background for SDEs. In preparation of the notes a number of sources were used, mainly [44, 15, 49, 50, 54, 46]. The list of references has both sources used for preparing the course and for further reading.

The prerequisites include good background in Calculus/Mathematical Analysis and basic knowledge of Probability. Previous study of numerical integration of (deterministic) ODEs is helpful.

The notes should be viewed as the material accompanying the lectures – some of the material included in the lecture notes will be skipped on lectures, while some places in the notes will be covered in more depth on lectures. The last 1.5-2 lectures will use separate slides and will cover more advanced material, mainly related to geometric integration of SDEs.

2 Preliminaries: revision of Probability

This section contains a brief summary of some basics from the Probability theory.

Definition 2.1 *Outcomes of an experiment ω are called **elementary events** or **sample points** and their collection Ω is called the **space of elementary events** or the **sample space**.*

Definition 2.2 ***Events** are all subsets $A \subset \Omega$, for which under the condition of the experiment, one can conclude that either 'the outcome $\omega \in A$' or 'the outcome $\omega \notin A$'.*

Definition 2.3 *Let Ω be a non-empty set and $\mathcal{F}$ be a collection of subsets of Ω. We say that $\mathcal{F}$ is a **σ-algebra** provided that*

1. $\Omega \in \mathcal{F}$;
2. *if $A_n \in \mathcal{F}$, $n = 1, 2, \ldots$, then $\cup A_n \in \mathcal{F}$, $\cap A_n \in \mathcal{F}$;*
3. $A \in \mathcal{F} \Rightarrow \overline{A} \in \mathcal{F}$.

Definition 2.4 *The space Ω together with a σ-algebra $\mathcal{F}$ of its subsets is a **measurable space** $(\Omega, \mathcal{F})$.*

Definition 2.5 *Let $(\Omega, \mathcal{F})$ be a measurable space. A **probability measure** $P = P(A)$ is a function that assigns a number in $[0, 1]$ to every set $A \in \mathcal{F}$ and satisfies the following axioms:*

1. $P(\Omega) = 1$;
2. *(**countable additivity**) whenever $A_1, A_2, \ldots$ is a sequence of pairwise disjoint sets in $\mathcal{F}$, then*

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

*$P(A)$ is called the **probability** of an event A.*

We can now formulate **Kolmogorov's** universally accepted **axiomatic system**.

Definition 2.6 *An ordered triple $(\Omega, \mathcal{F}, P)$, where*

1. *Ω is a set of points ω,*
2. *$\mathcal{F}$ is a σ-algebra of subsets of Ω and*
3. *P is a probability measure on $\mathcal{F}$,*

*is called a **probabilistic model** or a **probability space**. Here, Ω is the sample space or space of elementary events, the sets A in $\mathcal{F}$ are events and $P(A)$ is the probability of the event A.*

In what follows we will always assume that we are given a sufficiently rich probability space $(\Omega, \mathcal{F}, P)$.

2.1 Random variables

We now remind you about the definition of a random variable, its characteristics and properties.

We first need to recall what the Borel σ-algebra is and consider the *measurable space* $(\mathbf{R}, \mathcal{B}(\mathbf{R}))$.

Let $\mathcal{A}$ be the system of subsets of the real line $\mathbf{R}$ consisting of finite unions of disjoint intervals of the form $(a, b]$ together with the empty set $\emptyset$:

$$A \in \mathcal{A} \text{ if } A = \bigcup_{i=1}^{n} (a_i, b_i], \quad n < \infty.$$

Denote by $\mathcal{B}(\mathbf{R})$ the smallest σ-algebra $\sigma(\mathcal{A})$ containing $\mathcal{A}$. It is called the **Borel σ-algebra** of subsets of the real line and its sets are called **Borel sets**. We have

$$(a,b) = \bigcup_{n=1}^{\infty} (a, b - \frac{1}{n}], \quad a < b;$$

$$[a,b] = \bigcap_{n=1}^{\infty} (a - \frac{1}{n}, b], \quad a < b; \quad \{a\} = \bigcap_{n=1}^{\infty} (a - \frac{1}{n}, a].$$

Then the Borel σ-algebra contains not only intervals of the form $(a,b]$ but also points (singletons) $\{a\}$ and all sets of the following forms

$$(a,b), \quad [a,b], \ [a,b), \ (-\infty,b), \ (-\infty,b], \ (a,\infty). \tag{2.1}$$

We also note that we could construct the Borel σ-algebra $\mathcal{B}(\mathbf{R})$ by starting with any of the six kinds of intervals from (2.1) instead of $(a,b]$.

Definition 2.7 *A real-valued **random variable** $\xi = \xi(\omega)$ is a real-valued function on Ω that is $\mathcal{F}$-measurable that means we require*

$$\{\omega : \xi(\omega) \in B\} \in \mathcal{F} \tag{2.2}$$

for every $B \in \mathcal{B}(\mathbf{R})$.

Note the importance of the condition (2.2): if a probability measure P is defined on $(\Omega, \mathcal{F})$, (2.2) then makes sense to speak of the probability of the event $\{\xi \in B\}$ since we know how to assign probabilities to events from $\mathcal{F}$.

Definition 2.8 *Let a random variable ξ be defined on $(\Omega, \mathcal{F})$ and consider a probability space $(\Omega, \mathcal{F}, P)$. A probability measure P_ξ on $(\mathbf{R}, \mathcal{B}(\mathbf{R}))$ defined as*

$$P_\xi(B) = P\{\omega : \xi(\omega) \in B\}, \quad B \in \mathcal{B}(\mathbf{R}),$$

*is called the **probability distribution** of ξ on $(\mathbf{R}, \mathcal{B}(\mathbf{R}))$.*

The function

$$F_\xi(x) = P\{\omega : \xi(\omega) \le x\}, \quad x \in \mathbf{R},$$

*is called **the distribution function** of ξ.*

Example 2.1 *(Bernoulli distribution). Consider a random variable ξ that takes values from $X = \{a, b\}$, $a, b \in \mathbf{R}$, and*

$$p_1 = P(\{\omega : \xi = a\}) = p, \qquad p_2 = P(\{\omega : \xi = b\}) = 1 - p,$$

where $p \in [0,1]$. We call such ξ a Bernoulli random variable.

In the next definition we introduce a classification of random variables.

Definition 2.9 *A random variable ξ is called*

- ***discrete** if it takes values in a countable set $X = \{x_1, x_2, \ldots\}$;*
- ***continuous** if its distribution F_ξ is continuous for $x \in \mathbf{R}$;*
- ***absolutely continuous** if there is a non-negative function $\rho = \rho_\xi(x)$, called its **density**, such that*

$$F_\xi(x) = \int_{-\infty}^{x} \rho_\xi(z) dz, \quad x \in \mathbf{R}.$$

Example 2.2 *The widely accepted (although simplistic) model for stock prices is that they at a fixed time T are log-normally distributed. Let ξ be a normally distributed (Gaussian) random variable with mean μ and variance σ^2: $\xi \sim \mathcal{N}(\mu, \sigma^2)$, i.e. ξ is a continuous random variable with the probability density*

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}.$$

The log-normal assumption means that the log of the stock price S_T during a time period T changes by ξ:

$$\ln S_T = \ln S_0 + \xi \tag{2.3}$$

or

$$S_T = S_0 \exp(\xi).$$

It is said that S_T has a log-normal distribution. Gaussian and log-normal random variables are examples of absolute continuous random variables.

Definition 2.10 *We call random variables $\eta_1, \eta_2, \ldots, \eta_n$* ***independent*** *if any of the following holds:*

1. *For any n and any $x_1, x_2, \ldots, x_n$: the joint distribution function*

$$\begin{aligned} F_{\eta_1,\ldots,\eta_n}(x_1, \ldots, x_n) &= P(\eta_1 \le x_1, \ldots, \eta_n \le x_n) \\ &= \prod_{k=1}^{n} P(\eta_k \le x_k) = \prod_{k=1}^{n} F_{\eta_k}(x_k); \end{aligned}$$

2. *In the case of absolutely continuous random variables defining the joint density*

$$\rho_{\eta_1,\ldots,\eta_n}(x_1, \ldots, x_n) := \frac{\partial^n F_{\eta_1,\ldots,\eta_n}(x_1, \ldots, x_n)}{\partial x_1, \ldots \partial x_n},$$

we get

$$\rho_{\eta_1,\ldots,\eta_n}(x_1, \ldots, x_n) = \prod_{k=1}^{n} \rho_{\eta_k}(x_k).$$

2.2 Expectations

In the discrete case, when the space Ω is discrete, expectation can be defined as

$$E\xi(\omega) := \sum_{i=1}^{M} \xi(\omega_i) P(\omega_i) \tag{2.4}$$

and also for discrete random variables it can be computed as

$$E\xi = \sum_{i=1}^{L} x_i P\{\xi(\omega) = x_i\}. \tag{2.5}$$

In the absolute continuous case we can define the expectation of ξ via the Riemann integral as

$$E\xi := \int_{-\infty}^{\infty} x \rho_\xi(x) dx$$

or more generally

$$Eg(\xi) := \int_{-\infty}^{\infty} g(x) \rho_\xi(x) dx, \tag{2.6}$$

where ρ_ξ is the density of ξ and $g(x)$ is a 'good' function.

A generic definition of expectation is based on the *Lebesgue integral*, which we introduce below (see also [49, 9, 50]). But we start with a reminder about the Riemann integral. Suppose $f(x)$ is a continuous function on a closed interval $[a, b]$. Let us partition this interval: $a = x_0 < x_1 < \cdots < x_n = b$ and denote the length of the longest subinterval in this partition by Δ, i.e. $\Delta = \max_{i=0,\ldots,n-1}(x_{i+1} - x_i)$. For each subinterval $[x_i, x_{i+1}]$, we set $m_i = \min_{x\in[x_i,x_{i+1}]} f(x)$ and $M_i = \max_{x\in[x_i,x_{i+1}]} f(x)$. The lower Riemann sum is

$$\underline{\mathrm{F}}_n = \sum_{i=1}^{n} m_i(x_{i+1} - x_i)$$

and the upper Riemann sum is

$$\bar{\mathrm{F}}_n = \sum_{i=1}^{n} M_i(x_{i+1} - x_i).$$

As Δ goes to zero, both Riemann sums converge to the same limit, which we call the **Riemann integral** and denote as $\int_a^b f(x)dx$. Unfortunately, we cannot use this construction for defining expectations because random variables are functions of $\omega \in \Omega$, which is often not a subset of $\mathbf{R}$ unlike the case of function $f(x)$ with $x \in [a, b]$. The sample space Ω is often an abstract space and there is no natural way to partition it as we did with the interval $[a, b]$. But we can put 'things upside down': instead of partitioning the domain of definition, partition the range of the function!

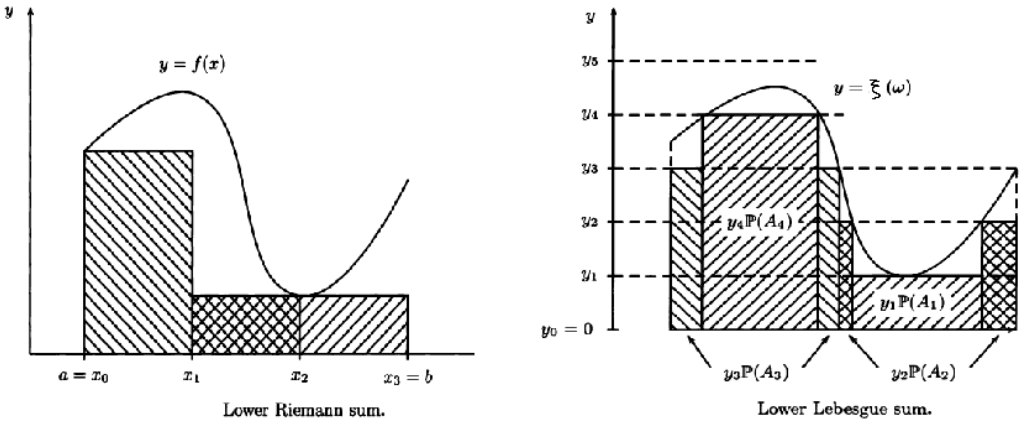

Figure 2.1: Riemann vs Lebesgue [Source: [50][Chapter 1]].

Suppose $0 \le \xi(\omega) < \infty$ for all $\omega \in \Omega$. Create a partition of the positive semiline: $0 = y_0 < y_1 < y_2 < \cdots$ with $\Delta = \max_{i=0,1,2\ldots,}(y_{i+1} - y_i)$. For each subinterval $[y_i, y_{i+1})$, we define the event

$$A_i = \{\omega \in \Omega : \ \xi(\omega) \in [y_i, y_{i+1})\}.$$

Then we can define the lower (and analogously the upper) Lebesgue sum as[1]

$$\underline{\mathrm{F}}_n = \sum_{i=1}^{n} y_i P(A_i).$$

As Δ goes to zero, this Lebesgue sum goes to a limit, which we call the **Lebesgue integral** and denote as $\int_\Omega \xi(\omega)dP(\omega)$. Note that the limit can be infinite as we have not put any conditions on $\xi(\omega)$. Figure 2.1 gives visual comparison of the definitions of Riemann and Lebesgue integrals.

[1] The requirement for random variables to be $\mathcal{F}$-measurable is used here.

Further, we need to consider when the assumption $0 \leq \xi(\omega) < \infty$ is violated. If the set of ω on which this condition is violated has zero probability, then the above definition does not change. If $P\{\omega \in \Omega : \xi(\omega) \geq 0\} = 1$ but $P\{\omega \in \Omega : \xi(\omega) = \infty\} > 0$, then we define that $\int_\Omega \xi(\omega) dP(\omega) = \infty$.

Ok, we defined the Lebesgue integral for positive functions. Now let us extend its definition. If $\xi(\omega)$ takes both positive and negative values, we define its positive and negative parts as

$$\xi^+(\omega) = \max\{\xi(\omega), 0\} \quad \text{and} \quad \xi^-(\omega) = \max\{-\xi(\omega), 0\},$$

which are both nonnegative random variables and $\xi(\omega) = \xi^+(\omega) - \xi^-(\omega)$ and $|\xi(\omega)| = \xi^+(\omega) + \xi^-(\omega)$. For both $\xi^+(\omega)$ and $\xi^-(\omega)$, the above definition of the Lebesgue integral works and provided these integrals are finite, we naturally define

$$\int_\Omega \xi(\omega) dP(\omega) = \int_\Omega \xi^+(\omega) dP(\omega) - \int_\Omega \xi^-(\omega) dP(\omega).$$

If both $\int_\Omega \xi^+(\omega) dP(\omega)$ and $\int_\Omega \xi^-(\omega) dP(\omega)$ are finite, then $\int_\Omega \xi(\omega) dP(\omega)$ is finite and we say that $\xi(\omega)$ is *integrable*. If $\int_\Omega \xi^+(\omega) dP(\omega) = \infty$ and $\int_\Omega \xi^-(\omega) dP(\omega)$ is finite, then we define $\int_\Omega \xi(\omega) dP(\omega) = \infty$. If $\int_\Omega \xi^-(\omega) dP(\omega) = \infty$ and $\int_\Omega \xi^+(\omega) dP(\omega)$ is finite, then we define $\int_\Omega \xi(\omega) dP(\omega) = -\infty$. If both $\int_\Omega \xi^+(\omega) dP(\omega)$ and $\int_\Omega \xi^-(\omega) dP(\omega)$ are infinite then $\int_\Omega \xi(\omega) dP(\omega)$ is not defined.

Definition 2.11 ***Expectation*** *$E(\cdot)$ of a random variable $\xi(\omega)$ on $(\Omega, \mathcal{F}, P)$ is defined as*

$$E\xi(\omega) = \int_\Omega \xi(\omega) dP(\omega). \tag{2.7}$$

We say that a random variable $\xi(\omega)$ is *integrable* if $E|\xi(\omega)| < \infty$.

The idea behind this definition is that we average values of $\xi(\omega)$ over the sample space Ω with appropriate weightings given by the probability $P(\omega)$.

Example 2.3 *If $\xi(\omega)$ takes only finite (or countable) number of values $\{x_1, \ldots, x_n\}$ then*

$$E\xi(\omega) = \int_\Omega \xi(\omega) dP(\omega) = \sum_{i=1}^n x_i P\{\xi = x_i\}, \tag{2.8}$$

which is obviously a very familiar formula to you! And in particular, if Ω is finite (or countable) then (cf. (2.4) and (2.5)):

$$E\xi(\omega) = \sum_{i=1}^n x_i P\{\xi = x_i\} = \sum_{\omega_i \in \Omega}^M \xi(\omega_i) P(\omega_i).$$

Let us recall properties of expectations.

Properties of expectations[2]

Let ξ and η be integrable random variables and a and b be some real numbers. The following properties hold:

1. $Ea = a$;
2. $E(a\xi + b\eta) = aE\xi + bE\eta$ (*linearity*);
3. If $\xi \leq \eta$, then $E\xi \leq E\eta$ (*comparison*);
4. If φ is a convex function on $\mathbf{R}$, then $\varphi(E\xi) \leq E\varphi(\xi)$ (Jensen′s inequality).

[2] See their proofs in, e.g., [49].

Also, recall the definition of variance

$$Var\xi = E\xi^2 - (E\xi)^2 = E\left(\xi - E\xi\right)^2.$$

The abstract nature of Definition 2.11 is useful for the unifying theory and for establishing properties of expectations. But computing Lebesgue integrals (2.7) over an abstract space Ω is too complex. In practice, instead we, as a rule, rely on distributions and densities of random variables of our interest and this way we switch from integrals over Ω to integrals over $\mathbf{R}$. To this end, we use the probability measure P_ξ on $(\mathbf{R}, \mathcal{B}(\mathbf{R}))$ induced by the random variable ξ from Definition 2.8. From your previous study of Probability, you know that most of the 'interesting' random variables have a density $\rho_\xi(x) = \rho(x)$, i.e. a nonnegative Borel-measurable function $\rho(x)$, $x \in R$, such that (cf. Definition 2.9):

$$P_\xi(B) = \int_B \rho(x)dx \quad \text{for any } B \in \mathcal{B}(\mathbf{R}).$$

The following proposition links integrals over Ω and over $\mathbf{R}$ (see its proof e.g. in [50, 49]).

Proposition 2.1 *Let $\xi(\omega)$ be a random variable on the probability space $(\Omega, \mathcal{F}, P)$ and $f(x)$ be a Borel-measurable function on $\mathbf{R}$. Then*

$$E|f(\xi)| = \int_{\mathbf{R}} |f(x)|dP_\xi(x).$$

If $E|f(\xi)| < \infty$ then

$$Ef(\xi) = \int_{\mathbf{R}} f(x)dP_\xi(x).$$

If in addition $\xi(\omega)$ has a density $\rho(x)$ then

$$Ef(\xi) = \int_{-\infty}^{\infty} f(x)\rho(x)dx. \tag{2.9}$$

The relationship (2.9) obviously coincides with (2.6), which is the usual way how we compute expectations of absolute continuous random variables.

We note that probability of an event is the expectation of the indicator function of this event, e.g. for an event $A \in \mathcal{F}$:

$$P(A) = E(I_A(\omega)).$$

Remark 2.1 *For a random variable ξ with $E\xi^2 < \infty$, the expectation $m = E\xi$ is the unique constant which gives the best estimate of ξ in the mean-square sense, i.e. m attains the least mean-square error $E(\xi - m)^2$ and hence is the best mean-square estimate among constants. In this context variance can be interpreted as the mean-square error of estimation of a random variable by its mean.*

2.3 Independence and conditional expectations

Earlier, in Definition 2.10, we recalled the meaning of independence of random variables. Let us introduce a couple of related notions.

Let a random variable $\xi(\omega)$ be defined on $(\Omega, \mathcal{F}, P)$. The sets $\{\omega : \xi(\omega) \in B\} \in \mathcal{F}$, $B \in \mathcal{B}(\mathbf{R})$, form a **$\sigma$-algebra generated by** ξ and denoted by $\sigma(\xi)$ or $\mathcal{F}^\xi$.

Definition 2.12 *Let $(\Omega, \mathcal{F}, P)$ be a probability space and $\mathcal{G}_1, \mathcal{G}_2, \ldots, \mathcal{G}_n$ be sub-σ-algebras of $\mathcal{F}$. We say that the σ-algebras $\mathcal{G}_1, \mathcal{G}_2, \ldots, \mathcal{G}_n$ are **independent** if for all $A_i \in \mathcal{G}_i$, $i = 1, \ldots, n$:*

$$P(A_1 \cap A_2 \cap \cdots \cap A_n) = P(A_1)P(A_2)\cdots P(A_n).$$

*We say that a random variable ξ defined on $(\Omega, \mathcal{F}, P)$ is **independent** of a sub-σ-algebra $\mathcal{G}$ of $\mathcal{F}$ if a σ-algebra $\sigma(\xi)$ generated by ξ and $\mathcal{G}$ are independent.*

We will also need a more complicated notion: *conditional expectation.*

Definition 2.13 *Let ξ be an integrable random variable defined on $(\Omega, \mathcal{F}, P)$ and $\mathcal{G}$ be a sub-σ-algebra of $\mathcal{F}$. The* ***conditional expectation*** *of ξ given $\mathcal{G}$, denoted as $E(\xi|\mathcal{G})$, is a random variable such that (i) $E(\xi|\mathcal{G})$ is $\mathcal{G}$-measurable and (ii) $E(\xi|\mathcal{G})$ satisfies the partial averaging*

$$\int_A E(\xi|\mathcal{G})(\omega)dP(\omega) = \int_A \xi(\omega)dP(\omega) \quad \text{for all } A \in \mathcal{G}.$$

It is always useful to have not only formal but also an intuitive understanding of definitions. In the case of Definition 2.13 the informal prospective is as follows. The sub-σ-algebra $\mathcal{G}$ plays here the role of a 'partial world': we are able to observe whether an event from $\mathcal{G}$ happened or not but we not see anything beyond $\mathcal{G}$. The property (i) corresponds to the interpretation that $E(\xi|\mathcal{G})$ is the best estimate for ξ given information $\mathcal{G}$, i.e. this random variable $E(\xi|\mathcal{G})$ is determined by the information from $\mathcal{G}$. The partial averaging means that the conditional expectation $E(\xi|\mathcal{G})$ and the random variable ξ give the same value when averaged over those parts of Ω that are sets in $\mathcal{G}$. We can say that the conditional expectation $E(\xi|\mathcal{G})$ is the expectation of a random variable ξ taken over events of those parts of Ω which are not in $\mathcal{G}$.

If ξ and η are integrable random variables defined on $(\Omega, \mathcal{F}, P)$, then the conditional expectation $E(\xi|\eta)$ is defined as

$$E(\xi|\eta) = E(\xi|\sigma(\eta)), \tag{2.10}$$

where $\sigma(\eta)$ is the minimal σ-algebra generated by η (i.e., by events $\{\omega \in \Omega : \eta(\omega) \in B\}$ for $B \in \mathcal{B}(\mathbf{R})$).

The following proposition takes place.

