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(Ph.D. Thesis)

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Numerical Solution of Stochastic Differential Equations

Chien–Cheng Chang

Abstract

We present numerical methods of high order accuracy for solving stochastic differential equations with constant diffusion coefficients. Our analysis is performed in the L_2 norm, which has the advantage of exhibiting the non-anticipating property of stochastic differential equations.

For the scalar case, a second order method of Runge-Kutta type is derived, and in the case of a system, a similar method of order $1\frac{1}{2}$ is presented. By a method of Runge-Kutta type, we mean a one-step method where one needs only to evaluate the function involved at several different points.

For the case of a system, we also present a method of Taylor series type, in which the derivatives of the function involved appear explicitly. The analysis of this method in turn leads us to conjecture that the method of order $1\frac{1}{2}$ mentioned above and another simpler method of Runge-Kutta type have a second order accuracy in a weak sense.

Finally, variance reduction techniques for evaluating the expectations of functionals of the solution are discussed, and numerical examples are presented.

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Contents

Introduction

In this thesis, we consider the following d-dimensional stochastic differential equation

$$d\underline{x} = \underline{f}(t,\underline{x})\,dt + \nu\,d\underline{w}_t\,,\quad 0 \le t \le T \qquad (0\text{-}1)$$

where $\nu \ge 0$ is a constant, $\underline{f}(t,\underline{x})$ is a sufficiently smooth function satisfying a Lipshitz condition with respect to t, and $\underline{w}_t (t \ge 0)$ is a Wiener process (Brownian motion). This equation can be interpreted either in Ito's sense or in Stratonovich's sense (see chapter 1).

Equation (0-1) occurs in the study of several physical phenomena, e.g., the motion of a particle in the collision theory of chemical reactions (Benson [2]), in blood clotting (Fogelson [11]), in stellar dynamics (Chandrasekhar [4]), signal modeling in communication systems (Jazwinski [15]), and the stochastic behavior of fluid particles in turbulence theory (Chorin [7]).

By introducing t as a first component of $\underline{x}$, we can simplify equation (0-1) as the $d+1$-dimensional equation

$$d\underline{y} = \underline{g}(\underline{y})\,dt + d\underline{v}_t\,,\quad 0 \le t \le T$$

with $\underline{y} = (t, \underline{x})$, $\underline{v} = (0, \underline{w})$ and $\underline{g} = (1, \underline{f}(\underline{x}))$. Hence it suffices to consider

$$d\underline{x} = \underline{f}(\underline{x})\,dt + \nu\,d\underline{w}_t\,,\quad 0 \le t \le T\,. \qquad (0\text{-}2)$$

We develop and analyze high order accurate methods of constructing sample solutions of equation (0-2) and we further consider variance reduction techniques for evaluating accurately expectations of functionals of these sample solutions.

Most of the methods derived in this thesis are of Runge-Kutta type, i.e., one-step method where one need only, at each time step, to evaluate the function $\underline{f}$ at several points without involving its derivatives. For the sake of brevity, if a scheme is of Runge-Kutta type, we call it a Runge-Kutta method. Consider the partition of the interval $[0, T]$:

$$\Pi = (0,\cdots,t_{n+1} = t_n + h,\cdots,t_l = T) . \qquad (0\text{-}3)$$

Let E denote the expectation and $\|\cdot\|$ denote the 2-norm in R^d space. We say that a numerical scheme is of order h^p in the L_q sense, if there exists a constant C such that, for sufficiently small h,

$$\left[E\|\underline{X}_n - \underline{x}(t_n)\|^q \right]^{\frac{1}{q}} \leq C\, h^p \qquad (0\text{-}4)$$

where $\underline{X}_n$ is the numerical solution and $\underline{x}(t_n)$ is the exact solution of the differential equation (0-2) at t_n. Futhermore, a stochastic quantity $\underline{z}$ is said to be of order h^p in the L_q sense, if

$$\left[E\|\underline{z}\|^q \right]^{\frac{1}{q}} \textit{ is of order } h^p . \qquad (0\text{-}5)$$

The difficulty in solving equation (0–2) arises from the nondifferentiability of the Wiener process $\underline{w}_t$. To take a close look at this difficulty, we define the variable:

$$\underline{y}(t) = \underline{x}(t) - \nu\, \underline{w}_t\,, \quad 0 \leq t \leq T$$

Equation (0-2) reduces then to an infinite set of ordinary differential equations:

$$\frac{d\underline{y}}{dt} = \underline{f}(\underline{y} + \nu\, \underline{w}_t)\,, \quad 0 \leq t \leq T \qquad (0\text{-}6)$$

one for each sample path of the Wiener process $\underline{w}_t$. The theory of ordinary differential equations assures the existence of the solutions $y(t)$ of these equations, which are only once differentiable as functions of t.

Since the error estimates of high order accurate methods involve high order derivatives of $\underline{y}(t)$, it is not clear how one is able to obtain high order accurate methods for solving equations (0−6), or equation (0-2).

In fact, the fundamental question that must be answered before one proceeds to analyze numerical methods for solving stochastic differential equation is: how does one measure the accuracy of numerical methods, i.e., in which norm should one deal with convergence?

We are dealing with stochastic schemes, and it is natural to consider the accuracy of numerical methods only in a probabilistic senses. However, different definitions of convergence lead to different error estimates. Error estimates in the L_1 norm lead to what are apparantly the simplest estimates, and indeed, L_1 analysis is a very useful tool when one is dealing with the local truncation error of numerical methods (see section 2.1 and 3.1). However, L_1 analysis fails to exhibit one very important effect: the nonanticipating property of the solution of the stochastic differential equation.

It will turn out that the analysis in the L_2 norm does exibit the effect of the nonanticipating property. L_2 convergence implies L_1 convergence by Liapunov's inequality. For an example of the contrast between the L_1 and the L_2 analysis and an explanation why the latter is superior to the former, we refer to section 2.2.

Let us start considering numerical methods for solving the stochastic differential equation (0-2). The most popular methods are splitting schemes (see Chorin [8,9], Franklin [12]). For these schemes, at each time step, one approximates, for each sample path of the Wiener process, the differential equation

$$d\underline{x} = \underline{f}(t\ \underline{x})\ dt \tag{0-7}$$

by a method for solving ordinary differential equations, then one adds to the approximate solution an independent increment of the Wiener process $\nu\,\underline{w}_t$.

The simplest example of a splitting scheme is Euler's method which is given by

$$\underline{X}_{n+1} = \underline{X}_n + h\underline{f}(\underline{X}_n) + \nu\,\Delta_n\underline{w} \qquad \text{(0-8)}$$

where $\Delta_n\underline{w} \equiv \Delta\underline{w}_{t_{n+1}} - \Delta\underline{w}_{t_n}$. One more example of a splitting scheme, based on mid-point rule, is

$$\underline{X}_{n+1} = \underline{X}_n + h\underline{f}(\,\underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n)\,) + \nu\,\Delta_n\underline{w}\,. \qquad \text{(0-9)}$$

This type of splitting schemes is only first order accurate in the L_2 sense no matter how accurately one solves the nonrandom part (0-7) (see section 2.2).

To obtain more accurate numerical schemes, McShane [17,18] has extended the idea of Runge-Kutta methods to stochastic differential equation. For equation (0-2), he proposed

$$\underline{Q}_n = \underline{X}_n + h\underline{f}(\underline{X}_n) + \nu\,\Delta_n\underline{w} \qquad \text{(0-10)}$$

$$\underline{X}_{n+1} = \underline{X}_n + \nu\,\Delta_n\underline{w} + \frac{1}{2}h[\,\underline{f}(\underline{X}_n) + \underline{f}(\underline{Q}_n)\,]\,.$$

However, this scheme has the same accuracy as the splitting scheme mentioned above (see also section 2.2).

The major difference between McShane's approach and that of splitting schemes is that the former interlaces the function $\underline{f}$ and the Wiener process while the latter does not. By interlacing, we mean that the function $\underline{f}$ and the Wiener process $\underline{w}_t$ interact with each other at each time step.

The main purpose of this thesis is to present more accurate numerical methods for solving the stochastic differential equation (0-2). For the scalar case, we derive a second order (in the L_2 sense) Runge-Kutta method. However, this method does not give a second order accuracy when extended to a system. For the case of a system, we derive a Runge-Kutta method of order

$h^{1.5}$ in the L_2 sense. We also develop a Runge-Kutta method which computer experiments show to have second order accuracy, but in a different sense (defined below).

All our analyses are based on a Taylor expansion of the solution, followed by the derivation of an approximation formula whose Taylor expansion coincides to some order with the expansion of the solution. This device is similar to the method used by Chorin [5] in the approximation of Wiener integrals.

We start by considering the scalar case of the splitting scheme (0-9) and find the following Runge-Kutta method (in (2-55)):

$$P_n = \nu \sqrt{\vartheta' - \beta'^2} \tag{0-11}$$

$$Q_n = X_n + \frac{1}{2} h f(X_n) + \nu \sqrt{h}\, \beta'$$

$$X_{n+1} = X_n + \nu \Delta_n w + \frac{1}{2} h [\, f(Q_n + \sqrt{h} P_n) + f(Q_n - \sqrt{h} P_n)\,]$$

where the random variables β' and ϑ' are integrals of increments of the Wiener process $\underline{w}_t$ (see (2-44)). We prove that scheme (0-11) has second order accuracy in the L_2 sense. However, the scheme (0-11) fails to maintain its accuracy when extended to a system of stochastic differential equations.

For the case of a system, we prove that the following numerical scheme is of order $h^{1.5}$ in the L_2 sense (see (2-83) and (3-64)):

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2} h \underline{f}(\underline{X}_n) \tag{0-12}$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2} h \underline{f}(\underline{X}_n) + \frac{3}{2} \nu \sqrt{h}\, \underline{\beta}'$$

$$\underline{X}_{n+1} = \underline{X}_n + \nu \Delta_n w + \frac{1}{3} h \,[\, \underline{f}(\underline{Q}_n) + 2 \cdot \underline{f}(\underline{Q}_n')\,]$$

where $\underline{\beta}' = \{\beta'^j\}$ is a set of independent Gaussian random variables and each of them has mean 0 and variance $\frac{1}{3}$. Scheme (0−10) is a particular case of the one-parameter family of numerical schemes with the same accuracy:

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + k\,\nu\,\sqrt{h}\,\underline{\beta}' \qquad \text{(0-13)}$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + l\,\nu\,\sqrt{h}\,\underline{\beta}'$$

$$\underline{X}_{n+1} = \underline{X}_n + \nu\,\Delta_n\underline{w} + h[\,a\underline{f}(\underline{Q}_n) + b\underline{f}(\underline{Q}_n')\,]$$

where the parameters satisfies the conditions:

$$a + b = 1\,,\; a\cdot k + b\cdot l = 1\,,\; a\cdot k^2 + b\cdot l^2 = \frac{3}{2}.$$

Scheme (0-12) corresponds to the parameter values,

$$a = \frac{1}{3},\; b = \frac{2}{3},\; k = 0\,,\; l = \frac{3}{2}.$$

For the case of a system of stochastic differential equations, we also develop the the following scheme of Runge-Kutta type (see (3-59)):

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) \qquad \text{(0-14)}$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + \nu\,\sqrt{h}\,\underline{\xi}$$

$$\underline{X}_{n+1} = \underline{X}_n + \nu\sqrt{h}\,\underline{\xi} + \frac{1}{2}h\,[\,\underline{f}(\,\underline{Q}_n\,) + \underline{f}(\,\underline{Q}_n')\,]$$

where $\underline{\xi} = \{\xi^j\}$ is a set of Gaussian variables and each of them has mean 0 and variance 1. The computer experiments (in chapter 5) show that scheme (0-14) is a second order method, but in a slightly weaker sense, i.e., there exists a constant C such that, for sufficiently small h,

$$|\,E\varphi(\underline{x}(t_n)) - E\varphi(\underline{X}_n)\,| \le C\,h^2 \qquad \text{(0-15)}$$

where φ is a sufficiently smooth functional satisfying a Lipshitz condition. I have been not able to provide a proof that scheme (0-14) has second order accuracy in the sense of (0-15). For a heuristic discussion of the accuracy and the principle underlying scheme (0−14), see section 3.4. One may notice that in schemes (0−11), (0−12) and (0-14), the function $\underline{f}$ and the Wiener process $\underline{w}_t$ are interlaced.

All the schemes discussed above lend themselves to Monte-Carlo sampling with effective variance reduction. The main purpose of variance reduction is to substantially increase the accuracy of computed expectations of functionals of sample solutions with only a small increase in computational effort. We discuss, in chapter 4, several variance reduction techniques which are suitable for stochastic differential equations. We introduce the concept of partial variance reduction and show how to implement the technique based on Hermite polynomial expansions, as suggested by Chorin [6]. Finally, we present some computational results and compare them with analytical solutions.

This thesis is organized as follows. In Chapter 1, we give the needed probability background. In Chapter 2, we derive Runge-Kutta methods for scalar stochastic differential equations. In Chapter 3, we derive Runge-Kutta methods for a system of stochastic differential equations. Chapter 4 is devoted to the study of techniques of variance reduction. Finally, in Chapter 5, we present computational results.

Chapter 1

Preliminary Probability Background

In this chapter we develop the probabilistic tools needed for our work in later chapters and we follow closely the notations in Arnold [1]. We start by giving various definitions of convergences used most often in probability theory. Let $\underline{x} = \{x^1, \cdots, x^d\}$ be an R^d-valued vector and $\|\cdot\|$ denote the two norm in the R^d space, $\|\underline{x}\| = [\sum_j (x^j)^2]^{\frac{1}{2}}$.

Convergence Concepts

Let $\underline{x}$ and $\underline{x}_n$, $n \geq 1$ be R^d-valued random variables defined on a probability space $(\Omega, \mathbf{M}, P)$. Four basic convergence concepts are defined in the following:

(i) If there exists exists a set $N \in \mathbf{M}$ of measure 0, such that, for $\omega \in N^c$, the sequence of the $\underline{x}_n(\omega) \in R^d$ converges to $\underline{x}(\omega) \in R^d$, then $\{\underline{x}_n\}$ is said to converge certainly or with probability 1 to $\underline{x}$. We write

$$ac\text{-}\lim_{n \to \infty} \underline{x}_n = \underline{x} \,. \tag{1-1}$$

(ii) If, for every $\varepsilon > 0$, $P[\omega |\ \|\underline{x}_n(\omega) - \underline{x}(\omega)\| > \varepsilon] \longrightarrow 0$, $as\ n \longrightarrow \infty$, then $\{\underline{x}_n\}$ is said to converge stochastically or in probability to $\underline{x}$. We write

$$st\text{-}\lim_{n \to \infty} \underline{x}_n = \underline{x} \,. \tag{1-2}$$

(iii) If $\underline{x}_n$ and $\underline{x}$ lie in L_p, i.e., $E\|\underline{x}\|^p \leq \infty$ and $E\|\underline{x}_n - \underline{x}\|^p \longrightarrow 0$, then $\{\underline{x}_n\}$ is said to converge in p^{th} mean to $\underline{x}$. We write

$$pm\text{-}\lim_{n \to \infty} \underline{x}_n \longrightarrow \underline{x} \,. \tag{1-3}$$

(iv) Let F_n and F denote the distribution of $\underline{x}_n$ and $\underline{x}$. If

$$\lim_{n \to \infty} \int_{R^d} g(x)\, dF_n(x) = \int_{R^d} g(x)\, dF(x) . \tag{1-4}$$

for every real-valued continuous bounded function g defined on R^d. Then the sequence $\{\underline{x}_n\}$ is said to converge in distribution to $\underline{x}$.

These convergence concepts are related to each other in the following fashion:

convergence in q^{th} mean

$\Downarrow$

convergence in p^{th} mean $(p \leq q)$

$\Downarrow$

a.c. convergence => s.t. convergence => convergence in dist. .

Conditional expectations. Let $\underline{x} \in L_1$ be a R^d-valued random variable, and $\mathbf{N} \subseteq \mathbf{M}$ be a sub-sigma-algebra of $\mathbf{M}$. There exists an N-measurable $\underline{y}$ such that

$$\int_A \underline{y}\, dP = \int_A \underline{x}\, dP . \tag{1-5}$$

which is assured by the Radon-Nikodynm theorem. We call $\underline{y}$ the conditional expectation of $\underline{x}$ under the condition $\mathbf{N}$ and write $\underline{y} = E(\underline{x} \mid \mathbf{N})$.

Conditional Probabilities. The conditional probability $P(A \mid \mathbf{N})$ of an event $A \in \mathbf{M}$ under the condition $\mathbf{N} \subseteq \mathbf{M}$ is defined by

$$P(A \mid \mathbf{N}) = E(I_A \mid \mathbf{N}) \tag{1-6}$$

where I_A is the indicator of the set A. Being a conditional expectation, a conditional probability is a N-measurable function on Ω.

Stochastic processes

Definition. Let $I = [t_0, T]$ nonempty index set and let $(\Omega, \mathbf{M}, P)$ be a probability space. Then, a family of $(\underline{x}_t, t \in [t_0, T])$ of R^d-valued random variables is called a stochastic process (random process, random function) with parameter set (index set) I and state space R^d.

If $(\underline{x}_t, t \in [t_0, T])$ is a stochastic process, then $\underline{x}_t(\cdot)$ is, for every fixed $t \in [t_0, T]$, a R^d-valued random variable and, for every fixed $\omega \in \Omega$, $\underline{x}_\cdot(\omega)$ is a R^d-valued function defined on I. It is called a **sample function** (realization, trajectory, path) of the stochastic process.

One interesting question is how we can tell whether a process has continuous sample functions or not. A very simple criterion is given as follows: is

Komolgorov's criterion. Let $(\underline{x}_t, t \in [t_0, T])$ be a stochastic process: if there exist three positive numbers p, q and r such that, for each t and s in $[t_0, T]$,

$$E\|\underline{x}_t - \underline{x}_s\|^p \le r\,|t-s|^{1+q} . \tag{1-7}$$

Then, $\underline{x}_t$ possesses with probability 1 continuous sample functions.

Martingales. Let $(\Omega, \mathbf{M}, P)$ be a probability space, and $(\underline{x}_t; t \in [t_0, T])$ be a real-valued stochastic process on $(\Omega, \mathbf{M}, P)$. Let $(\mathbf{M}_t)$ denote an increasing family of sub-sigma-algebra of $\mathbf{M}$, i.e.,

$$\mathbf{M}_s \subset \mathbf{M}_t \quad \text{for} \quad t_0 \le s \le t \le T.$$

If $\underline{x}_t$ is $\mathbf{M}_t$-measurable and integrable then the pair $(\underline{x}_t, \mathbf{M}_t)$ is called a *martingale* if

$$E(\underline{x}_t \mid \mathbf{M}_s) = \underline{x}_s \quad \textit{almost certainly} \tag{1-8}$$

for all s and t in $[t_0, T]$, where $s \le t$. Martingales are an abstract presentation of the concept of *fair game*. As we shall see, Ito's stochastic integrals have the advantage of being martingales.

In the following discussion, we shall assume that the state space R^d is endowed with the sigma-algebra $\mathbf{B}^d$ of all Borel (measurable) sets.

Markov processes Let $(\Omega, \mathbf{M}, P)$ be a probability space, a stochastic process $(\underline{x}_t, t \in [t_0, T])$ defined on it with state space R^d is called a *Markov process* if it satisfies the following *Markov property*:

$$P(\underline{x}_t \in B \mid \mathbf{N}[t_0, s]) = P(\underline{x}_t \in B \mid \underline{x}_s) \quad \textit{almost certainly} \tag{1-9}$$

for $t_0 \le s \le t \le T$ and $B \in \mathbf{M}$, where $\mathbf{N}([t_0, s])$ is the smallest sub-sigma-algebra of $\mathbf{M}$ with respect to which all the random variables $\underline{x}_t$, $t_0 \le t \le s$ are measurable.

The Markov property states that: if the state of a system is known at a particular time, then the past information has no effect on our knowledge of the later development of the system. Some useful conditions equivalent to the Markov property are (see Arnold [1] pp. 29)

(i) For $t_0 \le s \le t \le T$ and $A \in \mathbf{N}([t_0, T])$,

$$P[A \mid \mathbf{N}([t_0, s])] = P(A \mid \underline{x}_s), \tag{1-10}$$

(ii) for $t_0 \le s \le t \le T$ and $\underline{y}$ $\mathbf{N}[t_0, T]$-measurable and integrable,

$$E[\underline{y} \mid \mathbf{N}([t_0, s])] = E(\underline{y} \mid \underline{x}_s), \tag{1-11}$$

(iii) for $t_0 \le s \le t \le u \le T$, $A \in \mathbf{N}([t_0, s])$ and $B \in \mathbf{N}([u, T])$,

$$P(A \cap B \mid \underline{x}_t) = P(A \mid \underline{x}_t) \cdot P(B \mid \underline{x}_t), \tag{1-12}$$

(iv) for $n \ge 1$, $t_0 \le t_1 \le \cdots \le t_n < t < T$ and $B \in \mathbf{B}^d$,

$$P(\underline{x}_t \in B \mid \underline{x}_{t_1}, \cdots, \underline{x}_{t_n}) = P(\underline{x}_t \in B \mid \underline{x}_{t_n}). \tag{1-13}$$

Transition probabilities. Let $\underline{x}_t$, for $0 \le t \le T$, be a Markov process and $P(s, \underline{x}_s, t, B)$ be the conditional distribution corresponding to the conditional probability $P(\underline{x}_t \in B \mid \underline{x}_s)$. Then $P(s, \underline{x}, t, B)$ has the following properties:

(i) For fixed $s \le t$ and $B \in \mathbf{B}^d$, the equality

$$P(s, \underline{x}_s, t, B) = P(\underline{x}_t \in B \mid \underline{x}_s)$$

holds with probability 1.

(ii) $P(s, \underline{x}, t, \cdot)$ is a probability for fixed $s \le t$ and $B \in \mathbf{B}^d$.

(iii) $P(s, \cdot, t, B)$ is $\mathbf{B}^d$ measurable for fixed $s \le t$ and $B \in \mathbf{B}^d$.

(iv) the Chapman-Komolgorov equation holds:

$$P(s, \underline{x}, t, B) = \int_{R^d} P(u, \underline{y}, t, B) P(s, \underline{x}, u, d\underline{y}) \tag{1-14}$$

(1-14)

We call the function $P(s, \underline{x}, t, B)$ the transition probability of the Markov process $\underline{x}_t$. In fact, any function P satisfying the properties (ii)-(iv) is called a transition probability function.

Diffusion processes A R^d-valued Markov process $\underline{x}_t$, $t_0 \le t \le T$ with almost certainly continuous sample functions is called a diffusion process if the transition probability $P(s, \underline{x}, t, B)$ satisfies the following conditions: for $s \in [t_0, T)$, $x \in R^d$, and $\varepsilon > 0$, (i)

$$\lim_{t \downarrow s} \int_{|y - x| > \varepsilon} P(s, \underline{x}, t, d\underline{y}) = 0 , \tag{1-15}$$

(ii) there exists a R^d-valued function $\underline{f}(s, \underline{x})$ such that

$$\lim_{t \downarrow s} \int_{|y - x| \le \varepsilon} (\underline{y} - \underline{x}) P(s, \underline{x}, t, d\underline{y}) = \underline{f}(s, \underline{x}) , \tag{1-16}$$

(iii) there exists a $d \times d$ matrix-valued function $\underline{B}(s, \underline{x})$ such that

$$\lim_{t \downarrow s} \int_{|y - x| \le \varepsilon} (\underline{y} - \underline{x})(\underline{y} - \underline{x})^T P(s, \underline{x}, t, d\underline{y}) = \underline{B}(s, \underline{x}) \tag{1-17}$$

where the superscript T denote the transpose. The function $\underline{f}$ and $\underline{B}$ are called, respectively, the drift vector and diffusion matrix of the diffusion process $\underline{x}_t$.

Wiener processes. Next we will discuss a remarkable Markov process, the Wiener process (or Brownian motion), which plays a fundamental role in in stochastic integrals and stochastic differential equations.

A R^d-valued *Wiener process* or a *Brownian motion* is a stochastic process $\underline{w}_t \equiv \underline{w}(t),\ t \geq 0$ satisfying

(i) $\underline{w}(0) = 0$,

(ii) for $0 \leq t_1 \leq t_2 \leq \cdots \leq t_n$

$\underline{w}(t_1),\ \underline{w}(t_2) - \underline{w}(t_1), \cdots, \underline{w}(t_n) - \underline{w}(t_{n-1})$ *are independent*;

(iii) for $s \leq t$, $\underline{w}(t) - \underline{w}(s)$ has the normal distribution $(0, (t-s)I_d)$ where I_d is the $d \times d$ identity matrix, i.e., it has the probability density:

$$[2\pi(t-s)]^{-\frac{d}{2}} \exp\left[\frac{-\|y-x\|^2}{2(t-s)}\right]. \tag{1-18}$$

The property (ii) states that a Wiener process has independent increments, and by (iii), the increments are stationary since the distribution of $\underline{w}(t) - \underline{w}(s)$ depends only on $t-s$. We have

Lemma 1.1. (i) A Wiener process $\underline{w}_t$ is a Gaussian stochastic process with mean $E(\underline{w}_t) = 0$ and covariance $E[\underline{w}_s\ \underline{w}_t{}^T] = [\min(s, t)]I_d$

(ii) If $\underline{w}_t$ is a Wiener process, the processes $-\underline{w}_t$, $c^{-1}\underline{w}_{c^2t}\ (c \neq 0)$, and $\underline{w}_{t+s} - \underline{w}_s$ (s is fixed) are also Wiener processes.

Now let $\mathbf{B}_t = \mathbf{B}(\underline{w}_s, 0 \leq s \leq t)$, i.e., the smallest sub-sigma-algebra of $\mathbf{M}$ with respect to which all the random variables $\underline{w}_s$, $0 \leq s \leq t$ are measurable. Then, for $s \leq t$, $E(\underline{w}_t \mid \mathbf{B}_s) = E(\underline{w}_t \mid \underline{w}_s) = \underline{w}_s$, therefore, $(\underline{w}_t, \mathbf{B}_t)$ is a martingale.

Since $E(|\underline{w}_t - \underline{w}_s|^4) = (d^2 + 2d)(t-s)^2$, it follows from Komolgorov's criterion that there exists a version of a Wiener process with continuous sample functions. We will use this version throughout this thesis.

Even though almost all sample functions of a Wiener process are continuous, they are nowhere differentiable.

Lemma 1.2. Let $\underline{w}_t$ be a Wiener process; we have

$$qm\text{-}\lim_{\Delta_n \to 0} \sum_{k=1}^{n} \|\underline{w}_{t_k} - \underline{w}_{t_{k-1}}\|^2 = t - s$$

where qm means quadratic mean, $\{t_k\}$ is a partition of the interval $[s, t]$ and $\Delta_n = \max (t_k - t_{k-1})$ (see Arnold [1] pp. 49)

By this lemma, we deduce from the following inequality

$$\sum_k \|\underline{w}_{t_k} - \underline{w}_{t_{k-1}}\|^2 \le \max_k \|\underline{w}_{t_k} - \underline{w}_{t_{k-1}}\| \cdot \sum_k \|\underline{w}_{t_k} - \underline{w}_{t_{k-1}}\|$$

that

$$\sum_k \|\underline{w}_{t_k} - \underline{w}_{t_{k-1}}\| \to \infty \quad as \ \Delta_n \to \infty$$

with probability 1. This is equivalent to saying that almost every sample function of a Wiener process is of unbounded variation in a finite interval of time.

Stochastic integrals

Now we start to define the stochastic integral

$$\underline{J}(t) = \int_{t_0}^{t} \underline{G}(s)\, d\underline{w}_s \tag{1-19}$$

where $\underline{w}_t$ is a m-dimensional Wiener process and $\underline{G}$ is a $d \times m$-matrix valued function. Since $\underline{w}_t$ is nowhere differentiable, the integral $\int_{t_0}^{t} \underline{G}(s)\, d\underline{w}_s$ cannot be defined in the usual Lebesque Stieltjes sense. If $\underline{G} = \underline{G}(t)$ is absolutely continuous, we may define

$$\underline{J}(t) = \underline{G}(t)\underline{w}(t) - \int_{t_0}^{t} \frac{d\underline{G}(s)}{ds} \underline{w}(s)\, ds \; . \tag{1-20}$$

However, if $\underline{G}$ is only a continuous or an integrable function, this definition does not make any sense.

The general definition of stochastic integral is through the use of step functions. For this purpose, we will introduce the concept of nonanticipating functions.

Let $\underline{w}_t = \underline{w}(t)$, $t \geq 0$ be a Wiener process on a probability space $(\Omega, \mathbf{M}, P)$, (M_t) be an increasing family of sub-sigma-algebras of $\mathbf{M}$ such that

(i) $\mathbf{B}(\underline{w}_s,\ 0 \leq s \leq t) \subseteq \mathbf{M}_t$,

(ii) $\underline{w}(t) - \underline{w}(s)$ *is independent of* $\mathbf{M}_s$

for $t \geq s$, then $\mathbf{M}$ is said to be **nonanticipating** with respect to the m-dimensional Wiener process $\underline{w}_t$. One may well just take the class: $\mathbf{M}_t = \mathbf{B}_t = \mathbf{B}(\underline{w}(s), 0 \leq s \leq t)$ (defined in the text following lemma 1).

We let $\mathbf{M}_2^{d,m}[t_0, t] = \mathbf{M}_2[t_0, t]$ denote the set of all nonanticipating functions $\underline{G}$ defined on $[t_0, T]\times\Omega$ for which the functions $\underline{G}(\cdot, \omega)$ are with probability 1 in $L^2[t_0, t]$.

A function $\underline{G} \in \mathbf{M}_2[t_0, t]$ is called a *step function* if there exists a partition $[0 = t_0, t_1, \cdots, t_n = t]$ such that $\underline{G}(s) = \underline{G}(t_{i-1})$ for all $s \in [t_{i-1}, t_i)$. The stochastic integral of a step function is defined as follows:

$$\int_{t_n}^{t} \underline{G}\, d\underline{w} \equiv \int_{t_0}^{t} \underline{G}(s)\, d\underline{w}_s = \sum_i \underline{G}(t_{i-1})\, (\underline{w}_{t_i} - \underline{w}_{t_i-1}) . \tag{1-21}$$

To define the stochastic integral for arbitrary function in $M_2[0, t]$, we need the following lemma. Note that a $d\times m$-matrix valued function can be understood as a $R^{d\times m}$-valued function.

Lemma 1.3. For every function $\underline{G} \in \mathbf{M}_2[t_0, t]$, there exists a series of step function $\underline{G}_n \in \mathbf{M}_2[t_0, t]$ such that $ac\text{-}\lim_{n\to\infty} \int_{t_0}^{t} \|\underline{G}_n(s) - \underline{G}(s)\|^2\, ds = 0$.

Lemma 1.4 Let $\underline{G} \in \mathbf{M}_2[t_0, t]$ and that $\underline{G}_n \in \mathbf{M}_2[t_0, t]$ be a sequence of step functions for which

$$st\text{-}\lim_{n\to\infty}\int_{t_0}^{t} \|\underline{G}_n(s) - \underline{G}(s)\|^2\, ds \longrightarrow 0\,.$$

then

$$st\text{-}\lim_{n\to\infty}\int_{t_0}^{t} \underline{G}_n(s)\, d\underline{w}_s = I(\underline{G}) \tag{1-22}$$

where $I(\underline{G})$ is a random variable that does not depend on the specific choice of the sequence of step functions $\underline{G}_n$ (see Arnold [1] pp. 69).

Definition For every $d\times m$-matrix valued function $\underline{G} \in \mathbf{M}_2[t_0, t]$, the stochastic (Ito's) integral of $\underline{G}$ with respect to the m dimensional Wiener process $\underline{w}_t$ over the interval is defined by $I(\underline{G})$ in (1–18), which is almost certainly determined uniquely. The integrals so defined are martingales.

Stochastic Differential Equations

In terms of Ito's stochastic integrals, we can define a stochastic differential equation:

$$d\underline{x}_t = \underline{f}(t,\underline{x})\, dt + \underline{G}(t,\underline{x})\, d\underline{w}_t\,, \quad 0 \le t \le T < \infty\,, \tag{1-23}$$
$$\underline{x}(t_0) = \underline{x}_{t_0} = \underline{c}$$

by its integral form:

$$\underline{x}_t(\omega) = \underline{x}(t_0) + \int_{t_0}^{t} \underline{f}(s,\omega)\, ds + \int_{t_0}^{t} \underline{G}(s,\underline{w})\, d\underline{w}_s(\omega) \tag{1-24}$$

where $\underline{w}_t$ is a m-dimensional Wiener process, $\underline{f}$ is a R^d-valued function and $\underline{G}$ is a $d\times m$ matrix-valued function.

Suppose that $\underline{f}$ (R^d-valued) and $\underline{G}$ ($d\times m$-matrix valued) are defined on $[t_0, T]\times R^d$ and satisfy the following conditions: there exists a constant $L > 0$ such that

(i) (Restriction on growth) for all $t \in [t_0, T]$ and $\underline{x} \in R^d$,

$$\|\underline{f}(t,\underline{x})\|^2 + \|\underline{G}(t,\underline{x})\|^2 \le L^2(1 + \|\underline{x}\|)^2 .$$

(ii) (Lipshitz condition) for all $t \in [t_0, T]$ and $\underline{x}, \underline{y} \in R^d$,

$$\|\underline{f}(t,\underline{x}) - \underline{f}(t,\underline{y})\| + \|\underline{G}(t,\underline{x}) - \underline{G}(t,\underline{y})\| \le L\,\|\underline{x} - \underline{y}\| .$$

These conditions assure the existence and uniqueness of the solution of the stochastic differential equation (1-24). We have

Theorem 1.1. Under the assumptions (i) and (ii) in the above, then equation (1-24) has on $[t_0, T]$ a unique R^d-valued solution $\underline{x}(t)$ which is continuous with probability 1 and satisfies the initial condition $\underline{x}_{t_0} = \underline{c}$ (see Arnold [1] pp. 105).

Theorem 1.2. Suppose equation (1-20) satisfies the same conditions of theorem 1, then the solution of the equation for arbitrary initial condition is a Markov process on the interval $[t_0, T]$ with the transition probability

$$P(s,\underline{x},t,B) = P[\,\underline{x}_t \in B \mid \underline{x}_s = \underline{x}\,] = P[\underline{x}_t(s,\underline{x}) \in B]$$

(see Arnold [1] pp. 146).

Theorem 1.3. In addition to the assumptions in theorem 1, suppose that the functions $\underline{f}$ and $\underline{G}$ are continuous with respect to t, then the solution of equation (1-20) is a d dimensional diffusion process on $[0, T]$ with drift vector $\underline{f}(t,\underline{x})$ and diffusion matrix $\underline{B}(t,\underline{x}) = \underline{G}(t,\underline{x})\underline{G}^T(t,\underline{x})$ (see Arnold [1] pp. 152).

In this thesis, we consider the stochastic differential equation with constant diffusion matrix $\underline{B}(t,\underline{x}) = \nu I_d$ where I_d is the $d \times d$ identity matrix.

Wiener integrals. The expectations of Brownain motion's functionals are called Wiener integrals which can be evaluated in the function space $C[0, 1]$ of all continuous R^d-valued functions defined on $0 \le t \le 1$.

Actually, every solution of equation (1–24) is a functional of Brownain motion. The variance reduction techniques in chapter 4 are devoted to accurate evaluation of Wiener integrals of functionals of the solution of equation (1-24).

For some classes of Wiener integrals that play a role in physics (see Feynman/Hibbs [10] and Jaffe/Glimm [14]), accurate interpolation formulae have been derived (see Cameron [3] and Chorin [5]).

Remark. There is one another useful definition of stochastic integral which is in the sense of **Stratonovich** (see Arnold [1] pp. 168). Different senses of definitions of stochastic integrals lead to different definitions of equation (1–23). However, for the case (constant diffusion) that we consider in this thesis, there is no difference in explaining equation (1-23) in Ito's or in Stratonovich's sense.

Chapter 2

Runge–Kutta Methods in One Dimension

In this chapter we will derive a second order (in the L_2 sense) Runge-Kutta method and a class of Runge-Kutta methods of order $1\frac{1}{2}$ (in the L_2 sense) for solving the scalar stochastic differential equation:

$$dx = f(x)\,dt + \nu\,dw_t\,,\quad 0 \le t \le T \tag{2-1}$$

where $\nu \ge 0$ is a constant and $f = f(x)$ is a sufficiently smooth function satisfying a Lipshitz condition. The main results are stated in Theorem 2.1 (in section 2.3) and Theorem 2.2 (in section 2.5).

We start in section 2.1 by analyzing the local truncation error of the splitting scheme based on the mid-point rule. Then, in section 2.2, we demonstrate that this splitting scheme is not a second order method in any L_p sense ($p \ge 2$) and explain why L_2 analysis is preferred to the L_1 analysis.

In section 2.3, we construct a Runge-Kutta method by interlacing the function f and the Wiener process w_t. For technical reasons, a Taylor series method is developed as an intermediate step. In section 2.4 we prove that the Runge-Kutta method derived in section 2.3 has second order accuracy in the L_2 sense. However, this result does not generalize to the system case.

Finally, in section 2.5, we derive a class of Runge-Kutta methods of order $1\frac{1}{2}$ (in the L_2 sense), which are easy to implement and will maintain their accuracy for the case of a system (discussed in section 3.5).

2.1 Analysis of a Splitting Scheme Based on the Mid–Point Rule

Consider a partition of the interval $[\,0,\ T\,]$

$$\Pi = [\,0\,,\cdots,t_{n+1} = t_n + h,\cdots\, t_l \,=\, T\,] \tag{2-2}$$

and the splitting scheme based on mid-point rule

$$X_{n+1} = X_n + hf\,(\,X_n + \frac{1}{2}hf\,(X_n)\,) + \nu\,\Delta_n w \tag{2-3}$$

where $\Delta_n w = w_{t_{n+1}} - w_{t_n}$. From the theory of ordinary differential equations we see that, if the random effect disappears (i.e. $\nu = 0$), then the scheme (2-3) is a second order method for the equation (2−1) with $\nu = 0$. However, in this section, we show that if $\nu \neq 0$, scheme (2-3) is not a second order method in any L_p sense ($p \geq 2$) for the stochastic differential equation (2-1).

Without loss of generality, we assume that $\nu = 1$ in the following discussion. That is, we consider the stochastic differential equation:

$$dx = f\,(x)dt + dw_t\,,\ \ 0 \leq t \leq T \tag{2-4}$$

and the splitting scheme for it:

$$X_{n+1} = X_n + \Delta_n w + hf\,(\,X_n + \frac{1}{2}hf\,(X_n)\,)\,. \tag{2-5}$$

In analogy with the analysis of numerical methods for ordinary differential equations, we analyze the local truncation error D_n of (2-5), which is defined by the equation:

$$x(t_{n+1}) = x(t_n) + \Delta_n w + hf\,(\,x(t_n) + \frac{1}{2}hf\,(x(t_n))\,) - D_n\,. \tag{2-6}$$

To facilitate our discussion, for each specified subinterval, say, $[t_n,\ t_{n+1}]$, we define the variable:

$$y(t) = x(t) - \Delta w_t\ ,\ \ t_n \leq t \leq t_{n+1} = t_n + h \tag{2-7}$$

where $\Delta w_t = w_t - w_{t_n}$. From this definition, it follows immediately that

$$y(t_n) = x(t_n) \tag{2-8}$$

for the specified interval. Substituting the definitions in (2-7) into (2−4) and (2-6), we obtain, respectively

$$\frac{dy}{dt} = f(y + \Delta w_t), \quad t_n < t < t_{n+1} = t_n + h \tag{2-9}$$

and

$$-D_n = y(t_{n+1}) - y(t_n) - hf(x(t_n) + \frac{1}{2}hf(x(t_n))) . \tag{2-10}$$

For convenience of analysis, we will rewrite D_n in an integral form. Integrating equation (2-9) from t_n to $t_n + h$, we obtain

$$y(t_{n+1}) - y(t_n) = \int_{t_n}^{t_n+h} f(y(s) + \Delta w_s)\, ds \tag{2-11}$$

and since $x(t_n)$ is a random variable for fixed time t_n, we have

$$hf(x(t_n) + \frac{1}{2}hf(x(t_n))) = \int_{t_n}^{t_n+h} f(x(t_n) + \frac{1}{2}hf(x(t_n)))\, ds . \tag{2-12}$$

Substituting the results in (2−11) and (2−12) into D_n of (2−10), we obtain

$$-D_n = \int_{t_n}^{t_n+h} [\, f(y(s) + \Delta w_s) - f(x(t_n) + \frac{1}{2}hf(x(t_n)))\,]\, ds . \tag{2-13}$$

With D_n in this form, further analysis can be made because of the differentiability of the function f.

In the following discussion, we will analyze D_n in the L_1 sense, which is apparently the simplest way of estimation. And as we shall see, many conclusions in the L_2 sense can be drawn from the results derived in the L_1 sense.

Our next task is to show that D_n is of order $h^{1.5}$ in the L_1 sense, i.e., $E|D_n| \leq const. \cdot h^{1.5}$. From now on, the notation $O(h^p)$ will be employed to denote a stochastic quantity whose order is h^p in the L_1 sense or in the L_2 sense.

We expand each term in the integrand of D_n of (2-10) in a Taylor series in $\Delta x_s \equiv y(s) - y(t_n) + \Delta w_s$ around $x(t_n) = y(t_n)$. We find:

$$f(y(s) + \Delta w_s) = f(x(t_n) + [y(s) - y(t_n) + \Delta w_s]) \tag{2-14}$$

$$= f(x(t_n)) + f_x(x(t_n))\Delta x_s + \frac{1}{2} f_{xx}(x(t_n))\Delta x_s^2 + \frac{1}{6} f_{xxx}(x(t_n))\Delta x_s^3$$

$$+ \frac{1}{24} f_{xxxx}(x(t_n))\Delta x_s^4 + \frac{1}{120} f_{xxxxx}(x'(t_n))\Delta x_s^5$$

where the last term is the Cauchy expression of remainder of the Taylor expansion. In the same way, we have

$$f(x(t_n) + \frac{1}{2} h f(x(t_n))) = f(x(t_n)) \tag{2-15}$$

$$+ \frac{1}{2} h f_x(x(t_n)) f(x(t_n)) + \frac{1}{8} h^2 f_{xx}(x(t_n)) f^2(x(t_n))$$

$$+ \frac{1}{48} h^3 f_{xxx}(x''(t_n)) f^3(x(t_n))$$

where, again, we use the Cauchy expression of the remainder. To estimate these remainders, we make the assumption:

$$\sup_x \left| \frac{\partial^\mu}{\partial x^\mu} f(x) \right| \textit{ are bounded}, \quad 0 \le \mu \le 5 \tag{2-16}$$

to assure that the expectations involved exist (in the following discussion). From this assumption, it follows that the remainder in (2-15) is of order h^3 in the L_1 sense. That is, we can write (2-15) in the form:

$$f(x(t_n) + \frac{1}{2} h f(x(t_n))) = f(x(t_n)) \tag{2-17}$$

$$+ \frac{1}{2} h f_x(x(t_n)) f(x(t_n))$$

$$+ \frac{1}{8} h^2 f_{xx}(x(t_n)) f^2(x(t_n)) + O(h^3) .$$

To analyze the order of the remainder of the expansion (2-14), more work is needed. Let E denote the expectation, as in the previous chapter. Recall that Δw_s is a Gaussian random variable with mean 0 and variance $\Delta s = s - t_n$ by the definition of the Wiener process (see Chapter 1), then

$$E|\Delta w_s| = \frac{1}{\sqrt{2\pi\Delta s}} \int_{-\infty}^{\infty} |u| \, e^{-\frac{u^2}{2\Delta s}} du \tag{2-18}$$

$$= 2 \cdot \frac{1}{\sqrt{2\pi\Delta s}} \int_0^\infty u \, e^{-\frac{u^2}{2\Delta s}} du$$

$$= \sqrt{\frac{2}{\pi}} \int_0^\infty e^{-v} \sqrt{\Delta s} \, dv \quad (v = \frac{u^2}{2\Delta s})$$

$$= \sqrt{\frac{2}{\pi}} \sqrt{\Delta s} = \sqrt{\frac{2}{\pi}} \sqrt{s - t_n} \le \sqrt{h}$$

which says that the increment Δw_s of the Wiener process w_t is of order $h^{½}$ in in the L_1 sense. In general, the random variable Δw_s^p is of order $h^{\frac{p}{2}}$ in the L_1 sense since

$$E|\Delta w_s|^p = \frac{1}{\sqrt{2\pi\Delta s}} \int_{-\infty}^{\infty} |u|^p \, e^{-\frac{u^2}{2\Delta s}} du \tag{2-19}$$

$$= 2 \cdot \frac{1}{\sqrt{2\pi\Delta s}} \int_0^\infty u^p \, e^{-\frac{u^2}{2\Delta s}} du$$

$$= \sqrt{\frac{1}{\pi}} \int_0^\infty [2\Delta s]^{\frac{p}{2}} e^{-v} \, v^{\frac{p-1}{2}} dv \quad (v = \frac{u^2}{2\Delta s})$$

$$= \sqrt{\frac{1}{\pi}} \, \Gamma[\frac{p+1}{2}] \cdot [2\Delta s]^{\frac{p}{2}} \le \Gamma[\frac{p+1}{2}] \cdot [2h]^{\frac{p}{2}}$$

where Γ is the gamma function. Observe further that

$$y(s) - y(t_n) = \int_{t_n}^{s} f(y(r) + \Delta w_r) \, dr \tag{2-20}$$

which is obtained by integrating equation (2–9) from t_n to s. Since f is bounded by assumption (2-16), we have the estimate:

$$E|y(s) - y(t_n)| = \int_{t_n}^{s} E|f(y(r) + \Delta w_r)| \, dr \le const. \; h \tag{2-21}$$

which means that $y(s) - y(t_n)$ is of order h in the L_1 sense.