Proposition 2.2 *Let ξ and η be integrable random variables defined on $(\Omega, \mathcal{F}, P)$ and ξ be $\sigma(\eta)$-measurable. Then there exists a deterministic function $g(x)$ such that*

$$\xi = g(\eta).$$

Example 2.4 *Consider the conditional expectation $E(\xi|\eta)$ given by (2.10). By Definition 2.13, $E(\xi|\eta)$ is $\sigma(\eta)$-measurable random variable. Then by Proposition 2.2 there is a function $g(x)$ such that*

$$E(\xi|\eta) = g(\eta). \tag{2.11}$$

It can be proved (see, e.g., [49, 58, 50]) that conditional expectations have the following properties. Assume that random variables ξ and η defined on $(\Omega, \mathcal{F}, P)$ are integrable and $a, b \in \mathbf{R}$ are some constants. Let $\mathcal{G}$ be a sub-σ-algebra of $\mathcal{F}$. Then

1. $E\xi = E(E(\xi|\mathcal{G}))$;
2. If $\mathcal{F}_0 = \{\varnothing, \Omega\}$ is the trivial algebra, then $E(\xi|\mathcal{F}_0) = E\xi$.
3. If $\mathcal{G}_2$ is a sub-σ-algebra of sub-σ-algebra $\mathcal{G}_1 \subset \mathcal{F}$ (i.e., $\mathcal{G}_2 \subset \mathcal{G}_1 \subset \mathcal{F}$), then $E(E(\xi|\mathcal{G}_1)|\mathcal{G}_2) = E(\xi|\mathcal{G}_2)$ (*iterated conditioning or tower property*);
4. $E(\xi|\mathcal{F}) = \xi$.
5. If ξ and $\mathcal{G}$ are independent, then $E(\xi|\mathcal{G}) = E\xi$ (*independence*);
6. The conditional expectation $E(\xi|\mathcal{G})$ can be interpreted as a prediction of ξ given the information $\mathcal{G}$;
7. If ξ is $\mathcal{G}$-measurable, then $E(\xi\eta|\mathcal{G}) = \xi E(\eta|\mathcal{G})$ (*taking out what is known*);
8. $E(a\xi + b\eta|\mathcal{G}) = aE(\xi|\mathcal{G}) + bE(\eta|\mathcal{G})$ (*linearity*);

9. $E(a|\mathcal{G}) = a$;
10. If $\xi \le \eta$, $E(\xi|\mathcal{G}) \le E(\eta|\mathcal{G})$ (*comparison*);
11. If φ is a convex function on $\mathbf{R}$, then $\varphi(E(\xi|\mathcal{G})) \le E(\varphi(\xi)|\mathcal{G})$ (*conditional Jensen's inequality*);
12. $|E(\xi|\mathcal{G})| \le E(|\xi|\ |\mathcal{G})$.

Further facts about conditional expectations are also useful.

Proposition 2.3 *Let $X_1, \dots, X_n$ and $Y_1, \dots, Y_m$ be integrable random variables defined on $(\Omega, \mathcal{F}, P)$. Let $\mathcal{G}$ be a sub-σ-algebra of $\mathcal{F}$ and $X_1, \dots, X_n$ be $\mathcal{G}$-measurable and $Y_1, \dots, Y_m$ be independent of $\mathcal{G}$. For a 'good' function $f(x_1, \dots, x_n, y_1, \dots, y_m)$, define a function*

$$g(x_1, \dots, x_n) = Ef(x_1, \dots, x_n, Y_1, \dots, Y_m).$$

Then

$$E(f(X_1, \dots, X_n, Y_1, \dots, Y_m)|\mathcal{G}) = g(X_1, \dots, X_n).$$

We note that conditional probability of an event is the conditional expectation of the indicator function of this event, e.g. for an event $A \in \mathcal{F}$ and σ-algebra $\mathcal{G} \subset \mathcal{F}$:

$$P(A|\mathcal{G}) = E(I_A(\omega)|\mathcal{G}). \tag{2.12}$$

We can use properties of conditional expectations to compute them. The other possible way to compute them is to move from integration over an abstract space Ω in Definition 2.13 to integration over $\mathbf{R}$ as we did in the case of usual expectations in the previous section. Suppose two random variables ξ and η have a joint density $\rho_{\xi\eta}(x, y)$ (see Definition 2.10) then one can introduce the conditional density

$$\rho_\xi(x|\eta = y) = \frac{\rho_{\xi\eta}(x, y)}{\rho_\eta(y)}$$

and

$$E[f(\xi, \eta)|\eta = y] = \int_{-\infty}^{\infty} f(x, y)\rho_\xi(x|\eta = y)dx. \tag{2.13}$$

Note that $E[f(\xi, \eta)|\eta = y]$ is deterministic while $E[f(\xi, \eta)|\eta]$ is random.

Remark 2.2 *The conditional expectation $E(\xi|\eta)$ is the mean-square optimal estimate of ξ obtained via observations of η.*

In future we will also need the following notion.

Definition 2.14 *Consider a probability space $(\Omega, \mathcal{F}, P)$. Let $\tilde{\Omega} \in \mathcal{F}$ and $P(\Omega \backslash \tilde{\Omega}) = 0$. If a property holds for all $\omega \in \tilde{\Omega}$, we say that it holds **almost everywhere** (a.e.) or that it holds with probability 1 or almost surely (a.s.).*

2.4 Two limit theorems

Let us recall two limit theorems (Kolmogorov's law of large numbers and Central Limit theorem), which are needed for justifying the Monte Carlo technique in Section 8).

Theorem 2.1 ***(Kolmogorov's strong law of large numbers (SLLN))*** *Let $\xi_1, \xi_2, \dots$ be a sequence of independent random numbers sampled from the same distribution, which has mean μ. Introduce the arithmetic average of the sequence up to the n^{th} term:*

$$S_n = \frac{1}{n}\sum_{i=1}^{n} \xi_i.$$

Then $S_n \to \mu$ as $n \to \infty$ with probability 1, i.e. the arithmetical average of outcomes tends towards the expectation with certainty.

You can find the proof of SLLN in, e.g. [49].

Theorem 2.2 ***(Central Limit Theorem (CLT))*** *Let $\eta_1, \eta_2, \dots$ be a sequence of independent identically distributed (i.i.d.) random variables under the probability measure P with finite mean m and finite non-zero variance ν^2 and let*

$$\theta_n := \eta_1 + \cdots + \eta_n.$$

Then

$$\hat{\theta}_n := \frac{\theta_n - nm}{\sqrt{n\nu^2}} \tag{2.14}$$

converges in distribution to an $\mathcal{N}(0,1)$ random variable as $n \to \infty$, i.e. for any $-\infty \le a < b \le \infty$

$$P(a < \hat{\theta}_n < b) \to \Phi(b) - \Phi(a), \tag{2.15}$$

where $\Phi(x)$ is the normal distribution function given by

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{z^2}{2}} dz.$$

In a concise way, we can say that the distribution of $\hat{\theta}_n$ tends to the normal distribution with zero mean and unit variance when n goes to infinity. You can find the proof of CLT in, e.g. [49, 58]. We denote convergence in distribution as

$$\hat{\theta}_n \Longrightarrow \hat{\theta}$$

and here the random variable $\hat{\theta} \sim \mathcal{N}(0,1)$.

3 Brownian Motion (Wiener Process)

In 1827 Scottish botanist Robert Brown reported that he observed an irregular motion of pollen grains in water [5][3]. Albert Einstein gave a mathematical explanation of this phenomenon [8]. A rigorous mathematical construction of the random process known as Brownian motion or Wiener process was done by Nobert Wiener [57]. The work was motivated by Physics. At the same time, as early as 1900, Bachilier [1] proposed Brownian motion as a model for stock price behaviour.

Consider random variables on a probability space $(\Omega, \mathcal{F}, P)$. In market models, physical and biological models and any other dynamic models, we usually deal with families of random variables depending on a parameter (e.g., S_n stock price at $t = t_n$ has n as a parameter).

Definition 3.1 ***Random function*** *$\zeta_t(\omega)$ is a family of random variables, depending on the parameter $t \in \mathbb{T}$. When the set $\mathbb{T}$ is a subset of a real line $\mathbf{R}$ and the parameter t is interpreted as time, we say that $\zeta_t(\omega)$ is a* ***random (stochastic) process*** *(instead of a random function).*

If $\mathbb{T}$ consists of integers, one often says that $\zeta_t(\omega)$ is a *random sequence* or a *discrete-time stochastic process*. If we fix the elementary event in $\zeta_t(\omega)$ we obtain the non-random function $\zeta_t(\cdot)$ which is called the **trajectory** or **realisation** of the random process. Note that if we fix t then we obtain a random variable.

[3] You can read a paper by Brian J. Ford on Brown's experiment [10] and see its recreation at the website http://www.sciences.demon.co.uk/wbbrowna.htm.

Example 3.1 *The stochastic process η_n, $n = 0, \dots, N$, is a symmetric random walk under the measure P if $\eta_0 = 0$ and $\eta_n = \sum_{i=1}^n \zeta_i$, where the ζ_i can take only the values $\{-1, 1\}$ and are i.i.d. random variables under the measure P with*

$$P(\zeta_i = \pm 1) = \frac{1}{2}.$$

This process is often motivated as a model of the gains from repeated plays of a fair game. For example, suppose we play a game in which each play is equivalent to tossing a fair coin. If it comes up heads I pay you £1, otherwise you pay me £1. For each n, the η_n is equal to my net gain after n plays. It is easy to compute (please do these calculations yourself) that

$$E_P \eta_n = 0 \quad \textit{and} \quad Var_P \eta_n = n.$$

The random variables

$$\Delta\eta_n := \eta_n - \eta_{n-1}, \quad n = 1, 2, \dots,$$

are called increments of the random walk. We see that $\Delta\eta_n = \zeta_n$ and thus the increments $\Delta\eta_n$ are independent under P. We say that this process is a ***process with independent increments****.*

Definition 3.2 ***Standard Wiener process*** *$W(t)$, $t \geq 0$, is a random process such that*

1. *$W(0) = 0$;*
2. *For any $0 \leq t_0 < t_1 < \cdots < t_n$, the increments $W(t_1) - W(t_0), W(t_2) - W(t_1), \dots, W(t_n) - W(t_{n-1})$ are independent;*
3. *The random variable $W(t) - W(s)$, $s < t$, has the normal distribution with zero mean, $E(W(t) - W(s)) = 0$, and variance $Var(W(t) - W(s)) = t - s$, i.e. the distribution function of this random variable is such that*

$$P(a < W(t) - W(s) < b) = \frac{1}{\sqrt{2\pi(t-s)}} \int_a^b \exp\left(-\frac{z^2}{2(t-s)}\right) dz;$$

4. *The trajectories of $W(t)$ are continuous.*

There are different proofs for the existence of this mathematical object[4]. We will not consider them.

3.1 Properties of the Wiener process

From the second property in Definition 3.2 we see that, like the simple random walk, the Wiener process is a process with independent increments. Consequently, the joint density of Wiener increments has the form

$$\begin{aligned}\rho(x_1, \dots, x_n) &= \prod_{k=1}^n \frac{1}{\sqrt{2\pi(t_k - t_{k-1})}} \exp\left(-\frac{x_k^2}{2(t_k - t_{k-1})}\right) \\ &= \frac{1}{(2\pi)^{\frac{n}{2}} \prod_{k=1}^n \sqrt{t_k - t_{k-1}}} \exp\left\{-\sum_{k=1}^n \frac{x_k^2}{2(t_k - t_{k-1})}\right\}.\end{aligned}$$

The Wiener process also has the following properties.

1. $EW(t) = 0$, $E[W(t)]^2 = t$;
2. Trajectories of $W(t)$ are not differentiable (almost everywhere);

[4] See, e.g., Section 1.5 in [23].

3. *Quadratic variation.* Let $t_0 < \cdots < t_N = T$ be an arbitrary discretization on an interval $[t_0, T]$ into N parts and $h := \max_k(t_{k+1} - t_k)$. Introduce the quadratic variation of the Wiener process:

$$\vartheta_h := \sum_{k=0}^{N-1} [W(t_{k+1}) - W(t_k)]^2.$$

Then

$$E(\vartheta_h - (T - t_0))^2 \to 0 \ \text{ as } \ h \to 0. \tag{3.1}$$

The limit we have in (3.1) is called *mean-square convergence* and we say that ϑ_h converges to $T - t_0$ in the mean-square sense.

Example 3.2 *We prove the second equality in Property 1:*

$$E[W(t)]^2 = E[W(t) - W(0)]^2 = t - 0 = t.$$

Exercise 3.1 *Prove the first equality in Property 1.*

Heuristic argument for justification of Property 2:
Define

$$\eta_h(t) := \frac{W(t+h) - W(t)}{h}.$$

Obviously, $\eta_h(t) \sim \mathcal{N}(0, 1/h)$. Hence $\eta_h(t)$ cannot have a limit as $h \to 0$ in any probabilistic sense. Note that although the Wiener process is continuous everywhere, it is (with probability 1) differentiable nowhere.

Example 3.3 *(Hint for the proof of the property about quadratic variation). First, show that*

$$E\vartheta_h = T - t_0 \ \ \textit{and} \ \ Var\,(\vartheta_h) = 2\sum_{k=0}^{N-1} (t_{k+1} - t_k)^2. \tag{3.2}$$

Then

$$\begin{aligned} E(\vartheta_h - (T - t_0))^2 &= E(\vartheta_h - E\vartheta_h)^2 = Var\,(\vartheta_h) \\ &= 2\sum_{k=0}^{N-1} (t_{k+1} - t_k)^2 \to 0 \quad \textit{as} \ \ h \to 0. \end{aligned}$$

Exercise 3.2 *Derive (3.2) and thus complete the above proof.*

Remark 3.1 *Let us pay attention that the quadratic variation property of the Wiener process is rather unusual. For a smooth function, quadratic variation (i.e. sum of squares of increments) tends to zero as $h \to 0$ (Exercise. Check that this is right). For functions changing by some finite jumps, such a sum tends to the sum of squares of jumps on the interval $[t_0, T]$ and the limit does not depend on t_0, T in a continuous manner (Exercise. Check that this is right).*

Remark 3.2 *The convergence of the quadratic variation in the mean-square sense (3.1) (also called L_2-convergence) does not imply that for almost all trajectories of the Wiener process the limit*

$$\lim_{h \to 0} \sum_{k=0}^{N-1} [W(t_{k+1}) - W(t_k)]^2$$

exists. The mean-square convergence implies that there is a subsequence of partitions of the interval $[t_0, T]$ along which the convergence to $T - t_0$ is almost sure (i.e. for almost all trajectories or, in other words, the convergence takes place for all trajectories except for a set of them having probability zero on which the assertion might be not true). See further details in, e.g., [27, 56, 59].

Corollary to Property 3. *For almost all trajectories of the Wiener process $W(t)$ the (first-order) variation $\sum_{k=0}^{N-1} |W(t_{k+1}) - W(t_k)|$ is unbounded on any interval.*

Proof. Let us consider a subsequence of partitions of the interval $[t_0, T]$ for which $\lim_{h\to 0} \sum_{k=0}^{N-1} [W(t_{k+1}) - W(t_k)]^2$ equals $T - t_0$ almost surely (see Remark 3.2). We have

$$\sum_{k=0}^{N-1} [W(t_{k+1}) - W(t_k)]^2 \le \max_k |W(t_{k+1}) - W(t_k)| \times \sum_{k=0}^{N-1} |W(t_{k+1}) - W(t_k)|. \tag{3.3}$$

Due to the continuity of $W(t)$, $\max_k |W(t_{k+1}) - W(t_k)| \to 0$ as $h \to 0$. The quadratic variation in the left-hand side of (3.3) goes to the finite $T - t_0$ as $h \to 0$ (see Property 3 of the Wiener process and Remark 3.2). Then the variation $\sum_{k=0}^{N-1} |W(t_{k+1}) - W(t_k)| \to \infty$ as $h \to 0$ which proves the corollary.

The consequence of this result is absolutely astonishing. Variation basically gives you the length of the trajectory, therefore, a trajectory of the Wiener process has infinite length on any finite time interval!

Some other properties.

4. A trajectory of the Wiener process will eventually take any (whatever large or small) value.
5. At every scale a trajectory of the Wiener process looks the same. It is a fractal[5].

A typical trajectory of the Wiener process is plotted in Fig. 3.1.

Exercise 3.3 *Using the in-built function randn() for generating random numbers with standard normal distribution in MatLab, simulate trajectories of the Wiener process. Plot the trajectories and zoom-in to visualise the fractal nature of the Wiener process.*

Thus we see that the Wiener process has rather unusual properties from the point of view of standard Analysis. Between 1940 and 1950, Calculus based on the Wiener process arose. This Calculus we often now call *Ito Calculus* and the theory of stochastic differential equations. This theory was created independently by K. Ito (Japan) and I.I. Gichman (USSR) during the Second World War. They continued the study undertaken by S.N. Bernstein (USSR) and N. Wiener (USA).

3.2 Filtration

As usual, we assume that we have a probability space $(\Omega, \mathcal{F}, P)$ which is sufficiently rich for our experiment.

Definition 3.3 ***Filtration*** *$\{\mathcal{F}_t\}_{t\ge 0}$ is a set of σ-algebras $\mathcal{F}_t$ such that $\mathcal{F}_s \subseteq \mathcal{F}_t$ for $s < t$ and $\mathcal{F}_t \subseteq \mathcal{F}$ for all t.*

A *natural filtration* $\{\mathcal{F}_t^X\}_{t\ge 0}$ associated with a stochastic process $X(t)$ encodes the information generated by this process on the interval $[0, t]$. We say that an event $A \in \mathcal{F}_t^X$ if, having observed the trajectory $X(s)$ for $s \in [0, t]$, we can answer the question of whether or not A has occurred. Obviously, more than one process can be associated with the same filtration.

Example 3.4 *The natural filtration $\mathcal{F}_t$ of the Wiener process $W(t)$ is a σ-algebra generated by all $W(s)$, $0 \le s \le t$. The increments $W(t') - W(t)$, $t' > t$, are independent of $\mathcal{F}_t$. Not that the random variable $W(t')$ with $t' > t$ is not independent of $\mathcal{F}_t$ (explain why).*

Definition 3.4 *We say that a stochastic process $X(t)$ is* ***adapted*** *to the filtration $\{\mathcal{F}_t\}_{t\ge 0}$ if $X(t)$ is measurable with respect to $\mathcal{F}_t$ for all $t \ge 0$.*

[5] A geometric pattern that is repeated at even smaller scales to produce irregular shapes and surfaces that cannot be represented by classical Geometry.

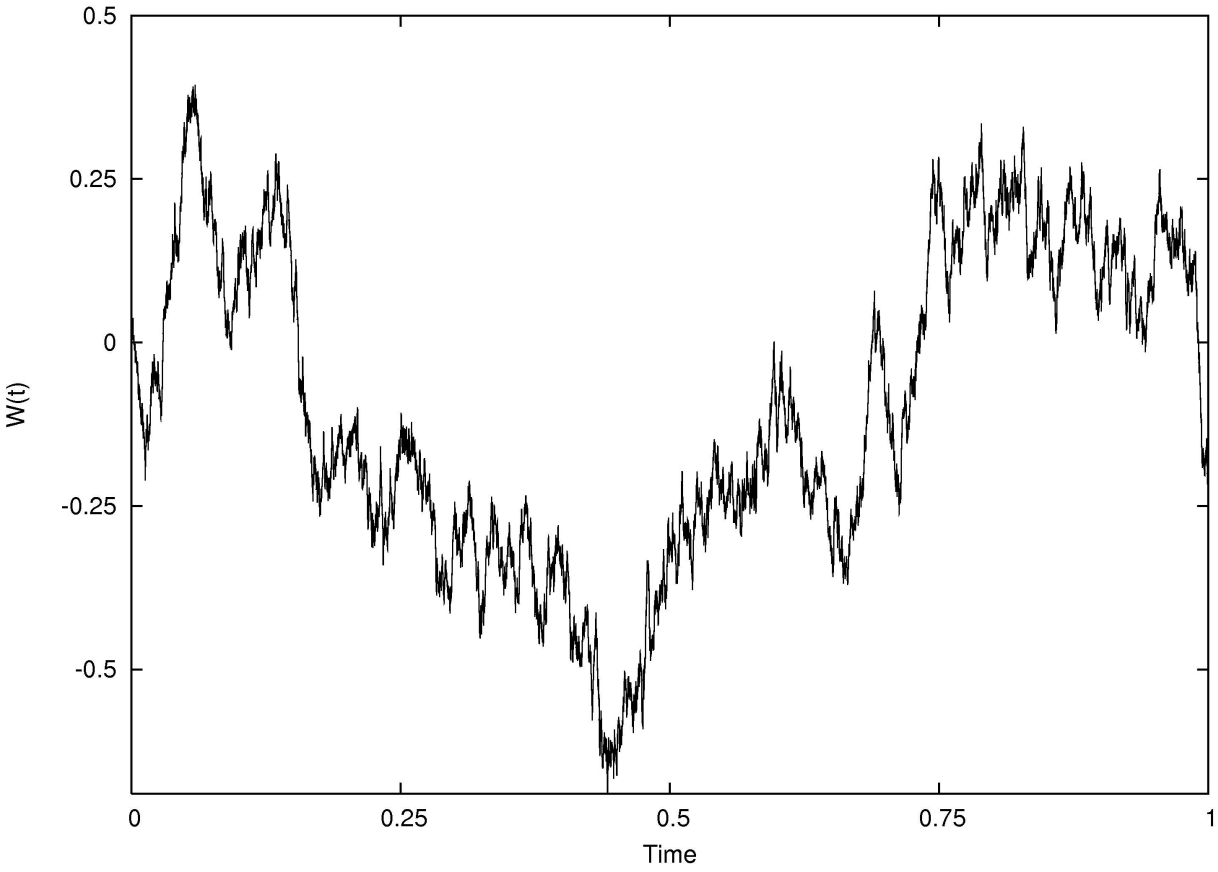

Figure 3.1: A typical trajectory of the Wiener process.

Example 3.5 *The process* $Y(t) := \max_{0 \le s \le t} W(s)$ *is adapted to the filtration* $\{\mathcal{F}_t^W\}_{t \ge 0}$ *generated by the Wiener process* $W(t)$*, whereas the process* $Z(t) := W^2(t+1) - W^2(t)$ *is not adapted to* $\{\mathcal{F}_t^W\}_{t \ge 0}$.

Example 3.6 *Let* $W(t)$ *be a standard Wiener process with the natural filtration* $\mathcal{F}_t$*. The stochastic process defined by*

$$S(t) = S_0 e^{\mu t + \sigma W(t)}, \ t \ge 0, \tag{3.4}$$

is called ***geometric Brownian motion (GBM).*** *Here* $S_0 > 0$, μ, *and* $\sigma > 0$ *are some constants. Obviously,* $\mathcal{F}_t$ *is the natural filtration for* $S(t)$ *as well. Geometric Brownian motion is the basic reference model for stock prices in continuous time. In particular, it is the model underlying the Black–Scholes–Merton pricing theory.*

Exercise 3.4 *Continuing Exercise 3.3, plot trajectories of GBM in MatLab.*

Definition 3.5 *The quadruple* $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t \ge 0}, P)$ *is called a* ***filtered probability space****.*

Definition 3.6 *Let* $X(t)$ *and* $Y(t)$, $t \in [t_0, T]$, *be two real-valued stochastic processes defined on a probability space* $(\Omega, \mathcal{F}, P)$*. We say that they are* ***independent*** *if the events* $\{(X(t_1), \ldots, X(t_n)) \in A\}$ *and* $\{(Y(s_1), \ldots, Y(s_m)) \in B\}$ *are independent for all* n, m, *all times* $(t_1, \ldots, t_n) \in [t_0, T]^n$ *and* $(s_1, \ldots, s_m) \in [t_0, T]^m$ *and all sets* $A \in \mathcal{B}(\mathbf{R}^n)$ *and* $B \in \mathcal{B}(\mathbf{R}^m)$.