Now we are ready to deal with the remainder in (2–14). The above analysis shows that the leading order term of this remainder is $f_{xxxxx}(x^*(t_n))\Delta w_s^5$ and it is of order $h^{2.5}$ in the L_1 sense. Furthermore, the same analysis can also be applied to other terms of the expansion (2-14) and this enable us to rewrite (2-14) in a more compact form:

$$f(y(s)+\Delta w_s) = f(x(t_n)) + f_x(x(t_n))(y(s)-y(t_n)+\Delta w_s) \qquad (2\text{-}22)$$
$$+\frac{1}{2}f_{xx}(x(t_n))(y(s)-y(t_n)+\Delta w_s)^2$$
$$+\frac{1}{2}f_{xxx}(x(t_n))\,(y(s)-y(t_n))\,\Delta w_s^{\,2}$$
$$+\frac{1}{6}f_{xxx}(x(t_n))\Delta w_s^{\,3} + \frac{1}{24}f_{xxxx}(x(t_n))\Delta w_s^{\,4} + O(h^{\frac{5}{2}}).$$

Substituting the results in (2-17) and (2-22) into D_n of (2-13), we can, after some cancellation, write D_n in increasing power of Δw_s:

$$-D_n = f_x(x(t_n))\int_{t_n}^{t_n+h}\Delta w_s\,ds + \frac{1}{2}f_{xx}(x(t_n))\int_{t_n}^{t_n+h}\Delta w_s^{\,2}ds - R_n \qquad (2\text{-}23)$$

where we keep in $-D_n$ only the two terms of the expansion (2-6) with leading order in Δw_s, and group all the other terms in a lengthy remainder:

$$-R_n = f_x(x(t_n))\int_{t_n}^{t_n+h}(y(s)-y(t_n)-\frac{1}{2}hf(x(t_n)))\,ds \qquad (2\text{-}24)$$
$$+f_{xx}(x(t_n))\int_{t_n}^{t_n+h}[(y(s)-y(t_n))\Delta w_s + \frac{1}{2}(y(s)-y(t_n))^2]\,ds$$
$$+\frac{1}{2}f_{xxx}(x(t_n))\int_{t_n}^{t_n+h}(y(s)-y(t_n))\Delta w_s^{\,2}\,ds$$
$$+\frac{1}{6}f_{xxx}(x(t_n))\int_{t_n}^{t_n+h}\Delta w_s^{\,3}\,ds - \frac{1}{8}h^3 f_{xx}(x(t_n))f^2(x(t_n))$$
$$+\frac{1}{24}f_{xxxx}(x(t_n))\int_{t_n}^{t_n+h}\Delta w_s^{\,4}\,ds + O(h^{\frac{7}{2}}).$$

Now let us examine the orders of the first two terms of $-D_n$ in (2-23). The analyses in (2-18) and in (2-19) show that

(a) $\int_{t_n}^{t_n+h} \Delta w_s \, ds$ is of order $h^{1.5}$ in the L_1 sense.

(b) $\int_{t_n}^{t_n+h} \Delta w_s^{\,2} \, ds$ is of order h^2 in the L_1 sense.

Hence, we can assure that $-D_n$ (in (2-21)) is at least of order $h^{1.5}$ in the L_1 sense. However, it is still not clear, at this stage, what the order of $-D_n$ is in the L_1 sense because the orders of the first three terms of $-R_n$ (in (2-24)) cannot be seen readily. To investigate this question, we need the following lemma.

Lemma 2.1. For the first three terms in $-R_n$ of (2-22), we have the following estimates:

(i)

$$\int_{t_n}^{t_n+h} [\, y(s)-y(t_n)-\frac{1}{2}hf(x(t_n)) \,] \, ds$$

$$= f_x(x(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r \, drds + \frac{1}{6}h^3 f_x(x(t_n)) f(x(t_n))$$

$$+ \frac{1}{2} f_{xx}(x(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r^{\,2} \, drds + O(h^{\frac{7}{2}}) \, .$$

(ii)

$$\int_{t_n}^{t_n+h} (y(s) - y(t_n)) \Delta w_s \, ds$$

$$= f(x(t_n)) \int_{t_n}^{t_n+h} (s - t_n) \Delta w_s \, ds + f_x(x(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r \Delta w_s \, drds + O(h^{\frac{7}{2}}) \, .$$

(iii)

$$\int_{t_n}^{t_n+h} (y(s)-y(t_n))^2\, ds = \frac{1}{3}h^3 f^2(x(t_n)) + O(h^{\frac{7}{2}}) .$$

(iv)

$$\int_{t_n}^{t_n+h} (y(s)-y(t_n))\Delta w_s^2\, ds = f(x(t_n)) \int_{t_n}^{t_n+h} (s-t_n)\Delta w_s^2 ds + O(h^{\frac{7}{2}}) .$$

Proof. Since Δw^p is a stochastic quantity of order $h^{\frac{p}{2}}$, we can derive the equality (i) by considering the sequences of equalities:

$$\int_{t_n}^{t_n+h} [y(s)-y(t_n)-\frac{1}{2}hf(x(t_n))]\, ds$$

$$= \int_{t_n}^{t_n+h}\int_{t_n}^{s} [f(y(r)+\Delta w_r)-f(y(t_n))]\, drds \quad (by\ (2\text{-}20))$$

$$= \int_{t_n}^{t_n+h}\int_{t_n}^{s} [f_x(y(t_n))(y(r)-y(t_n)+\Delta w_r)]\, drds$$

$$+ \int_{t_n}^{t_n+h}\int_{t_n}^{s} [\frac{1}{2}f_{xx}(y(t_n))(y(r)-y(t_n)+\Delta w_r)^2 + O(h^{\frac{3}{2}})]\, drds$$

$$= f_x(x(t_n))\int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r\, drds + f_x(x(t_n))\int_{t_n}^{t_n+h}\int_{t_n}^{s} [y(r)-y(t_n)]\, drds$$

$$+ \frac{1}{2}f_{xx}(x(t_n))\int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r^2\, drds + O(h^{\frac{7}{2}})$$

while the second term on the right hand side of the last equality can rewritten further:

$$f_x(x(t_n))\int_{t_n}^{t_n+h}\int_{t_n}^{s} [y(r)-y(t_n)]\, drds$$

$$= f_x(x(t_n))\int_{t_n}^{t_n+h}\int_{t_n}^{s} [(r-t_n)f(x(t_n)) + O(h^{\frac{3}{2}})]\, drds$$

$$= \frac{1}{6}h^3 f_x(x(t_n))f(x(t_n)) + O(h^{\frac{7}{2}}) .$$

To prove the second equality (ii), it is more convenient to consider the difference of the left hand side and the first term on the right hand side of it. Using (2-20), we have

$$\int_{t_n}^{t_n+h} [\, y(s)-y(t_n)-(s-t_n)f(x(t_n))\,]\Delta w_s\, ds$$

$$= \int_{t_n}^{t_n+h}\int_{t_n}^{s}[\, f(y(r)+\Delta w_r)-f(y(t_n))\,]\Delta w_s\, drds$$

$$= \int_{t_n}^{t_n+h}\int_{t_n}^{s}[\, f_x(y(t_n))(y(r)-y(t_n)+\Delta w_r)+O(h)\,]\Delta w_s\, drds$$

$$= \int_{t_n}^{t_n+h}\int_{t_n}^{s}[\, f_x(y(t_n))\Delta w_r+O(h)\,]\Delta w_s\, drds$$

$$= f_x(x(t_n))\int_{t_n}^{t_n+h}\int_{t_n}^{s}\Delta w_r\Delta w_s\, drds + O(h^{\frac{7}{2}}).$$

The justification of the equalities (iii) and (iv) can be made by merely recalling the estimate following equation (2–19). This completes the proof of Lemma 1.

From the expression of $-R_n$ in (2-24), we see that equality (i) in Lemma 1 corresponds to the first term of $-R_n$, (ii) and (iii) to the second term, and (iv) to the third term of $-R_n$. Substituting the results in the Lemma into $-R_n$ of (2-24), we obtain

$$-R_n = f_x^2(x(t_n))\int_{t_n}^{t_n+h}\int_{t_n}^{s}\Delta w_r\, drds + \frac{1}{6}h^3 f_x^2(x(t_n))f(x(t_n)) \qquad (2\text{-}25)$$

$$+\frac{1}{2}f_x(x(t_n))f_{xx}(x(t_n))\int_{t_n}^{t_n+h}\int_{t_n}^{s}\Delta w_r^2\, drds$$

$$+f_{xx}(x(t_n))f(x(t_n))\int_{t_n}^{t_n+h}(s-t_n)\Delta w_s ds + f_x(x(t_n))f_{xx}(x(t_n))\int_{t_n}^{t_n+h}\int_{t_n}^{s}\Delta w_r\Delta w_s drds$$

$$+ \frac{1}{2} f(x(t_n)) f_{xxx}(x(t_n)) \int_{t_n}^{t_n+h} (s - t_n) \Delta w_s^2 \, ds$$

$$+ \frac{1}{24} h^3 f^2(x(t_n)) f_{xx}(x(t_n)) + \frac{1}{6} f_{xxx}(x(t_n)) \int_{t_n}^{t_n+h} \Delta w_s^3 \, ds$$

$$+ \frac{1}{24} f_{xxxx}(x(t_n)) \int_{t_n}^{t_n+h} \Delta w_s^4 \, ds + O(h^{\frac{7}{2}}) .$$

where all but the last three terms are obtained from these substitutions.

Let us examine the orders each term of $-R_n$ of (2-25). We find:

(c) the first and the fourth and the eighth term are of order $h^{2.5}$ in the L_1 sense.

(d) all the remaining terms except the last one are of order h^3 in the L_1 sense.

These observations imply that $-R_n$ is a stochastic quantity of order $h^{2.5}$ in the L_1 sense. Therefore, by recalling the comments in (a) and (b), following (2-24), we conclude that $-D_n$ is a stochastic quantity of order $h^{1.5}$ in the L_1 sense and

$$-D_n = f_x(x(t_n)) \int_{t_n}^{t_n+h} \Delta w_s \, ds + \frac{1}{2} f_{xx}(x(t_n)) \int_{t_n}^{t_n+h} \Delta w_s^2 \, ds + O(h^{2.5}) . \quad (2\text{-}26)$$

Remark. In the above discussion, we encountered expressions of remainders whose orders are half integers of the form $k + 0.5$ ($k > 0$, an integer). Since Δw_s^p is of order $h^{\frac{p}{2}}$ in the L_1 sense, in the leading terms of the remainders, the increments of the Brownian motion must appear with odd power. Recall the nonanticipating property of the solution of stochastic differential equation (see [..]), and we conclude that the expectation of the leading terms are zero. We will use this fact repeatedly in the later development. Here we would like to illustrate this fact by considering an example.

Suppose we wish to evaluate the expectation of $f_x(x(t_n))\Delta w_r \Delta w_s \Delta w_t$ where $t_n \le r \le s \le t \le t_{n+1} = t_n + h$. Because of the nonanticipating property, $f_x(x(t_n))$ is independent of the remaining part of the stochastic quantity considered. Thus, the expectation sought equals to the product of the expectations of these two parts.

Now we expand the increments Δw_r, Δw_s, Δw_s in the following way:

$$\Delta w_r = \; = w_r - w_{t_n}$$

$$\Delta w_s = (w_s - w_r) + (w_r - w_{t_n})$$

$$\Delta w_t = (w_t - w_s) + (w_s - w_r) + (w_r - w_{t_n})$$

This results in

$$\Delta w_r \Delta w_s \Delta w_t = (w_r - w_{t_n})^3$$

$$+ 2\cdot(w_r - w_{t_n})^2(w_s - w_r) + (w_r - w_{t_n})(w_s - w_r)^2$$

$$+ (w_r - w_{t_n})^2(w_t - w_s) + (w_r - w_{t_n})(w_s - w_r)(w_t - w_s)$$

where, in each term, one factor is independent of the other and at least one factor has odd multiplicity. Therefore, the expectation of each individual term on the right hand side of the above equation is zero, and thus the expectation of the stochastic quantity considered is zero.

2.2 Accuracy of the Splitting Scheme

Different ways of analyzing the accuracy of numerical schemes for stochastic differential equations may produce very different results. In this section, we consider this problem by answering the following two questions:

(i): is the scheme (2–5) a second order method in some L_p sense ($p \ge 2$)? and (ii): why is the L_2 analysis superior to the L_1 analysis?

The answer to the first question is no. This can be seen by taking, for example, $f(x) = x$ and $x(0) = 0$ in equation (2-4). That is, we have the Langevin equation with initial datum 0:

$$dx = x\,dt + dw_t\,,\quad 0 \le t \le T \tag{2-27}$$

the solution $x(t)$ of which, for each fixed t, is known to be a Gaussian variable with mean 0 and variance $\frac{1}{2}(e^{2t} - 1)$ (see Arnold [1] pp. 134). Therefore, all the moments of $x(t)$ exist, and thus the analysis in the previous section is also valid here even though the assumption (2–16) does not hold in this case (see the comment following the assumption (2-16)).

Let $-d_n$ be the local truncation error of scheme (2-5) in this particular case. From the expression of D_n in (2-23) and that of $-R_n$ in (2-25), we see that

$$-d_n = \int_{t_n}^{t_n+h} \Delta w_s\, ds + \int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r\, dr ds + \frac{1}{6}h^3 x(t_n)\,, \tag{2-28}$$

or from (2-26), we have

$$-d_n = \int_{t_n}^{t_n+h} \Delta w_s\, ds + O(h^{2.5})\,. \tag{2-29}$$

Define $e_n = X_n - x(t_n)$. Subtracting equation (2-6) from equation (2-5) with $f = x$, we obtain

$$e_{n+1} = a(h)\, e_n + d_n \tag{2-30}$$

where $a(h) = 1 + h + \frac{1}{2}h^2$. Equation (2-30) has the solution

$$e_n = a^{n-1}(h) d_0 + \cdots + a(h) d_{n-2} + d_{n-1} \tag{2-31}$$

provided that the initial condition is imposed exactly. Note that the leading terms of d_n, i.e., $\int_{t_n}^{t_n+h} \Delta w_s\, ds$, are independent of each other. Then the expectation of a product of any two of them is zero since the individual expectations are zero, i.e., for $m \neq n$,

$$E\left[\int_{t_m}^{t_m+h} \Delta w_s \, ds \cdot \int_{t_n}^{t_n+h} \Delta w_s \, ds\right] = E\left[\int_{t_m}^{t_m+h} \Delta w_s \, ds\right] \cdot E\left[\int_{t_n}^{t_n+h} \Delta w_s \, ds\right] \tag{2-32}$$

$$= \int_{t_m}^{t_m+h} E[\Delta w_s] \, ds \cdot \int_{t_n}^{t_n+h} E[\Delta w_s] \, ds = 0 \, .$$

Furthermore, an easy analysis shows that

$$E\left[\int_{t_n}^{t_n+h} \Delta w_s \, ds\right]^2 = E\left[\int_{t_n}^{t_n+h}\int_{t_n}^{t_n+h} \Delta w_r \Delta w_s \, drds\right] \tag{2-33}$$

$$= 2\cdot \int_{t_n}^{t_n+h}\int_{s}^{t_n+h} E[\Delta w_r \Delta w_s] \, drds = 2\cdot\int_0^h\int_s^h r \, drds = \frac{1}{3}h^3$$

Recalling the nonanticipating property of the solution $x(t_n)$, then, from (2-28), for sufficiently small h, we have the leading term estimate:

$$E[e_n^2] \approx a^{n-2}(h)E[d_0^2] + \cdots + a^2(h)E[d_{n-2}^2] + E[d_{n-1}^2]$$

$$\approx [\, a^{2n-2}(h) + \cdots + a^2(h) + 1 \,]\cdot \frac{1}{3}h^3$$

$$\approx \frac{a^{2n} - 1}{a^2 - 1}h^3 \approx \frac{e^{2t_n} - 1}{e^{2h} - 1}h^3 \approx (e^{2t_n})\cdot h^2$$

since $A(h) \approx e^h$, where we use the notation $P \approx Q$ to denote that P and Q are of same order in h. It follows from this estimate that

$$\sqrt{[E(e_n^2)]} \approx e^{t_n}\cdot h \tag{2-34}$$

which implies that, for $f = x$, the scheme (2-5) is of order h in the L_2 sense. And by Liapunov inequality

$$\left[E(e_n^p)\right]^{\frac{1}{p}} \leq \left[E(e_n^q)\right]^{\frac{1}{q}}, \quad 1 < p \leq q < \infty \tag{2-35}$$

i.e., the L_p norm of e_n is not greater than its L_q norm for $1 < p \leq q < \infty$, we conclude that scheme (2-5) is not a second order method for the equation (2-

4) in any L_p sense for $p \geq 2$.

Now we answer the second question (ii) above by considering, again, the same example. By applying the triangle inequality to the right hand side of (2-30), we obtain, after taking expectations,

$$E|e_{n+1}| \leq a(h)E|e_n| + E|d_n|$$

Since $E|d_n|$ is of order $h^{1.5}$, the above estimate can be rewritten as

(a)

$$E|e_{n+1}| \leq a(h)E|e_n| + O(h^{1.5})$$

On the other hand, by squaring both sides of equation (2–30), we obtain, after taking expectation,

$$E[e_{n+1}^2] = a^2(h)E[e_n^2] + 2a(h)E[e_n d_n] + E[d_n{}^2]$$

And since $E[d_n{}^2]$ is of order h^3, this estimate can be written as

(b)

$$E[e_{n+1}^2] = a^2(h)E[e_n^2] + 2a(h)E[e_n d_n] + O(h^3)$$

These two types of analyses in (a) and (b) are, for brevity, called the L_1 and the L_2 analysis respectively. There is an extreme difference between these two analyses in that, we shall see, the existence of the second term on the right hand side of equation (b) plays only a minor role in error contributions.

Recalling the nonanticipating property, we see from the expression (2-28) that

$$2a(h)E[e_n d_n] = -2a(h)\cdot E[e_n]\cdot E[\int_{t_n}^{t_n+h} \Delta w_s \, ds] \tag{2-36}$$

$$- 2a(h)\cdot E[e_n]\cdot E\left[\int_{t_n}^{t_n+h}\int_{t_n}^{s}\Delta w_r\, drds\right] - \frac{1}{3}h^3 a(h)\cdot E[e_n x(t_n)]$$

In the first and second term on the right hand side of this equality, we can put the expectation E inside the integral and find that the resultant integrals are zero and obtain

$$2a(h)E[e_n d_n] = \frac{1}{3}h^3 a(h)E[e_n x(t_n)] \le 2\varepsilon h a(h)E[e_n^2] + \frac{1}{72}a(h)\varepsilon^{-1}h^5 E[x^2(t_n)]$$

where ε is an appropriate positive number and the last inequality is obtained by applying once the arithmetic inequality $2\, a\cdot b \le a^2 + b^2$. The number ε is used to keep track of the interaction between the (accumulating) error e_n and the local truncation error d_n. Substituting the result in (2-37) into (b), we obtain

$$E[e_{n+1}^2] \le [a^2(h) + \varepsilon h a(h)]\cdot E[e_n^2] + O(h^3) + \varepsilon^{-1}h^5 E[x^2(t_n)] \qquad (2\text{-}38)$$

from which we see that $2a(h)E[e_n d_n]$ does not play a main role in the error contributions as $\varepsilon h a(h)$ is dominated by $a^2(h)$ and $\frac{1}{72}a(h)\varepsilon^{-1}h^5 E[x^2(t_n)]$ by $O(h^3)$.

Suppose that the initial condition is imposed exactly. It follows from (b) and the theory of difference equations

$$E|e_n| \text{ is of order } h^{0.5} \qquad (2\text{-}39)$$

and from (2-38) that

$$\sqrt{E[e_n^2]} \text{ is of order } h \qquad (2\text{-}40)$$

Comparing these results ((2−39),(2−40)) with that in (2−33), we find that only the L_2 analysis gives the order of the scheme considered. In fact, $E|e_n|$ is also of order of order h, which is seen from, by Liapunov inequality,

$$E|e_n| \le \sqrt{E[e_n^2]} \approx h$$

Therefore, we conclude that the L_2 analysis is superior to the L_1 analysis since the former exploits the nonanticipating property and thus provide a more precise estimate than the latter. As we see from the above discussion, the techniques used do not depend on the specific choice of the function f, this conclusion holds also for the class of functions f satisfying the condition (2-16). This important observation provides the basis for the analysis in section 2.3-5, 3.3 and 3.5.