Example 3.7 *In future we will often consider a number of independent standard Wiener processes.*

3.3 Markov processes

Most of stochastic models used in Financial Mathematics, in molecular dynamics and other applications are Markovian, i.e. their solution is a Markov process. In this section we introduce this important notion.

On the physical level of rigour, one can define the Markov property of a stochastic process $\zeta(t)$ is that the future behaviour of $\zeta(t)$ after time t depends only on its value at the time t and does not depend on its history before the time t. In other words, a Markov process has no memory: the future depends on the past through the present. The models (random walks, Wiener process, GBM) are Markovian. Now the mathematical definition[6].

Definition 3.7 *Let $\zeta(t)$ be a stochastic process defined on a filtered probability space $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}, P)$. The process $\zeta(t)$ satisfies the **Markov property** if, for any bounded Borel-measurable function f and for any time moments s and t with $s \le t$, the following relationship holds:*

$$E(f(\zeta(t))|\mathcal{F}_s) = E(f(\zeta(t))|\zeta(s)). \tag{3.5}$$

It follows from this definition (see also Example 2.4) that if $\zeta(t)$ is Markovian, then for every bounded Borel-measurable function $f(x)$ there is another function $g(x)$ (depending on s and f) such that

$$E(f(\zeta(t))|\mathcal{F}_s) = g(\zeta(s)).$$

Instead of $f(x)$ and $g(x)$, we can write $f(t,x)$ and $f(s,x)$ and thus

$$E(f(t,\zeta(t))|\mathcal{F}_s) = f(s,\zeta(s)). \tag{3.6}$$

Example 3.8 *Let us prove that a standard Wiener process $W(t)$ defined on $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}, P)$ is Markovian. Take an arbitrary bounded Borel-measurable function $f(x)$ and form a function $h(x,y) := f(x+y)$. Then $f(x) = h(x-y, y)$ and we can write for any time moments s and t with $s \le t$:*

$$E(f(W(t))|\mathcal{F}_s) = E(h(W(t) - W(s), W(s))|\mathcal{F}_s).$$

Since $W(s)$ is $\mathcal{F}_s$-measurable and $W(t) - W(s)$ is independent of $\mathcal{F}_s$, we get by Proposition 2.3:

$$E(h(W(t) - W(s), W(s))|\mathcal{F}_s) = g(W(s))$$

for some function $g(x)$, which proves that $W(t)$ is Markovian.

If $\zeta(t)$ is a Markov process then we have for $A \in R$:

$$\begin{aligned} P(\zeta(t) \in A|\mathcal{F}_s) &\overset{(2.12)}{=} E(I_{\zeta(t)\in A}(\omega)|\mathcal{F}_s) \\ \overset{(3.5)}{=} E(I_{\zeta(t)\in A}(\omega)|\zeta(s)) &\overset{(2.12)}{=} P(\zeta(t) \in A|\zeta(s)) := P(s,\zeta(s);t,A) \text{ a.s.}, \end{aligned} \tag{3.7}$$

where $P(s,x;t,y)$ is called the **Markov transition function**.

4 Simplistic Introduction to Ito Calculus

Let us start with a simple example. Consider a bank account, for which we use the model

$$B(t) = B_0 e^{rt}, \tag{4.1}$$

where $r \ge 0$ is a constant interest rate. Equivalently, we can say that $B(t)$ is the solution of the following initial value problem for the ordinary differential equation (ODE):

$$\dot{B} = rB, \quad B(0) = B_0, \tag{4.2}$$

[6] A more traditional definition of the Markov property is via transition probabilities. If it is defined via transition probabilities then the definition below is a property.

or

$$dB = rBdt, \quad B(0) = B_0,$$

or in the integral form

$$B(t) = B_0 + \int_0^t rB(s)ds.$$

In real life interest rates are not constant and (4.2) can be generalised by substituting the constant r with a short rate depending on time $r(t)$ and possibly on randomness $r(t) = r(t, \omega)$ and some other variables:

$$\dot{B} = r(t)B, \quad B(0) = B_0. \tag{4.3}$$

Now let us try to answer the question: what kind of differential equation can we write for geometric Brownian motion

$$S(t) = S_0 e^{\mu t + \sigma W(t)}? \tag{4.4}$$

Take a 'nice' (smooth) function $g(t, x)$ of two independent ('dummy') variables. Due to the Taylor theorem, we have

$$g(t + \Delta t, x + \Delta x) - g(t, x) = \frac{\partial g}{\partial t}\Delta t + \frac{\partial g}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 g}{\partial x^2}(\Delta x)^2 + \cdots. \tag{4.5}$$

If in (4.5) we substitute a smooth function $x(t)$ instead of the dummy variable x and $\Delta x = x(t+\Delta t) - x(t)$, the last term of the right-hand side of (4.5) is of order[7] $O((\Delta t)^2)$ and the omitted terms in (4.5) are of order $O((\Delta t)^2)$ or higher. Then, as $\Delta t \to 0$, we get the differential[8]

$$dg = \frac{\partial g}{\partial t}dt + \frac{\partial g}{\partial x}dx$$

or

$$\frac{dg}{dt}(t, x(t)) = \frac{\partial g}{\partial t} + \frac{\partial g}{\partial x}\frac{dx}{dt},$$

which is just the chain rule.

Let

$$g(t, x) = S_0 e^{\mu t + \sigma x}. \tag{4.6}$$

Then we can write $S(t) = g(t, W(t))$ and obtain

$$\begin{aligned} &g(t + \Delta t, W(t + \Delta t)) - g(t, W(t)) \\ &= \frac{\partial g}{\partial t}\Delta t + \frac{\partial g}{\partial x}(W(t + \Delta t) - W(t)) + \frac{1}{2}\frac{\partial^2 g}{\partial x^2}(W(t + \Delta t) - W(t))^2 + \cdots. \end{aligned} \tag{4.7}$$

We know (see Definition 3.2) that

$$E[W(t + \Delta t) - W(t)]^2 = \Delta t.$$

Hence, the last term on the right-hand side of (4.7) is, in fact, of order Δt and we cannot ignore it, i.e. we cannot ignore the term containing the second derivative as we did above in the case of a smooth $x(t)$. Taking this into account and assuming that we can do the transition in (4.7) as $\Delta t \to 0$ rigorously, the differential equation governing $S_t = g(t, W_t)$ will take the form

$$dS = \frac{\partial g}{\partial t}(t, W(t))dt + \frac{\partial g}{\partial x}(t, W(t))dW(t) + \frac{1}{2}\frac{\partial^2 g}{\partial x^2}(t, W(t))dt. \tag{4.8}$$

[7] Please check.

[8] The differential of a function is the principal (linear) part in the increment of a function.

Due to (4.6), we have

$$\frac{\partial g}{\partial t} = S_0 \mu e^{\mu t + \sigma x} = \mu g, \quad \frac{\partial g}{\partial x} = S_0 \sigma e^{\mu t + \sigma x} = \sigma g, \quad \frac{\partial^2 g}{\partial x^2} = \sigma^2 g.$$

Thus, we heuristically get the **stochastic differential equation (SDE)** for geometric Brownian motion:

$$dS = (\mu + \frac{\sigma^2}{2}) S dt + \sigma S dW(t), \ S(0) = S_0, \tag{4.9}$$

or

$$\frac{dS}{dt} = (\mu + \frac{\sigma^2}{2}) S + \sigma S \dot{W}(t), \ S(0) = S_0. \tag{4.10}$$

However, we still have a major problem here: how to interpret $dW(t)$ given that $W(t)$ is a 'bad' function (it is not differentiable, its variation is unbounded). Due to this, (4.9) actually has no sense in the form it is written[9]. It is just a formal writing of a mathematical object. There are at least two ways to interpret it. One is simple but less productive, the other is more productive but less simple.

The first way
Consider an ODE:

$$\dot{x} = g(t, x), \ x(0) = x_0,$$

and forget that you know what derivative is and what the definition of this object is based on the notion of derivatives for the moment. Then we can view this ODE as a limiting object of the (well-defined) difference equation (the Euler method[10]):

$$x_{k+1} = x_k + \delta g(t_k, x_k)$$

with a discretization step $\delta = T/N$ of the time interval $[0, T]$ with $0 = t_0 < t_1 < \cdots < t_N = T$. If the limit of x_k exists when $\delta \to 0$, we can say that the ODE is such an object for which solution $x(t)$ is the obtained limit.

We can do something similar with the stochastic differential equation (4.9) – we can view it as a limit of one or another discrete scheme, e.g., of the (weak) Euler method:

$$S_{k+1} = S_k + (\mu + \frac{\sigma^2}{2}) S_k \delta + \sigma S_k \sqrt{\delta} \xi_{k+1}, \tag{4.11}$$

where ξ_k are i.i.d. with $P(\xi_k = \pm 1) = 1/2$ or we can take ξ_k as i.i.d. Gaussian random variables with zero mean and unit variance (this may ensure a stronger convergence). The scheme (4.11) converges in some sense to a continuous process $S(t)$ which can be viewed as a solution of (4.9). This approach can be justified rigorously (it was first considered by S.N. Bernstein in the 1930s [3]).

The second way
This is more complicated. It is based on *Stochastic Calculus*. Due to this, a rigorous sense may be given to (4.9) if we re-write it in the integral form:

$$S(t) = S_0 + \int_0^t (\mu + \frac{\sigma^2}{2}) S(s) ds + \int_0^t \sigma S(s) dW(s). \tag{4.12}$$

Then, the equation (4.9) is used as the symbolic writing of (4.12). The first integral in (4.12) is just a usual Riemann integral because $S(s)$ is continuous. However, the second integral requires a rigorous mathematical interpretation. It is the so-called **Ito stochastic integral**. It was introduced by K. Ito [22].

[9] More precisely, it is so if we look at it from the position of standard Analysis. The modern theory of white noise (see, e.g., [20] and references therein) gives a rigorous interpretation to (4.10).
[10] See, e.g., [6].

4.1 Ito Integral and SDEs

To complete the definition of (4.12), we need to give the meaning to an expression such that $\int_0^T h(t)dW(t)$, where $h(t) = h(t,\omega)$ is $\mathcal{F}_t$-measurable function for all $t > 0$.

Example 4.1 *How to give the meaning to the integrals* $\int_0^T W(t)dW(t)$ *or* $\int_0^T S(t)dW(t)$?

Assume for a moment that $W(t)$ is differentiable. Then, obviously

$$dW(t) = \dot{W}(t)dt, \quad W(0) = 0,$$

and for 'good' functions h

$$\int_0^T h(t)dW(t) = \int_0^T h(t)\dot{W}(t)dt,$$

where the integral on the right would be a well-defined Riemann integral. However, $W(t)$ is not differentiable as we know. If variation of $W(t)$ would be bounded, this integral can be interpreted as the Stieltjes (Riemann–Stieltjes) integral[11]. However, variation of $W(t)$ is unbounded. So, we need to do something else.

Let $h(t)$ be a continuous stochastic process adapted to $\mathcal{F}_t$ such that

$$\int_0^T E[h(t)]^2 dt < \infty.$$

Then the **Ito stochastic integral** is defined as the mean-square limit:

$$\int_0^T h(t)dW(t) := \underset{h\to 0}{\text{l.i.m.}} \sum_{i=0}^{N-1} h(t_i) \times (W(t_{i+1}) - W(t_i)), \tag{4.13}$$

where $0 = t_0 < t_1 < \cdots < t_N = T$ is a discretization of the time interval $[0,T]$, $\delta := \max_i(t_{i+1} - t_i)$ and l.i.m. means the limit in the mean-square sense, i.e.

$$E\left[\int_0^T h(t)dW(t) - \sum_{i=0}^{N-1} h(t_i) \times (W(t_{i+1}) - W(t_i))\right]^2 \to 0 \quad \text{as } \delta \to 0. \tag{4.14}$$

Remark 4.1 *Ito integral exists for any continuous, bounded (and some unbounded)* $h(t)$ *(see a proof in, e.g., [56, 27, 30, 59]).*

Remark 4.2 *It is essential that* $h(t_i)$ *in (4.13) must always be evaluated at the left point, in contrast to the Riemann–Stieltjes integral (see Footnote 11) which does not depend on the point* $t \in [t_i, t_{i+1}]$ *at which* h *is evaluated. If we allow* $h(t)$ *to be evaluated at a different point in (4.13), the limit will be different and we will get another type of stochastic integral (see also Exercise 4.2 and Remark 4.4). This is again unusual from the point of view of standard Analysis and is a consequence of, in particular, unbounded variation of the Wiener process.*

Exercise 4.1 *Using the definition of the Ito integral show that*

$$\int_0^T W(t)dW(t) = \frac{W^2(T)}{2} - \frac{T}{2}.$$

This is not what one would predict from the classical integration theory. The extra term $-T/2$ *arises due to the fact that the quadratic variation of the Wiener process is not zero.*

[11] The Riemann–Stieltjes integral of a continuous function $g(t)$ with respect to a function $f(x)$ of bounded variation on $[0,T]$ is defined as

$$\int_0^T g(t)df(t) := \lim_{h\to 0} \sum_{i=0}^{N-1} g(s_i^*) \times (f(t_{i+1}) - f(t_i)),$$

where s_i^* is an arbitrary point in the interval $[t_i, t_{i+1}]$.

Exercise 4.2 *Compute* $l.i.m._{h\to 0}\sum_{i=0}^{N-1} W(t_{i+1})(W(t_{i+1})-W(t_i))$ *and compare with the answer from Exercise 4.1 (also compare with Remarks 4.2 and 4.4).*

Properties of Ito integral

1. $E\int_0^T h(t)dW(t)=0;$
2. $E\left[\int_0^T h(t)dW(t)\right]^2=\int_0^T E[h(t)]^2dt.$

Proofs of these properties can be found, e.g., in [30, 59].

Exercise 4.3 *Let* $W(t)$ *be a standard Wiener process. Compute*

$$E\int_0^t W^2(s)dW(s) \quad \textit{and} \quad E\int_0^t W^2(s)ds.$$

Remark 4.3 *If* $h(t)$ *does have a continuous first derivative (note that the integrands in Example 4.1 are not differentiable), then, e.g.,*

$$\begin{aligned} & l.i.m._{h\to 0}\sum_{i=0}^{N-1} h(t_i)\times(W(t_{i+1})-W(t_i)) \qquad (4.15)\\ = \; & l.i.m._{h\to 0}\sum_{i=0}^{N-1} h(t_{i+1})\times(W(t_{i+1})-W(t_i)) \end{aligned}$$

or, more precisely, the definition of the stochastic integral in this case does not depend on the point $t\in[t_i,t_{i+1}]$ *at which* h *is evaluated (cf. Footnote 11). Further, one can show that for differentiable* $h(t)$*:*

$$\int_0^T h(t)dW(t)=h(T)dW(T)-\int_0^T W(t)h'(t)dt. \qquad (4.16)$$

Exercise 4.4 *(i) Show that (4.15) is true. (ii) Show that (4.16) is true.*

Based on the definition of the Ito integral, we can now properly define SDE. Assume that $a(t,x)$ and $b(t,x)$ have some good analytical properties. The solution of the stochastic differential equation

$$dX=b(t,X)dt+\sigma(t,X)dW(t),\quad X(t_0)=x, \qquad (4.17)$$

is a stochastic process $X(t)$ such that for every t the random variable $X(t)$ is measurable with respect to $\mathcal{F}_t$ and $X(t)$ satisfies the integral equation

$$X(t)=x+\int_{t_0}^t b(s,X_{t_0,x}(s))ds+\int_{t_0}^t \sigma(s,X_{t_0,x}(s))dW(s), \qquad (4.18)$$

where the first integral is a Riemann integral and the second one – an Ito integral. A proof of the existence and uniqueness of solutions of SDEs under some assumptions on the functions $b(t,x)$ and $\sigma(t,x)$ can be found in, e.g., [27, 56, 18, 30, 59]. The notation $X_{t_0,x}(s)$ means that $X(t_0)=x$.

We can analogously introduce multidimensional Ito SDEs:

$$dX=b(t,X)dt+\sum_{r=1}^q \sigma_r(t,X)dW_r(t),\quad X(t_0)=x, \qquad (4.19)$$

where $b(t,x)$ and $\sigma_r(t,x)$, $r=1,\dots,q$, are 'good' d-dimensional vector-functions and $W_r(t)$, $r=1,\dots,q$, are independent standard Wiener processes on the filtered probability space $(\Omega,\mathcal{F},P,\{\mathcal{F}_t\})$, and it is again understood in the integral form

$$X_{t_0,x}(t) = x + \int_{t_0}^{t} b(s, X_{t_0,x}(s))ds + \sum_{r=1}^{q}\int_{t_0}^{t}\sigma_r(s, X_{t_0,x}(s))dW_r(s), \tag{4.20}$$

where the first integral is a (component-wise) Riemann integral and the integrals in the last term are (component-wise) Ito integrals.

Property. *The solution $X_{t_0,x}(t)$ of the SDE (4.19) is a Markovian process.*

A proof of this property can be found e.g. in [56, 60].

Remark 4.4 ***(Ito vs Stratonovich)***. *We discussed already (see Exercises 4.1 and 4.2 and Remark 4.2) that a definition of stochastic integral depends on the points at which the integrand is evaluated in the approximate sum. In applications we normally use two interpretations of stochastic integrals and, consequently, of SDEs. They are Ito and Stratonovich interpretations:*
Ito:

$$\int_0^T b(t,X(t))dW(t) = \underset{\delta\to 0}{l.i.m.}\sum_{i=0}^{N-1} b(t_i,X(t_i))\times(W(t_{i+1})-W(t_i)),$$

Stratonovich:

$$\int_0^T b(t,X(t))\circ dW(t) = \underset{\delta\to 0}{l.i.m.}\sum_{i=0}^{N-1} b\left(t_i,\frac{X(t_i)+X(t_{i+1})}{2}\right)(W(t_{i+1})-W(t_i)).$$

In Financial Mathematics one uses the Ito interpretation. Stratonovich interpretation is often used in applications from physics and also within stochastic geometry.

Exercise 4.5 *Using the definition of Stratonovich integral, compute* $\int_0^T W(t)\circ dW(t)$.

The relationship between Ito and Stratonovich SDEs. Consider the Ito SDEs (4.19). It can be re-written as the SDE in the sense of Stratonovich as

$$dX = \left(b(t,X) - \frac{1}{2}\sum_{r=1}^{q}\frac{\partial\sigma_r}{\partial x}(t,X)\sigma_r(t,X)\right)dt + \sum_{r=1}^{q}\sigma_r(t,X)\circ dW_r(t)\,. \tag{4.21}$$

Here $\partial\sigma_r/\partial x$ is the matrix with entry $\partial\sigma_r^i/\partial x^j$ at the intersection of the i-th row and j-th column. Obviously, if we are given an SDE in the sense of Stratonovich, we can re-write it in the Ito sense. Note that in the case of SDEs with additive noise (i.e., $\sigma_r(t,x)=\sigma_r(t,)$, $r=1,\dots,q$) Ito and Stratonovich interpretations coincide.

4.2 Examples of SDEs

The first set of examples are from Financial Engineering:

- Geometric Brownian motion (see e.g. [4, 24, 50, 54]):

$$dS = \mu S dt + \sigma S dW. \tag{4.22}$$

- Orstein-Uhlenbeck process/Vasicek model (see e.g. [4, 24, 50]):

$$dr = a\,[b-r]\,dt + \sigma dW^Q,\ r(0)=r_0. \tag{4.23}$$

- Cox-Ingersoll-Ross (CIR) model (see e.g. [4, 24, 50]):

$$dr = a\,[b - r]\,dt + \sigma\sqrt{r}dW^Q,\ r(0) = r_0 > 0, \tag{4.24}$$

- Heston stochastic volatility model [19]:

$$\begin{aligned} dS &= \mu S dt + \sqrt{v} S dW_1(t), \\ dv &= \kappa(\theta - v)dt + \sigma\sqrt{v}\left(\rho dW_1(t) + \sqrt{1-\rho^2}dW_2(t)\right). \end{aligned} \tag{4.25}$$

- SABR stochastic volatility model [17]:

$$\begin{aligned} dF &= \sigma(t)F^\beta\left(\rho dW_1(t) + \sqrt{1-\rho^2}dW_2(t)\right), \\ d\sigma &= \alpha\sigma dW_1(t). \end{aligned}$$

- LIBOR market model: the LIBOR rates $L(t, T_{i-1})$, $1 \le i \le n$, $0 \le t \le T_{i-1} \wedge T_k$ satisfy the SDEs (see e.g. [4, 50]):

$$dL(t,T_{i-1}) = L(t,T_{i-1})\sigma^\top(t,T_{i-1}) \begin{cases} -\sum\limits_{l=i}^{k-1} \frac{\delta L(t,T_l)}{\delta L(t,T_l)+1}\sigma(t,T_l)dt + dW_j^{T_k}(t),\ i<k, \\ dW^{T_k}(t),\quad i=k, \\ \sum\limits_{l=k}^{i-1} \frac{\delta L(t,T_l)}{\delta L(t,T_l)+1}\sigma(t,T_l)dt + dW^{T_k}(t),\quad i>k. \end{cases} . \tag{4.26}$$

The second set of examples are from molecular dynamics:

- Langevin equations (see e.g. [26, 25]):

$$\begin{aligned} d\mathbf{R} &= \frac{\mathbf{P}}{m}dt,\ \ \mathbf{R}(0) = \mathbf{r}, \\ d\mathbf{P} &= \nabla U(\mathbf{R})dt - \gamma\mathbf{P}dt + \sqrt{\frac{2m\gamma}{\beta}}d\mathbf{w}(t),\ \ \mathbf{P}(0) = \mathbf{p},\ j = 1,\ldots,n. \end{aligned} \tag{4.27}$$

- Stochastic gradient system:

$$d\mathbf{R} = -\nabla U(\mathbf{R})dt + \sqrt{\frac{2}{\beta}}d\mathbf{w}(t),\ \mathbf{R}(0) = \mathbf{r}. \tag{4.28}$$

SDEs are also used in Bayesian statistics, population dynamics, chemical reactions, engineering applications, economics and so on.

4.3 Ito Formula

In this section we consider the Ito formula which is one of the most important results in Stochastic Calculus. We give here its heuristic justification. Its rigorous proof can be found in, e.g., [27, 56, 30, 59].

First, we recall (see also the beginning of Section 4) that if $g(t,x)$, $x \in \mathbf{R}$, is a smooth deterministic function and $X(t)$ is a solution of the ODE

$$dX = b(t, X(t))dt,$$

then the differential of $g(t, X(t))$ is found as

$$dg(t,X(t)) = \left[\frac{\partial g}{\partial t}(t,X(t)) + b(t,X(t))\frac{\partial g}{\partial x}(t,X(t))\right]dt. \tag{4.29}$$

Consider the (one-dimensional) SDE

$$dX = b(t,X)dt + \sigma(t,X)dW(t), \quad X(t_0) = x. \tag{4.30}$$

Let us find a formula for $g(t,X(t))$ with $X(t)$ from (4.30) analogous to (4.29).