2.3 A Second Order Runge–Kutta Method

In the previous section, we showed that the Runge-Kutta method based on mid-point rule fails to have second order accuracy in the L_2 sense. In this section, we will develop a method of Runge-Kutta type for the stochastic differential equation (2-4). The information contained in (2–5), (2-6), (2-23) and (2-24) suggests to us to consider first the following Taylor series method:

$$Q_n = X_n + \frac{1}{2} h f(X_n) \tag{2-41}$$

$$X_{n+1} = X_n + \Delta_n w + h f(Q_n) + f_x(X_n) \int_{t_n}^{t_n+h} \Delta w_s \, ds + \frac{1}{2} f_{xx}(X_n) \int_{t_n}^{t_n+h} \Delta w_s^2 \, ds$$

The local truncation error of the scheme is given by R_n in (2-23), i.e., the exact solution $x = x(t)$ of the stochastic differential equation (2-4) satisfies

$$x(t_{n+1}) = x(t_n) + \Delta_n w + h f(q(t_n)) \tag{2-42}$$

$$+ f_x(x(t_n)) \int_{t_n}^{t_n+h} \Delta w_s ds + \frac{1}{2} f_{xx}(x(t_n)) \int_{t_n}^{t_n+h} \Delta w_s^2 ds - R_n$$

where we define

$$q(t_n) = x(t_n) + \frac{1}{2} h f(x(t_n)) \tag{2-43}$$

As we know from the discussion in section 3 that R_n is of order $h^{2.5}$ in the L_1 sense, we would expect that the scheme (2-42) has the order $h^{1.5}$ in that sense, due to the accumulation of the local truncation errors.

The question is whether we can have a better estimate, i.e., could scheme (2-41) has higher order accuracy (better than $h^{1.5}$)? For we have seen a successful example in section 2 where we employed the L_2 analysis.

Therefore, in the following discussion, we will adopt L_2 analysis instead of L_1's since it exploits the nonanticipating property. However, our L_2 analysis will not be made directly to the scheme (2-41).

Scheme (2-41) is an intermediate step which leads to a more satisfying method of Runge-Kutta type. The main idea is to interlace the function f and the Wiener process w_t, i.e., to let them interact with each other at each time step.

Before we go further, let us define some useful random variables:

$$\beta \equiv h^{\frac{3}{2}}\beta' \equiv \int_{t_n}^{t_n+h} \Delta w_s ds, \qquad \vartheta \equiv h^2\vartheta' \equiv \int_{t_n}^{t_n+h} \Delta w_s{}^2 ds \tag{2-44}$$

From these definitions, it is obvious that the random variables β' and ϑ' are of order 1 in the L_1 sense and scheme (2–41) can be rewritten as

$$Q_n = X_n + \frac{1}{2}hf(X_n) \tag{2-45}$$

$$X_{n+1} = X_n + \Delta w_n + hf(Q_n) + h^{\frac{3}{2}}\beta' f_x(X_n) + \frac{1}{2}h^2\vartheta' f_{xx}(X_n)$$

which has a more convenient form that we can work on to obtain a Runge-Kutta method. The first step is to add a term involving β' to Q_n so that the first derivative term in X_{n+1} will appear implicitly. Observe that

$$hf(Q_n + \sqrt{h}\beta')$$

$$= hf(Q_n) + h^{\frac{3}{2}}\beta' f_x(Q_n) + \frac{1}{2}h^2\beta'^2 f_{xx}(Q_n) + O(h^{\frac{5}{2}})$$

$$= hf(Q_n) + h^{\frac{3}{2}}\beta' f_x(X_n) + \frac{1}{2}h^2\beta'^2 f_{xx}(X_n) + O(h^{\frac{5}{2}})$$

which leads us to consider the following scheme:

$$Q_n' = X_n + \frac{1}{2}hf(X_n) + \sqrt{h}\,\beta' \tag{2-46}$$

$$X_{n+1} = X_n + \Delta w_n + hf(Q_n') + \frac{1}{2}h^2[\vartheta' - \beta'^2]f_{xx}(X_n)\,.$$

the local truncation error T_n' of which is defined in the equation:

$$x(t_{n+1}) = x(t_n) + \Delta w_n + hf(q'(t_n)) + \frac{1}{2}h^2[\vartheta' - \beta'^2]f_{xx}(x(t_n)) - T_n' \tag{2-47}$$

where we define

$$q'(t_n) = q(t_n) + \sqrt{h}\,\beta' = x(t_n) + \frac{1}{2}hf(x(t_n)) + \sqrt{h}\,\beta'\,. \tag{2-48}$$

Here we have been careful in making the local truncation error T_n' of scheme (2-46) have the same order (in the L_1 sense) as that, i.e., R_n of scheme (2-41) (or (2–45)). This can be seen by analyzing T_n' further. As a starting point, for seeing that T_n' and R_n are of the same order, we carry out the Taylor expansion:

$$hf(q'(t_n)) = hf(\,q(t_n) + \sqrt{h}\,\beta'\,) \tag{2-49}$$

$$= hf(q(t_n)) + h^{\frac{3}{2}}\beta' f_x(q(t_n)) + \frac{1}{2}h^2\beta'^2 f_{xx}(q(t_n))$$

$$+ \frac{1}{6}h^{\frac{5}{2}}\beta'^3 f_{xxx}(q(t_n)) + \frac{1}{24}h^3\beta'^4 f_{xxxx}(q(t_n)) + O(h^{\frac{7}{2}})\,.$$

Recall the definition of $q(t_n)$ in (2-43). Each term on the right hand side of the above equation is then expanded in a Taylor series about $x(t_n)$ and this gives

$$hf(q'(t_n)) = hf(q(t_n)) + h^{\frac{3}{2}}\beta' f_x(x(t_n))$$

$$+ \frac{1}{2}h^{\frac{5}{2}}\beta' f(x(t_n))f_{xx}(x(t_n)) + \frac{1}{2}h^2\beta'^2 f_{xx}(x(t_n))$$

$$+ \frac{1}{8}h^3 f^2(x(t_n)) f_{xx}(x(t_n)) + \frac{1}{6}h^{\frac{5}{2}}\beta'^3 f_{xxx}(x(t_n))$$

$$+ \frac{1}{4}h^3\beta'^2 f(x(t_n)) f_{xxx}(x(t_n)) + \frac{1}{24}h^3\beta'^4 f_{xxxx}(x(t_n)) + O(h^{\frac{7}{2}})$$

Substituting this result into (2-47), we obtain, after some cancellation,

$$x(t_{n+1}) = x(t_n) + \Delta_n w + hf(q(t_n)) \tag{2-51}$$

$$+ h^{\frac{3}{2}}\beta' f_x(x(t_n)) + \frac{1}{2}h^2\vartheta' f_{xx}(x(t_n))$$

$$+ \frac{1}{2}h^{\frac{5}{2}}\beta' f(x(t_n)) f_{xx}(x(t_n)) + \frac{1}{8}h^3 f^2(x(t_n)) f_{xx}(x(t_n)) + \frac{1}{6}h^{\frac{5}{2}}\beta'^3 f_{xxx}(x(t_n))$$

$$+ \frac{1}{4}h^3\beta'^2 f(x(t_n)) f_{xxx}(x(t_n)) + \frac{1}{24}h^3\beta'^4 f_{xxxx}(x(t_n)) + T_n' + O(h^{\frac{7}{2}})$$

Recalling the definitions of β' and ϑ' in (2-44) and comparing this expression with that in (2-42), we can relate T_n' and R_n in the equation:

$$-R_n = -T_n' + \frac{1}{2}h^{\frac{5}{2}}\beta' f(x(t_n)) f_{xx}(x(t_n)) + \frac{1}{8}h^3 f^2(x(t_n)) f_{xx}(x(t_n)) \tag{2-52}$$

$$+ \frac{1}{6}h^{\frac{5}{2}}\beta'^3 f_{xxx}(x(t_n)) + \frac{1}{4}h^3\beta'^2 f(x(t_n)) f_{xxx}(x(t_n)) + \frac{1}{24}h^3\beta'^4 f_{xxxx}(x(t_n)) + O(h^{\frac{7}{2}}),$$

in short,

$$-R_n = -T_n' + O(h^{\frac{5}{2}}) \tag{2-53}$$

Recall that R_n is of order $h^{\frac{5}{2}}$ in the L_2 sense, thus so is T_n'. In other words, T_n' and R_n have the same order in h in the L_2 sense.

At this stage, it is still not clear how one is able to derive a Runge-Kutta method from the scheme (2–46). For there exists a second derivative term of f with a coefficient containing $\vartheta' - \beta'^2$. However, from the definition of the random variables β' and ϑ', we find a very interesting relationship: $\beta'^2 \le \vartheta'$, since the inequality

$$h^3\beta'^2 = (h^{\frac{3}{2}}\beta')^2 = \left[\int_{t_n}^{t_n+h} \Delta w_s ds\right]^2 \leq h \int_{t_n}^{t_n+h} \Delta w_s{}^2 ds = h[h^2\vartheta'] = h^3\vartheta' \quad (2\text{-}54)$$

holds by the Cauchy-Schwartz inequality. Hence, the random variable $\vartheta' - \beta'^2$ is positive. It is this fortunate observation that leads us to succeed in deriving the Runge-Kutta method:

$$P_n = \sqrt{\vartheta' - \beta'^2} \quad (2\text{-}55)$$

$$Q_n' = X_n + \frac{1}{2}hf(X_n) + \sqrt{h}\,\beta'$$

$$X_{n+1} = X_n + \Delta_n w + \frac{1}{2}h[\,f(Q_n' + \sqrt{h}P_n) + f(Q_n' - \sqrt{h}P_n)\,]$$

with β' and ϑ' defined in (2-44). This scheme is obtained by a symmetry consideration so that we need only to evaluate one intermediate value, i.e., Q_n' at each time step. Now we state the main result of this chapter.

Theorem 2.1. Let f be a sufficiently smooth function satisfying a Lipshitz condition and the condition stated in (2-16). Then the above scheme is second order in the L_2 sense, i.e., there exists two constants C and h_0 such that

$$\left[E(x(t_n) - X_n)^2\right]^{\frac{1}{2}} \leq C\,h^2\,, \quad h \leq h_0$$

for all $h \leq h_0$, provided that the initial condition is imposed exactly or to second order in the L_2 sense (say, $[E(x(0) - x_0)^2]^{1/2} \leq C_0\,h^2$). The constant C depends on the bounds for the function f and its first few derivatives.

Remark. In scheme (2-55), if we replace β' by $\nu\,\beta'$, ϑ' by $\nu^2\vartheta'$, and P_n by $\nu\,P_n$, then we obtain the corresponding scheme (0–9) for solving equation (0–2). As ν tends to zero, this scheme reduces to the ordinary mid-point Runge-Kutta method as we expect.

Before we prove Theorem 2.1, we devote the rest of this section to analyzing the local truncation error T_n of scheme (2-55), which is defined in the equation:

$$x(t_{n+1}) = x(t_n) + \Delta_n w + \frac{1}{2}h[\, f(q'(t_n) + \sqrt{h}P_n) + f(q'(t_n) - \sqrt{h}P_n)\,] + T_n \,. \tag{2-56}$$

Recall the definition of $q_n'(t_n)$ in (2-48). We start by considering a Taylor expansion of $f(q'(t_n) + \sqrt{h}P_n)$ about $q(t_n)$:

$$f(q'(t_n) + \sqrt{h}P_n) = f(q'(t_n)) + \sqrt{h}P_n f_x(q'(t_n)) + \frac{1}{2}hP_n{}^2 f_{xx}(q'(t_n)) + \frac{1}{6}h^{\frac{3}{2}}P_n{}^3 f_{xxx}(q'(t_n)) + \frac{1}{24}h^2 P_n{}^4 f_{xxxx}(q'(t_n)) + O(h^{\frac{5}{2}}) \tag{2-57}$$

and a Taylor expansion of $f(q'(t_n) + \sqrt{h}P_n)$ about $q'(t_n)$:

$$f(q'(t_n) - \sqrt{h}P_n) = f(q'(t_n)) - \sqrt{h}P_n f_x(q'(t_n)) + \frac{1}{2}hP_n{}^2 f_{xx}(q'(t_n)) - \frac{1}{6}h^{\frac{3}{2}}P_n{}^3 f_{xxx}(q'(t_n)) + \frac{1}{24}h^2 P_n{}^4 f_{xxxx}(q'(t_n)) + O(h^{\frac{5}{2}}) \,. \tag{2-58}$$

Summing up the results in (2-57) and (2-58), we obtain, after some cancellation,

$$\frac{1}{2}h[\, f(q'(t_n) + \sqrt{h}P_n) + f(q'(t_n) - \sqrt{h}P_n)\,] = hf(q'(t_n)) + \frac{1}{2}h^2 P_n{}^2 f_{xx}(q'(t_n)) + \frac{1}{24}h^3 P_n{}^4 f_{xxxx}(q'(t_n)) + O(h^{\frac{7}{2}}) \,. \tag{2-59}$$

The second term on the right hand side is then expanded in a Taylor series about $q(t_n)$. We obtain:

$$\begin{aligned} \frac{1}{2}h^2 P_n{}^2 f_{xx}(q'(t_n)) &= \frac{1}{2}h^2 P_n{}^2 f_{xx}(q(t_n) + \sqrt{h}\,\beta') \\ &= \frac{1}{2}h^2 P_n{}^2 f_{xx}(x(t_n)) + \frac{1}{2}h^{\frac{5}{2}}\beta' P_n{}^2 f_{xxx}(x(t_n)) \\ &\quad + \frac{1}{4}h^3 P_n{}^2 f(x(t_n)) f_{xxx}(x(t_n)) + \frac{1}{4}h^3 \beta'^2 P_n{}^2 f_{xxxx}(x(t_n)) + O(h^{\frac{7}{2}}) \,. \end{aligned} \tag{2-60}$$

In a similar way, the third term on the right hand can be expanded as

$$\frac{1}{24}h^3 P_n^4 f_{xxxx}(q'(t_n)) = \frac{1}{24}h^3 P_n^4 f_{xxxx}(x(t_n)) + O(h^{\frac{7}{2}}) .$$

Substituting this result and that in (2-60) into (2-59), we obtain:

$$\frac{1}{2}h[\, f(q'(t_n)+\sqrt{h}P_n)+ f(q'(t_n)-\sqrt{h}P_n)\,] \tag{2-61}$$

$$= hf(q'(t_n))+ \frac{1}{2}h^2 P_n^2 f_{xx}(x(t_n)) + \frac{1}{2}h^{\frac{5}{2}}\beta' P_n^2 f_{xxx}(x(t_n))$$

$$+ \frac{1}{4}h^3 P_n^2 f(x(t_n))f_{xxx}(x(t_n)) + \frac{1}{4}h^3\beta'^2 P_n^2 f_{xxxx}(x(t_n)) + \frac{1}{24}h^3 P_n^4 f_{xxxx}(x(t_n)) + O(h^{\frac{7}{2}})$$

Recalling the definition $P_n = \sqrt{\vartheta' - \beta'^2}$ and substituting the result in (2-61) into (2-56), we obtain:

$$x(t_{n+1}) = x(t_n) + \Delta_n w + hf(q'(t_n)) + \frac{1}{2}h^2[\vartheta' - \beta'^2]f_{xx}(x(t_n)) \tag{2-62}$$

$$+ \frac{1}{2}h^{\frac{5}{2}}\beta' P_n^2 f_{xxx}(x(t_n)) + \frac{1}{4}h^3 P_n^2 f(x(t_n))f_{xxx}(x(t_n))$$

$$+ \left[-\frac{1}{8}h^3\beta'^4 + \frac{1}{6}h^3\beta'^2\vartheta' + \frac{1}{24}h^3\vartheta'^2 \right] f_{xxxx}(x(t_n)) - T_n + O(h^{\frac{7}{2}}) .$$

By comparing this expression with that in (2-47), we can relate T_n and T_n' in the equation:

$$-T_n' = -T_n + \frac{1}{2}h^{\frac{5}{2}}[\beta'\vartheta' - \beta'^3]f_{xxx}(x(t_n))$$

$$+ \frac{1}{4}h^3[\vartheta' - \beta'^2]f(x(t_n))f_{xxx}(x(t_n))$$

$$+ \left[-\frac{5}{24}h^3\beta'^4 + \frac{1}{6}h^3\beta'^2\vartheta' + \frac{1}{24}h^3\vartheta'^2 \right] f_{xxxx}(x(t_n)) + O(h^{\frac{7}{2}}) . \tag{2-63}$$

Now we are ready to write down explicitly the local truncation error T_n of scheme (2–55), since we have the relationship (2-52) between R_n and T_n' and the relationship (2-63) between T_n' and T_n.

Again, for convenience of analysis, let us define some useful variables:

$$\gamma \equiv h^{\frac{5}{2}}\gamma' \equiv \int_{t_n}^{t_{n+1}} (s-t_n)\Delta w_s \, ds \, ,$$

$$\tau \equiv h^{\frac{5}{2}}\tau' \equiv \int_{t_n}^{t_n+h} \Delta w_s{}^3 \, ds \, , \qquad (2\text{-}64)$$

$$\delta \equiv h^{\frac{5}{2}}\delta' \equiv \int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r \, drds \, .$$

From these definitions, it is clear that the random variables γ', δ', τ' are all of order 1 in the L_1 sense. With these definitions, we find from R_n in (2-23), (2-52) and (2-63) that the local truncation error T_n can be written in the form:

$$\begin{aligned} -T_n \equiv\ & \frac{1}{2}h^{\frac{5}{2}}(2\gamma'-\beta')f(x(t_n))f_{xx}(x(t_n)) \\ & + h^{\frac{5}{2}}\delta' f_x^2(x(t_n)) \qquad (2\text{-}65) \\ & + \frac{1}{6}h^{\frac{5}{2}}(\tau'-3\beta'\vartheta'+2\beta'^3)f_{xxx}(x(t_n)) - V_n \end{aligned}$$

in which we keep only those terms of order $h^{2.5}$ (e.g. 1^{st}, 4^{th} and 9^{th} terms in R_n) and collect the remaining terms in

$$\begin{aligned} -V_n =\ & \frac{1}{6}h^3 f(x(t_n))f_x^2(x(t_n)) + \frac{1}{2}f_x(x(t_n))\, f_{xx}(x(t_n)) \int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r{}^2 \, drds \qquad (2\text{-}66) \\ & + f_x(x(t_n))\, f_{xx}(x(t_n)) \int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r \Delta w_s \, drds - \frac{1}{12}h^3 f^2(x(t_n))\, f_{xx}(x(t_n)) \\ & + \frac{1}{2}f(x(t_n))f_{xxx}(x(t_n)) \int_{t_n}^{t_n+h} (s-t_n)\Delta w_s{}^2 ds - \frac{1}{4}h^3\vartheta' f(x(t_n))\, f_{xxx}(x(t_n)) \\ & + \left[\frac{1}{6}h^3\beta'^4 - \frac{1}{6}h^3\beta'^2\vartheta' - \frac{1}{24}h^3\vartheta'^2 + \frac{1}{24}\int_{t_n}^{t_n+h} \Delta w_s{}^4 \, ds\right] f_{xxxx}(x(t_n)) + O(h^{\frac{7}{2}}) \, . \end{aligned}$$

2.4 Convergence of the Second Order Runge–Kutta Method

In this section, we will prove Theorem 2.1, i.e., scheme (2–55) with the local truncation error T_n in (2-65) is of order h^2 in the L_2 sense under the conditions stated in the theorem. For this purpose, let us write down the following equations: the numerical scheme (2-55):

$$X_{n+1} = X_n + \Delta_n w + \frac{1}{2}h[\, f(Q_n' + \sqrt{h}P_n) + f(Q_n' - \sqrt{h}P_n)\,] \quad (2\text{-}67)$$

and the exact equation with local truncation error:

$$x(t_{n+1}) = x(t_n) + \Delta_n w + \frac{1}{2}h[\, f(q'(t_n) + \sqrt{h}P_n) + f(q'(t_n) - \sqrt{h}P_n)\,] - T_n \quad (2\text{-}68)$$

Let e_n denote $X_n - x(t_n)$. Like in the theory of ordinary differential equations, we subtract equation (2-68) from equation (2-67). This gives

$$e_{n+1} = e_n + \frac{1}{2}h\, v_n + T_n \quad (2\text{-}69)$$

where we define

$$v_n = v_{n,+} + v_{n,-} \quad (2\text{-}70)$$

and

$$v_{n,+} = f(q'(t_n) + \sqrt{h}P_n) - f(Q_n' + \sqrt{h}P_n),$$

$$v_{n,-} = f(q'(t_n) - \sqrt{h}P_n) - f(Q_n' - \sqrt{h}P_n).$$

To make an L_2 norm analysis, let us square both sides of equation (2-67), then

$$e_{n+1}^2 = e_n^2 + h e_n v_n + \frac{1}{4}h^2 v_n^2 + 2e_n T_n + h\, v_n T_n + T_n^2 .$$

We now estimate the expectations of the last five terms on the right hand side of the above equation. Let f satisfy the following Lipshitz condition:

$$|f(x) - f(y)| \le L\, |x - y|, \quad x, y \in R .$$

where $L \ge 0$ is a constant. Consider $v_{n,+}$, $v_{n,-}$; and apply the Lipshitz condition of f to them. We find

$$|v_{n,+}| = |f(q(t_n)+\sqrt{h}(\beta'+P_n)) - f(Q_n+\sqrt{h}(\beta'+P_n))|$$
$$\leq L|q(t_n) - Q_n|$$
$$= L|(x(t_n)+\frac{1}{2}hf(x(t_n))) - (X_n+\frac{1}{2}hf(X_n))|$$
$$\leq L(1+\frac{1}{2}hL)|e_n|$$

and

$$|v_{n,-}| = |f(q(t_n)+\sqrt{h}(\beta'-P_n)) - f(Q_n+\sqrt{h}(\beta'-P_n))|$$
$$\leq L|q(t_n) - Q_n|$$
$$= L|(x(t_n)+\frac{1}{2}hf(x(t_n))) - (X_n+\frac{1}{2}hf(X_n))|$$
$$\leq L(1+\frac{1}{2}hL)|e_n|\ .$$