Following the Taylor theorem, we formally have (see also (4.5) and (4.7)):

$$\begin{aligned} dg(t,X(t)) &= \frac{\partial g}{\partial t}(t,X)dt + \frac{\partial g}{\partial x}(t,X)dX \\ &+ \frac{1}{2}\frac{\partial^2 g}{\partial x^2}(t,X) \times (dX)^2 + \cdots \\ &= \frac{\partial g}{\partial t}(t,X)dt + \frac{\partial g}{\partial x}(t,X)\ b(t,X)dt + \frac{\partial g}{\partial x}(t,X)\ \sigma(t,X)dW(t) \\ &+ \frac{1}{2}\frac{\partial^2 g}{\partial x^2}(t,X)\ \sigma^2(t,X)\ (dW)^2 + \cdots, \end{aligned} \tag{4.31}$$

where the omitted terms contain factors of the form $(dW)^3$, $(dW)^2dt$, $(dt)^2$, $(dt)^2dW$, etc. Mean-square orders of smallness of all these terms are higher than dt. We already know that $E[dW(t)]^2 = dt$ and that the last term in (4.31) cannot be omitted: it becomes, after integration,

$$\frac{1}{2}\int_{t_0}^{t} \frac{\partial^2 g}{\partial x^2}(s,X)\ \sigma^2(s,X)ds.$$

Finally, integrating (4.31), we obtain (we assume here that we can do the transition rigorously):

$$\begin{aligned} g(t,X(t)) - g(t_0,x) = \int_{t_0}^{t} &\left[\frac{\partial g}{\partial t}(s,X(s)) + b(s,X(s))\frac{\partial g}{\partial x}(s,X(s))\right. \\ &\left. + \frac{\sigma^2(s,X(s))}{2}\frac{\partial^2 g}{\partial x^2}(s,X(s))\right] ds \\ &+ \int_{t_0}^{t} \sigma(s,X(s))\frac{\partial g}{\partial x}(s,X(s))\ dW(s) \end{aligned} \tag{4.32}$$

or in the form of differentials

$$\begin{aligned} dg(t,X(t)) = &\left[\frac{\partial g}{\partial t}(t,X(t)) + b(t,X(t))\frac{\partial g}{\partial x}(t,X(t))\right. \\ &\left. + \frac{\sigma^2(t,X(t))}{2}\frac{\partial^2 g}{\partial x^2}(t,X(t))\right] dt \\ &+ \sigma(t,X(t))\frac{\partial g}{\partial x}(t,X(t))\ dW(t), \end{aligned} \tag{4.33}$$

which is the **Ito formula**. It is also known as the formula of the change of variables in the stochastic integral.

Example 4.2 *Let $g(x) = x^2$ and $S(t)$ be a solution of (4.12). Find the SDE for $\xi(t) := g(S(t))$ and then compute $ES^2(t)$.*

Answer. Applying the Ito formula, we obtain

$$\begin{aligned} dg(S(t)) &= \left[(\mu + \frac{\sigma^2}{2})S(t)\frac{\partial g}{\partial x}(S(t)) + \frac{\sigma^2}{2}S^2(t)\frac{\partial^2 g}{\partial x^2}(S(t))\right] dt \\ &+ \sigma S(t)\frac{\partial g}{\partial x}(S(t))\ dW(t) \\ &= 2\left[\mu + \sigma^2\right] S^2(t)dt + 2\sigma S^2(t)\ dW(t), \end{aligned}$$

i.e.

$$d\xi = 2\left[\mu + \sigma^2\right]\xi dt + 2\sigma\xi dW(t), \quad \xi(0) = S^2(0).$$

Formally taking expectations from the left and right hand sides of the above equation and taking into account that the expectation of the Ito integral is zero, we obtain

$$dE\xi = 2\left[\mu + \sigma^2\right]E\xi dt, \quad E\xi(0) = S^2(0).$$

Hence

$$E\xi(t) = \xi(0)\exp(2\left[\mu + \sigma^2\right]t),$$

i.e.

$$ES^2(t) = S^2(0)\exp(2\left[\mu + \sigma^2\right]t).$$

Exercise 4.6 *Let $S(t)$ be from (4.22). Find an SDE for $\ln S(t)$ and then solve (4.22).*

Exercise 4.7 *Solve (4.23) using the integrating factor method.*

Exercise 4.8 *Using the Ito formula, show that*

$$\int_0^t sdW(s) = tW(t) - \int_0^t W(s)ds$$

(here $W(s)$ is a standard Wiener process).

Exercise 4.9 *Let $g_n(x) = x^n$, where n is a positive integer, and let $W(t)$ be a standard Wiener process. Using the Ito formula, derive the equation for $\xi^{(n)}(t) := g_n(W(t))$ and compute $EW^{2n}(t)$.*

Let us now introduce the multidimensional Ito formula. Introduce the two operators associated with the SDEs (4.19):

$$\begin{aligned} Lu(t,x) &:= \frac{\partial}{\partial t}u(t,x) + \frac{1}{2}\sum_{r=1}^{q}\sum_{i,j=1}^{d}\sigma_r^i\sigma_r^j\frac{\partial^2}{\partial x^i\partial x^j}u(t,x) + \sum_{i=1}^{d}b^i\frac{\partial}{\partial x^i}u(t,x), \qquad (4.34)\\ \Lambda_r u(t,x) &:= \sum_{i=1}^{d}\sigma_r^i\frac{\partial}{\partial x^i}u(t,x). \end{aligned}$$

Let $f(t,x)$ be a smooth 'good' function. Then we can write the multidimensional Ito (change of variables) formula in the form:

$$df(t,X(t)) = Lf(t,X(t))dt + \sum_{r=1}^{q}\Lambda_r f(t,X(t))dW_r(t) \qquad (4.35)$$

or in the integral form

$$f(t,X_{t_0,x}(t)) = f(t_0,x) + \int_{t_0}^{t}Lf(s,X)ds + \sum_{r=1}^{q}\int_{t_0}^{t}\Lambda_r f(s,X(s))dW_r(s). \qquad (4.36)$$

A justification (not proof!) of the multidimensional Ito formula can be found in [50] and a proof in [56].

Let $u(t,x)$ be a (classical) solution of the Cauchy (initial-value) problem for the linear parabolic partial differential equation (PDE) associated with the SDE (4.19):

$$\begin{aligned} Lu &= 0, \quad t < T,\ x \in R^d, \qquad (4.37)\\ u(T,x) &= f(x),\ x \in R^d. \qquad (4.38) \end{aligned}$$

Note that the equation (4.37) is written with negative direction of time and (4.38) is actually the terminal condition. This PDE associated with the SDEs (4.19) is usually called the *backward Kolmogorov equation.*

Example 4.3 ***(Feynman-Kac formula)*** *Let us apply the Ito formula to $u(t, X_{t_0,x}(t))$, where $u(t,x)$ is the solution of (4.37)-(4.38) and $X(t)$ is the solution of (4.19). We obtain*

$$u(t, X_{t_0,x}(t)) = u(t_0, x) + \int_{t_0}^{t} Lu(s, X)ds + \sum_{r=1}^{q} \int_{t_0}^{t} \Lambda_r u(s, X(s))dW_r(s). \tag{4.39}$$

Taking expectation of the left and right hand sides of (4.39), using properties of Ito integrals and (4.37), we get

$$u(t_0, x) = Eu(t, X_{t_0,x}(t)).$$

Then using (4.38), we arrive at

$$u(t_0, x) = Eu(T, X_{t_0,x}(T)) = Ef(X_{t_0,x}(T)).$$

Thus, we have obtained the probabilistic representation of the solution to the problem (4.37)-(4.38) (the famous Feynman-Kac formula):

$$u(t_0, x) = Ef(X_{t_0,x}(T)), \tag{4.40}$$

where $X_{t_0,x}(t)$, $t \geq t_0$, is the solution of (4.19).

Exercise 4.10 *Consider the Cauchy problem*

$$\begin{aligned} Lu + c(t,x)u &= 0, \quad t < T,\ x \in R^d, & (4.41)\\ u(T,x) &= f(x),\ x \in R^d. & (4.42) \end{aligned}$$

Using the Ito formula, show that its solution has the following probabilistic representation

$$u(t_0, x) = E\left[f(X_{t_0,x}(T))Y_{t_0,x,1}(T)\right], \tag{4.43}$$

where $X_{t_0,x}(t)$, $t \geq t_0$, is the solution of (4.19) and the scalar $Y_{t_0,x,y}(t)$, $t \geq t_0$, satisfies the equation

$$dY = c(t, X)Y dt,\ Y(t_0) = y. \tag{4.44}$$

Remark 4.5 *We can analogously derive probabilistic representations for boundary value problems (Dirichlet and with some extra effort - Neumann) and also for linear elliptic PDEs [11, 56] (and also [44]).*

Example 4.4 *Since $X_{t_0,x}(t)$ is a Markovian process, we have for $t_0 \leq t \leq T$:*

$$E(f(X_{t_0,x}(T))|\mathcal{F}_t) = E(f(X_{t_0,x}(T))|X_{t_0,x}(t)) = E(f(X_{t,X_{t_0,x}(t)}(T))|X_{t_0,x}(t)) = u(t, X_{t_0,x}(t)).$$

Thus

$$E(f(X_{t_0,x}(T))|\mathcal{F}_t) = u(t, X_{t_0,x}(t)), \tag{4.45}$$

where $X(t)$ is the solution of (4.19) and $u(t,x)$ is the solution of (4.37)-(4.38).

Exercise 4.11 *Consider the Cauchy problem for partial differential equation*

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial x^2} - cu = 0, \quad t \in [0,1),\ x \in \mathbf{R},\\ u(1,x) = x, \quad x \in \mathbf{R}, \end{aligned}$$

where c is some constant. Using a probabilistic representation for this problem, find the solution $u(t,x)$.

5 Stochastic numerics – initial thoughts

In this section we have preliminary discussion about numerical methods for SDEs. One can consider this topic as a generalisation of numerical schemes for (deterministic) ordinary differential equations. Of course, the SDE case is more complicated. Dependence of $X(t) = X(t;\omega)$ on ω ("randomness") raises the question how to measure closeness between the exact solution and its approximation. As we will see, this can be done in various ways and the answer on this question largely depends on the question what you would like to compute. Another problem we face here in comparison with deterministic ODEs is that trajectories $X(t)$ are not differentiable. In the deterministic numerical analysis we rely on smoothness of ODEs solution to prove a convergence order of a numerical scheme. Consequently, the deterministic numerical analysis results are no longer applicable here though many ideas from it are certainly very useful for the stochastic case.

Before we proceed to the stochastic case, you might wish to do a 'deterministic' exercise.

Exercise 5.1 *Consider the ODE*

$$\dot{x} = b(t,x),\ x(t_0) = x_0.$$

The simplest numerical method for solving ODEs is the Euler method:

$$x_{k+1} = x_k + b(t_k, x_k)h\,, \tag{5.1}$$

where $h > 0$ is a discretization time step of an interval $[t_0, T]$ and $h = (T - t_0)/N$. Show that this method has second order of accuracy on a single step, i.e. that

$$|x_1 - x(t+h)| \le Kh^2,$$

for some constant $K > 0$ independent of h.

Note that the global error of the Euler method (5.1) is of first order:

$$|x_k - x(t_k)| \le Kh, \quad k = 1, \dots, N,$$

for some constant $K > 0$ independent of h.

Consider the system of Ito SDEs:

$$dX = b(t,X)dt + \sum_{r=1}^{q} \sigma_r(t,X)dW_r(t), \quad X(t_0) = x. \tag{5.2}$$

The simplest approximate method for solving (5.2) is *Euler's method*:

$$X_{k+1} = X_k + \sum_{r=1}^{q} \sigma_{rk}\Delta_k w_r(h) + b_k h\,, \tag{5.3}$$

where $\Delta_k w_r(h) = w_r(t_{k+1}) - w_r(t_k)$, and the index k at σ_r and b indicates that these functions are evaluated at the point (t_k, X_k). We see that (5.3) is a natural generalisation of the Euler method (5.1) for ODEs to the stochastic case.

Under some conditions on the functions $b(t,x)$ and $\sigma_r(t,x)$ G. Marujama [34] showed the mean-square convergence of this method, while I.I. Gichman and A.V. Skorokhod [12] proved that the order of accuracy of Euler's method is 1/2, i.e.,

$$(E(X(t_k) - X_k)^2)^{1/2} \le Ch^{1/2}\,, \tag{5.4}$$

where C is a constant not depending on k and h.

In order to realise the Euler method on a computer, we observe that (i) increments $\Delta_k w_r(h)$ of Wiener process are independent; (ii) $\Delta_k w_r(h)$ are Gaussian random variables $\sim \mathcal{N}(0,h)$; (iii) Gaussian random variables have the following scaling property:

$$\Delta_k w_r(h) = \sqrt{h}\xi_{rk}, \tag{5.5}$$

where $\xi_{rk} \sim \mathcal{N}(0,1)$.

Exercise 5.2 *Show that (5.5) is true.*

Then we can re-write the Euler scheme as the following algorithm:

$$\begin{aligned} X_0 &= x, \\ X_{k+1} &= X_k + \sqrt{h}\sum_{r=1}^{q}\sigma_{rk}\xi_{rk} + b_k h\,, \end{aligned} \tag{5.6}$$

where ξ_{rk} are i.i.d random variables $\sim \mathcal{N}(0,1)$.

6 Mean-square approximation

In this section we consider stronger type of convergence of numerical schemes for SDEs, namely mean-square convergence and a.s. convergence.

Let $(X(t),\mathcal{F}_t)$, $t_0 \le t \le T$, be a solution of the system (5.2) with $E|X(t_0)|^2 < \infty$. The *one-step approximation* $\bar{X}_{t,x}(t+h)$, $t_0 \le t < t+h \le T$, depends on x, t, h, and $\{w_1(\theta)-w_1(t),\dots,w_q(\theta)-w_q(t),\ t \le \theta \le t+h\}$ and is defined as follows:

$$\bar{X}_{t,x}(t+h) = x + A(t,x,h; w_i(\theta)-w_i(t),\ i=1,\dots,q,\ t\le\theta\le t+h). \tag{6.1}$$

Using the one-step approximation, we recurrently construct the approximations $(\bar{X}_k,\mathcal{F}_{t_k})$, $k = 0,\dots,N$, $t_{k+1}-t_k = h_{k+1}$, $T_N = T$:

$$\begin{aligned} &\bar{X}_0 = X_0 = X(t_0),\ \bar{X}_{k+1} = \bar{X}_{t_k,\bar{X}_k}(t_{k+1}) \\ &= \bar{X}_k + A(t_k,\bar{X}_k,h_{k+1}; w_i(\theta)-w_i(t_k),\ i=1,\dots,q,\ t_k\le\theta\le t_{k+1}). \end{aligned} \tag{6.2}$$

We will use the following notation. An approximation of $X(t_k)$ will be denoted by $\bar{X}(t_k)$, $\bar{X}_k$, or simply by X_k. By $\bar{X}_{t_k,X}(t_i)$, $t_i \ge t_k$, we denote an approximation of the solution at step i such that $\bar{X}_k = X$. Clearly,

$$\bar{X}_{k+1} = \bar{X}_{t_k,\bar{X}_k}(t_{k+1}) = \bar{X}_{t_0,\bar{X}_0}(t_{k+1}).$$

Everywhere below we put $\bar{X}_0 = X(t_0)$. For simplicity, we assume that $t_{k+1}-t_k = h = (T-t_0)/N$.

Definition 6.1 *If for a method for (5.2) we have the error estimate*

$$(E(X(t_k)-X_k)^2)^{1/2} \le Ch^p\,, \tag{6.3}$$

then we say that ***the mean-square order of accuracy*** *of the method is p.*

The Euler method (5.3) is an example of mean-square methods. In the case of general SDEs (5.2) it converges with mean-square $p = 1/2$ as we previously already mentioned.

6.1 Fundamental theorem on mean-square convergence

In the deterministic numerical analysis, if the local order of ODE one-step approximation is equal to $p+1$ then the corresponding numerical method has the global order p (see e.g. [6]). In this section we look at a similar result in the case of mean-square approximations of SDEs.

Assume that the functions $b(t,x)$ and $\sigma_r(t,x)$ are defined and continuous for $t \in [t_0, T]$, $x \in \mathbf{R}^d$, and satisfy the following *globally Lipschitz condition*: for all $t \in [t_0, T]$, $x \in \mathbf{R}^d$, $y \in \mathbf{R}^d$ there is an inequality

$$|b(t,x) - b(t,y)| + \sum_{r=1}^{q} |\sigma_r(t,x) - \sigma_r(t,y)| \le K|x-y|\,. \tag{6.4}$$

Here and below we denote by $|x|$ the Euclidean norm of the vector x and by $x^{\intercal}y$ or by (x,y) the scalar (inner) product of two vectors x and y.

The following theorem was proved in [39] (see also [40] and [44, Chapter 1]).

Theorem 6.1 *Suppose the one-step approximation $\bar{X}_{t,x}(t+h)$ has order of accuracy p_1 for expectation of the deviation and order of accuracy p_2 for the mean-square deviation; more precisely, for arbitrary $t_0 \le t \le T-h$, $x \in \mathbf{R}^d$ the following inequalities hold:*

$$|E(X_{t,x}(t+h) - \bar{X}_{t,x}(t+h))| \le K(1+|x|^2)^{1/2} h^{p_1}\,, \tag{6.5}$$

$$\left[E|X_{t,x}(t+h) - \bar{X}_{t,x}(t+h)|^2\right]^{1/2} \le K(1+|x|^2)^{1/2} h^{p_2}\,. \tag{6.6}$$

Also let

$$p_2 \ge \frac{1}{2}\,,\ p_1 \ge p_2 + \frac{1}{2}\,. \tag{6.7}$$

Then for any N and $k = 0, 1, \ldots, N$ the following inequality holds:

$$\left[E|X_{t_0,X_0}(t_k) - \bar{X}_{t_0,X_0}(t_k)|^2\right]^{1/2} \le K(1+E|X_0|^2)^{1/2} h^{p_2-1/2}\,, \tag{6.8}$$

i.e., the order of accuracy of the method constructed using the one-step approximation $\bar{X}_{t,x}(t+h)$ is $p = p_2 - 1/2$.

We note that all the constants K mentioned above, as well as the ones that will appear in the sequel, depend on the system (5.2) and the approximation (6.1) only and do not depend on X_0 and N.

Remark 6.1 *Often the notion of **strong order of accuracy** is used (see, e.g., [29]): if for some method*

$$E\,|X(t_k) - X_k| \le K h^p,$$

where K is a positive constant independent of k and h, then we say that the strong order of accuracy of the method is equal to p. Clearly, if the mean-square order of a method is p, then the method has the same strong order.

Let us prove the fundamental theorem.

Lemma 6.1 *There is a representation*

$$X_{t,x}(t+h) - X_{t,y}(t+h) = x - y + Z \tag{6.9}$$

for which

$$E|X_{t,x}(t+h) - X_{t,y}(t+h)|^2 \le |x-y|^2(1+Kh)\,, \tag{6.10}$$

$$EZ^2 \le K|x-y|^2 h\,. \tag{6.11}$$

Proof. Ito's formula implies that for $0 \le \theta \le h$:

$$E|X_{t,x}(t+\theta) - X_{t,y}(t+\theta)|^2 = |x-y|^2$$
$$+2E\int_t^{t+\theta}(X_{t,x}(s) - X_{t,y}(s))^\intercal (a(s, X_{t,x}(s)) - a(s, X_{t,y}(s)))ds$$
$$+E\int_t^{t+\theta}\sum_{r=1}^{q}|\sigma_r(s, X_{t,x}(s)) - \sigma_r(s, X_{t,y}(s))|^2 ds.$$

It follows from here and (6.4) that

$$E|X_{t,x}(t+\theta) - X_{t,y}(t+\theta)|^2 \le |x-y|^2 + K\int_t^{t+\theta} E|X_{t,x}(s) - X_{t,y}(s)|^2 ds. \tag{6.12}$$

In turn, this implies

$$E|X_{t,x}(t+\theta) - X_{t,y}(t+\theta)|^2 \le |x-y|^2 \times e^{Kh}\,,\ 0 \le \theta \le h, \tag{6.13}$$

from which (6.10) follows. Further, noting that

$$Z = \int_t^{t+h}\sum_{r=1}^{q}(\sigma_r(s, X_{t,x}(s)) - \sigma_r(s, X_{t,y}(s)))dw_r(s)$$
$$+\int_t^{t+h}(a(s, X_{t,x}(s)) - a(s, X_{t,y}(s)))ds\,,$$

and using (6.13), it is not difficult to obtain (6.11). □

Remark 6.2 *Below we will use a conditional version of the inequalities (6.5), (6.6), (6.10), (6.11). In these conditional versions the deterministic variables x, y are replaced by $\mathcal{F}_t$-measurable random variables X, Y. For example, the conditional version of (6.5) reads:*

$$|E(X_{t,X}(t+h) - \bar{X}_{t,X}(t+h)|\mathcal{F}_t)| \le K(1+|X|^2)^{1/2}h^{p_1}\,. \tag{6.14}$$

We will also use simple consequences of these inequalities. For example, (6.14) implies

$$E|E(X_{t,X}(t+h) - \bar{X}_{t,X}(t+h)|\mathcal{F}_t)|^2 \le K(1+E|X|^2)h^{2p_1}\,. \tag{6.15}$$

The proof of these conditional versions rests on an assertion of the following kind: if ζ is $\tilde{\mathcal{F}}$-measurable, $\tilde{\mathcal{F}} \subset \mathcal{F}$, $f(x,\omega)$ does not depend on $\tilde{\mathcal{F}}$, $\omega \in \Omega$, and $Ef(x,\omega) = \phi(x)$, then $E(f(\zeta,\omega)|\tilde{\mathcal{F}}) = \phi(\zeta)$ (see [12]). In the case under consideration the increments of the Wiener processes $w_1(\theta) - w_1(t), \dots, w_q(\theta) - w_q(t)$, $t \le \theta \le t+h$, do not depend on $\mathcal{F}_t$ (see, e.g. [12]), and neither does $\bar{X}_{t,x}(t+h)$, which is formed so that it depends on x, t, h, and the mentioned increments only.

Lemma 6.2 *For all natural N and all $k = 0, \dots, N$ the following inequality holds:*

$$E|\bar{X}_k|^2 \le K(1+E|X_0|^2). \tag{6.16}$$

Proof. Suppose that $E|\bar{X}_k|^2 < \infty$. Then using the conditional version of (6.6), we obtain

$$E|X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1})|^2 \le K(1+E|\bar{X}_k|^2)h^{2p_2}\,. \tag{6.17}$$

It is well known [12] that if an $\mathcal{F}_t$-measurable random variable X has bounded second moment, then the solution $X_{t,X}(t+\theta)$ also has bounded second moment. Therefore, $E|X_{t_k,\bar{X}_k}(t_{k+1})|^2 < \infty$. This and (6.17) imply that $E|\bar{X}_{k+1}|^2 < \infty$ (recall that $\bar{X}_{t_k,\bar{X}_k}(t_{k+1}) = \bar{X}_{k+1}$). Since $E|\bar{X}_0|^2 < \infty$, we have proved the existence of all $E|\bar{X}_k|^2 < \infty$, $k = 0, \dots, N$.