Therefore, the second term on the right hand side of equation (2-71) can be estimated as:

$$|E[he_n v_n]| \leq hE|e_n v_n| \leq hE(|e_n||v_{n,+}+v_{n,-}|) \leq 2hL(1+\frac{1}{2}hL)E[e_n^2]\ .$$

The estimation of the third term is quite similar and we have, by the Lipschitz condition for f,

$$E[\frac{1}{4}h^2 v_n{}^2] \leq \frac{1}{4}h^2 E[v_n^2] \leq h^2 L^2 (1 + \frac{1}{2}hL)^2 E[e_n^2]\ . \qquad (2\text{-}73)$$

Next comes the fourth term where we need to take into account T_n given in (2-65), thus V_n in (2-66). Recall that those terms in which the independent increment Δw appears in odd power will vanish after taking the expectation. Thus

$$-E[T_n] = -E[V_n] \qquad (2\text{-}74)$$
$$= E\left\{\frac{1}{6}ff_x{}^2 + \frac{1}{12}f_x f_{xx} + \frac{1}{6}f_x f_{xx} - \frac{1}{12}f^2 f_{xx} + \frac{1}{6}ff_{xxx}\right\}\cdot h^3$$

$$+ E\left\{\left\{-\frac{1}{8}ff_{xxx} + [\frac{1}{6}\cdot\frac{1}{3} - \frac{1}{6}\cdot\frac{13}{30} - \frac{1}{24}\cdot\frac{7}{12} + \frac{1}{24}] f_{xxxx}\right\}h^3 + O(h^4)\right\}$$

$$= E\left\{\left\{\frac{1}{6}f_x^2 + \frac{1}{4}f_x f_{xx} + \frac{1}{24}f^2 f_{xx} + \frac{1}{24}ff_{xxx} + \frac{1}{1440}f_{xxxx}\right\}h^3 + O(h^4)\right\}.$$

where all the functions' values are evaluated at $x(t_n)$. The detailed derivation of (2–74) is carried out in lemma 3 of appendix A. This result suggests that we write $E[V_n] = h^3 E[V_n']$, where $V_n' = h^{-3}V_n$ is of order h^0 in the L_2 sense. Therefore, the independence of e_n and the increments of a Wiener process leads to the following estimate:

$$|E[2e_n T_n]| = 2h^3 |E[e_n V_n']| \le \varepsilon_1 hLE[e_n^2] + \varepsilon_1^{-1}L^{-1}h^5 E[V_n'^2] \qquad (2\text{-}75)$$

where we use twice the arithmetic inequality $2ab \le a^2 + b^2$ with

$$a = (\varepsilon_1 hL)^{\frac{1}{2}} e_n \quad \text{and} \quad b = (\varepsilon_1 hL)^{-\frac{1}{2}} h^2 V_n'$$

and ε_1 is an appropriate positive number. A similar trick can be applied to the fifth term, and yields

$$|E[hv_n T_n]| \le \frac{1}{2}[\ \varepsilon_2 hL^{-1}E(v_n^2) + \varepsilon_2^{-1}hLE(T_n^2)\ ] \qquad (2\text{-}76)$$

$$\le \frac{1}{2}\varepsilon_2\, hL(1 + \frac{1}{2}hL)^2\ E[e_n^2] + O(h^6)$$

where again ε_2 is an appropriate positive number and $E[T_n^2]$ is of order h^5 (see below). Finally we arrive at the estimation of the expectation $E[T_n^2]$. By the Cauchy-Schwartz inequality, we have $(a+b+c)^2 \le 3\ (a^2+b^2+c^2)$, and if we apply this result to T_n^2, we find the estimate:

$$E[T_n^2] \le 3\cdot\frac{1}{4}h^5 E[(2\gamma' - \beta')^2] E[f^2 f_{xx}^2] \qquad (2\text{-}77)$$

$$+ 3\cdot E(\delta'^2)h^5 E[f_x^4] + 3\cdot\frac{1}{36}h^5 E[(\tau' - 3\beta'\vartheta' + 2\beta'^3)^2] E[f_{xxx}^2] + O(h^6)$$

$$= 3\cdot\frac{1}{4}\,\frac{1}{30}h^5E[f^2f_{xx}^2] + 3\cdot\frac{1}{20}h^5E[f_x^4] + 3\cdot\frac{1}{36}\,\frac{11}{2520}h^5E[f_{xxx}^2] + O(h^6)\,.$$

where all the functions' values are evaluated at $x(t_n)$. Therefore we have the following estimate:

$$E[T_n^2] \le \left\{ \frac{1}{40}E[f^2f_{xx}^2] + \frac{3}{20}E[f_x^4] + \frac{11}{30240}E[f_{xxx}^2] \right\} h^5 + O(h^6)$$

which, for convenience, will be written as

$$E[T_n^2] \le E[G_n^2]\,h^5 + O(h^6)\,. \tag{2-78}$$

where

$$G_n^2 = \frac{1}{40}E[f^2f_{xx}^2] + \frac{3}{20}E[f_x^4] + \frac{11}{30340}E[f_{xxx}^2]$$

is of order h^0. For a detailed calculation involved in (2-77), we refer to Lemma 4 of Appendix A. Finally, we reach the stage of estimating the whole equation (2−71). By collecting the results from (2−72)–(2−78) and taking expectations on both sides of equation (2-71), we obtain:

$$E[e_{n+1}^2] \le B(h)E[e_n^2] + [E(G_n^2) + \frac{1}{2}\varepsilon_1^{-1}L^{-1}E(V_n^2)]h^5 + O(h^6) \tag{2-79}$$

where

$$B = B(h) = 1 + (2 + \varepsilon_1 + \varepsilon_2)hL + (2 + \frac{\varepsilon_2}{2})h^2L^2 + [1 + \frac{1}{8}\varepsilon_2]h^3L^3 + \frac{1}{4}h^4L^4\,.$$

To have a common bound for all time steps, let us define

$$G \equiv \max_n E[G_n^2] \quad \text{and} \quad V \equiv \max_n E[\,V_n^2\,]$$

and let $M = G + \varepsilon_1^{-1}L^{-1}V$, the inequality (2-79) becomes

$$E[e_{n+1}^2] \le e^{(2+\varepsilon)hL}E[e_n^2] + M\,h^5 + O(h^6) \tag{2-80}$$

where we set $\varepsilon = \varepsilon_1 + \varepsilon_2$ so that $B(h) \le e^{(2+\varepsilon)hL}$. This is a recursive relation we encounter often in the theory of ordinary differential equations. An elementary calculation shows that the solution of (2-80) is

$$E[e_n^2] \le \frac{e^{(2+\varepsilon)t_n L} - 1}{(2+\varepsilon)L} M\, h^4 + e^{(2+\varepsilon)t_n L} E[e_0^2] + O(h^5)\,. \qquad \text{(2-81)}$$

The right hand side of this inequality is of order h^4 provided that the initial condition is properly imposed. Suppose that $E[e_0^2] \le C_0^2\, h^4$, where C_0 is a constant. Substituting this into the above equation and taking square root on both sides of the resultant inequality, we complete the proof of Theorem 2.1 with

$$C = \sup_{h \le h_0} \left\{ \frac{M}{(2+\varepsilon)L} (e^{(2+\varepsilon)TL} - 1) + C_0^2 \cdot e^{(2+\varepsilon TL)} + O(h) \right\}^{\frac{1}{2}}. \qquad \text{(2-82)}$$

Remark. The reason of introducing the two positive numbers ε_1 and ε_2 is twofold: to keep track of the 'interaction' between T_n and e_n (see (2-75)) or v_n (see (2–76)), and to balance the error contributions from the initial error and local truncation errors (see (2-81)) in hope that the constant C can be minimized with suitable choice of ε.

2.5 Runge–Kutta Methods of Order One and Half

There are two main difficulties with scheme (2-55): the first one is that we do not have an efficient way to sample systematically the Gaussian variables β', $\Delta \underline{w}_n$ and the non-Gaussian random variable ϑ' (defined in (2-44)); and the second one is that it will not be a second order method when extended to the case of a system. To see the complexity of the distribution of ϑ', we refer to Levy [16].

To sample only Gaussian random variables, one should be content with schemes with less accuracy. In this section, we provide such schemes of order $h^{1.5}$ in the L_2 sense. The main advantage with these schemes is that they will maintain the order of accuracy when extended to a system of stochastic differential equations.

To design a scheme of order $h^{1.5}$, we have several choices. Let us consider first the following theorem.

Theorem 2.2. Under the same conditions of Theorem 1, the following scheme

$$Q_n = X_n + \frac{1}{2}hf(X_n) \tag{2-83}$$

$$Q_n^* = X_n + \frac{1}{2}hf(X_n) + \frac{3}{2}\sqrt{h}\,\beta'$$

$$X_{n+1} = X_n + \Delta_n w + \frac{1}{3}h\,[\,f(Q_n) + 2\cdot f(Q_n^*)\,]$$

has 1.5 order accuracy in the L_2 sense (see (0-4) for the definition).

Proof. There is no substantial difference between this proof and that of Theorem 1. We need only to assure whether the techniques used in the latter can be applied in this case. The key point is to examine the local truncation error of scheme (2-83). Let us define

$$q^*(t_n) = x(t_n) + \frac{1}{2}hf(x(t_n)) + \frac{3}{2}\sqrt{h}\,\beta' \,. \tag{2-84}$$

Then the local truncation error T_n' of the scheme (2-83) is defined in the equation:

$$x(t_{n+1}) = x(t_n) + \Delta_n w + \frac{1}{3}h[\,f(q(t_n)) + 2\cdot f(q^*(x(t_n))\,] + T_n' \,. \tag{2-85}$$

To make an error analysis, let us carry out the following Taylor expansion of $f(q^*(t_n))$:

$$hf(q^*(t_n)) = hf(q(t_n) + \frac{3}{2}\sqrt{h}\,\beta') \tag{2-86}$$

$$= hf(q(t_n)) + \frac{3}{2}h^{\frac{3}{2}}\beta' f_x(x(t_n)) + \frac{9}{8}h^2\beta'^2 f_{xx}(x(t_n)) + O(h^{\frac{5}{2}})$$

$$= hf(q(t_n)) + \frac{3}{2}f_x(x(t_n))\int_{t_n}^{t_n+h}\Delta w_s\, ds + \frac{9}{8}h^2\beta'^2 f_{xx}(x(t_n)) + O(h^{\frac{5}{2}}) .$$

Replacing $f(q^*(t_n))$ in (2-85) by the above expression, we obtain

$$x(t_{n+1}) = x(t_n) + \Delta_n w + hf(q(t_n)) \tag{2-87}$$
$$+ f_x(x(t_n))\int_{t_n}^{t_n+h}\Delta w_s\, ds + \frac{3}{4}h^2\beta'^2 f_{xx}(x(t_n)) + T_n' + O(h^{\frac{5}{2}}) .$$

Comparing the above expression with that in (2-42) and recalling that R_n is of order $h^{2.5}$, we arrive at

$$T_n' = \frac{1}{2}f_{xx}(x(t_n))\int_{t_n}^{t_n+h}\Delta w_s^2\, ds - \frac{3}{4}h^2\beta'^2 f_{xx}(x(t_n)) + O(h^{\frac{5}{2}}) . \tag{2-88}$$

One major fact about T_n' is that its expectation is of order h^3. The reason is that (i) the expectations of those terms of order $h^{2.5}$ is zero, and (ii) $E[(\beta')^2] = \frac{1}{3}$ (see appendix A.) and

$$E[\int_{t_n}^{t_n+h}\Delta w_s^2\, ds\ ] = \int_0^h s\ ds = \frac{1}{2}h^2 \tag{2-89}$$

which make the expectations of the leading terms in in T_n' cancel each other. With this fact in mind, the rest of the proof proceeds exactly in the same way as in the proof of theorem 1.

The general idea in designing a scheme of order $h^{1.5}$ like (2-83) is to consider the family of schemes:

$$Q_n = X_n + \frac{1}{2}hf(X_n) + k\sqrt{h}\,\beta' \tag{2-90}$$

$$Q_n' = X_n + \frac{1}{2}hf(X_n) + l\sqrt{h}\,\beta'$$

$$X_{n+1} = X_n + \Delta_n w + h[\ af(Q_n) + bf(Q_n')\ ]$$

where a, b, k, l are parameters to be determined. In a similar way as we did in theorem 2, we find that the exact solution of of stochastic equation satisfies:

$$x(t_{n+1}) = x(t_n) + \Delta_n w + h(a+b)f(q(t_n)) \tag{2-91}$$

$$+ h(a\cdot k + b\cdot l)\beta' f_x(x(t_n)) + \frac{1}{2}h(a\cdot k^2 + b\cdot l^2)\beta'^2 f_{xx}(x(t_n)) + O(h^{\frac{5}{2}}) + T_n^*.$$

By comparing the above expression and (2-26), we are led to choose

$$a + b = 1 \ , \quad a\cdot k + b\cdot l = 1 \tag{2-92}$$

in order that scheme (2–90) have first order accuracy. With these choices, the local truncation error T_n^* of scheme (2-80) is

$$T_n^* = \frac{1}{2}f_{xx}(x(t_n))\int_{t_n}^{t_n+h} \Delta w_s{}^2 ds - \frac{1}{2}h(a\cdot k^2 + b\cdot l^2)\beta'^2 f_{xx}(x(t_n)) + O(h^{\frac{5}{2}}) \, . \tag{2-93}$$

However, as we understand from the proofs of theorem 2 (or 1), we may wish to minimize the contribution of the local truncation error T_n^*. One way to achieve this is to choose the parameters so that the expectations of the leading terms of T_n^* are zero (e.g. in (2-88)). This leads to

$$a\cdot k^2 + b\cdot l^2 = \frac{3}{2}. \tag{2-94}$$

The case corresponding to scheme (2-83) is $a = \frac{1}{3}$, $b = \frac{2}{3}$, $k = 0$, $l = \frac{3}{2}$. We make this choice so that we need only three function's evaluations at each time step, and all parameters are rational numbers with a, b positive.

Chapter 3

Runge–Kutta Methods for a System

In this chapter, we consider the following d dimensional system of stochastic differential equations (see chapter 1):

$$d\underline{x} = \underline{f}(\underline{x})\, dt + \nu\, d\underline{w}_t\ , \quad 0 \le t \le T\ , \tag{3-1}$$

where $\nu \ge 0$ is a constant and $\underline{f} = \underline{f}(\underline{x})$ is a smooth function satisfying a Lipshitz condition. The main results are stated in theorem 3.1 (in section 3.2) and theorem 3.2 (in section 3.3).

We start, in section 3.1, by analyzing the local truncation error of the splitting scheme based on the mid-point rule, an analysis that parallels section 2.1. Then, in section 3.2, we derive a Taylor series method which we prove to have second order accuracy in the L_2 sense, and explain why the Runge-Kutta method derived in section 2.3 does not generalize to the system of equations (3-1).

On the basis of this Taylor series method, in section 3.3, we develop Runge-Kutta methods under the consideration of the weak convergence sense, defined in (0–14). Finally, in section 3.4, we extend the Runge-Kutta methods derived in section 2.5, and prove that they maintain their accuracy for the system case. We also discuss the convergence of these methods in the weak sense.

3.1 Analysis of a Splitting Scheme Based on the Mid–Point Rule

Consider a partition of the interval $[0,\ T]$:

$$\Pi = [\ 0, \cdots, t_{n+1} = t_n + h, \cdots, t_l = T\ ]$$

and the splitting scheme based on the mid-point rule

$$\underline{X}_{n+1} = \underline{X}_n + \Delta_n \underline{w} + h\underline{f}(\underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n)) \tag{3-2}$$

for solving the stochastic differential equation (3-1), where $\Delta_n \underline{w} = \underline{w}_{t_{n+1}} - \underline{w}_{t_n}$.

In analogy with the analysis of numerical methods for ordinary differential equations, we analyze the local truncation error $-\underline{D}_n$ of the scheme (3–2), which is defined by the equation

$$\underline{x}(t_n) = \underline{x}(t_n) + \Delta_n \underline{w} + h\underline{f}(\underline{x}(t_n) + \frac{1}{2}h\underline{f}(\underline{x}(t_n))) - \underline{D}_n \, . \tag{3-3}$$

To facilitate the discussion, we define, for each specified interval, say $[t_n, t_{n+1}]$, the variable:

$$\underline{y}(t) = \underline{x}(t) - \Delta \underline{w}_t \, , \quad t_n \le t \le t_{n+1} = t_n + h \, , \tag{3-4}$$

where $\Delta w_t = \underline{w}_t - w_{t_n}$. From this definition, it follows immediately that

$$\underline{y}(t_n) = \underline{x}(t_n) \tag{3-5}$$

for the specified interval. Substituting the definitions in (3-4) into equation (3-1) and the scheme (3-4), we obtain respectively

$$\frac{d\underline{y}}{dt} = \underline{f}(\underline{y} + \Delta \underline{w}_t) \, , \quad t_n < t < t_n + h \tag{3-6}$$

$$\underline{y}(t_n) = \underline{x}(t_n)$$

and

$$-\underline{D}_n = \underline{y}(t_n) - \underline{y}(t_n) - h\underline{f}(\underline{x}(t_n) + \frac{1}{2}h\underline{f}(\underline{x}(t_n))) \, . \tag{3-7}$$

For convenience of analysis, we will write $-\underline{D}_n$ in an integral form. Integrating equation (3-6) from t_n to $t_n + h$, we find

$$\underline{y}(t_{n+1}) - \underline{y}(t_n) = \int_{t_n}^{t_n+h} \underline{f}(\underline{y}(s) + \Delta \underline{w}_s) \, ds \, , \tag{3-8}$$

and since $\underline{x}(t_n)$ is a random variable for fixed t_n, we have

$$h\underline{f}(\underline{x}(t_n) + \frac{1}{2}h\underline{f}(\underline{x}(t_n))) = \int_{t_n}^{t_n+h} \underline{f}(\underline{x}(t_n) + \frac{1}{2}h\underline{f}(\underline{x}(t_n)))\, ds . \qquad (3\text{-}9)$$

Substituting the results in (3-8) and (3-9) into $-\underline{D}_n$ of (3-7), we obtain

$$-\underline{D}_n = \int_{t_n}^{t_n+h} [\, \underline{f}(\underline{y}(s) + \Delta\underline{w}_s) - \underline{f}(\underline{x}(t_n) + \frac{1}{2}h\underline{f}(\underline{x}(t_n)))\,]\, ds . \qquad (3\text{-}10)$$

With $-\underline{D}_n$ in this form, further analysis can be made because of the differentiability of the function $\underline{f}$.

As we did in section 2.1, we will show that each component $-D_n^i$ of $-\underline{D}_n$ is of order $h^{1.5}$ in the L_1 sense and in the L_2 sense.

In the following, we will adopt the *summation convention*, which says that any repeated subscript or superscript in a multiplication term is to be summed over its range, e.g., $a_j^i b^j = \sum_j [a_j^i b^j]$ (there is no summation over i).

Let us stipulate that a superscript specifies the component, and subscripts with a comma in the first place denote differentiation, e.g., $f^i_{,jk}$ means differentiation of f^i with respect to its j^{th} and k^{th} arguments.