Consider the equation

$$E|\bar{X}_{k+1}|^2 = E|\bar{X}_k|^2 + E|X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k|^2 \tag{6.18}$$
$$+ E|X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1})|^2 + 2E\bar{X}_k^{\intercal}(X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k)$$
$$+ 2E\bar{X}_k^{\intercal}(\bar{X}_{t_k,\bar{X}_k}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1}))$$
$$+ 2E(X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k)^{\intercal}(\bar{X}_{t_k,\bar{X}_k}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1}))\,.$$

We have (see [12])

$$E|X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k|^2 \le K(1 + E|\bar{X}_k|^2)h\,. \tag{6.19}$$

Further, we obtain from (6.17) and (6.19):

$$2|E(X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k)^{\intercal}(\bar{X}_{t_k,\bar{X}_k}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1}))\,| \tag{6.20}$$
$$\le 2(E|X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k|^2)^{1/2}(E|X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1})|^2)^{1/2}$$
$$\le K(1 + E|\bar{X}_k|^2)h^{\,p_2+1/2}\,.$$

It is not difficult to prove the inequality

$$E|E(X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k|\mathcal{F}_{t_k})|^2 \le K(1 + E|\bar{X}_k|^2)h^2\,. \tag{6.21}$$

Therefore

$$2|E\bar{X}_k^{\intercal}(X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k)| = 2|E\bar{X}_k^{\intercal}E(X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k|\mathcal{F}_{t_k})| \tag{6.22}$$
$$\le 2(E|\bar{X}_k|^2)^{1/2}(E|E(X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_k|\mathcal{F}_{t_k})|^2)^{1/2} \le K(1 + E|\bar{X}_k|^2)h\,.$$

Similarly, but referring to (6.15) instead of (6.21), we obtain

$$2|E\bar{X}_k^{\intercal}(\bar{X}_{t_k,\bar{X}_k}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1}))| \le K(1 + E|\bar{X}_k|^2)h^{p_1}\,. \tag{6.23}$$

Applying the inequalities (6.19), (6.17), (6.22), (6.23), and (6.20) to the equality (6.18) and recalling that $p_1 \ge 1,\ p_2 \ge 1/2$, we arrive at the inequality (taking, without loss of generality, $h \le 1$) :

$$E|\bar{X}_{k+1}|^2 \le E|\bar{X}_k|^2 + K(1 + E|\bar{X}_k|^2)h = (1 + Kh)E|\bar{X}_k|^2 + Kh\,. \tag{6.24}$$

Hence, using the well-known result (a variant of Gronwall's lemma) which, for the sake of reference, is stated as Lemma 6.3 below, we obtain (6.16). □

Lemma 6.3 *Suppose that for arbitrary N and $k = 0, \ldots, N$ we have*

$$u_{k+1} \le (1 + Ah)u_k + Bh^p\,, \tag{6.25}$$

where $h = T/N,\ A \ge 0,\ B \ge 0,\ p \ge 1,\ u_k \ge 0,\ k = 0, \ldots, N$. Then

$$u_k \le e^{AT}u_0 + \frac{B}{A}(e^{AT} - 1)h^{p-1} \tag{6.26}$$

(where for $A = 0$ we put $(e^{AT} - 1)/A$ equal to zero).

Let us proceed to the proof of Theorem 6.1 itself. We have

$$X_{t_0,X_0}(t_{k+1}) - \bar{X}_{t_0,X_0}(t_{k+1}) = X_{t_k,X(t_k)}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1}) \tag{6.27}$$
$$= (X_{t_k,X(t_k)}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1})) + (X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1}))\,.$$

The first difference in the right-hand side of (6.27) is the error of the solution arising due to the error in the initial data at time t_k, accumulated at the k-th step. The second difference is the one-step error at the $(k+1)$-step. Taking the square of both sides of the equation, we obtain

$$\begin{aligned} & E|X_{t_0,X_0}(t_{k+1}) - \bar{X}_{t_0,X_0}(t_{k+1})|^2 \\ & = EE(|X_{t_k,X(t_k)}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1})|^2|\mathcal{F}_{t_k}) \\ & +EE(|X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1})|^2|\mathcal{F}_{t_k}) \\ & +2EE((X_{t_k,X(t_k)}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1}))^\intercal (X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1}))|\mathcal{F}_{t_k}) \, . \end{aligned} \tag{6.28}$$

By the conditional version of Lemma 6.1, we get

$$\begin{aligned} & EE(|X_{t_k,X(t_k)}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1})|^2|\mathcal{F}_{t_k}) \\ & \le E|X(t_k) - \bar{X}_k|^2 \times (1+Kh) \, . \end{aligned} \tag{6.29}$$

By the conditional version of (6.6) and Lemma 6.2, we have

$$\begin{aligned} & EE(|X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1})|^2|\mathcal{F}_{t_k}) \\ & \le K(1+E|\bar{X}_k|^2)h^{2p_2} \le K(1+E|X_0|^2)h^{2p_2} \, . \end{aligned} \tag{6.30}$$

The difference $X_{t_k,X(t_k)}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1})$ in the last summand in (6.28) can be treated using Lemma 6.1:

$$X_{t_k,X(t_k)}(t_{k+1}) - X_{t_k,\bar{X}_k}(t_{k+1}) := X(t_k) - \bar{X}_k + Z \, .$$

Then we obtain two terms each of which can be estimated individually. Using (6.15) and Lemma 6.2, we get

$$\begin{aligned} & |EE((X(t_k) - \bar{X}_k)^\intercal (X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1}))|\mathcal{F}_{t_k})| \\ & = |E((X(t_k) - \bar{X}_k)^\intercal E(X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1})|\mathcal{F}_{t_k}))| \\ & \le (E|X(t_k) - \bar{X}_k|^2)^{1/2} K(1+E|X_0|^2)^{1/2} h^{p_1} \, . \end{aligned} \tag{6.31}$$

Finally, using Lemma 6.2 and the inequality (6.6), we obtain

$$\begin{aligned} & |E(Z^\intercal (X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1})))| \\ & \le (EE(|Z|^2|\mathcal{F}_{t_k}))^{1/2} (EE(|X_{t_k,\bar{X}_k}(t_{k+1}) - \bar{X}_{t_k,\bar{X}_k}(t_{k+1})|^2|\mathcal{F}_{t_k}))^{1/2} \\ & \le K(E|X(t_k) - \bar{X}_k|^2)^{1/2} (1+E|X_0|^2)^{1/2} h^{p_2+1/2} \, . \end{aligned} \tag{6.32}$$

Introduce the notation $\varepsilon_k^2 := E|X(t_k) - \bar{X}_k|^2$. The relations (6.28) – (6.32) and the condition $p_1 \ge p_2 + 1/2$ then lead to the inequality (we take $h < 1$) :

$$\varepsilon_{k+1}^2 \le \varepsilon_k^2 (1+Kh) + K(1+E|X_0|^2)^{1/2} \varepsilon_k h^{p_2+1/2} + K(1+E|X_0|^2) h^{2p_2} \, .$$

Using the elementary relation

$$(1+E|X_0|^2)^{1/2} \varepsilon_k h^{p_2+1/2} \le \frac{\varepsilon_k^2 h}{2} + \frac{1+E|X_0|^2}{2} h^{2p_2} \, ,$$

we get

$$\varepsilon_{k+1}^2 \le \varepsilon_k^2 (1+Kh) + K(1+E|X_0|^2) h^{2p_2} \, .$$

The inequality (6.8) follows from this, taking into account Lemma 6.3 and the fact that $\varepsilon_0^2 = 0$. This proves Theorem 6.1. □

6.2 Discussion

The rule:

> "if, in a single step, the mean-square error has order h^{p_2} (i.e., inequality (6.6) holds), then it has order $h^{p_2-1/2}$ on the whole interval"

is not true without the additional condition $p_1 \geq p_2 + 1/2$. A simple example in which this can be seen is given by the method

$$\bar{X}_{k+1} = \bar{X}_k + \sigma(t_k, \bar{X}_k)\Delta_k w(h) \tag{6.33}$$

for the scalar version of system (5.2). It is easy to see that here $p_2 = 1$ while the method diverges for $a \neq 0$.

Exercise 6.1 *Show that p_2 for (6.33) is indeed equal to* 1.

The rule:

> "if, in a single step, the mean-square deviation has order h^{p_2}, then it has order h^{p_2-1} on the whole interval"

is true, but a bit rough. Following this rule, we cannot prove the convergence of the Euler method, in which $p_2 = 1$. Moreover, a more efficient rule for the mean-square deviation cannot be found if we are guided only by the mean-square characteristic of the one-step approximation. The rule following from Theorem 6.1 is based on properties of both the *mean* and the *mean-square deviation* of the one-step approximation. In particular, for Euler's method $p_1 = 2,\ p_2 = 1$ (see the next subsection), and so it follows from Theorem 6.1 that Euler's method has order of accuracy 1/2.

Properties of the mean are used at a single place in the proof of the theorem (and at a "delicate" place indeed), more precisely, when deriving the inequality (6.31).

Let us consider an example which warn against a noncritical use of "sufficiently natural" methods motivated by deterministic ODE methods (see further examples in [44, Chapter 1] and [40]).

Example 6.1 *We consider the linear Stratonovich SDE*

$$dX = aXdt + \sigma X \circ dw,\ 0 \leq t \leq T\,, \tag{6.34}$$

and the implicit method (trapezium method) for it:

$$X_{k+1} = X_k + a\frac{X_k + X_{k+1}}{2}h + \sigma\frac{X_k + X_{k+1}}{2}\Delta_k w(h)\,. \tag{6.35}$$

So,

$$X_{k+1} = X_k + X_k\frac{ah + \sigma\Delta_k w(h)}{1 - ah/2 - \sigma\Delta_k w(h)/2}\,. \tag{6.36}$$

Since the mathematical expectation of the right-hand side does not exist, it is clear that the approximation (6.35) cannot converge in mean-square to the solution of (6.34).

Exercise 6.2 *Explain why expectation of the right-hand side of (6.36) does not exist.*

Fully explicit numerical methods for (5.2) were proposed in [42] (see also [44, Chapter 1]). To resolved the problem illustrated in the above counterexample, truncated random variables instead of Gaussian random variables are used in [42].

6.3 The explicit Euler method

For the system (5.2) we consider the one-step approximation (6.1) of the form

$$\bar{X}_{t,x}(t+h) = x + b(t,x)h + \sum_{r=1}^{q} \sigma_r(t,x)\Delta_t w_r(h)\,, \tag{6.37}$$

where $\Delta_t w_r(h) = w_r(t+h) - w_r(t)$.

As we already know, by (6.2), this approximation generates the *Euler method*:

$$X_0 = X(t_0)\,,\ X_{k+1} = X_k + b_k h + \sum_{r=1}^{q} \sigma_{rk}\Delta_k w_r(h)\,, \tag{6.38}$$

where b_k, σ_{rk} are the values of the coefficients b and σ_r at the point (t_k, X_k), and $\Delta_k w_r(h) = w_r(t_k + h) - w_r(t_k)$.

For (6.37) we can find p_1 and p_2 satisfying the estimates (6.5) and (6.6). To this end we term-wise subtract (6.38) from the SDE solution

$$X_{t,x}(t+h) = x + \int_t^{t+h} b(s, X_{t,x}(s))ds + \sum_{r=1}^{q} \int_t^{t+h} \sigma_r(s, X_{t,x}(s))dw_r(s)\,. \tag{6.39}$$

We obtain

$$\begin{aligned} X_{t,x}(t+h) - \bar{X}_{t,x}(t+h) &= \int_t^{t+h} (b(s, X_{t,x}(s)) - b(t,x))ds \\ &\quad + \sum_{r=1}^{q} \int_t^{t+h} (\sigma_r(s, X_{t,x}(s)) - \sigma_r(t,x))dw_r(s)\,. \end{aligned} \tag{6.40}$$

Calculation of the expectation leads to

$$E(X_{t,x}(t+h) - \bar{X}_{t,x}(t+h)) = E\int_t^{t+h} (b(s, X_{t,x}(s)) - b(t,x))ds\,. \tag{6.41}$$

Taking the square of both sides of (6.40) and then evaluating expectation, we obtain

$$\begin{aligned} E|X_{t,x}(t+h) - \bar{X}_{t,x}(t+h)|^2 &\le 2E\Big|\int_t^{t+h} (b(s, X_{t,x}(s)) - b(t,x))ds\Big|^2 \\ &\quad + 2\sum_{r=1}^{q} \int_t^{t+h} E|\sigma_r(s, X_{t,x}(s)) - \sigma_r(t,x)|^2 ds\,. \end{aligned} \tag{6.42}$$

We assume that, in addition to (6.4), the functions $b(t,x)$ and $\sigma_r(t,x)$ have partial derivatives with respect to t that grow at most as linear functions of x as $|x| \to \infty$. Then a and σ_r satisfy an inequality of the form

$$\begin{aligned} |b(s, X_{t,x}(s)) - b(t,x)| &\le |b(s, X_{t,x}(s)) - b(s,x)| + |b(s,x) - b(t,x)| \\ &\le K|X_{t,x}(s) - x| + K(1 + |x|^2)^{1/2}(s-t)\,. \end{aligned} \tag{6.43}$$

By the Bunyakovsky–Schwarz inequality we have

$$\Big|\int_t^{t+h} (b(s, X_{t,x}(s)) - b(t,x))ds\Big|^2 \le h\int_t^{t+h} |b(s, X_{t,x}(s)) - b(t,x)|^2 ds\,,$$

and due to (6.43) and (6.19) the first term of the right-hand side of (6.42) is bounded by $K(1+|x|^2)h^3$. Using the inequality (6.43) for σ_r and (6.19), we see that the second term of the right-hand side of (6.42)

is bounded by $K(1+|x|^2)h^2$. Thus $p_2 = 1$. Note that this value of p_2 is determined by the second term at the right-hand side of (6.42).

To find p_1, we turn to (6.41). We assume in addition that the derivatives $\partial a^i/\partial x^j$ and $\partial^2 a^i/\partial x^j \partial x^k$, $i,j,k = 1,\dots,d$, are uniformly bounded. We write

$$\begin{aligned} & b(s, X_{t,x}(s)) - b(t,x) \qquad (6.44)\\ = \;& b(t, X_{t,x}(s)) - b(t,x) - (b(t, X_{t,x}(s)) - b(s, X_{t,x}(s)))\\ = \;& \frac{\partial b}{\partial x}(t,x)(X_{t,x}(s) - x) + \rho_1 + \rho_2\,, \end{aligned}$$

where $\partial b/\partial x$ is the $d \times d$-matrix with entries $\partial b^i/\partial x^j$ at the intersection of the i-th row and j-th column, and

$$|\rho_1| \le K|X_{t,x}(s) - x|^2\,,\ |\rho_2| \le K(1 + |X_{t,x}(s)|^2)^{1/2}(s-t)\,. \qquad (6.45)$$

It follows from

$$E(X_{t,x}(s) - x) = E\int_t^s b(\theta, X_{t,x}(\theta))d\theta \qquad (6.46)$$

and (6.4) for $y = 0$ that for all $t_0 \le \theta \le T$

$$|b(\theta, X_{t,x}(\theta))| \le |b(\theta,0)| + |b(\theta, X_{t,x}(\theta)) - b(\theta,0)| \le K(1 + |X_{t,x}(\theta)|)\,.$$

Then it is not difficult to obtain the estimate

$$|\int_t^{t+h} E(X_{t,x}(s) - x)ds| \le K(1+|x|^2)^{1/2}h^2\,.$$

This and (6.41), (6.44), (6.45) imply (6.5) with $p_1 = 2$.

By Theorem 6.1, under the given assumptions regarding the coefficients a and σ_r, *Euler's method is a method of order* $p = p_2 - 1/2 = 1/2$.

Now we consider Euler's method for the system with additive noise:

$$dX = b(t,X)dt + \sum_{r=1}^q \sigma_r(t)dw_r(t)\,. \qquad (6.47)$$

Exercise 6.3 *Show that in the case of (6.47) the second term at the right-hand side of (6.42) can be bounded by* $K(1+|x|^2)h^3$. *Then confirm that* $p_2 = 3/2$ *and that Theorem 6.1 implies that the order of Euler's method for systems with additive noise is* 1.

6.4 The Milstein method

It is interesting to note that in the case of general SDEs (4.13) there is no known (applicably useful!) scheme of higher order than 1/2. In particular cases (we have already mentioned the additive noise case) it is possible to have constructive numerical schemes with mean-square order higher than 1/2. For instance, *a method of first order* (the Milstein method proposed in [36]) has the form

$$X_{k+1} = X_k + \sum_{r=1}^q \sigma_{r_k}\Delta_k w_r(h) + b_k h + \sum_{i=1}^q\sum_{r=1}^q (\Lambda_i\sigma_r)_k \int_{t_k}^{t_{k+1}} (w_i(\theta) - w_i(t_k))dw_r(\theta)\,. \qquad (6.48)$$

Note that in the case of additive noise (i.e., $\sigma_r(t,x) = \sigma_r(t)$, $r = 1,\dots,q$) the Milstein and Euler methods coincide.

In the general case we face with the difficulty of simulating the Ito integral in (6.48). But for a single noise ($q = 1$), the integral in (6.48) can be expressed in terms of $\Delta_k w$ and the formula takes the following constructive form, e.g. in the scalar case ($d = 1$):

$$X_{k+1} = X_k + \sigma_k\Delta_k w + b_k h + \frac{1}{2}(\sigma\frac{\partial\sigma}{\partial x})_k\Delta_k^2 w - \frac{1}{2}(\sigma\frac{\partial\sigma}{\partial x})_k h\,. \qquad (6.49)$$

Exercise 6.4 *Show that in the scalar case (6.48) becomes (6.49).*

Exercise 6.5 *Using the fundamental theorem, prove that the Milstein method is of mean-square order* 1.

6.5 3/2 mean-square method SDEs with additive noise

For SDEs with additive noise (i.e., $\sigma_r(t,x) = \sigma_r(t)$, $r = 1,\ldots,q$), there are constructive (i.e. they can be realised without need of simulating complicated random variables arising due to iterative Ito integrals like in the Milstein method) methods of mean-square order 3/2. For example, the Taylor-type 3/2 mean-square method has the form [40, 44, 29]:

$$\begin{aligned} X_{k+1} &= X_k + \sum_{r=1}^{q} \sigma_{r_k} \Delta_k w_r(h) + a_k h + \sum_{r=1}^{q} (\Lambda_r a)_k \int_{t_k}^{t_{k+1}} (w_r(\theta) - w_r(t_k)) d\theta \\ &\quad + \sum_{r=1}^{q} \sigma'_{r_k} \int_{t_k}^{t_{k+1}} (\theta - t_k) dw_r(\theta) + (La)_k \frac{h^2}{2}\,. \end{aligned} \tag{6.50}$$

Exercise 6.6 *Using the fundamental theorem, prove that the method for SDEs with additive noise is of mean-square order* 3/2.

The method (6.50) can be re-written in the following form ready for implementation

$$\begin{aligned} X_{k+1} &= X_k + \sum_{r=1}^{q} \sigma_r(t_k) \xi_{rk} h^{1/2} + a(t_k, X_k) h \\ &\quad + \sum_{r=1}^{q} \Lambda_r a(t_k, X_k) (\frac{1}{2} \xi_{rk} + \frac{1}{\sqrt{12}} \eta_{rk}) h^{3/2} \\ &\quad + \sum_{r=1}^{q} \frac{d\sigma_r}{dt}(t_k) (\frac{1}{2} \xi_{rk} - \frac{1}{\sqrt{12}} \eta_{rk}) h^{3/2} + La(t_k, X_k) \frac{h^2}{2}\,, \end{aligned} \tag{6.51}$$

where ξ_{rk}, η_{rk} are i.i.d. $\mathcal{N}(0,1)$ random variables.

Exercise 6.7 *Explain how (6.51) follows from (6.50).*

Remark 6.3 *Many other mean-square (explicit and implicit) schemes can be found in [29, 44], including methods for special classes of SDEs (e.g. with additive noise, coloured, noise, small noise, etc.).*

6.6 Nonglobally Lipschitz conditions

Among the conditions of Theorem 6.1, globally Lipschitz conditions (6.4) are most restrictive. SDEs with nonglobally Lipschitz conditions, for which there exist unique extendable solutions, make up a very broad and important class in applications.

Example 6.2 *Consider the SDE (see [52, 32] and also [44]):*

$$dX = -X^3 dt + dw(t)\,. \tag{6.52}$$

Let us start, for instance, at $X(0) = X_0 = 1/h$ (we can do so without loss of generality since we always reach a similar position with a positive probability). Hence

$$X_1 = X_0 - X_0^3 h + \Delta_0 w(h) = \frac{1}{h} - \frac{1}{h^2} + \Delta_0 w(h)$$

with a large probability is a negative number which can be approximately considered as $\approx -1/h^2$. *Then*

$$X_2 = -\frac{1}{h^2} + \frac{1}{h^5} + \Delta_1 w(h) \approx \frac{1}{h^5},\ X_3 \approx -\frac{1}{h^{14}}\,,$$

and so on. In numerical experiments one can observe that the explicit Euler method leads to computer overflows. Indeed, numerical experiments show that a typical trajectory of the explicit Euler method for (6.52) blows up at times t *between* 2.5 *and* 800 *for the time step* $h = 0.36$, $X_0 = 0$. *A decrease of the time step improves the situation, e.g., for* $h = 0.25$ *a typical trajectory blows up at times from* 33 *to* 8×10^4.

The above example demonstrates that the explicit Euler scheme can be divergent for SDEs with nonglobally Lipschitz conditions. It was shown (see e.g. [21, 55] and references therein) that many implicit schemes and also some special explicit schemes are convergent for interesting cases of SDEs with nonglobally Lipschitz conditions.

Exercise 6.8 *Consider the SDE in the Stratonovich sense:*

$$dX = (1 - X^5)\,dt + X^2 \circ dw, \quad X(0) = 0. \tag{6.53}$$

In Ito's sense, the drift of the equation becomes $b(t,x) = 1 - x^5 + x^3$. *Apply to this equation the explicit Euler method (6.38), the drift-implicit Euler method [40, 44, 29]*

$$X_{k+1} = X_k + b(t_k, X_{k+1})h + \sum_{r=1}^{q} \sigma_r(t_k, X_k)\Delta_k w_r(h) \tag{6.54}$$

and the explicit balanced method from [55]

$$X_{k+1} = X_k + \frac{b(t_k, X_k)h + \sum_{r=1}^{m} \sigma_r(t_k, X_k)\Delta_k w_r(h)}{1 + h|b(t_k, X_k)| + \sum_{r=1}^{m} |\sigma_r(t_k, X_k)\Delta_k w_r(h)|}. \tag{6.55}$$

Implement in MatLab all these three methods (note that (6.54) requires to use a nonlinear solver at every step, e.g. Newton's method can be used). Compare qualitative behaviour of the three methods by doing numerical experiments. The outcomes can be compared with the results in [55].

6.7 Almost sure convergence

As one can see from the definition (6.3), mean-square methods guarantee closeness of the exact trajectory and its approximation in the mean-square sense (L_2-norm). Mean-square methods are useful for direct simulation of stochastic trajectories, when one needs to look at qualitative behaviour of the model.

We can also consider a stronger type of convergence and require that for almost every trajectory $W(\cdot)$ and any $\varepsilon > 0$ the method converges *almost surely* with order γ, i.e.

$$|X(t_k) - X_k| \le C(\omega)h^\gamma \quad a.s., \tag{6.56}$$

where C is an a.s. bounded random variable independent of k and h.

For instance, we can prove that the following estimate holds for the Euler scheme (6.37) (see e.g. [13] and also [55]): for some $p \ge 1$:

$$\left[E|X(t_k) - X_k|^{2p}\right]^{1/(2p)} \le Kh^{1/2}. \tag{6.57}$$

Denote $R := |X(t_k) - X_k|$. The estimate (6.57) and Markov's inequality imply

$$P(R > h^\gamma) \le \frac{ER^{2p}}{h^{2p\gamma}} \le C(x)h^{p(1-2\gamma)}.$$

Then for any $\gamma = 1/2 - \varepsilon$ there is a sufficiently large $p \ge 1$ such that (recall that $h = T/N$)

$$\sum_{N=1}^{\infty} P\left(R > \frac{T^\gamma}{N^\gamma}\right) \le C(x)T^{p(1-2\gamma)} \sum_{N=1}^{\infty} \frac{1}{N^{p(1-2\gamma)}} < \infty.$$

Hence, due to the Borel-Cantelli lemma[12], the random variable $\varkappa := \sup_{h>0} h^{-\gamma}|R|$ is a.s. finite which implies

$$|X(t_k) - X_k| \le C(\omega)h^{1/2-\varepsilon} \quad a.s., \tag{6.58}$$

where C is an a.s. finite random variable independent of h. Note that $C(\omega)$ depends on ε.