Now we expand each term in the integrand of $\underline{D}_n$ of (3-10) in a Taylor series around $\underline{x}(t_n) = \underline{y}(t_n)$. Define the variable $\Delta\underline{x}_s = \Delta\underline{y}(s) - \underline{y}(t_n) + \Delta\underline{w}_s$, we have

$$f^i(\underline{y}(s) + \Delta\underline{w}_s) = f^i(\underline{x}(t_n) + [\underline{y}(s) - \underline{y}(t_n) + \Delta\underline{w}_s]) = \qquad (3\text{-}11)$$

$$f^i(\underline{x}(t_n)) + f^i_{,j}(\underline{x}(t_n))\Delta x_s{}^j + \frac{1}{2}f^i_{,jk}(\underline{x}(t_n))\Delta x_s{}^j\Delta x_s{}^k + \frac{1}{6}f^i_{,jkl}(\underline{x}(t_n))\Delta x_s{}^j\Delta x_s{}^k\Delta x_s{}^l$$

$$+ \frac{1}{24}\int_0^1 f^i_{,jklm}(\underline{x}(t_n))\Delta x_s{}^j\Delta x_s{}^k\Delta x_s{}^l\Delta x_s{}^m$$

$$+ \frac{1}{120}f^i_{,jklmn}(\underline{x}'(\underline{x}(t_n))\Delta x_s{}^j\Delta x_s{}^k\Delta x_s{}^l\Delta x_s{}^m\Delta x_s{}^n$$

where the last term is the Lagrangian expression of remainder ot the Taylor expansion. In the same way, we have

$$f^i(\underline{x}(t_n) + \frac{1}{2}h\underline{f}(\underline{x}(t_n))) = \underline{f}(\underline{x}(t_n)) \tag{3-12}$$

$$+ \frac{1}{2}hf^i_{;j}(\underline{x}(t_n))\underline{f}^j(\underline{x}(t_n)) + \frac{1}{8}h^2f^i_{;jk}(\underline{x}(t_n))f^j(\underline{x}(t_n))f^j(\underline{x}(t_n))$$

$$+ \frac{1}{48}h^3f^i_{;jkl}(\underline{x}''(t_n))f^j(\underline{x}(t_n))f^k(\underline{x}(t_n))f^l(\underline{x}(t_n))$$

where, again, we use the Cauchy expression of the remainder. To estimate these remainders, we make the following assumptions:

$$\sup_{\underline{x}} \left| \frac{\partial^{\mu_1 + \cdots + \mu_n}}{\partial^{\mu_1}x_1 \cdots \partial^{\mu_n}x_n} f^i(\underline{x}) \right| \ \textit{are bounded}\,, \tag{3-13}$$

$$\text{for } 0 \le \mu_1 + \cdots + \mu_n \le 5, \quad 0 \le i \le d\,.$$

From this definition, it follows immediately that the remainder in (3-12) is of order h^3 in the L_1 and L_2 sense . Thus we can write (3-12) in the form:

$$f^i(\underline{x}(t_n) + \frac{1}{2}h\underline{f}(\underline{x}(t_n))) = f^i(\underline{x}(t_n)) \tag{3-14}$$

$$+ \frac{1}{2}f^i_{;j}(\underline{x}(t_n))f^j(\underline{x}(t_n))$$

$$+ \frac{1}{6}h^2f^i_{;j}(\underline{x}(t_n))f^j(\underline{x}(t_n))f^k(\underline{x}(t_n)) + O(h^3)$$

To analyze the order of the remainder of the expansion (3-11), more work is needed. Let E denote the expectation, as before. Recalling that $\Delta\underline{w}_s$ is a Gaussian random vector of which each component has mean 0 and variance $\Delta s = s - t_n$ and is independent of each other, we see from (2-18) that

$$E|\Delta w_s^{j_1} \cdots \Delta w_s^{j_d}| = E|\Delta w_s^{j_1}| \cdots E|\Delta w_s^{j_d}| \tag{3-15}$$

$$= [\frac{2}{\pi}\Delta s]^{\frac{1}{2}d} \le [\frac{2}{\pi}]^{\frac{1}{2}d} \cdot [s - t_n]^{\frac{1}{2}d} \le const. \cdot h^{\frac{1}{2}d}\,.$$

which says that the product $\Delta w_s^{j_1} \cdots \Delta w_s^{j_d}$ is of order $h^{\frac{1}{2}d}$. In general, $[\Delta w_s^{j_1}]^{l_1} \cdots [\Delta w_s^{j_d}]^{l_d}$ is of order $h^{\frac{1}{2}(l_1 + \cdots + l_d)}$, since

$$E|[\Delta w_s^{j_1}]^{l_1} \cdots [\Delta w_s^{j_d}]^{l_d}| = E|\Delta w_s^{j_1}|^{l_1} \cdots E|\Delta w_s^{j_d}|^{l_d} \tag{3-16}$$

$$= (\frac{1}{\pi})^d (2\Delta s)^{\frac{1}{2}(l_1+\cdots+l_d)} \cdot \Gamma[\frac{l_1+1}{2}] \cdots \Gamma[\frac{l_d+1}{2}]$$

$$\leq const. \cdot h^{\frac{1}{2}(l_1+\cdots+l_d)} \quad (\Delta s = s - t_n)$$

where Γ is the gamma function. Observe further that

$$(\underline{y}(s) - \underline{y}(t_n))^i = \int_{t_n}^{s} f^i(\underline{y}(r) + \Delta\underline{w}_r)\, dr \qquad (3\text{-}17)$$

which is obtained by integrating (3-6) from t_n to s. Since f^i is bounded by assumption (3-13), we have the estimate:

$$E|(\underline{y}(s) - \underline{y}(t_n))^i| \leq \int_{t_n}^{t_n+h} E|f^i(\underline{y}(r) + \Delta\underline{w}_r)|\, dr \leq const. \cdot h \qquad (3\text{-}18)$$

which shows that $(\underline{y}(s) - \underline{y}(t_n))^i$ is of order h in the L_1 and L_2 sense.

Now we are ready to deal with the remainder in (3-11). The above analysis shows that the leading term of this remainder is

$$f^i_{jklmn}(\underline{x}'(t_n))\Delta w_s{}^j \Delta w_s{}^k \Delta w_s{}^l \Delta w_s{}^m \Delta w_s{}^n$$

and is of order order $h^{2.5}$ in the L_1 and L_2 sense. Furthermore, the same analysis can also be applied to other terms of expansion (3−11) and this enables us to rewrite (3−11) in a more compact form:

$$f^i(\underline{y}(s) + \Delta\underline{w}_s) = f^i(\underline{x}(t_n)) + f^i_{,j}(\underline{x}(t_n))(\underline{y}(s) - \underline{y}(t_n) + \Delta w_s)^j \qquad (3\text{-}19)$$

$$+ \frac{1}{2} f^i_{,jk}(\underline{x}(t_n))(\underline{y}(s) - \underline{y}(t_n) + \Delta w_s)^j (\underline{y}(s) - \underline{y}(t_n) + \Delta w_s)^k$$

$$+ \frac{1}{2} f^i_{,jkl}(\underline{x}(t_n))(\underline{y}(s) - \underline{y}(t_n))^j \Delta w_s{}^k \Delta w_s{}^l + \frac{1}{6} f^i_{,jkl}(\underline{x}(t_n))\Delta w_s{}^j \Delta w_s{}^k \Delta w_s{}^l$$

$$+ \frac{1}{24} f^i_{,jklm}(\underline{x}(t_n))\Delta w_s{}^j \Delta w_s{}^k \Delta w_s{}^l \Delta w_s{}^m + O(h^{\frac{5}{2}})$$

Substituting the results in (3-14) and (3-18) into $-D_n$ of (2-10), we can write, after some cancellations,

$$-D_n^i = f^i_{,j}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \Delta w_s{}^j\, ds + \frac{1}{2} f^i_{,jk}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \Delta w_s{}^j \Delta w_s{}^k\, ds - R_n^i \quad (3\text{-}20)$$

where we keep in $-D_n^i$ only the two terms of expansion (3-11) and put all the other terms in the following remainder

$$-R_n^i = f^i_{,j}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} (\underline{y}(s)-\underline{y}(t_n)-\frac{1}{2}h\underline{f}(\underline{x}(t_n))\,)^j ds \tag{3-21}$$

$$+ f^i_{,jk}(x(t_n)) \int_{t_n}^{t_n+h} [(\underline{y}(s)-\underline{y}(t_n))^j \Delta w_s{}^k + \frac{1}{2}(\underline{y}(s)-\underline{y}(t_n))^j(\underline{y}(s)-\underline{y}(t_n))^k]\, ds$$

$$+ \frac{1}{2} f^i_{,jkl}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} (\underline{y}(s)-\underline{y}(t_n))^j \Delta w_s{}^k \Delta w_s{}^l ds$$

$$+ \frac{1}{6} f^i_{,jkl}(\underline{x}(t_n)) \int_{t_n}^{t_n+n} \Delta w_s{}^j \Delta w_s{}^k \Delta w_s{}^l ds - \frac{1}{8}h^3 f^i_{,jk}(\underline{x}(t_n)) f^j(\underline{x}(t_n)) f^k(\underline{x}(t_n))$$

$$+ \frac{1}{24} f^i_{,jklm}(x(t_n)) \int_{t_n}^{t_n+h} \Delta w_s{}^j \Delta w_s{}^k \Delta w_s{}^l \Delta w_s{}^m ds + O(h^{\frac{7}{2}})\,.$$

Now let us examine the orders of the first two terms of $-D_n^i$ (in (3-20)) in the L_1 sense. From the analyses in (3-15) and (3-16), we see that

(a) $\int_{t_n}^{t_n+h} \Delta w^j \, ds$ is of order $h^{1.5}$ in the L_1 and L_2 sense.

(b) $\int_{t_n}^{t_n+h} \Delta w^j \Delta w^k \, ds$ is of order h^2 in the L_1 and L_2 sense.

Hence, we can assure that $-D_n^i$ (in (3-20)) is at least of order $h^{1.5}$ in the L_1 sense. However, it is still not clear, at this stage, what the order of $-D_n^i$ is in the L_1 sense because the orders of the first three terms of $-R_n^i$ (in (3-21)) cannot be seen readily. Before we go further, we need the following lemma.

Lemma 3.1. For the first three terms in $-R_n^i$ of (3-21), we have the following estimates:

(i)

$$\int_{t_n}^{t_n+h} (y(s)-y(t_n)-\frac{1}{2}hf(\underline{x}(t_n)))^j \, ds$$

$$= f^j_k(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r{}^k \, drds + \frac{1}{6}h^3 f^j_k(\underline{x}(t_n)) f^k(\underline{x}(t_n))$$

$$+ \frac{1}{2} f^j_{kl}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r{}^k \Delta w_r{}^l \, drds + O(h^{\frac{7}{2}})$$

(ii)

$$\int_{t_n}^{t_n+h} (\underline{y}(s)-\underline{y}(t_n))^j \Delta w_s{}^k \, ds$$

$$= f^j(x(t_n)) \int_{t_n}^{t_n+h} (s-t_n)\Delta w_s{}^k \, ds + f^j_l(x(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r{}^k \Delta w_s{}^l \, drds + O(h^{\frac{7}{2}})$$

(iii)

$$\int_{t_n}^{t_n+h} (\underline{y}(s)-\underline{y}(t_n))^j (\underline{y}(s)-\underline{y}(t_n))^k \, ds = \frac{1}{3}h^3 f^j(\underline{x}(t_n)) f^k(\underline{x}(t_n)) + O(h^{\frac{7}{2}})$$

(iv)

$$\int_{t_n}^{t_n+h} (\underline{y}(s)-\underline{y}(t_n))^j \Delta w_s{}^k \Delta w_s{}^l \, ds = f^j(x(t_n)) \int_{t_n}^{t_n+h} (s-t_n)\Delta w_s{}^k \Delta w_s{}^l \, ds + O(h^{\frac{7}{2}}) .$$

Proof. From the analyses in (3-15) and (3-16), we see that the equality (i) can be derived by considering the sequences of equalities:

$$\int_{t_n}^{t_n+h} (\underline{y}(s)-\underline{y}(t_n)-\frac{1}{2}h\underline{f}(\underline{x}(t_n)))^j \, ds$$

$$= \int_{t_n}^{t_n+h} \int_{t_n}^{s} (\underline{f}(\underline{y}(r)+\Delta\underline{w}_r)-\underline{f}(\underline{y}(t_n)))^j \, drds$$

$$= \int_{t_n}^{t_n+h} \int_{t_n}^{s} [\, f^j_k(\underline{y}(t_n))\Delta x^k_r + \frac{1}{2} f^j_{kl}(\underline{y}(t_n))\Delta x^k_r \Delta x^l_r \, drds + O(h^{\frac{7}{2}})$$

$$= f^j_{.k}(x(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r^k \, drds + f^j_{.k}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} (\underline{y}(r) - \underline{y}(t_n))^k \, drds$$

$$+ \frac{1}{2} f^j_{.kl}(x(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r{}^k \Delta w_r{}^l \, drds + O(h^{\frac{7}{2}})$$

where $\underline{x}_r = \underline{y}(r) - \underline{y}(t_n) + \Delta \underline{w}$ as we used in (3-11). The second term on the right hand side of the last equality can be rewritten further:

$$f^j_{.k}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} (\underline{y}(r) - \underline{y}(t_n))^k \, drds$$

$$= f^j_{.k}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} [(r - t_n) f^k(\underline{x}(t_n)) + O(h^{\frac{3}{2}})] \, drds$$

$$= \frac{1}{6} h^3 f^j_{.k}(\underline{x}(t_n)) f^k(\underline{x}(t_n)) + O(h^{\frac{7}{2}}).$$

To prove the second equality (ii), it is more convenient to consider the difference of the left hand side and the first term on the right hand side of it. We have

$$\int_{t_n}^{t_n+h} [\underline{y}(s) - \underline{y}(t_n) - (s - t) \underline{f}(\underline{x}(t_n))]^j \Delta w_s{}^k \, ds$$

$$= \int_{t_n}^{t_n+h} \int_{t_n}^{s} [\underline{f}(\underline{y}(r) + \Delta w_r) - \underline{f}(\underline{y}(t_n))]^j \Delta w_s{}^k \, drds$$

$$= \int_{t_n}^{t_n+h} \int_{t_n}^{s} [f^j_{.l}(\underline{y}(t_n))(\underline{y}(r) - \underline{y}(t_n) + \Delta w_r)^l + O(h)] \Delta w_s{}^k \, drds$$

$$= \int_{t_n}^{t_n+h} \int_{t_n}^{s} [f^j_{.l}(x(t_n)) \Delta w_r{}^l + O(h)] \Delta w_s{}^k \, drds$$

$$= f^j_{.l}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r{}^k \Delta w_s{}^l \, drds + O(h^{\frac{7}{2}})$$

The justification of the equalities (iii) and (iv) can be made by merely recalling the estimate in (3-17). This complete the proof of lemma 1.

From the expression of $-R_n^i$ in (3-21), we see that equality (i) corresponds to the first term of $-R_n^i$, (ii) and (iii) to the second term, and (iv) to the third term of $-R_n^i$. Substituting the results in the lemma into $-R_n^i$ of (3-21), we obtain

$$-R_n^i = f^i_{;j}(\underline{x}(t_n))f^j_{;k}(\underline{x}(t_n)) \int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r{}^k \, drds \tag{3-22}$$

$$+ \frac{1}{6}h^3 f^i_{;j}(\underline{x}(t_n))f^j_{;k}(\underline{x}(t_n))f^k(\underline{x}(t_n)) + \frac{1}{2}f^i_{;j}(\underline{x}(t_n))f^j_{;kl}(\underline{x}(t_n)) \int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r{}^k \Delta w_r{}^l drds$$

$$+ f^i_{;jk}(\underline{x}(t_n))f^j(\underline{x}(t_n)) \int_{t_n}^{t_n+h} (s-t_n)\Delta w_s{}^k ds + f^i_{;jk}(\underline{x}(t_n))f^j_{;l}(\underline{x}(t_n)) \int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r{}^k \Delta w_s{}^l drds$$

$$+ \frac{1}{2}f^i_{;jkl}(\underline{x}(t_n))f^j(\underline{x}(t_n)) \int_{t_n}^{t_n+h} (s-t)\Delta w_s{}^k \Delta w_s{}^l ds$$

$$+ \frac{1}{24}h^3 f^i_{;jk}(\underline{x}(t_n))f^j(\underline{x}(t_n))f^k(\underline{x}(t_n)) + \frac{1}{6}f^i_{;jkl}(x(t_n)) \int_{t_n}^{t_n+h} \Delta w_s{}^j \Delta w_s{}^k \Delta w_s{}^l ds$$

$$+ \frac{1}{24}f^i_{;jklm}(x(t_n)) \int_{t_n}^{t_n+h} \Delta w_s{}^j \Delta w_s{}^k \Delta w_s{}^l \Delta w_s{}^m \, ds + O(h^{\frac{7}{2}}).$$

where all but the last three terms are obtained from the equalities in lemma 1. Examining each term on the right hand side of (3–22), we find that the leading terms are the 1^{st}, 4^{th} and 8^{th} term, which are of order $h^{\frac{5}{2}}$. This observation enables us to write

$$-R_n^i = f^i_{;j}(\underline{x}(t_n))f^j_{;k}(\underline{x}(t_n)) \int_{t_n}^{t_n+h}\int_{t_n}^{s} \Delta w_r^k \, drds \tag{3-23}$$

$$+ f^i_{;jk}(\underline{x}(t_n))f^j(\underline{x}(t_n)) \int_{t_n}^{t_n+h} (s-t_n)\Delta w_s^k \, ds$$

$$+ \frac{1}{6}f^i_{;jkl}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \Delta w_s^j \Delta w_s^k \Delta w_s^l \, ds + O(h^3).$$

Thus $-R_n^i$ is of order $h^{2.5}$ in the L_1 sense, and we conclude that $-D_n^i$ is of order

$h^{1.5}$ in the L_1 sense.

Actually, the above conclusions also hold for the L_2 analysis, i.e., $-\underline{D}_n$ and $-\underline{R}_n$ are of order $h^{1.5}$ and $h^{2.5}$, respectively. We need only to make sure that the expectations involved in above discussion also exist if taken in the L_2 sense, which is guaranteed by the assumption (3-13).

For the sake of brevity and convenience in later discussion, we introduce the variables:

$$\beta^j \equiv h^{\frac{3}{2}}\beta'^j \equiv \int_{t_n}^{t_n+h} \Delta w^j \, ds \ , \quad \vartheta^{jk} \equiv h^2 \vartheta'^{jk} \equiv \int_{t_n}^{t_n+h} \Delta w^j \Delta w^k \, ds \ . \qquad (3\text{-}24)$$

Then the expression of $-D_n^i$ in (3-20) can be written as

$$-D_n^i = f^i_{,j}(\underline{x}(t_n))\beta^j + \frac{1}{2} f^i_{,jk}(\underline{x}(t_n))\vartheta^{jk} - R_n^i \qquad (3\text{-}25)$$

Furthermore, we introduce

$$\vartheta^{jkl} = \int_{t_n}^{t_n+h} \Delta w_s^j \Delta w_s^k \Delta w_s^l \, ds \qquad (3\text{-}26)$$

and

$$\gamma^k = \int_{t_n}^{t_n+h} \int_{t_n}^{s} \Delta w_r{}^k \, dr ds \ , \quad \delta^k = \int_{t_n}^{t_n+h} (s - t_n)\Delta w_s^k \, ds \ . \qquad (3\text{-}27)$$

The expression of $-R_n^i$ in (3-23) can be rewritten as

$$-R_n^i = f^i_{,j}(\underline{x}(t_n)) f^j_{,k}(\underline{x}(t_n))\gamma^k \qquad (3\text{-}28)$$
$$+ f^i_{,jk}(\underline{x}(t_n)) f^j(\underline{x}(t_n))\delta^k + \frac{1}{6} f^i_{,jkl}(\underline{x}(t_n))\vartheta^{jkl} + O(h^3) \ .$$

Remark. Recall the estimates in (3-15), (3-16) and the nonanticipating property of the solution of stochastic differential equation. As we have done in the remark of section 2.1, we conclude that any stochastic quantity whose order is of the form: $k + 0.5$ (k is an integer) in the L_1 sense has zero expectation, since the components of the Wiener process are independent of each other and these components, as a whole, must appear with odd power in the stochastic quantity considered. This important observation suggests to us to consider the convergence of a stochastic scheme in the L_2 sense instead of the L_1 sense since L_2 analysis exploits the nonanticipating property while the latter does not.

3.3 A Second Order Taylor Series Method

In this section, we will prove second order accuracy (in the L_2 sense) of a Taylor series method and explain why the result in theorem 2.1 of section 2.2 does not generalize to a system of stochastic differential equations. This Taylor series is derived as an intermediate step and will serve as a basis for the Runge-Kutta method.

A close look at equation (3-3), (3-7) and the expressions of $-D_n^i$ and $-R_n^i$ given in (3-10) and (3–21) leads us to consider the following Taylor series method:

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) \tag{3-29}$$

$$\underline{X}_{n+1} = \underline{X}_n + \Delta\underline{w}_n + h\underline{f}(\underline{Q}_n)$$

$$+ \underline{f}_{,j}(\underline{X}_n)\int_{t_n}^{t_n+h} \Delta\underline{w}_s{}^j\, ds + \frac{1}{2}\underline{f}_{,jk}(\underline{X}_n)\int_{t_n}^{t_n+h} \Delta w_s{}^j \Delta w_s{}^k\, ds$$

with the local truncation error $-R_n^i$ given in (3-22) (or (3–23)), where we note the appearance of cross derivative terms of $\underline{f}$ in this scheme and these cross terms, as we shall see, will eventually destroys the second order accuracy of the Runge-Kutta method (2-55) when extended to the system case.

Now we prove the following theorem:

Theorem 3.1. Let $\underline{f}$ be a smooth function satisfying a Lipshitz condition and the conditions stated in (3–13). In addition, suppose that each component of $\underline{f}$ and each of its first and second partial derivatives satisfy a Lipshitz condition with the same Lipshitz constant. Then the scheme (3-25) is of second order in the L_2 sense: there exists two constants h_0 and C so that

$$\left[E\|\underline{X}_n - \underline{x}(t_n)\|^2\right]^{\frac{1}{2}} \le C\,h^2$$

for all $h \le h_0$, provided that the initial condition is exactly imposed or accurate to the second order in the L_2 sense. The constants C on depends the global bounds for the function $\underline{f}$ and its partial derivatives to the fifth order.

Proof. First, let us define

$$\underline{q}(t_n) = \underline{x}(t_n) + \frac{1}{2}h\underline{f}(\underline{x}(t_n)) \,. \tag{3-30}$$

By combining (3-3) with (3.20) we see that the exact solution $\underline{x}(t)$ satisfies

$$\begin{aligned} \underline{x}(t_{n+1}) &= \underline{x}(t_n) + \Delta\underline{w}_s + h\underline{f}(\underline{q}(t_n)) \\ &\quad + \underline{f}_{,j}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \Delta w_s{}^j \, ds + \frac{1}{2}\underline{f}_{,jk}(\underline{x}(t_n)) \int_{t_n}^{t_n+h} \Delta w_s{}^j \Delta w_s{}^k \, ds - \underline{R}_n \end{aligned} \tag{3-31}$$

where the remainder $-\underline{R}_n$ is of order $h^{2.5}$ either in the L_1 or in the L_2 sense. Let $\underline{e}_n = \underline{X}_n - \underline{x}(t_n)$. Subtracting the above equation from the second equation in (3-29), we obtain immediately

$$\begin{aligned} \underline{e}_{n+1} &= \underline{e}_n + h(\underline{f}(\underline{Q}_n) - \underline{f}(\underline{q}(t_n))) \\ &\quad + [\,\underline{f}_{,j}(\underline{X}_n) - \underline{f}_{,j}(\underline{x}(t_n))\,] \int_{t_n}^{t_n+h} \Delta w_s{}^j \, ds \\ &\quad + \frac{1}{2}[\,\underline{f}_{,jk}(\underline{X}_n) - \underline{f}_{,jk}(\underline{x}(t_n))\,] \int_{t_n}^{t_n+h} \Delta w_s{}^j \Delta w_s{}^k \, ds - R_n \,. \end{aligned} \tag{3-32}$$

For the sake of brevity, we introduce the notations:

$$\underline{v} \equiv \underline{f}(\underline{Q}_n)) - \underline{f}(\underline{q}(t_n)) \,. \qquad (3\text{-}33)$$

and

$$\underline{v}_j \equiv \underline{f}_{,j}(\underline{X}_n) - \underline{f}_{,j}(\underline{x}(t_n)) \,, \quad \underline{v}_{jk} \equiv \underline{f}_{,jk}(\underline{X}_n)) - \underline{f}_{,jk}(\underline{x}(t_n)) \,,$$

where we may notice that there is no comma (which means differentiation) in the subscripts for either v^i or v^i_{jk}. Then, recalling the definitions in (3-24), we can write equation (3-32) in the (component) form:

$$e^i_{n+1} = e^i_n + hv^i + v^i_j \beta^j + \frac{1}{2} v^i_{jk} \vartheta^{jk} - R^i_n \,. \qquad (3\text{-}34)$$

To make an L_2 norm analysis, we are led to square both sides of this equation and take a sum over the index i on both sides of the resultant equality. This results in

$$\begin{aligned} \|\underline{e}_{n+1}\|^2 = \|\underline{e}_n\|^2 &+ \sum_{i=1}^{d} [\, h^2(v^i)^2 + (v^i_j\beta^j)^2 + \frac{1}{4}(v^i_{jk}\vartheta^{jk})^2 \,] \\ &+ 2\sum_{i=1}^{d} [\, he^i_n v^i + e^i_n v^i_j \beta^j + \frac{1}{2} e^i_n v^i_{jk} \vartheta^{jk} \,] \qquad (3\text{-}35) \\ &+ 2\sum_{i=1}^{d} [\, hv^i v^i_j \beta^j + \frac{1}{2} hv^i v^i_{jk} \vartheta^{jk} + \frac{1}{2} v^i_{j_1} v_{j_2 k} \beta^{j_1} \vartheta^{j_2 k} \,] \\ &- 2\sum_{i=1}^{d} [\, e^i_n R^i_n + hv^i R^i_n + v^i_j \beta^j R^i_n + \frac{1}{2} v^i_{jk} \vartheta^{jk} R^i_n \,] + \|R_n\|^2 \end{aligned}$$

In all, there are fifteen terms on the right hand side of the above equation to be estimated. However, by the nonanticipating property, the expectations of the 6^{th}, 8^{th} and 10^{th} terms are zero.

Therefore, we need only to deal with the remaining twelve terms. Let each component of $\underline{f}$ and its partial derivatives up to second order ($\underline{f}_{,j}$, $\underline{f}_{,jk}$) satisfy the Lipschitz condition:

$$|g(\underline{x}) - g(\underline{y})| \leq L \, \|\underline{x} - \underline{y}\| \qquad (3\text{-}36)$$

where g can be any one of the functions stated above. Now consider

$$\|\underline{Q}_n - \underline{q}(t_n)\| = \|\underline{X}_n - \underline{x}(t_n) + \frac{1}{2}h[\underline{f}(\underline{X}_n) - \underline{f}(\underline{x}(t_n))]\| \tag{3-37}$$

$$\le \|\underline{X}_n - \underline{x}(t_n)\| + \frac{1}{2}hL\|\underline{f}(\underline{X}_n) - \underline{f}(\underline{x}(t_n))\| = (1 + \frac{1}{2}\sqrt{d}hL)\|\underline{e}_n\|$$

Then the second and the third term on the right hand side of (3-35) can be estimated respectively as:

$$E\left[\sum_{i=1}^{d} h^2(v^i)^2\right] \le dh^2L^2E\|\underline{Q}_n - \underline{q}(t_n)\|^2 \le dh^2L^2(1 + \frac{1}{2}\sqrt{d}hL)^2\, E\|\underline{e}_n\|^2 \tag{3-38}$$

and

$$E[\sum_{i=1}^{d}(v_j^i\beta^j)^2] = E[\sum_{i=1}^{d}(v_{j_1}^i v_{j_2}^i \beta^{j_1}\beta^{j_2})] = E\sum_{i=1}^{d}[v_{j_1}^i v_{j_2}^i]E[\beta^{j_1}\beta^{j_2}] \tag{3-39}$$

$$= E[\sum_{i=1}^{d}(v_{j_1}^i v_{j_2}^i)]\cdot \frac{1}{3}h^3\delta^{j_1 j_2} = \frac{1}{3}h^3E[\sum_{i,j}(v_j^i)^2]$$

$$\le \frac{1}{3}h^3 \cdot d^2L^2\sum_{i=1}^{d}[E\|\underline{e}_n\|^2] = \frac{1}{3}dL^2h^3\cdot E\|\underline{e}_n\|^2 .$$

The analysis of the fourth term is somewhat complicated. Consider the expression:

$$E[\sum_{i=1}^{d}(v_{jk}^i \vartheta^{jk})^2] = E[\sum_{i=1}^{d}(v_{j_1k_1}^i v_{j_2k_2}^i \vartheta^{j_1k_1}\vartheta^{j_2k_2})] \, .$$

If one index (of j_1, k_1, j_2, k_2) appears singly, then the expectation of the corresponding term is zero. This observation leads us to consider the following four cases:

(i) $j_1 = k_1 = j_2 = k_2$: there are d possibilities and in this case

$$E[\vartheta^{j_1k_1}\vartheta^{j_2k_2}] = E[\vartheta^{jj}\vartheta^{jj}] = \frac{7}{12}h^4$$

(ii) $j_1 = k_1 \ne j_2 = k_2$: there are $d(d-1)$ possibilities and we have

$$E[\vartheta^{j_1k_1}\vartheta^{j_2k_2}] = E[\vartheta^{j_1j_1}]E[\vartheta^{j_2j_2}] = \frac{1}{4}h^4$$

(iii) $j_1 = j_2 \ne k_1 = k_2$: there are $d(d-1)$ possibilities and we have

$$E[\vartheta^{j_1k_1}\vartheta^{j_2k_2}] = E[\vartheta^{jk}\vartheta^{jk}] = \frac{1}{6}h^4$$

(iv) $j_1 = k_2 \neq k_1 = j_2$: this case is completely the same as the case (iii).

All the above calculations can be found in the appendix *A*. With these results, the expectation of the fourth term can be estimated as:

$$E[\sum_{i=1}^{d}(v^i_{j_1k_1}v^i_{j_2k_2}\vartheta^{j_1k_1}\vartheta^{j_2k_2})] \tag{3-40}$$
$$\leq d\cdot\left[\frac{7}{12}d+(\frac{1}{4}+2\cdot\frac{1}{6})d(d-1)\right]h^4L^2E\|e_n\|^2 = \frac{7}{12}d^3h^4L^2E\|e_n\|^2 .$$

We estimate the fifth and the seventh term by applying the Cauchy-Schwartz inequality in the following way:

$$E[\sum_{i=1}^{d}(he^i_nv^i)] \leq hE\left[(\sum_{i=1}^{d}(e^i_n)^2)^{\frac{1}{2}}(\sum_{i=1}^{d}(v^i)^2)^{\frac{1}{2}}\right] \tag{3-41}$$
$$\leq hE\left[\|e_n\|\cdot\sqrt{d}L(1+\frac{1}{2}\sqrt{d}hL)\|e_n\|\right]$$
$$\leq \sqrt{d}hL(1+\frac{1}{2}\sqrt{d}hL)E\|e_n\|^2$$

and

$$E[\sum_{i=1}^{d}(e^i_nv^i_{jk}\vartheta^{jk})] = E[\sum_{i=1}^{d}(e^i_nv^i_{jk})]E(\vartheta^{jk}) = E[\sum_{i=1}^{d}(e^i_nv^i_{jk})]\cdot\frac{1}{2}h^2\delta^{jk} \tag{3-42}$$
$$= \frac{1}{2}h^2E\left[\sum_{j=1}^{d}\sum_{i=1}^{d}(e^i_nv^i_{jj})\right]$$
$$\leq \frac{1}{2}h^2E\left\{\sum_{j=1}^{d}\left[(\sum_{i=1}^{d}(e^i_n)^2)^{\frac{1}{2}}(\sum_{i=1}^{d}(v^i_{jj})^2)^{\frac{1}{2}}\right]\right\} \leq \frac{1}{2}d\sqrt{d}h^2LE\|e_n\|^2 .$$

The estimation of the ninth term on the right side of (3-35) is similar to that of the seventh term. The result is

$$E[\sum_{i=1}^{d}(hv^iv^i_{jk}\vartheta^{jk})] = h\cdot E\sum_{i=1}^{d}[v^iv^i_{jk}\cdot\frac{1}{2}h^2\delta^{jk}] \tag{3-43}$$
$$= \frac{1}{2}h^3\cdot E[\sum_{i,j}v^iv^i_{jj}] \leq \frac{1}{2}d\sqrt{d}h^3L^2(1+\frac{1}{2}\sqrt{d}hL)E\|e_n\|^2 .$$

Now we estimate the last five terms, each of which contains the factor $-\underline{R}_n$-the local truncation error. Hence, to estimate these terms, the expression of $-\underline{R}_n$ either in (3-22) or in (3-28) will be used.

Let us start by considering the expectation of $-R_n^i$ (see (3-22)). Remember that those terms in which the components of $\Delta\underline{w}$ appears with odd power (the 1st, 4th and 8th term) will vanish after taking expectations.

All the expectations in (3-22) of remaining terms can be easily evaluated except the second before last term in which we need to consider two cases:

(i) j,k,l,m are all equal: there are d possibilities,

(ii) j,k,l,m are equal in pairs, but are not all equal: there are $d(d-1)$ possibilities. Then, by a simple calculation, we find

$$-E[R_n^i] = E\left[\frac{1}{6}h^3 f^i_{,j} f^j_{,k} f^k + \frac{1}{2} f^i_{,j} f^j_{,kl} \cdot \frac{1}{6}h^3\delta^{kl} + f^i_{,jk} f^j_{,l} \cdot \frac{1}{6}h^3\delta^{kl}\right] \tag{3-44}$$

$$+ E\left[\frac{1}{2} f^i_{,jkl} f^j \cdot \frac{1}{3}h^3\delta^{kl} + \frac{1}{24}h^3 f^i_{,jk} f^j f^k\right]$$

$$+ E\left[\frac{1}{24}\sum_{j=1}^{d}[f^i_{,jjjj} \cdot h^3] + \frac{1}{24}\sum_{j\neq k}[f^i_{,jjkk} \cdot \frac{1}{3}h^3]\right] + O(h^4)$$

where all functions' value are evaluated at $\underline{x}(t_n)$. Finishing the arithmetic by letting $-R_n^i = h^3 M_n^i$, where M_n^i is a stochastic quantity of order h^0 in the L_1 sense or in the L_2 sense, we have

$$E[M_n^i] = E[\ \frac{1}{6} f^i_{,j} f^j_{,k} f^k + \frac{1}{12}\sum_{k=1}^{p} f^i_{,j} f^j_{,kk} + \frac{1}{6}\sum_{k=1}^{p} f^i_{,jk} f^j_{,k}\ ] \tag{3-45}$$

$$+ E[\ \frac{1}{6}h^3\sum_{k=1}^{p} f^i_{,jkk} f^j + \frac{1}{24} f^i_{,jk} f^j f^k + \frac{1}{24}\sum_{j=1}^{p} f^i_{,jjjj} + \frac{1}{72}\sum_{j\neq k} f^i_{,jjkk} + O(h)\ ].$$

With this result, we can now estimate the eleventh and twelfth term on the right hand side of $(3-35)$ as:

$$-E[\sum_{i=1}^{d}(e_n^i R_n^i)] = h^3 E[\sum_{i=1}^{d}(e_n^i M_n^i)] \tag{3-46}$$

$$\leq \frac{1}{2}\left[\varepsilon_1 h L E[\sum_{i=1}^{d}(\underline{e}_n^i)^2] + \varepsilon_1^{-1} L^{-1} h^5 E[\sum_{i=1}^{d}(M_n^i)^2]\right]$$

$$\leq \frac{1}{2}\left[\varepsilon_1 h L E\|\underline{e}_n\|^2 + \varepsilon_1^{-1} L^{-1} B_1^2 h^5\right]$$

and

$$-E[\sum_{i=1}^{d}(h v^i R_n^i)] = h^4 E[\sum_{i=1}^{d}(v^i M_n^i)] \tag{3-47}$$

$$\leq \frac{1}{2}\left[\varepsilon_1 d h^2 L^2 (1+\frac{1}{2}hL)^2 E\|\underline{e}_n\|^2 + \varepsilon_1^{-1} B_1^2 h^6\right]$$

where ε_1 is an appropriate positive number and

$$B_1^2 \equiv \sup_n E[\sum_{i=1}^{d}(M_n^i)^2]$$

Now we estimate the thirteenth term $-v_j^i \beta^j R_n^i$ on the right hand side of (3-35). Replacing $-R_n^i$ by its expression in (3-23), we find that only the 1^{st}, 4^{th} and 7^{th} term will remain after taking expectations. The only difficult point is evaluating the expectation of the 7^{th} term in which two cases need to be considered: (i) all four dummy indexes are the same or (ii) they are equal in pairs. The result is

$$-E[v_j^i \beta^j R_n^i] = E[v_j^i f^i_{,j_1} f^{j_1}_{,k}] \cdot \frac{1}{6} h^3 \delta^{jk} + E[v_j^i f^i_{,j_1 k} f^{j_1}] \cdot \frac{1}{3} h^3 \delta^{jk} \tag{3-48}$$

$$+ \frac{1}{6} E[\sum_{j=1}^{d} v_j^i f^i_{,jjj} \cdot h^3] + \frac{1}{6} E[3 \cdot \sum_{j \neq k} v_j^i f^i_{,jkk} \cdot \frac{1}{3} h^3] + E[v_j^i \cdot O(h^4)]$$

$$= E\left\{\sum_{j=1}^{d} v_j^i \left[\frac{1}{6} h^3 [f^i_{,j_1} f^{j_1}_{,j} + 2 f^i_{,j_1 j} f^{j_1} + \sum_{k=1}^{d} f^i_{,jkk}] + O(h^4)\right]\right\}$$

$$\equiv h^3 E[\sum_{j=1}^{d} v_j^i M_{jn}^i]$$

where $M_{jn}^i \equiv h^{-3} \beta^j R_n^i$ is a stochastic quantity of order h^0 in the L_1 or L_2 sense. Then we have the estimate:

$$-E[\sum_{i=1}^{d}[v_j^i\beta^j R_n^i]] = h^3 E[\sum_{i=1}^{d}[\sum_{j=1}^{d} v_j^i M_{jn}^i]] \tag{3-49}$$

$$\leq \frac{1}{2}\varepsilon_2 d^{-2}L^{-1}hE[\sum_{i,j}(v_j^i)^2] + \frac{1}{2}\varepsilon_2^{-1}Ld^2h^5E[\sum_{i,j}(M_{jn}^i)^2]$$

$$\leq \frac{1}{2}\varepsilon_2 hLE|\underline{e}_n|^2 + \frac{1}{2}d^2\varepsilon_2^{-1}LB_2{}^2h^5$$

where, again, ε_2 is an appropriate positive number and

$$B_2^2 \equiv \sup_n E[\sum_{i,j}(M_{jn}^i)^2]$$

There are still two terms remain to be treated. From the above discussion, we see that what really matters in a estimation is the order of the stochastic quantity. Therefore for a much complicated term like $v_{jk}^i\vartheta^{jk}R_n^i$, we may set $M_{jkn}^i = h^{-4}\vartheta^{jk}R_n^i$ and write

$$-E\sum_{i=1}^{d}[v_{jk}^i\vartheta^{jk}R_n^i] = h^4\sum_{i,j,k}[v_{jk}^i\vartheta^{jk}M_{jkn}^i] \tag{3-50}$$

since ϑ^{jk} is of order h^2 and $-R_n^i$ is of order $h^{2.5}$ and the expectations of a term of order $h^{4.5}$ is zero. Hence, the expectation of the second last term on the right hand side of (3–35) can be estimated as

$$-E[v_{jk}^i\vartheta^{jk}R_n^i] \leq \frac{1}{2}[h^2E[\sum_{i,j,k}(v_{jk}^i)^2] + h^6E[\sum_{i,j,k}(M_{jkn}^i)^2]] \tag{3-51}$$

$$\leq \frac{1}{2}d^3h^2L^2E|\underline{e}_n|^2 + \frac{1}{2}h^6B_3{}^2$$

where the first inequality is obtained by applying the Cauchy-Schwartz inequality to the right hand side of (3-50) once and

$$B_3^2 = \sup_n E[\sum_{i,j,k}(M_{jkn}^i)^2]$$

The estimation of the last term: $|R_n|^2$ can be done in a similar way. Squaring both sides of the expression of R_n^i in (3-28) and taking sum over the index i, we find:

$$\|R_n\|^2 = E[\sum_{i=1}^{d}(R_n^i)^2] = h^5 E\left[\sum_{i=1}^{d}[f^i_{\cdot j} f^j_{\cdot k}\delta^k + f^i_{\cdot jk} f^j \gamma^k + \frac{1}{6} f^i_{\cdot jkl}\vartheta^{jkl}]^2\right] + O(h^6)$$

$$\leq 3 \cdot h^5 E\left[\sum_{i=1}^{d}[f^i_{\cdot j} f^j_{\cdot k}\delta^{'k}]^2 + \sum_{i=1}^{d}[f^i_{\cdot jk} f^j \gamma^{'k}]^2 + \frac{1}{36}\sum_{i=1}^{d}[f^i_{\cdot jkl}\vartheta^{'jkl}]^2\right] + O(h^6)$$

$$\leq B_R{}^2 h^5 + O(h^6) \tag{3-52}$$

where the definition of $B_R{}^2$, similar to those of B_1^2, B_2^2 and B_3^2, is clear from the last inequality.

To complete the proof of theorem 3.1, we need to summarize all the estimates that have been made in the above. Taking into account all the coefficients in (3-35) and collecting the estimates from (3–36) to (3-52), we obtain

$$E\|e_{n+1}\|^2 \leq \left[1 + G_1 hL + \frac{1}{2}G_2^2 h^2 L^2 + \frac{1}{6}G_3^3 h^3 L^3 + \frac{1}{24}G_4^4 h^4 L^4\right] \cdot E\|e_n\|^2$$

$$+ B\, h^5 + O(h^6) \tag{3-53}$$

where

$$G_1 = 2\sqrt{d} + \varepsilon_1 + \varepsilon_2\,,$$

$$G_2{}^2 = 2\cdot[\,2d + \varepsilon_1 dL^{-2} + \frac{1}{2}d\sqrt{d}L^{-1}\,]$$

$$G_3{}^3 = 6\cdot[\,p\sqrt{p} + \frac{1}{3}dL^{-1} + \frac{1}{2}d\sqrt{d}L^{-2} + \varepsilon_1 d\sqrt{d}L^{-2}\,]\,,$$

$$G_4{}^4 \equiv 24\cdot[\,\frac{1}{4}d^2 + \frac{1}{4}d^2L^{-2} + \frac{1}{4}\varepsilon_1 d^2 L^{-2} + \frac{7}{48}d^3L^{-2}\,]$$

and

$$B \equiv (1 + \varepsilon_1{}^{-1}L^{-1})B_1^2 + \varepsilon_2{}^{-1}\, Ld^2 B_2{}^2 + B_R{}^2\,.$$

With this expression, if we choose $\varepsilon \equiv \varepsilon_1 + \varepsilon_2$ so that G_1 is greater than G_1, G_2, G_3 and G_4. Then for equation (3–53), we have the following estimate:

$$E\|e_{n+1}\|^2 \leq e^{(2\sqrt{d} + \varepsilon)hL} E\|e_n\|^2 + B\, h^5 + O(h^6) \tag{3-54}$$

An elementary calculation shows that the solution of this recursive relation is given by

$$E\|e_n\|^2 \leq \frac{e^{t_n(2\sqrt{d}+\varepsilon)}-1}{(2\sqrt{d}+\varepsilon)L} B\, h^4 + e^{(2\sqrt{d}+\varepsilon)t_n L} E\|\underline{e}_0\|^2 + O(h^5) \qquad \text{(3-55)}$$

Let $E\|\underline{e}_0\|^2 \leq C_0^2\, h^4$. By squaring both sides of the above inequality, we complete the proof of theorem 3.1 with

$$C = \sup_{h\leq h_0} \left\{ \frac{B}{(2\sqrt{d}+\varepsilon)L}(e^{(2\sqrt{d}+\varepsilon)TL}-1) + C_0^2\, e^{(2\sqrt{d}+\varepsilon)TL} + O(h) \right\}^{\frac{1}{2}}.$$

From the proof, we see that the local truncation error of a numerical scheme for solving equation (3-1) must be of order $h^{2.5}$ or even higher in order that the scheme itself be of order h^2 in the L_2 sense.

Now we can explain why the theorem 2.1 does not generalize to a system of stochastic differential equations. A natural extension of (2–55) to a system is

$$P_n^i = \sqrt{\vartheta^{ii} - \beta^{i2}} \qquad \text{(3-57)}$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + \sqrt{h}\,\underline{\beta}$$

$$\underline{X}_{n+1} = \underline{X}_n + \frac{1}{2}h[\,\underline{f}(\underline{Q}_n' + \sqrt{h}\underline{P}_n) + \underline{f}(\underline{Q}_n' - \sqrt{h}\underline{P}_n)\,].$$

A simple analysis shows that the local truncation error of the above scheme contains a term:

$$h^2\, \underline{f}_{jk}(\underline{x}_n)\, P_n^j\, P_n^k\,, \quad j \neq k \qquad \text{(3-58)}$$

which is of order h^2 (in the L_2 sense, and thus destroys the second order accuracy of the scheme (2–57) in the L_2 sense. In other words, we may say that the appearance of the cross derivative terms of $\underline{f}$ make the scheme (3–57) fail to be a second order method in the L_2 sense.