Exercise 6.9 *Consider the linear SDE*

$$dS = rSdt + \sigma Sdw, \quad S(0) = S_0, \tag{6.59}$$

where r and σ are some positive constants. This is an SDE for GBM (see Section 4). Apply the Euler scheme and Milstein scheme to (6.59) and realise the corresponding algorithms in MatLab. Solve (6.59) exactly. Run MatLab simulations of (6.59) using the exact formula for $S(t_k)$ and the two methods along the same Wiener paths and compute the corresponding errors $|S(t_k) - X_k|$. Study experimentally the a.s. convergence of the Euler and Milstein methods.

Exercise 6.10 *Continue the previous exercise and experimentally study the mean square errors of the Euler and Milstein methods. Use the Monte Carlo technique (see Section 8) to evaluate the errors, i.e.*

$$\sqrt{E\left|S(t_k) - S_k\right|^2} \approx \sqrt{\frac{1}{M}\sum_{m=1}^{M}\left|S^{(m)}(t_N) - S_N^{(m)}\right|^2},$$

where $S^{(m)}(t_N)$ and $S_N^{(m)}$ are realisations of the exact solution to (6.59) and of one of the two numerical methods along mth independent Wiener path. To observe the expected mean-square order, M should be sufficiently large to make the Monte Carlo error negligible. Read further about the Monte Carlo technique in Section 8, in particular about the need to report the Monte Carlo error.

7 Approximation in the weak-sense

Weak (or more precisely, weak-sense) methods are sufficient for evaluation of averages and are often simpler than mean-square ones. This type of convergence is of interest for solving linear PDEs (discussed in Section 8.2) and it is in most cases sufficient for applicable problems, e.g. in financial engineering and molecular dynamics. The first paper on weak approximation of SDEs is by Milstein [37].

As before, we consider the system

$$dX = b(t, X)dt + \sum_{r=1}^{q}\sigma_r(t, X)dw_r(t)\,, \tag{7.1}$$

where X, b, and σ are vectors of dimension d with components X^i, b^i, σ_r^i. We assume that the functions $b(t, x)$ and $\sigma_r(t, x)$ are sufficiently smooth with respect to the variables t, x and satisfy a global Lipschitz condition with respect to x: for all $t \in [t_0, T]$, $x \in \mathbf{R}^d$, $y \in \mathbf{R}^d$ the following inequality holds:

$$|b(t, x) - b(t, y)| + \sum_{r=1}^{q}|\sigma_r(t, x) - \sigma_r(t, y)| \le K|x - y|\,. \tag{7.2}$$

Here and below $|x|$ denotes the Euclidean norm of the vector x, and we denote by $x^\intercal y$ or by (x, y) the scalar (inner) product of two vectors x and y.

Definition 7.1 *If an approximation $\bar{X}$ is such that*

$$|Ef(\bar{X}(T)) - Ef(X(T))| \le Kh^p \tag{7.3}$$

*for f from a class of functions with polynomial growth at infinity, then we say that the **weak order of accuracy** of the approximation $\bar{X}$ (the method $\bar{X}$) is p. The constant K depends on the coefficients of (7.1), on the function f and on T.*

[12] See it e.g. in [49].

It can be proved (see, e.g. [44, Chapter 2]), for example, that the weak order of accuracy of Euler's method (5.3) is 1. Note that numerical integration in the mean-square sense with some order of accuracy guarantees an approximation in the weak sense with the same order of accuracy, since if $(E|\bar{X}(t) - X(t)|^2)^{1/2} = O(h^p)$ then for every function f satisfying a Lipschitz condition we have $E(f(\bar{X}(T)) - f(X(T))) = O(h^p)$. Moreover, an increase in the order of accuracy in the mean-square sense does not, in general, imply an increase of the weak order of accuracy. For example, the Milstein method (6.48) has first weak order of accuracy as Euler's method does. At the same time, a crude method like

$$X_{k+1} = X_k + b_k h + \sqrt{h} \sum_{r=1}^{q} \sigma_{rk} \eta_{rk} \,, \tag{7.4}$$

where $\eta_{rk},\ r = 1, \ldots, q,\ k = 0, \ldots, N-1$, are independent random variables taking the values $+1$ and -1 with probabilities $1/2$, also has first order of accuracy in the sense of weak approximation. We usually call (7.4) as the *weak Euler scheme*.

The main interest in weak approximations lies in the hope to obtain simpler methods and, in particular, methods not requiring modeling of complicated random variables. We recall that, e.g., the mean-square Milstein method (6.48), which is of the first order only, requires to solve the difficult problem of modeling complicated random variables of the type $\int_0^h w_i(\theta) dw_j(\theta)$. These problems of modeling complicated random variables can be avoided by integrating in the weak sense, which gives an impetus for the development of methods for constructing weak approximations. In addition we note that while in the deterministic theory the one-dimensional case differs but little from the multi-dimensional one, for the numerical integration of stochastic differential equations the multi-dimensional case, especially when several noises are involved, is essentially more complicated than the one-dimensional case.

7.1 The general convergence theorem

Along with the system (7.1), we consider the approximation

$$\bar{X}_{t,x}(t+h) = x + A(t, x, h; \xi) \,, \tag{7.5}$$

where ξ is a random variable (in general, a vector) having moments of a sufficiently high order, and A is a vector function of dimension d. Partition the interval $[t_0, T]$ into N equal parts with step $h = (T - t_0)/N$: $t_0 < t_1 < \cdots < t_N = T$, $t_{k+1} - t_k = h$. According to (7.5), we construct the sequence

$$\bar{X}_0 = X_0 = X(t_0),\ \bar{X}_{k+1} = \bar{X}_k + A(t, \bar{X}_k, h; \xi_k),\ k = 0, \ldots, N-1, \tag{7.6}$$

where ξ_0 is independent of $\bar{X}_0$, while ξ_k for $k > 0$ is independent of $\bar{X}_0, \ldots, \bar{X}_k$, $\xi_0, \ldots, \xi_{k-1}$. As before, we write $\Delta = X - x = X_{t,x}(t+h) - x$, $\bar{\Delta} = \bar{X} - x = \bar{X}_{t,x}(t+h) - x$. Let $X(t) = X_{t_0,X_0}(t)$ be a solution of (7.1) and $\bar{X}_{t_0,X_0}(t_k) = \bar{X}_k$.

Following [37], one usually consider the following class of functions within the weak-sense approximation context.

Definition 7.2 *We say that a function $f(x)$ belongs to the class $\mathbf{F}$, written as $f \in \mathbf{F}$, if we can find constants $K > 0$, $\kappa > 0$ such that for all $x \in \mathbf{R}^d$ the following inequality holds:*

$$|f(x)| \le K(1 + |x|^{\kappa}) \,. \tag{7.7}$$

If a function $f(s, x)$ depends not only on $x \in \mathbf{R}^d$ but also on a parameter $s \in S$, then we say that $f(s, x)$ belongs to $\mathbf{F}$ (with respect to the variable x) if an inequality of the type (7.7) holds uniformly in $s \in S$.

The following theorem was proved in [38] (see also [40, 44]).

Theorem 7.1 *Assume that*

(*a*) *the coefficients of equation* (7.1) *are continuous, satisfy the Lipschitz condition* (7.2) *and together with their partial derivatives with respect to* x *of order up to* $2p+2$, *inclusively, belong to* $\mathbf{F}$;

(*b*) *the method* (7.5) *is such that*

$$|E(\prod_{j=1}^{s}\Delta^{i_j}-\prod_{j=1}^{s}\bar{\Delta}^{i_j})|\le K(x)h^{p+1},\ s=1,\dots,2p+1,\ K(x)\in\mathbf{F}\,, \tag{7.8}$$

$$E\prod_{j=1}^{2p+2}|\bar{\Delta}^{i_j}|\le K(x)h^{p+1},\ K(x)\in\mathbf{F}\,; \tag{7.9}$$

(*c*) *the function* $f(x)$ *together with its partial derivatives of order up to* $2p+2$, *inclusively, belong to* $\mathbf{F}$;

(*d*) *for a sufficiently large* m (*specified below*) *the expectations* $E|\bar{X}_k|^{2m}$ *exist and are uniformly bounded with respect to* N *and* $k=0,1,\dots,N$.

Then, for all N *and all* $k=0,1,\dots,N$ *the following inequality holds:*

$$|Ef(X_{t_0,X_0}(t_k))-Ef(\bar{X}_{t_0,X_0}(t_k))|\le Kh^p\,, \tag{7.10}$$

i.e., the method (7.6) *has order of accuracy* p *in the sense of weak approximations.*

Proof. First of all we note that the Lipschitz condition (7.2) implies that for any $m>0$ the expectations $E|X(\theta)|^{2m}$ exist and are uniformly bounded with respect to $\theta\in[t_0,T]$ if only $E|X(t_0)|^{2m}<\infty$ (see [12]). Moreover, the same (7.2) implies

$$E\prod_{j=1}^{2p+2}|\Delta^{i_j}|\le K(x)h^{p+1},\ K(x)\in\mathbf{F}\,. \tag{7.11}$$

Further, suppose that $u(x)$ is a function that together with its partial derivatives of order up to $2p+2$, inclusively, belong to $\mathbf{F}$. Then

$$|Eu(X_{t,x}(t+h))-Eu(\bar{X}_{t,x}(t+h))|\le K(x)h^{p+1},\ K(x)\in\mathbf{F}\,. \tag{7.12}$$

Exercise 7.1 *Using (7.8), (7.9), (7.11), prove (7.12).*

We introduce the function

$$u(s,x)=Ef(X_{s,x}(t_{k+1}))\,.$$

By the conditions (a) and (c), u has partial derivatives with respect to x of order up to $2p+2$, inclusively; moreover, these derivatives belong to $\mathbf{F}$ (see [12]). Therefore the function $u(s,x)$ satisfies an estimate of the form (7.12) uniformly with respect to $s\in[t_0,t_{k+1}]$.

Further, since $\bar{X}_0=X_0$, $X_{t_0,X_0}(t_1)=X(t_1)$, $X_{t_1,X_{t_0,\bar{X}_0}(t_1)}(t_{k+1})=X(t_{k+1})$, we have

$$Ef(X(t_{k+1}))=Ef(X_{t_1,X_{t_0,\bar{X}_0}(t_1)}(t_{k+1}))-Ef(X_{t_1,\bar{X}_1}(t_{k+1}))+Ef(X_{t_1,\bar{X}_1}(t_{k+1}))\,. \tag{7.13}$$

Similarly, since $X_{t_1,\bar{X}_1}(t_{k+1})=X_{t_2,X_{t_1,\bar{X}_1}(t_2)}(t_{k+1})$, we have

$$Ef(X_{t_1,\bar{X}_1}(t_{k+1}))=Ef(X_{t_2,X_{t_1,\bar{X}_1}(t_2)}(t_{k+1}))-Ef(X_{t_2,\bar{X}_2}(t_{k+1}))+Ef(X_{t_2,\bar{X}_2}(t_{k+1}))\,. \tag{7.14}$$

Now (7.13) and (7.14) imply

$$\begin{aligned}Ef(X(t_{k+1})) &= Ef(X_{t_1,X_{t_0,\bar{X}_0}(t_1)}(t_{k+1}))-Ef(X_{t_1,\bar{X}_1}(t_{k+1}))\\ &\quad +Ef(X_{t_2,X_{t_1,\bar{X}_1}(t_2)}(t_{k+1}))-Ef(X_{t_2,\bar{X}_2}(t_{k+1}))+Ef(X_{t_2,\bar{X}_2}(t_{k+1}))\,.\end{aligned}$$

Proceeding further, we obtain

$$\begin{aligned} Ef(X(t_{k+1})) &= \sum_{i=0}^{k-1} Ef(X_{t_{i+1},X_{t_i,\bar{X}_i}(t_{i+1})}(t_{k+1})) - \sum_{i=0}^{k-1} Ef(X_{t_{i+1},\bar{X}_{i+1}}(t_{k+1})) \\ &\quad + Ef(X_{t_k,\bar{X}_k}(t_{k+1}))\,. \end{aligned} \tag{7.15}$$

This immediately implies (recall that $\bar{X}_{i+1} = \bar{X}_{t_i,\bar{X}_i}(t_{i+1})$) that

$$\begin{aligned} &Ef(X(t_{k+1})) - Ef(\bar{X}_{k+1}) \\ &= \sum_{i=0}^{k-1} (EE(f(X_{t_{i+1},X_{t_i,\bar{X}_i}(t_{i+1})}(t_{k+1}))|X_{t_i,\bar{X}_i}(t_{i+1})) \\ &\quad - EE(f(X_{t_{i+1},\bar{X}_{t_i,\bar{X}_i}(t_{i+1})}(t_{k+1}))|\bar{X}_{t_i,\bar{X}_i}(t_{i+1})) \\ &\quad + Ef(X_{t_k,\bar{X}_k}(t_{k+1})) - Ef(\bar{X}_{t_k,\bar{X}_k}(t_{k+1}))\,. \end{aligned} \tag{7.16}$$

According to the definition of $u(s,x)$, (7.16) implies

$$\begin{aligned} &|Ef(X(t_{k+1})) - Ef(\bar{X}_{k+1})| \\ &= |\sum_{i=0}^{k-1} (Eu(t_{i+1}, X_{t_i,\bar{X}_i}(t_i+h)) - Eu(t_{i+1}, \bar{X}_{t_i,\bar{X}_i}(t_i+h))) \\ &\quad + (Ef(X_{t_k,\bar{X}_k}(t_{k+1})) - Ef(\bar{X}_{t_k,\bar{X}_k}(t_{k+1})))| \\ &\le \sum_{i=0}^{k-1} E|E(u(t_{i+1}, X_{t_i,\bar{X}_i}(t_i+h)) - u(t_{i+1}, \bar{X}_{t_i,\bar{X}_i}(t_i+h))|\bar{X}_i)| \\ &\quad + E|E(f(X_{t_k,\bar{X}_k}(t_{k+1})) - f(\bar{X}_{t_k,\bar{X}_k}(t_{k+1}))|\bar{X}_k)|\,. \end{aligned} \tag{7.17}$$

We note that the functions $u(s,x)$ and $f(x)$, which belong to class $\mathbf{F}$ and so satisfy an inequality of the form (7.12), also satisfy the conditional version of this inequality. Suppose that for both $u(s,x)$ and $f(x)$ we have a function $K(x)$ in this inequality with $\kappa = 2m$. Then (7.17) implies

$$|Ef(X(t_{k+1})) - Ef(\bar{X}_{k+1})| \le \sum_{i=0}^{k-1} K(1+E|\bar{X}_i|^{2m})h^{p+1} + K(1+E|\bar{X}_k|^{2m})h^{p+1}.$$

Assuming that the condition (d) holds for precisely this $2m$, we arrive at (7.10). □

Exercise 7.2 *Using the general convergence theorem (i.e. Theorem 7.1), prove that the Euler scheme is of weak order* 1.

7.2 Nonglobally Lipschitz conditions

As in the case of mean-square schemes (see Section 6.6), the most restrictive conditions of Theorem 7.1 are globally Lipschitz conditions imposed on the coefficients of the SDEs (see the assumption (a) of the theorem). In [45] *the concept of rejecting exploding trajectories* (CRE) was proposed and justified, which, in principle, allows us to apply any numerical method to SDEs with nonglobally Lipschitz coefficients for estimating a mean $Ef(X(T))$, where the time T is fixed. Following this concept, we do not take into account the approximate trajectories which leave a sufficiently large sphere $S_R := \{x : |x| < R\}$ during the time T. It was proved that accuracy of any method of weak order p is estimated by $\varepsilon + O(h^p)$, where ε can be made arbitrarily small with growing R. It turns out that in practice the error given by ε is much smaller than the error of numerical integration. Thus, due to CRE, we can choose a suitable method for solving a system of SDEs with nonglobally Lipschitz coefficients taking into account all the known methods of numerical integration.

The other restrictive condition is the assumption (c) requiring the function $f(x)$ to be smooth. It is particular restrictive for applications in Financial Engineering, where $f(x)$ has the meaning of a payoff function which is usually nonsmooth (e.g. in the case of digital options it is discontinuous). This assumption can be relaxed: in [2] weak convergence with order one of the Euler method is proved for any measurable $f(x)$.

7.3 Second-order weak schemes

Above we have given two variants of Euler schemes (5.3) and (7.4) of weak order one. The next scheme is of second weak order for the SDE (7.1):

$$\begin{aligned} X_{k+1} &= X_k + \sum_{r=1}^{q} \sigma_{rk}\xi_{rk}h^{1/2} + b_k h + \sum_{r=1}^{q}\sum_{i=1}^{q}(\Lambda_i\sigma_r)_k\xi_{irk}h \\ &\quad + \frac{1}{2}\sum_{r=1}^{q}(\Lambda_r b + L\sigma_r)_k\xi_{rk}h^{3/2} + (Lb)_k\frac{h^2}{2}\,, \end{aligned} \tag{7.18}$$

where

$$\xi_{irk} = \frac{1}{2}\xi_{ik}\xi_{rk} - \frac{1}{2}\gamma_{ir}\zeta_{ik}\zeta_{rk},\ \gamma_{ir} = \begin{cases} -1, & i < r, \\ 1 & i \geq r \end{cases}\,, \tag{7.19}$$

ξ_{rk} and ζ_{ik} are independent random variables which can be modeled by, e.g., the law $P(\xi = 0) = 2/3$, $P(\xi = \pm\sqrt{3}) = 1/6$ or $P(\xi = \pm\sqrt{1-\sqrt{6}/3}) = 3/8$, $P(\xi = \pm\sqrt{1+\sqrt{6}}) = 1/8$ and by $P(\zeta = \pm 1) = 1/2$, respectively.

Exercise 7.3 *Using the general convergence theorem (i.e., Theorem 7.1), prove that the scheme (7.18)-(7.19) is of weak order* 2.

Consider the system with additive noise

$$dX = b(t,X)dt + \sum_{r=1}^{q}\sigma_r dw_r(t),\ X(0) = x. \tag{7.20}$$

The Runge–Kutta method of weak order two for (7.20) has the form (see [44, p. 113]):

$$X_{k+1} = X_k + \sum_{r=1}^{q}\sigma_r\xi_{rk}h^{1/2} + \frac{h}{2}\left[b_k + b\left(t_{k+1}, X_k + \sum_{r=1}^{q}\sigma_r\xi_{rk}h^{1/2} + b_k h\right)\right]\,, \tag{7.21}$$

where $b_k = b(t_k, X_k)$ and ξ is, e.g., $\mathcal{N}(0,1)$-distributed or distributed by the law

$$P(\xi = 0) = 2/3, \quad P(\xi = \pm\sqrt{3}) = 1/6.$$

This method is often called the *Heun method*. It is of week order 2.

Exercise 7.4 *Using the general convergence theorem (i.e. Theorem 7.1), prove that the scheme (7.21) for (7.20) is of weak order* 2.

Remark 7.1 *Many other weak schemes can be found in [29, 44, 16], including methods for special classes of SDEs (e.g. with additive noise, coloured, noise, small noise, etc.).*

7.4 The Talay–Tubaro extrapolation method

It is possible to expand the global errors of weak methods for stochastic systems in powers of time increment h. The approach is analogous to the Richardson–Runge extrapolation method for deterministic ODEs which you might have seen in a deterministic numerical analysis course. It allows us to estimate the global error as well as to improve the accuracy of the method. In particular, we can construct a method of order two applying the Euler method twice with different time steps.

Here we suppose that the coefficients of (7.1) are sufficiently smooth and all their derivatives up to a sufficiently large order are bounded. The function f is assumed to be sufficiently smooth and with growth not faster than polynomial at infinity.

Theorem 7.2 *Let a one-step weak approximation $\bar{X}_{t,x}(t+h)$ of the solution $X_{t,x}(t+h)$ of (7.1) generate a method of order p. Then the global error*

$$R := Ef(X_{t_0,X_0}(T)) - Ef(\bar{X}_{t_0,X_0}(T))$$

of the method has the following expansion

$$R = C_0 h^p + \cdots + C_n h^{p+n} + O(h^{p+n+1}), \tag{7.22}$$

where the constants $C_0, \ldots, C_n$ are independent of h, and n is an integer, $n \geq 0$ (n can be anyhow large if the coefficients of (7.1) belong to C^∞ and their derivatives of any order are bounded).

In particular, for the Euler method

$$R = C_0 h + \cdots + C_n h^{1+n} + O(h^{n+2}). \tag{7.23}$$

The proof of this theorem can be found in [53, 44].

Due to Theorem 7.2, we obtain an extension of the well known in the case of deterministic differential equations extrapolation methods to the stochastic case. For example, simulating $u(t_0, x) = Ef(X_{t_0,x}(T))$ twice by the Euler scheme but with varying time steps $h_1 = h$, $h_2 = \alpha h$, $\alpha > 0$, $\alpha \neq 1$, we obtain

$$\bar{u}^{h_1} = Ef(\bar{X}^{h_1}_{t_0,x}(T))$$

and

$$\bar{u}^{h_2} = Ef(\bar{X}^{h_2}_{t_0,x}(T)).$$

We can expand (see (7.23)

$$\begin{aligned} u &= \bar{u}^{h_1} + Ch_1 + O(h^2), \\ u &= \bar{u}^{h_2} + Ch_2 + O(h^2), \end{aligned} \tag{7.24}$$

whence

$$C = -\frac{\bar{u}^{h_2} - \bar{u}^{h_1}}{h_2 - h_1} + O(h). \tag{7.25}$$

By (7.24) and (7.25) we get the improved value with error $O(h^2)$:

$$\bar{u}_{imp} = \bar{u}^{h_1}\frac{h_2}{h_2 - h_1} - \bar{u}^{h_2}\frac{h_1}{h_2 - h_1},\ u = \bar{u}_{imp} + O(h^2). \tag{7.26}$$

Thus, the obtained method has an accuracy of order two. In the same spirit, using three recalculations of $u = Ef(X_{t_0,x}(T))$ by the Euler method with varying time-steps, one can find C_0 and C_1 from (7.23) and, as a consequence, a method of order three can be constructed, and so on. On the other hand, Ch gives the leading term of the error which can be used for error estimation in practice like Richardson-Runge method in the case of ODEs.

8 The Monte Carlo technique

We start with an illustrative example to explain the basic idea behind the Monte Carlo technique. Consider the problem of numerical evaluation of the integral of a 'good' function $f(x)$ over a unit interval

$$I = \int_0^1 f(x)dx. \tag{8.1}$$

Let M be a positive integer. We know from the numerical analysis that, e.g., for twice continuously differentiable functions $f(x)$ the trapezoidal rule

$$I \approx \bar{I} = \frac{f(0)+f(1)}{2M} + \frac{1}{M}\sum_{m=1}^{M-1} f\left(\frac{m}{M}\right) \tag{8.2}$$

is of order two, i.e.

$$|I - \bar{I}| \le \frac{K}{M^2}\ , \tag{8.3}$$

where $K > 0$ is a constant which does not depend on M.

The trapezoidal rule (8.2) is one of the deterministic methods for approximation of definite integrals. Deterministic methods suffer from the 'curse of dimensionality'. Suppose we need to compute a d-dimensional integral over $[0,1]^d$. The error of a product trapezoidal rule in d dimension is $O(M^{-2/d})$ for twice continuously differentiable integrands. This degradation in convergence rate with increasing dimension is characteristic of deterministic integration methods and they are not practical in higher dimensions[13].

Now let us look at how we can numerically estimate the integral (8.1) using probabilistic ideas. Obviously, we can represent the integral as

$$I = Ef(\xi), \tag{8.4}$$

where ξ is a random variable with uniform distribution on $[0,1]$.

Exercise 8.1 *Explain why (8.4) is true.*

Using this (probabilistic) representation, we can propose a probabilistic algorithm (the *Monte Carlo method*) for evaluating this integral. To this end, suppose we have an algorithm (called *random number generator* (RNG)) which allows us to simulate a sample $\xi_1, \xi_2, \ldots, \xi_M$ from uniform distribution on $[0,1]$. Or in other words, we can say this RNG draws $\xi_1, \xi_2, \ldots, \xi_M$ independently and uniformly from $[0,1]$. Then we can obtain an approximation $\hat{I}_M$ of I (its Monte Carlo estimate) as follows

$$I = Ef(\xi) \simeq \hat{I}_M := \frac{1}{M}\sum_{m=1}^{M} f(\xi_m). \tag{8.5}$$

Let me pay your attention that the left-hand side of (8.5) is deterministic, it is just a certain number, while its right-hand side is random, it depends on a particular realisation of $\xi_1, \xi_2, \ldots, \xi_M$.

If $f(x)$ is integrable on $[0,1]$ then by the Kolmogorov strong law of large numbers (see Theorem 2.1) $\hat{I}_M$ converges to I with probability one as M tends to infinity.

Exercise 8.2 *Explain application of the strong law of large numbers here.*

[13] There are sparse grid deterministic integration methods which can work in moderate dimensions, see e.g. http://garcke.ins.uni-bonn.de/research/pub/sparse_grids_nutshell.pdf

As it is usual in numerical analysis, when you have a numerical method, we need to ask the question about its accuracy. In the case of (8.5) we need to ask how fast the random variable $\hat{I}_M$ approaches I when M increases. First, let us compute $E\hat{I}_M$:

$$E\hat{I}_M = E\frac{1}{M}\sum_{m=1}^{M} f(\xi_m) = \frac{1}{M}\sum_{m=1}^{M} Ef(\xi_m) = I,$$

i.e.

$$Bias(\hat{I}_M) := E\left(\hat{I}_M - I\right) = 0. \tag{8.6}$$

Thus, there is no systematic error in the approximation of I by $\hat{I}_M$.

Now we assume that $f(x)$ is square integrable and compute variance of the estimator

$$Var(\hat{I}_M) = \frac{1}{M}Var(f(\xi)). \tag{8.7}$$

Exercise 8.3 *Prove (8.7).*

We note that

$$Var(f(\xi)) = \int_0^1 \left(f(x) - I\right)^2 dx. \tag{8.8}$$

Exercise 8.4 *Show that (8.8) is true.*

Equations (8.6) and (8.7) and Central Limit Theorem (CLT, Theorem 2.2) imply (details are given in the next section) that under a sufficiently large M the error $\hat{I}_M - I$ is approximately normally distributed with zero mean (cf. (8.6)) and variance $Var(f(\xi))/M$:

$$\hat{I}_M - I \sim \mathcal{N}(0, Var(f(\xi))/M). \tag{8.9}$$

We note that the error of the estimator $\hat{I}_M$ is random while the error of a deterministic integration rule (like the trapezoidal rule) is deterministic.

The error of a Monte Carlo estimator, which is characterized by its variance, is called the *Monte Carlo error* or *statistical error*. Let us pay attention to the fact that in this example there is no systematic error (bias is equal to zero) and only the statistical error is present.

Using the CLT, we can say more (see details in the next section) that the (random) value we find in a particular run of our Monte Carlo algorithm is such that the true value I belongs to the confidence interval:

$$I \in (\hat{I}_M - c\frac{\sqrt{Var(f(\xi))}}{\sqrt{M}}, \hat{I}_M + c\frac{\sqrt{Var(f(\xi))}}{\sqrt{M}}) \tag{8.10}$$

with probability, e.g. 0.68 for $c = 1$, 0.95 for $c = 2$ (well, more precisely $c = 1.96$), and 0.997 for $c = 3$. Note that we assume that M is sufficiently large here in order to use CLT.

The length of the confidence interval (8.10) is decreasing with increase of M as $1/\sqrt{M}$. This form of the statistical error is the central feature of the Monte Carlo method. Adding one decimal place of precision requires 100 times as many sample points. If you compare this with the error (8.3) of the trapezoidal method, you will see that convergence of the Monte Carlo method is slow. Indeed, Monte Carlo methods are usually not competitive for one-dimensional integrals. The value of the Monte Carlo technique is that it can deal, in principle, with the 'curse of dimensionality'. This is based on the fact that the Monte Carlo rate of convergence $O(1/\sqrt{M})$ is not restricted to integrals over unit intervals. What was done in this example can be easily extended to estimating an integral over $[0,1]^d$ (one would need just to sample a d-dimensional random variable ξ uniformly distributed in the cube $[0,1]^d$) or any other domain in R^d. The standard error will still have the form $\dfrac{\sqrt{Var(f(\xi))}}{\sqrt{M}}$ for a Monte Carlo estimate

based on M draws from $[0,1]^d$. [14] So, the order of convergence of the Monte Carlo method is $O(1/\sqrt{M})$ for any dimension d while the convergence rate of deterministic methods, e.g. of the trapezoidal rule, degrade quickly with increase of d (recall that for the trapezoidal rule the order is $O(M^{-2/d})$). Thus, Monte Carlo methods are attractive in evaluating integrals in high dimension.

We see that to quantify the Monte Carlo error we need to know $Var(f(\xi))$, i.e. the integral (8.8). In practical applications it is unreasonable to expect that $Var(f(\xi))$ is known. But the variance can be estimated in the same experiment as

$$\sigma_f^2 := Var(f(\xi)) \simeq \hat{\sigma}_f^2 := \frac{1}{M}\sum_{m=1}^{M}[f(\xi_m)]^2 - \hat{I}_M^2 \tag{8.11}$$

(instead of $1/M$ factor one can put $1/(M-1)$ to get the unbiased sample variance but in the Monte Carlo simulations samples of a very large size are usually used and the difference between these two sample variances is negligible). Thus, from simulating M values of the function $f(x)$, we obtain not only an estimate for the integral I but also a measure of the error in this estimate.

At this point, we finish the illustrative example, which, in a sense, is sufficient for understanding the Monte Carlo technique and its further use in various practical situations.

In a broader sense than the above example, the Monte Carlo method is a statistical method by which one evaluates a nonrandom quantity as an expected value of a random variable. In other words, if you can find a probabilistic representation for a quantity of your interest (i.e., if you can express this quantity as an expectation of a certain random variable) then you can straightforwardly apply this statistical technique. I am sure you already guess that we can combine probabilistic representations of linear PDE problems, weak-sense approximation and the Monte Carlo technique in order to get probabilistic algorithms for solving linear PDEs and associated problems like those arising in Financial Engineering and molecular dynamics.

Historical Remark. The Monte Carlo method was proposed as a tool for evaluating high-dimensional integrals by John von Neumann and Stanislaw Ulam in March 1947 when they work on thermonuclear bomb in Los Alamos (US). The name 'Monte Carlo' for this statistical sampling technique was coined by Nicholas Metropolis – a friend and collaborator of von Neumann and Ulam. This name was related to the fact that Ulam had an uncle who was a gambler and would borrow money from relatives because he "just had to go to Monte Carlo" – a reference to the Monte Carlo Casino in Monaco[15]. See an account of these days by their direct participant in[16]. The Monte Carlo method owes its birth not only to the nuclear arms race and genius of von Neumann and Ulam but also and essentially to appearing of first computers in 1940s. It should be also noted that random methods in computation can be traced back to the earliest pioneers of Probability theory, and perhaps the earliest example of 'Monte Carlo' is Buffon's needle problem of 1777[17].

Applicable Remark. The Monte Carlo technique (in its huge varieties) is widely used in a large number of applications. As we saw in the previous remark, it started from application in physics and it is still one of the important computational tools in physics. With enormous computational power available now (distributed computer systems, parallel computers, clusters), the Monte Carlo technique is becoming more and more practical. E.g., it is used in molecular dynamical simulations including simulation of complex biomolecules and in statistical physics. Monte Carlo methods are also widely used in Statistics.

[14] Here a certain caution is needed. Note that when we change the dimension, we change the function $f(x)$ and, consequently, change $Var(f(\xi))$.

[15] See it at http://en.montecarloresort.com/Casino-de-Monte-Carlo,507.html

[16] N. Metropolis. The beginning of the Monte Carlo method. Los Alamos Science Special Issue, 1987, 125-130. Available at http://library.lanl.gov/cgi-bin/getfile?00326866.pdf

[17] See: G. Buffon. Editor's note concerning a lecture given 1733 by Mr. Le Clerc de Buffon to the Royal Academy of Sciences in Paris. Histoire de l'Acad. Roy. des Sci., 1733, 43-45;

Buffon, G. "Essai d'arithmétique morale." Histoire naturelle, générale er particulière, Supplément 4, 1777, 46-123.

It comes as no surprise that the Monte Carlo technique is a natural computational tool in Financial Engineering.

8.1 The Monte Carlo error

Introduce

$$\hat{\eta}_M := \frac{1}{M}\sum_{m=1}^{M}\eta_m,$$

which is a statistical estimate for $E\eta$ (compare with (8.5)). Here η_m are i.i.d. random variables with finite mean and finite non-zero variance. It follows from CLT (see (2.14)-(2.15)) that

$$\frac{\hat{\eta}_M - E\eta}{\sqrt{Var(\eta)}/\sqrt{M}} \Longrightarrow \hat{\theta} \sim \mathcal{N}(0,1).$$

Then for $0 \le a, b \le \infty$[18] the probability that an interval of the form $(\hat{\eta} - a\sqrt{Var(\eta)}/\sqrt{M}, \hat{\eta} + b\sqrt{Var(\eta)}/\sqrt{M})$ covers $E\eta$, i.e.

$$E\eta \in (\hat{\eta}_M - a\sqrt{Var(\eta)}/\sqrt{M}, \hat{\eta}_M + b\sqrt{Var(\eta)}/\sqrt{M}), \tag{8.12}$$

approaches $\Phi(b) - \Phi(-a)$ as $M \to \infty$.

Exercise 8.5 *How does (8.12) follow from (2.15)?*

We can choose a and b so that the limiting probability is δ with some prescribed $\delta > 0$ (of course, it is usually of interest to pick δ close to 1). Among all choices of a and b for which $\Phi(b) - \Phi(-a) = \delta$, the values minimizing the length of the interval $(-a, b)$ are given by $a = b = c_\delta$, where $2\Phi(c_\delta) - 1 = \delta$. For simplicity, we will skip the index δ at c in future. The interval

$$\hat{\eta}_M \pm c\frac{\sqrt{Var(\eta)}}{\sqrt{M}} \tag{8.13}$$

covers $E\eta$ with probability approaching δ as $M \to \infty$ and is in this sense an asymptotically valid confidence interval for $E\eta$. For instance, for $c = 3$ we have $\delta = 0.997$.

Exercise 8.6 *If you would like to have an interval to which $E\eta$ belongs with 99.99% confidence, what is the corresponding value of c?*

Obviously, the above application of CLT justifies the use of (8.10) in the previous section (just compare (8.10) with (8.13)). Furthermore, for any consistent estimator $\hat{\nu}_M$ of $\sqrt{Var(\eta)}$ (i.e., we require that $\hat{\nu}_M \Longrightarrow \sqrt{Var(\eta)}$), we have $\hat{\nu}_M/\sqrt{Var(\eta)} \Longrightarrow 1$. Then one can show (see, e.g. [15]) that

$$\frac{\hat{\eta}_M - E\eta}{\hat{\nu}_M/\sqrt{M}} \Longrightarrow \hat{\theta} \sim \mathcal{N}(0,1)$$

and hence the interval

$$\hat{\eta}_M \pm c\frac{\hat{\nu}_M}{\sqrt{M}} \tag{8.14}$$

covers $E\eta$ with the corresponding probability. We can take

$$\hat{\nu}_M = \sqrt{\frac{1}{M-1}\sum_{m=1}^{M}\eta_m^2 - \hat{\eta}_M^2}.$$

Thus, we provided the theoretical basis for the error analysis of the Monte Carlo method.

[18] Note that a and b here are not the same as in (2.15).

8.2 The use of probabilistic representations for PDEs

Based on the probabilistic representation (4.40) of the solution $u(t,x)$ to the problem (4.37)-(4.38) and the ideas of the Monte Carlo technique, we can construct the following numerical procedure to approximately evaluate $u(t_0,x)$. In comparison with the example at the start of Section 8, we usually cannot simulate $X_{t_0,x}(T)$ (and, consequently, $f(X_{t_0,x}(T))$) exactly[19]. Then, we first need to approximate $X_{t_0,x}(T)$ and thus obtain

$$u(t_0,x) = Ef(X_{t_0,x}(T)) \simeq \bar{u}(t_0,x) = Ef(\bar{X}_{t_0,x}(T)), \tag{8.15}$$

where $\bar{X}_{t_0,x}(T)$ approximates $X_{t_0,x}(T)$ in the weak sense (see Section 7).

To make (8.15) realisable on a computer, we apply the Monte Carlo technique to the right-hand side of (8.15):

$$\bar{u}(t_0,x) = Ef(\bar{X}_{t_0,x}(T)) \simeq \hat{u}(t_0,x) := \frac{1}{M}\sum_{m=1}^{M} f({}_m\bar{X}_{t_0,x}(T)), \tag{8.16}$$

where ${}_m\bar{X}_{t_0,x}(T)$, $m = 1,\dots,M$, are independent realisations of the random variable $\bar{X}_{t_0,x}(T)$. The approximation of $\bar{u}(t_0,x)$ by $\hat{u}(t_0,x)$ is similar to what we considered in the example at the beginning of Section 8 and it is associated with the statistical (Monte Carlo) error.

So, in this case we have two errors: the error of numerical integration $\bar{u}(t_0,x) - u(t_0,x)$, which is the bias of the estimator $\hat{u}(t_0,x)$:

$$\begin{aligned} Bias(\hat{u}(t_0,x)) &= E\frac{1}{M}\sum_{m=1}^{M} f({}_m\bar{X}_{t_0,x}(T)) - u(t_0,x) = Ef(\bar{X}_{t_0,x}(T)) - u(t_0,x) \\ &= \bar{u}(t_0,x) - u(t_0,x); \end{aligned} \tag{8.17}$$

and the statistical error measured via variance of the estimator $\hat{u}(t_0,x)$:

$$Var(\hat{u}(t_0,x)) = \frac{Var\left(f(\bar{X}_{t_0,x}(T))\right)}{M} \approx \frac{Var\left(f(X_{t_0,x}(T))\right)}{M}\ . \tag{8.18}$$

As we discussed in the previous sections, the (random) value $\hat{u}(t,x)$ we find in a particular run of our Monte Carlo algorithm is such that the value $\bar{u}(t,x) = Ef(\bar{X}_{t,x}(T))$ belongs to the confidence interval:

$$\begin{aligned} \bar{u}(t,x) &\in (\hat{u}(t,x) - \frac{c}{\sqrt{M}}\sqrt{\hat{D}}, \hat{u}(t,x) + \frac{c}{\sqrt{M}}\sqrt{\hat{D}}), \\ \hat{D} &:= \frac{1}{M}\sum_{m=1}^{M}\left[f({}_m\bar{X}_{t,x}(T))\right]^2 - \left[\hat{u}(t,x)\right]^2, \end{aligned} \tag{8.19}$$

with probability, e.g. 0.68 for $c=1$, 0.95 for $c=2$, and 0.997 for $c=3$.

Remark 8.1 ***(important)*** *By the Monte Carlo procedure we find the solution $u(t,x)$ at a single point only. This is in contrast to finite-difference and finite element methods which simulate the solution in the whole domain.*

Exercise 8.7 *Consider the linear SDE*

$$dS = rSdt + \sigma Sdw, \quad S(0) = S_0, \tag{8.20}$$

where $r \geq 0$ is a risk-free interest rate and $\sigma > 0$ is volatility. This is an SDE for GBM (see Section 4) written under the risk neutral measure. Consider a European call option and assume that the price

[19] Note that $X_{t_0,x}(T)$ can be simulated exactly if $X(t)$ is, e.g., a Wiener process or Geometrical Brownian motion.

process is described by GBM. The price of the call with maturity T and strike K at time $t = 0$ is equal to [4, 50, 54]:

$$\begin{aligned} u(0, S_0) &= e^{-rT} E(S(T) - K)_+ \\ &= S_0 \Phi\left(\frac{\ln(S_0/K) + (r + \sigma^2/2)T}{\sigma\sqrt{T}}\right) \\ &\quad - K e^{-rT} \Phi\left(\frac{\ln(S_0/K) + (r - \sigma^2/2)T}{\sigma\sqrt{T}}\right), \end{aligned} \tag{8.21}$$

where $(x)_+ = \max(x, 0)$ and $\Phi(x)$ is the standard normal distribution function. Apply the three methods (5.3), (7.4) and (7.18)-(7.19) to the price the call. In MatLab realise these methods accompanying them by the Monte Carlo technique and study their errors. By taking a large number of Monte Carlo runs, show that (5.3) and (7.4) are first weak order methods while (7.18)-(7.19) is of second order.

Exercise 8.8 *By using the Talay-Tubaro expansion from Section 7.4, improve accuracy of the results from the previous exercise.*

Exercise 8.9 *By solving (8.20) explicitly, find the exact expression of $S(T)$. Apply the Monte Carlo technique to $u(0, S_0) = e^{-rT} E(S(T) - K)_+$ with exact $S(T)$ and experimentally study convergence of the Monte Carlo technique. In all exercises do not forget to report the Monte Carlo error: please remember that reporting outcomes of Monte Carlo simulation without providing the corresponding statistical errors essentially has no value.*

8.3 Variance reduction

We have discussed two errors arising in solving PDEs via the probabilistic approach: numerical integration error and statistical error. We know from Section 7 that to reduce the integration error, we can reduce the time step or use a more effective numerical method, which for the same time step gives a smaller error. Now let us look again at the Monte Carlo error.

We also already know the form of the Monte Carlo error (cf. (8.18)):

$$\rho = c \frac{\sqrt{Var\left(f(\bar{X}_{t_0,x}(T))\right)}}{\sqrt{M}} \ . \tag{8.22}$$

where, e.g., the values $c = 1, 2, 3$ correspond to the probabilities 0.68, 0.95, 0.997, respectively. We obviously can reduce it by increasing the number of independent Monte Carlo runs. But if $Var\left(f(\bar{X}_{t_0,x}(T))\right)$ is large then to achieve a satisfactory accuracy we have to simulate a very large number of independent trajectories. We can try to somehow reduce the variance and, clearly, variance reduction is of crucial importance for effectiveness of any Monte Carlo procedure.

The main idea of the variance reduction is as follows. Find a random variable $\Gamma_{t_0,x}(T)$ such that

$$E\Gamma_{t_0,x}(T) = Ef(\bar{X}_{t_0,x}(T)) \tag{8.23}$$

and

$$Var(\Gamma_{t_0,x}(T)) < Var\left(f(\bar{X}_{t_0,x}(T))\right). \tag{8.24}$$

The question is, of course, how to find such $\Gamma_{t_0,x}(T)$. There are a variety of possibilities exist, which or which realisation is, as a rule, problem dependent. It is well said in [15, p. 185]: "The greatest gains in efficiency from variance reduction techniques result from exploiting specific features of a problem, rather than from generic applications of generic methods". Indeed, variance reduction to be efficient requires some extra knowledge about the problem under consideration.

Here we will discuss only one method to reduce variance in order to illustrate the main idea. More about variance reduction techniques can be found in [15, Chapter 4] and also [16, 44].

The method of **control variates** is among common and broadly applicable techniques. To describe the method, suppose we would like to compute EY for some random variable Y (e.g., with $Y = f(\bar{X}_{t_0,x}(T))$) and for this aim we simulate the sample ${}_1Y, \dots, {}_M Y$ and estimate EY as before:

$$\mu := EY \simeq \hat{\mu} := \frac{1}{M} \sum_{m=1}^{M} {}_mY \tag{8.25}$$

(i.e. ${}_mY$ are i.i.d. with the law of Y).

Suppose now that we know expectation of another random variable Z and can simulate random variables with the distribution as of (Y, Z), i.e., we can simulate a sample $({}_mY, {}_m Z)$, $m = 1, \dots, M$. Then we can propose another unbiased estimator for μ :

$$\mu := EY \simeq \check{\mu} := \frac{1}{M} \sum_{m=1}^{M} \left({}_mY - \lambda \left[{}_mZ - EZ \right] \right), \tag{8.26}$$

where λ is a parameter and $({}_mY, {}_m Z)$ are i.i.d. with the law (Y, Z). This is a *control variate estimator*; the observed error serves as a control in estimating.

Exercise 8.10 *Show that the control variate estimator (8.26) is unbiased.*

We have the free parameter λ in (8.26). How can we use it? Recall that the aim is to get $\Gamma = Y - \lambda \left[Z - EZ \right]$ such that

$$Var\Gamma < VarY.$$

Then we would like to have λ such that $Var\Gamma$ is minimal. We have

$$Var\Gamma = VarY - 2\lambda Cov(Y, Z) + \lambda^2 VarZ. \tag{8.27}$$

Performing elementary calculations, we get the optimal λ :

$$\lambda^* = \frac{Cov(Y, Z)}{VarZ}. \tag{8.28}$$

Exercise 8.11 *Check that (8.28) is true.*

Now substituting (8.28) in (8.27), we obtain for the optimal λ^* :

$$Var\Gamma = Var(Y)[1 - \rho_{YZ}^2], \tag{8.29}$$

where ρ_{YZ} is the correlation between Y and Z.

Exercise 8.12 *Check that (8.29) is true.*

We see from (8.29) that $Var\Gamma < VarY$ unless Y and Z are uncorrelated. The variance reduction factor $1/(1 - \rho_{YZ}^2)$ increases very sharply as $|\rho_{YZ}|$ approaches 1 and, accordingly, it drops off quickly as $|\rho_{YZ}|$ decreases away from 1. E.g., a correlation of 0.95 produces a ten-fold speed-up, for a correlation of 0.70 the speed-up drops to about a factor of two. Note that the sign of correlation is irrelevant, it is absorbed in λ^*.

Of course, in practice we do not know $Cov(Y, Z)$ and might not know $VarZ$ but we can evaluate (obviously approximately) λ^* in the same Monte Carlo experiment via computing estimators for $Cov(Y, Z)$ and $VarZ$ and thus find $\hat{\lambda}^*$ – an estimator for λ^*.

Exercise 8.13 *Write down an expression for* $\hat{\lambda}^*$.

For the control variate method to be efficient in practice, we need to be able to find a auxiliary random variable Z such that it has a high degree of correlation with Y. It is not an easy task and it is very problem dependent. Although for some problems there are recipes how to find such Z, in general it is an art.

Remark 8.2 *The other commonly used variance reduction techniques are importance sampling and antithetic variables [15, 16, 44].*

Remark 8.3 *There are other ways (i.e., not only variance reduction) how Monte Carlo methods can be made more efficient, namely quasi-Monte Carlo methods [47] and multi-level Monte Carlo methods [14].*

Exercise 8.14 *Within the setting of Exercise 8.7, use the Monte Carlo technique to price an Asian European-type call option, i.e., compute*

$$u(0,S_0)=e^{-rT}E\left(\frac{1}{T}\int_0^T S(t)dt-K\right)_+. \tag{8.30}$$

There is no closed-form solution for this option price. Use the knowledge of the plain-vanilla call price (8.21) to construct a control variate in order to reduce the Monte Carlo error in finding the Asian option price.

9 Computing ergodic limits

For many applications (in particular, molecular dynamics and Bayesian statistics), it is of interest to compute the mean of a given function with respect to the invariant law of the diffusion, i.e. the ergodic limit.

Consider the system of Ito SDEs

$$dX=b(X)dt+\sum_{l=1}^{q}\sigma_r(X)dw_r(t),\ X(0)=x, \tag{9.1}$$

where X, b, σ_r are d-dimensional column-vectors and $w_r(t)$, $l=1,\dots,q$, are independent standard Wiener processes. In this section we use the notation $X(t)$ and $X(t;x)$ for solutions of the problem (9.1).

In what follows we assume that the following conditions are imposed on (9.1).

(A1) The coefficients of (9.1) are sufficiently smooth functions in $\mathbf{R}^d$.

(A2) The solution of (9.1) is *regular*, i.e., it is defined for all $t\geq 0$.

(A3) The process $X(t)$ is *ergodic*, i.e., there exists a unique invariant measure μ of X and independently of $x\in\mathbf{R}^d$ there exists the limit

$$\lim_{t\to\infty}E\varphi(X(t;x))=\int\varphi(x)\,d\mu(x):=\varphi^{erg} \tag{9.2}$$

for any function $\varphi(x)$ with polynomial growth at infinity.

(A4) The Markov transition function[20] $P(t,x,dy)$ (it is homogeneous for (9.1)) and the invariant measure $\mu(dx)$ have sufficiently smooth densities $p(t,x,y)$ and $\rho(x)$, respectively.

Regularity. In connection with the condition (A2), we recall sufficient conditions for regularity of SDEs' solution. Denote by $\mathbf{C}^2$ the class of functions defined on $[0,\infty)\times\mathbf{R}^d$ and twice continuously differentiable with respect to x and once with respect to t. A sufficient condition of regularity (see [18]) consists in existing a nonnegative function $V\in\mathbf{C}^2$ which satisfies the inequality

$$LV(t,x)\leq c_0V(t,x)+c_1,\ (t,x)\in[0,\infty)\times\mathbf{R}^d, \tag{9.3}$$

and

$$\lim_{R\to\infty}\inf_{|x|\geq R}V(t,x)=\infty, \tag{9.4}$$

[20] Its meaning is $P(t,x,dy)=P(X(t)\in dy|X(0)=x)$, see also (3.7) in Section 3.3.

where c_0 and c_1 are some constants and L is the operator

$$L := \frac{\partial}{\partial t} + \mathcal{L}$$

and $\mathcal{L}$ is the generator for (9.1):

$$\mathcal{L} := \sum_{i=1}^{d} b^i(x) \frac{\partial}{\partial x^i} + \frac{1}{2} \sum_{i,j=1}^{d} a^{ij}(x) \frac{\partial^2}{\partial x^i \partial x^j}, \qquad a^{ij} := \sum_{l=1}^{r} \sigma_l^i \sigma_l^j.$$

Moreover, if (9.3) and (9.4) are fulfilled and if an initial distribution for x (x can be random) is such that $EV(0,x)$ exists, then $EV(t, X(t;x))$ exists for all $t \geq 0$. For instance, if V has an m-polynomial growth at infinity, then there exist moments of order m for X.

The transition density $p(t,x,y)$ from (A4) satisfies the *Fokker-Planck (forward Kolmogorov) equation*

$$\frac{\partial p}{\partial t}(t,x,y) + \sum_{i=1}^{d} \frac{\partial}{\partial y^i} \left(b^i(y)\, p(t,x,y) \right) - \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2}{\partial y^i \partial y^j} \left(a^{ij}(y)\, p(t,x,y) \right) = 0, \quad t > 0, \tag{9.5}$$

$$p(0,x,y) = \delta(y-x),$$

and the invariant density $\rho(x)$ satisfies the stationary Fokker-Planck equation

$$\sum_{i=1}^{d} \frac{\partial}{\partial x^i} \left(b^i(x)\, \rho(x) \right) - \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2}{\partial x^i \partial x^j} \left(a^{ij}(x)\, \rho(x) \right) = 0. \tag{9.6}$$

Ergodicity. We are interested here in systems which solutions satisfy a stronger condition than (A3):

(A3e) The process $X(t)$ is *exponentially ergodic*, i.e., for any $x \in \mathbf{R}^d$ and any function φ with a polynomial growth we have the following strengthening of (9.2):

$$|E\varphi(X(t;x)) - \varphi^{erg}| \leq Ce^{-\lambda t}, \quad t \geq 0, \tag{9.7}$$

where $C > 0$ and $\lambda > 0$ are some constants.

It follows from (9.7) (and (9.2)) that for any $\varepsilon > 0$ there exists $T_0 > 0$ such that for all $T \geq T_0$

$$|E\varphi(X(T;x)) - \varphi^{erg}| \leq \varepsilon. \tag{9.8}$$

Thus, the problem of computing the ergodic limit is reduced to evaluating the expectation $E\varphi(X(T))$ at a finite (though usually large) time T.

Example 9.1 *Consider the Langevin equations*

$$\begin{aligned} dP &= f(Q)dt - \gamma P dt + \sqrt{\frac{2\gamma}{\beta}} dw(t), \quad P(0) = P_0 = p, \\ dQ &= M^{-1} P dt, \quad Q(0) = Q_0 = q, \end{aligned} \tag{9.9}$$

where P, Q, $f(q) = -\nabla U(q)$ are n-dimensional column-vectors, $\gamma > 0$ is a friction parameter, M is a non-singular, diagonal matrix, and $w(t) = (w_1(t), \ldots, w_n(t))^\top$ and $w_l(t)$ are independent standard Wiener processes. Let the potential $U(q)$ satisfy the following assumptions: $U(q) \geq 0$ for all $q \in \mathbf{R}^n$ and there exists an $\alpha_1 > 0$ and $0 < \alpha_2 < 1$ such that

$$\frac{1}{2}(\nabla U(q), q) \geq \alpha_2 U(q) + \gamma^2 \frac{\alpha_2(2-\alpha_2)}{8(1-\alpha_2)} |q|^2 - \alpha_1. \tag{9.10}$$

Under these assumptions the authors of [32] prove exponential ergodicity of (9.9), i.e., the condition (A3e) holds. It can directly be verified that the Gibbs distribution

$$\rho(p,q) \propto \exp\left(-\beta\left\{\frac{1}{2}p^\top M^{-1}p + U(q)\right\}\right) \tag{9.11}$$

is a solution of the stationary Fokker-Planck equation (cf. (9.6)) corresponding to (9.9). The Langevin equations (9.9) are very popular in, e.g., molecular simulation, when one is interested in constant temperature dynamics.

Exercise 9.1 *Verify that $\rho(p,q)$ from (9.11) is a solution of the corresponding stationary Fokker-Planck equation.*

Example 9.2 *Assume that $\rho(y) > 0$, $y \in \mathbf{R}^d$, is a sufficiently smooth density function which is known up to a constant of proportionality. Consider the stochastic gradient system*

$$dY = \frac{1}{2}\nabla \log \rho(Y)dt + dw(t). \tag{9.12}$$

The solution $Y(t)$ of (9.12) is exponentially ergodic under the following conditions (see [48]): $\rho(y)$ is a bounded density,

$$\log \rho(y) \in C^2(\mathbf{R}^d), \tag{9.13}$$

and there exists $0 < \alpha < 1$ such that

$$\liminf_{|y|\to\infty} \left[(1-\alpha)|\nabla \log \rho(y)|^2 + \Delta \log \rho(y)\right] > 0, \tag{9.14}$$

where Δ is the Laplace operator. Stochastic gradient systems are widely used in Bayesian statistics and molecular dynamics.

Exercise 9.2 *Show that if the solution to (9.12) is an ergodic process, then its invariant measure is $\rho(y)$.*

Resting on (9.8), we can consider the following Monte Carlo estimate for the ergodic limit φ^{erg}:

$$\hat{\varphi}^{erg} = \frac{1}{M}\sum_{m=1}^{M} \varphi\left(\bar{X}^{(m)}(T;x)\right), \tag{9.15}$$

where M is the number of independent approximate realizations and $\bar{X}(T;x)$ is a weak approximation of $X(T;x)$ with order $p > 0$. The total error

$$R_{\hat{\varphi}^{erg}} := \hat{\varphi}^{erg} - \varphi^{erg} \tag{9.16}$$

consists of three parts: the error ε of the approximation (9.8); the error of numerical integration Kh^p; and the Monte Carlo error; i.e.,

$$R_{\hat{\varphi}^{erg}} \sim Kh^p + \varepsilon + O\left(\frac{1}{\sqrt{M}}\right).$$

More precisely,

$$Bias(\hat{\varphi}^{erg}) = |E\hat{\varphi}^{erg} - \varphi^{erg}| \le Kh^p + \varepsilon \tag{9.17}$$

and the estimator's variance is

$$Var(\hat{\varphi}^{erg}) = O(1/M). \tag{9.18}$$

Here, in this ensemble average approach to computing ergodic limits, each error is controlled by its own parameter: sufficiently large T ensures smallness of ε; time step h (as well as the choice of a numerical method) controls the numerical integration error; the statistical error is regulated by choosing an appropriate number of independent trajectories M.

There is also *another approach for calculating ergodic limits*, which is very popular in the physical and Bayesian statistics community. It is based on the known equality (**time averaging**):

$$\lim_{t\to\infty}\frac{1}{t}\int\limits_0^t \varphi(X(s;x))ds = \varphi^{erg} \quad a.s., \tag{9.19}$$

where the limit does not depend on x. Then by approximating a single trajectory, one gets for a sufficiently large $\tilde{T}$:

$$\frac{1}{\tilde{T}}\int\limits_0^{\tilde{T}} \varphi(X(s;x))ds \approx \breve{\varphi}^{erg} = \breve{\varphi}_L^{erg} := \frac{1}{L}\sum_{l=1}^{L}\varphi(\bar{X}(t_l;x)), \tag{9.20}$$

where $Lh = \tilde{T}$. It was rigorously treated in [51], where ergodicity of numerical methods is investigated in the case of ergodic SDEs with nondegenerate noise and globally Lipschitz coefficients (see also [33] and references therein). Let us emphasize that $\tilde{T}$ in (9.20) is much larger than T in (9.8) and (9.15) because $\tilde{T}$ should be such that it not just ensures the distribution of $X(t)$ to be close to the invariant distribution (like is required from T) but it should also guarantee smallness of variance of $\breve{\varphi}^{erg}$.

Under some conditions on the coefficients of (9.1), the estimator $\breve{\varphi}^{erg}$ has the following properties [51, 33]:

$$\mathrm{Bias}(\breve{\varphi}_L^{erg}) \le K_1 h^p + \frac{K_2}{\tilde{T}}\ ; \tag{9.21}$$

$$\mathrm{Var}(\breve{\varphi}_L^{erg}) \le \frac{K}{\tilde{T}}; \tag{9.22}$$

there exists a deterministic constant K so that for h sufficiently small, positive $\varepsilon > 0$, and $\tilde{T}$ sufficiently large one has:

$$|\breve{\varphi}_L^{erg} - \varphi^{erg}| \le Kh^p + \frac{C(\omega)}{\tilde{T}^{1/2-\varepsilon}} \quad \text{a.s.}, \tag{9.23}$$

where $C(\omega) > 0$ is an a.s. bounded random variable depending on ε and the particular φ.

In practice one usually estimates the statistical error of the time averaging estimator $\breve{\varphi}_L^{erg}$ as follows. We run a long trajectory $M\tilde{T}$ split into M blocks of a large length $\tilde{T} = hL$ each. We evaluate the estimators ${}_m\breve{\varphi}_L^{erg}$, $m = 1,\dots,M$, for each block. Since $\tilde{T}$ is big and a time decay of correlations is usually fast, ${}_m\breve{\varphi}_L^{erg}$ can be considered as almost uncorrelated. We compute the sampled variance

$$\hat{D} = \frac{1}{M-1}\sum_{m=1}^{M}\left({}_m\breve{\varphi}_L^{erg}\right)^2 - \Big(\frac{1}{M}\sum_{m=1m}^{M}\breve{\varphi}_L^{erg}\Big)^2.$$

For a sufficiently large $\tilde{T}$ and M, $\mathbf{E}\,\breve{\varphi}_L^{erg}$ belongs to the confidence interval

$$\mathbf{E}\,\breve{\varphi}_L^{erg} \in \big(\breve{\varphi}_{LM}^{erg} - c\frac{\sqrt{\hat{D}}}{\sqrt{M}}, \breve{\varphi}_{LM}^{erg} + c\frac{\sqrt{\hat{D}}}{\sqrt{M}}\big)\ ,$$

with probability, for example 0.95 for $c = 2$ and 0.997 for $c = 3$. Note that $\mathbf{E}\,\breve{\varphi}_L^{erg}$ contains the two errors forming the bias as explained in (9.21). We also pay attention to the fact that $\hat{D} \sim 1/\tilde{T}$, i.e., it is inverse proportional to the product hL.

To evaluate ergodic limits, one usually has to integrate a stochastic system over very long time intervals (even if the convergence to ergodic limits is exponential). This is a challenging problem from the computational point of view. To ensure that such simulations can be done with sufficient accuracy and with sensible computational costs. one uses so-called geometric integrators for approximating continuous dynamics. Geometric integrators are a class of numerical methods which preserve some structural properties of continuous dynamics they approximate. They are the methods which preserve some geometric features of the flow of differential equations. For geometric integrators within the stochastic context, see e.g. [44, 41, 43, 35, 7].

10 Further reading

For further study of Probability, [49, 58] can be used. The knowledge of stochastic processes and Ito Calculus can be enhanced using the introductory textbooks [28, 31, 9] and more comprehensive ones such as [56, 27, 30, 59]. To read on foundations of stochastic numerics, [44, 29, 16] can be used.

References

[1] L. Bachelier. Théorie de la Spéculation. *Annales Scientifique de l'Ecole Normale Supérieure* 3^e série, **17** (1900), 21–86.

[2] V. Bally, D. Talay. The law of the Euler scheme for stochastic differential equations I. Convergence rate of the distribution function. Probab. *Theory Relat. Fields* **104** (1996), 43-60.

[3] S. N. Bernstein. Principes de la theorie des equationnes differentielles stochastiques. *Travaux de I'lnstitut Physicow Mathematique de Stekloff* **5** (1934), 95–124.

[4] T. Björk. *Arbitrage Theory in Continuous Time.* Oxford University Press, 2004.

[5] R. Brown. A brief account of microscopical observations made in the months of June, July and August 1827, on the particles contained in the pollen of plants; and on the general existence of active molecules in organic and inorganic bodies. *Philosophical Magazine Series* 2, Vol. **4** (1828), 161–173.

[6] E. W. Cheney, D. R. Kincaid. *Numerical Mathematics and Computing.* Brooks/Cole-Thomson Learning, 2012.

[7] R.L. Davidchack, T.E. Ouldridge, M.V. Tretyakov. New Langevin and gradient thermostats for rigid body dynamics. *J. Chem. Phys.* **142** (2015), 144114.

[8] A. Einstein. Über die von der molekularkinetischen Theorie der Wärme gefordete Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen. *Annalen der Physik* **17** (1905), 132-148.

[9] L.C. Evans. *An Introduction to Stochastic Differential Equations.* AMS, 2013.

[10] B.J. Ford. Brownian movement in clarkia pollen: a reprise of the first observations. *Microscope* **40** (1992), 235–241.

[11] M.I. Freidlin. *Functional integration and partial differential equations.* Princeton Univ. Press, 1985.

[12] I.I. Gichman, A.V. Skorokhod, *Stochastic differential equations.* Naukova Dumka, Kiev, 1968; Springer, 1972.

[13] I. Gyöngy. A note on Euler's approximations. *Potential Anal.* **8** (1998), 205–216.

[14] M.B. Giles. Multilevel Monte Carlo path simulation. *Oper. Res.* **56** (2008), 607–617.

[15] P. Glasserman. *Monte Carlo Methods in Financial Engineering.* Springer, 2004.

[16] C. Graham, D. Talay. *Stochastic Simulation and Monte Carlo Methods.* Springer, 2013.

[17] P.S. Hagan, D. Kumar, A. S. Lesniewski, D. E. Woodward. Managing Smile Risk. *Wilmott Magazine*, September (2002) 84–108.

[18] R.Z. Hasminskii. *Stochastic Stability of Differential Equations.* Sijthoff & Noordhoff, 1980.

[19] S.L. Heston. A Closed-Form Solution for Options with Stochastic Volatility with Applications to Bond and Currency Options. *The Review of Financial Studies* **6** (1993), 327–343.

[20] H. Holden, B. Oksendal, J. Uboe, T. Zhang. *Stochastic Partial Differential Equations. A Modelling, White Noise Functional Approach.* Springer, 2010.Jentz

[21] M. Hutzenthaler, A. Jentzen. Numerical approximations of stochastic differential equations with non-globally Lipschitz continuous coefficients. *Mem. Amer. Math. Soc.* **236** (2015), no. 1112.

[22] K. Ito. Differential equations determining a Markov process (in Japanese). *Zenkoku Shijo Danwakai* **1077** (1942), 1352–1400.

[23] K. Ito, H. R. McKean. *Diffusion Processes and Their Sample Paths*. Springer, 1965.

[24] D. Lamberton, B. Lapeyre. *Introduction to Stochastic Calculus Applied to Finance*. Chapman & Hall, 1996.

[25] B. Leimkuhler, C. Matthews. *Molecular Dynamics with Deterministic and Stochastic Numerical Methods*. Springer, 2015.

[26] K. Lindenberg, B.J. West. *The Nonequilibrium Statistical Mechanics of Open and Closed Systems.* VCH Publishers, 1990.

[27] I. Karatzas, S.E. Shreve: *Brownian Motion and Stochastic Calculus*. Springer, 1991.

[28] F.C. Klebaner. *Introduction to Stochastic Calculus with Applications.* Imperial College Press, 2005.

[29] P.E. Kloeden, E. Platen. *Numerical solution of stochastic differential equations*. Springer, 1992.

[30] N.V. Krylov. *Introduction to the Theory of Random Processes*. AMS, 2002.

[31] X. Mao. *Stochastic Differential Equations and Applications*. Horwood, 2007.

[32] J.C. Mattingly, A.M. Stuart, D.J. Higham. Ergodicity for SDEs and approximations: Locally Lipschitz vector fields and degenerate noise. *Stoch. Proc. Appl.* **101** (2002), 185–232.

[33] J.C. Mattingly, A.M. Stuart, M.V. Tretyakov. Convergence of numerical time-averaging and stationary measures via Poisson equations. *SIAM J. Numer. Anal.* **48** (2010), 552–577.

[34] G. Marujama. Continuous Markov processes and stochastic equations. *Rend. Mat. Circ. Palermo*, Ser. 2, **4** (1955)**,** 48–90.

[35] J.H. Mentink, M.V. Tretyakov, A. Fasolino, M.I. Katsnelson, Th. Rasing. Stable and fast semi-implicit integration of the stochastic Landau-Lifshitz equation. *J. Phys.: Condens. Matter* **22** (2010), 176001.

[36] G.N. Milstein. Approximate integration of stochastic differential equations. *Theor. Prob. Appl.* **19** (1974), 583–588.

[37] G.N. Milstein. A method with second order accuracy for the integration of stochastic differential equations. *Theor. Prob. Appl.* **23** (1978), 414–419.

[38] G.N. Milstein. Weak approximation of solutions of systems of stochastic differential equations. *Theor. Prob. Appl.* **30** (1985), 706–721.

[39] G.N. Milstein. A theorem on the order of convergence of mean-square approximations of solutions of systems of stochastic differential equations. *Theor. Prob. Appl.* **32** (1987), 809–811.

[40] G.N. Milstein. *Numerical integration of stochastic differential equations*. Ural State University, Sverdlovsk, 1988. Engl. transl. by Kluwer Academic Publishers, 1995.

[41] G.N. Milstein, Yu.M. Repin, M.V. Tretyakov. Symplectic integration of Hamiltonian systems with additive noise. *SIAM J. Numer. Anal.* **39** (2002), 2066–2088.

[42] G.N. Milstein, Yu.M. Repin, M.V. Tretyakov. Numerical methods for stochastic systems preserving symplectic structure. *SIAM J. Num. Anal.* **40** (2002), 1583-1604

[43] G.N. Milstein, M.V. Tretyakov. Quasi-symplectic methods for Langevin-type equations. *IMA J. Numer. Anal.*, **23** (2003), 593–626.

[44] G.N. Milstein, M.V. Tretyakov. *Stochastic Numerics for Mathematical Physics*. Springer, 2004.

[45] G.N. Milstein, M.V. Tretyakov. Numerical integration of stochastic differential equations with non-globally Lipschitz coefficients. *SIAM J. Numer. Anal.* **43** (2005), 1139–1154.

[46] G.N. Milstein, M.V. Tretyakov. Computing ergodic limits for Langevin equations. *Phys. D* **229** (2007), 81–95.

[47] H. Niederreiter. *Random Number Generation and Quasi-Monte Carlo Methods*. SIAM, 1992.

[48] G.O. Roberts, R.L. Tweedie. Exponential convergence of Langevin distributions and their discrete approximations. *Bernoulli* **2** (1996), 341–363.

[49] A.N. Shiryaev. *Probability*. Springer, 1996.

[50] S.E. Shreve. *Stochastic Calculus for Finance II: continuous-time models*. Springer, 2004.

[51] D. Talay. Second-order discretization schemes for stochastic differential systems for the computation of the invariant law. *Stochastics and Stochastics Reports*, **29** (1990), 13–36.

[52] D. Talay. Approximation of the invariant probability measure of stochastic Hamiltonian dissipative systems with non-globally Lipschitz coefficients. In Bouc, R., Soize, C. (ed) Progress in Stochastic Structural Dynamics, Vol. 152, Publication du L.M.A.-CNRS, 1999.

[53] D. Talay, L. Tubaro. Expansion of the global error for numerical schemes solving stochastic differential equations. *Stoch.Anal.Appl.* **8** (1990), 483–509.

[54] M.V. Tretyakov. *Introductory Course on Financial Mathematics*. Imperial College Press, 2013.

[55] M.V. Tretyakov, Z. Zhang. A fundamental mean-square convergence theorem for SDEs with locally Lipschitz coefficients and its applications. *SIAM J. Numer. Anal.* **51** (2013), 3135–3162.

[56] A.D. Wentzell. *A Course in the Theory of Stochastic Processes*. McGraw-Hill, New York, 1981.

[57] N. Wiener. Differential space. *J. Math. Phys.* **2** (1923), 131–174.

[58] D. Williams. *Weighing the Odds*. Cambridge University Press, 2001.

[59] L.C.G. Rogers, D. Williams. *Diffusions, Markov Processes and Martingales*. Volume 1, Foundations. Cambridge University Press, 2000.

[60] L.C.G. Rogers, D. Williams. *Diffusions, Markov Processes and Martingales*. Volume 2, Ito Calculus. Cambridge University Press, 2000.