3.3 Runge–Kutta Methods of order One and Half

In this section, we will extend the results in section 3.5 to the system case. We need only to interpret the schemes in section 2.5 in vector notation. Consider the family of Runge-Kutta methods:

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + k\sqrt{h}\,\underline{\beta}' \tag{3-59}$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + l\sqrt{h}\,\underline{\beta}'$$

$$\underline{X}_{n+1} = \underline{X}_n + \Delta_n\underline{w} + h[\, a\underline{f}(\underline{Q}_n) + b\underline{f}(\underline{Q}_n')\,]$$

where $a + b = 1$, $a\cdot k + b\cdot l = 1$ and $a\cdot k^2 + b\cdot l^2 = \frac{3}{2}$. In particular, we will prove

Theorem 3.2. Let $\underline{f}$ be a smooth function satisfying the condition (3-13). In addition, assume that every component f^i of $\underline{f}$ satisfies a Lipshitz condition with the same Lipshitz constant. Then the following scheme

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) \tag{3-60}$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + \frac{3}{2}\sqrt{h}\,\underline{\beta}'$$

$$\underline{X}_{n+1} = \underline{X}_n + \Delta_n\underline{w} + \frac{1}{3}h[\,\underline{f}(\underline{Q}_n) + 2\cdot\underline{f}(\underline{Q}_n')\,]$$

is of order $h^{1.5}$ in the L_2 sense (see (0-4) or theorem 3.1 for the definition).

Proof. The proof is very similar to that of Theorem 2.2 in Chapter 2 except that we need to use the summation convention. The first step is to figure out the local truncation error of scheme (2-64). Let us define

$$\underline{q}'(t_n) = \underline{x}(t_n) + \frac{1}{2}h\underline{f}(\underline{x}(t_n)) + \frac{3}{2}\sqrt{h}\,\underline{\beta}' . \tag{3-61}$$

The local truncation error of scheme (3-64) is defined in the equation

$$\underline{x}(t_{n+1}) = \underline{x}(t_n) + \Delta_n \underline{w} + \frac{1}{3}h[\ \underline{f}(\underline{q}(t_n)) + 2\cdot \underline{f}(\underline{q}'(t_n))\ ] + \underline{T}_n' . \qquad (3\text{-}62)$$

To make an error analysis, let us carry out the following expansion of $\underline{f}(\underline{q}'(t_n))$:

$$hf^i(\underline{q}'(t_n)) = hf^i(\underline{q}(t_n) + \frac{3}{2}\sqrt{h}\,\underline{\beta}') \qquad (3\text{-}63)$$

$$= hf^i(\underline{q}(t_n)) + \frac{1}{2}h^{\frac{3}{2}} f^i_{,j}(\underline{x}(t_n))\beta'^j + \frac{9}{8}h^2 f^i_{,jk}(\underline{x}(t_n))\beta'^j\beta'^k + O(h^{\frac{5}{2}})$$

$$= hf^i(\underline{x}(t_n)) + \frac{3}{2}hf^i_{,j}(\underline{x}(t_n))\int_{t_n}^{t_n+h} \Delta w^j\, ds + \frac{9}{8}h^2 f^i_{,jk}(\underline{x}(t_n))\beta'^j\beta'^k + O(h^{\frac{5}{2}}) .$$

Replacing $\underline{f}(\underline{q}'(t_n))$ in (3-62) by the above expression, we obtain (in component form)

$$x^i(t_{n+1}) = x^i(t_n) + \Delta_n w^i + hf^i(\underline{q}(t_n)) \qquad (3\text{-}64)$$

$$+ f^i_{,j}(\underline{x}(t_n))\int_{t_n}^{t_n+h} \Delta w^j\, ds + \frac{3}{4}h^2 f^i_{,jk}(\underline{x}(t_n))\beta'^j\beta'^k + O(h^{\frac{5}{2}}) + T_n'^i .$$

Comparing the above expression with (3-27) and recalling that $-\underline{R}_n = \{-R_n^i\}$ is of order $h^{\frac{5}{2}}$, we arrive at

$$T_n'^i = \frac{1}{2}f^i_{,jk}(\underline{x}(t_n))\int_{t_n}^{t_n+h} \Delta w^j \Delta w^k\, ds - \frac{3}{2}h^2 f^i_{,jk}(\underline{x}(t_n))\beta'^j\beta'^k + O(h^{\frac{5}{2}}) . \qquad (3\text{-}65)$$

As in the scalar case, the main fact about $T_n'^i$ is that its expectation is of order h^3 despite of the appearance of the cross terms. The expectations of the cross terms are zero because of the independence between any two components of a (multi-dimensional) Wiener process. In fact,

$$E[T_n'^i] = \frac{1}{2}E[f^i_{,jk}(\underline{x}(t_n))]\cdot \frac{1}{2}h^2\delta^{jk} - \frac{3}{4}h^2\cdot E[f^i_{,jk}(\underline{x}(t_n))]\cdot \frac{1}{3}\delta^{jk} + O(h^3) \qquad (3\text{-}66)$$

$$= \frac{1}{4}h^2 E[\ \sum_{j=1}^{d} f^i_{,jj}(\underline{x}(t_n))\ ] - \frac{1}{4}h^2 E[\ \sum_{j=1}^{d} f^i_{,jj}(\underline{x}(t_n))\ ] + O(h^3) \equiv h^3 E[M_n'^i]$$

where $M_n'^i$ is an quantity of order h^0 in the L_1 sense. Let $e_n^i = x^i(t_n) - X_n^i$. Subtracting the third equation in (3-60) from (3-62), we have (in component form)

$$e_{n+1}^i = e_n^i + \frac{1}{3}h\ v^i + T_n'^i \qquad (3\text{-}67)$$

where we define

$$v_n^i = v_{n,1}^i + 2\cdot v_{n,2}^i$$

and

$$v_{n,1}^i = f^i(\underline{q}(t_n)) - f^i(\underline{Q}_n)\ ,$$

$$v_{n,2}^i = f^i(\underline{q}'(t_n) - f^i(\underline{Q}_n')\ .$$

Squaring equation (3-67) and taking sum over the index i, we obtain

$$\|\underline{e}_{n+1}\|^2 = \|\underline{e}_n\|^2 + \frac{2}{3}h\sum_{i=1}^{d}[e_n^i v_n^i] + \frac{1}{9}h^2\sum_{i=1}^{d}(v_n^i)^2 \qquad (3\text{-}68)$$

$$+ 2\cdot\sum_{i=1}^{d}[e_n^i T_n'^i] + \frac{2}{3}h\cdot\sum_{i=1}^{d}[v^i T_n'^i] + \|\underline{T}_n'\|^2\ .$$

Our analysis is based upon the estimation of the expectations of the terms on the right hand side of (3-68). Consider v_n^i defined above and apply the Lipshitz conditions on f; then

$$E[(v_n^i)^2] \le E[\ (v_{n,1}^i)^2 + 4\cdot v_{n,1}^i\cdot v_{n,2}^i + 4(v_{n,2})^2\ ] \le 9\cdot L^2 E\|\underline{e}_n\|^2\ . \qquad (3\text{-}69)$$

Using this fact and the Cauchy-Schwartz inequality on the right hand side of (3-68), for the fist and second term, we find

$$h^2 E[\sum_{i=1}^{d}(v_n^i)^2] \le 9h^2 E[\ \sum_{i=1}^{d} L^2\|\underline{e}_n\|^2\ ] \le 9\ dh^2 L^2 E\|\underline{e}_n\|^2 \qquad (3\text{-}70)$$

and

$$h\sum_{i=1}^{d}[e_n^i v_n^i] \le hE[\ [\sum_{i=1}^{d}(e_n^i)^2\ ]^{1/2}[\sum_{i=1}^{d}(v_n^i)^2\ ]^{1/2}\ ] \le 3\cdot\sqrt{d}hLE\|\underline{e}_n\|^2\ . \qquad (3\text{-}71)$$

Now note that the local truncation error $\underline{T}_n'$ appears in the last three terms on the right hand side of (3–68). Recall the nonanticipating property of the solution $\underline{x}(t_n)$. Using the fact in (3-66) to the term $\sum_{i=1}^{d}[e_n^i T_n'^i]$ and the arithmetic inequality $2\cdot a\cdot b \le a^2 + b^2$, we find

$$E[\sum_{i=1}^{d} e_n^i T_n^{'i}] = h^3 E[\sum_{i=1}^{d} e_n^i M_n^{'i}] \le \frac{1}{2}\varepsilon_1 hLE\|\underline{e}_n\|^2 + O(h^5). \qquad (3\text{-}72)$$

The same trick is also applied to the last two terms on the right hand side of (3-68), we have

$$E[h\sum_{i=1}^{d} v_n^i T_n^{'i}] \le h[\frac{3}{2}\varepsilon_2 L^{-1} E\sum_{i=1}^{d}(v_n^i)^2 + \frac{1}{3}\varepsilon_2^{-1} LE\sum_{i=1}^{d}(T_n^{'i})^2]$$

$$\le \frac{3}{2}\varepsilon_2 hLE\|\underline{e}_n\|^2 + O(h^5) \qquad (3\text{-}73)$$

since $E[\sum_{i=1}^{d}(T_n^{'i})^2] = E\|\underline{T}_n^{'}\|^2$ is of order h^4 in the L_1 sense as we shall see in a moment. Now we give an estimate of the leading terms of $\|\underline{T}_n^{'}\|^2$, which dominates the error of the scheme (3-60). Recalling the definition of $\vartheta^{'jk}$ in (3-24), we can write (3-65) in the form:

$$T_n^{'i} = h^2\cdot f^i_{,jk}(\underline{x}(t_n))[\frac{1}{2}\vartheta^{'jk} - \frac{3}{4}\beta^{'j}\beta^{'k}] + O(h^{\frac{5}{2}}). \qquad (3\text{-}74)$$

The remark at the end of section 3.3 and the independence between $\beta^{'j}$, $\vartheta^{'jk}$ and $f^i_{,jk}(\underline{x}(t_n))$ enable us to write

$$E[T_n^{'i}]^2 = \frac{1}{4}h^4 E[f^i_{,jk}(\underline{x}(t_n))(\vartheta^{'jk} - \frac{3}{2}\beta^{'j}\beta^{'k})]^2 + O(h^5) \qquad (3\text{-}75)$$

$$\le \frac{1}{4}h^4\cdot E[\sum_{j,k}(f^i_{,jk}(\underline{x}(t_n)))^2]\cdot E[\sum_{j,k}(\vartheta^{'jk} - \frac{3}{2}\beta^{'j}\beta^{'k})^2] + O(h^5)$$

$$\le \frac{1}{4}h^4\cdot [B_2^i]^2\cdot E[\sum_{j,k}[\vartheta^{'jk} - \frac{3}{2}\beta^{'j}\beta^{'k}]^2] + O(h^5)$$

where $[B_2^i]^2 \equiv \max_{0\le t\le T} E[\sum_{j,k}(f^i_{,jk})^2]$. In the last inequality of (3-75), let us consider two cases:

(i) $j = k$: there are d possibilities,

$$E[\vartheta^{'jk} - \frac{3}{2}\beta^{'j}\beta^{'k}]^2 = E[(\vartheta^{'jj})^2 - 3\cdot\vartheta^{'jj}\beta^{'j2} + \frac{9}{4}(\beta^{'j})^4] \qquad (3\text{-}76)$$

$$= \frac{7}{12} - 3\cdot\frac{13}{30} + \frac{9}{4}\cdot\frac{1}{3} = \frac{1}{30};$$

(ii) $j \neq k$: there are $d(d-1)$ possibilities, then

$$E[\,\vartheta'^{jk} - \frac{3}{2}\beta'^{j}\beta'^{k}\,]^2 = E[\,(\vartheta'^{jk})^2 - 3\cdot\vartheta'^{jk}\beta'^{j}\beta'^{k} + \frac{9}{4}(\beta'^{j})^2(\beta'^{k})^2\,] \tag{3-77}$$

$$= \frac{1}{6} - 3\cdot\frac{2}{15} + \frac{9}{4}\cdot\frac{1}{3}\cdot\frac{1}{3} = \frac{1}{60}.$$

Substituting the results in (3-76) and (3-77) into (3-75), and summing over the index i, we obtain

$$E\|\underline{T}_n'\|^2 \leq [\,\frac{1}{120}d + \frac{1}{240}d(d-1)\,]B_f^2h^4 = \frac{1}{240}d(d+1)B_f^2h^4 \tag{3-78}$$

where $B_f^2 \equiv \sum_{i=1}^{d}[B_f^i]^2$. Collecting the results from (3-70)-(3-73) and (3-78), and substituting them into (3-68), we obtain

$$E\|\underline{e}_{n+1}\|^2 \leq [\,1 + (2\sqrt{d} + \varepsilon)hL + d^2h^2L^2\,]\,E\|\underline{e}_n\|^2 + \frac{1}{240}d^2(d+1)h^4 + O(h^5)$$

where $\varepsilon \equiv \varepsilon_1 + \varepsilon_2$. Solving the recursive inequality (3−79), we arrive at the following estimate:

$$E\|\underline{e}_n\|^2 \leq \frac{1}{240}\cdot\frac{e^{(2\sqrt{d}+\varepsilon)t_nL} - 1}{(2\sqrt{d}+\varepsilon)L}d^2(d+1)B_f^2h^3 + e^{(2\sqrt{d}+\varepsilon)t_nL}\,E\|\underline{e}_0\|^2 + O(h^4).$$

Using the initial condition: $E\|\underline{e}_0\|^2 \leq C_0^2\,h^3$ in (3-80), we then complete the proof of theorem 3.2 with

$$\sqrt{E\|\underline{e}_n\|^2} \leq C\,h^{1.5} \tag{3-81}$$

where

$$C = \sup_{h\leq h_0}\left\{\frac{1}{240}\cdot\frac{e^{(2\sqrt{d}+\varepsilon)TL} - 1}{(2\sqrt{d}+\varepsilon)L}d^2(d+1)B_f^2 + C_0^2\,e^{(2\sqrt{d}+\varepsilon)TL} + O(h)\right\}^{\frac{1}{2}}.$$

From this expression we see that, if the initial error is sufficiently small, i.e., C_0 is a very small number, then for $h \geq \frac{1}{240} \approx .00417$, scheme (2−60) is practically of order h^2 (i.e. second order) in the L_2 sense.

3.4 Heuristic Second Order Runge–Kutta Methods

As we know from the discussion of section 3.2 that there are substantial difficulties in deriving second order Runge-Kutta method in the L_2 sense. From the practical point of view, L_2 convergence is a strong requirement, and one may be content with a convergence in a weaker sense.

In this section, we will consider the accuracy of numerical schemes in the weak sense (defined in (0-14)). Let φ be a smooth functional satisfying the Lipshitz condition:

$$|\varphi(\underline{x}) - \varphi(\underline{y})| \le L_\varphi \|\underline{x} - \underline{y}\| , \quad \underline{x}, \underline{y} \in R^d . \tag{3-82}$$

L_2 convergence implies weak convergence as can be seen from the following:

$$|E\varphi(\underline{x}(t_n)) - E\varphi(\underline{X}_n)| \le L_\varphi E\|\underline{e}_n\| \le L_\varphi \sqrt{E\|\underline{e}_n\|^2} \tag{3-83}$$

where the second inequality is obtained by applying the Cauchy-Schwartz inequality once. Moreover, from (3–83), we see that the rate of weak convergence is not less than that of L_2 convergence, and we may expect a faster convergence in the weak sense.

The purpose of this section is to consider the rate of convergence of numerical schemes in the weak sense in the hope that the Runge-Kutta methods of second order in that sense can be derived based on the Taylor series method (3–29).

Consider the (d-dimensional) stochastic differential equation:

$$d\underline{x} = \underline{f}(\underline{x})dt + d\underline{w}_t , \quad 0 \le t \le T . \tag{3-84}$$

Let us write down the second order (in the L_2 sense) Taylor series method (3-29) in terms of β^j and ϑ^{jk} defined in (3-24):

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(X_n), \tag{3-85}$$

$$\underline{X}_{n+1} = \underline{X}_n + \Delta_n \underline{w} + h\underline{f}(\underline{Q}_n) + \underline{f}_{,j}(\underline{X}_n)\beta^j + \frac{1}{2}\underline{f}_{,jk}(X_n)\vartheta^{jk}.$$

Define

$$\underline{B}_n = \underline{X}_n + h\,\underline{f}(\underline{Q}_n) \tag{3-86}$$

and

$$\underline{S}_n = \Delta_n \underline{w} + \underline{f}_{,j}(\underline{X}_n)\beta^j + \frac{1}{2}\underline{f}_{,jk}(\underline{X}_n)\vartheta^{jk} \tag{3-87}$$

then

$$\underline{X}_{n+1} = \underline{B}_n + \underline{S}_n.$$

Given a smooth functional φ, consider

$$\begin{aligned}\varphi(\underline{X}_{n+1}) &= \varphi(\underline{B}_n + \underline{S}_n) \\ &= \varphi(\underline{B}_n) + \varphi_{,j}(\underline{B}_n)\cdot S_n^j \\ &+ \frac{1}{2}\varphi_{,jk}(\underline{B}_n)\,[\Delta_n \underline{w} + \underline{f}_{,l}\beta^l]^j\cdot[\Delta_n \underline{w} + \underline{f}_{,m}\beta^m]^k \\ &+ \frac{1}{6}\varphi_{,jkl}(\underline{B}_n)\Delta_n w^j \Delta_n w^k \Delta_n w^l + \frac{1}{24}\varphi_{,jklm}(\underline{B}_n)\Delta_n w^j \Delta_n w^k \Delta_n w^l \Delta_n w^m + O(h^{\frac{5}{2}}).\end{aligned} \tag{3-88}$$

Note that the increment $\Delta_n \underline{w}$ is independent of the solution $\underline{x}(t_n)$ before and at time t_n (the nonanticipating property); we can thus carry out the calculation:

$$\begin{aligned}E[\varphi(\underline{X}_{n+1})] &= E[\varphi(\underline{B}_n)] + E[\sum_{j=1}^{p}\varphi_{,j}(\underline{B}_n)\cdot\frac{1}{2}h^2 f^j_{,kl}\delta^{kl}] \\ &+ \frac{1}{2}E[\varphi_{,jk}(\underline{B}_n)\cdot[h\,\delta^{jk} + \frac{1}{2}h^2(f^j_{,l}f^k_{,m}\delta^{lm} + f^k_{,m}f^j_{,l}\delta^{ml})]] \\ &+ \frac{1}{6}E[\sum_{j,k,l}\varphi_{,jkl}(\underline{B}_n)\cdot 0] + \frac{1}{24}E[\sum_{j=1}^{p}\varphi_{,jjjj}(\underline{B}_n)\cdot 3h^2 + \sum_{j\neq k}\varphi_{,jjkk}(\underline{B}_n)\cdot 3h^2] + O(h^3)\end{aligned} \tag{3-89}$$

where the function $\underline{f}$ and its partial derivatives are evaluated at t_n. Finishing the calculation by using the property of δ^{jk} (i.e., $\delta^{jk} = 1$, if $j = k$; $= 0$, otherwise) and combining the summations on the second last term on the right hand side, we obtain

$$E[\varphi(X_{n+1})] = E[\varphi(B_n)] + \frac{1}{2}h^2 E[\sum_{j,k}\varphi_{,j}(B_n)f^j_{,kk}] \quad (3\text{-}90)$$

$$+ \frac{1}{2}E[h\sum_{j=1}^{p}\varphi_{,jj}(B_n) + h^2\sum_{j,k,l}\varphi_{,jk}f^j_{,l}f^k_{,l}] + \frac{1}{8}h^2 E[\sum_{j,k}\varphi_{,jjkk}(B_n)] + O(h^3).$$

In obtaining the expression in (3-89) (or (3-90)), we use the following facts:

(i): $\Delta_n w^j$ is a Gaussian random variable with mean 0 and variance h;

(ii): $E[\beta^j] = 0$, $E[\beta^j \Delta_n w^k] = \frac{1}{2}h^2 \cdot \delta^{jk}$ and $E[\vartheta^{jk}] = \frac{1}{2}h^2 \cdot \delta^{jk}$.

Note that ϑ^{jk} (defined in (3–24)) is not a Gaussian random variable. These conditions can be satisfied by a single Gaussian random variable, if in the second equation of (3-85), we make the substitutions:

$$\left\{\Delta_n w^j\right\} \longrightarrow \left\{\sqrt{h}\,\xi^j\right\}, \quad \left\{\beta^j\right\} \longrightarrow \left\{\frac{1}{2}h^{1.5}\xi^j\right\}, \quad \left\{\vartheta^{jk}\right\} \longrightarrow \left\{\frac{1}{2}h^2\xi^j\xi^k\right\},$$

where $\{\xi^j\}$ is a set of k independent Gaussian random variable with mean 0 and variance 1. In other words, if we define

$$S'_n \equiv \sqrt{h}\,\xi + \frac{1}{2}h^{\frac{1}{2}}f_{,j}(B_n)\xi^j + \frac{1}{4}h^2 f_{,jk}(B_n)\xi^j\xi^k \quad (3\text{-}92)$$

and

$$X'_{n+1} = B_n + S'_n \quad (3\text{-}93)$$

where B_n is defined in (3-86) (note that we use the same X_n), then

$$E[\varphi(X'_{n+1})] = E[\varphi(B_n + S'_n)] \quad (3\text{-}94)$$

$$= E[\varphi(B_n)] + \frac{1}{2}h^2 E[\sum_{j=1}^{p}\varphi_{,j}(B_n)f^j_{,kk}]$$

$$+ \frac{1}{2}E[h\sum_{j=1}^{p}\varphi_{,jj}(B_n) + h^2\sum_{j,k,l}\varphi_{,jk}f^j_{,l}f^k_{,l}] + \frac{1}{8}h^2[\sum_{j,k}\varphi_{,jjkk}(B_n)] + O(h^3)$$

which has exact the same form as (3-90). Comparing (3-94) with (3–90), we find that they differ from each other with an amount of order h^3,i.e.,

$$|E\varphi(X_n) - E\varphi(X'_n)| \approx h^3 \quad (3\text{-}95)$$

With the substitutions in (3-91), we now consider the numerical scheme

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n), \tag{3-96}$$

$$\underline{X}_{n+1} = \underline{X}_n + \sqrt{h}\,\underline{\xi} + h\underline{f}(\underline{Q}_n) + \frac{1}{2}h^{\frac{3}{2}}\underline{f}_{,j}(\underline{X}_n)\xi^j + \frac{1}{4}h^2\underline{f}_{,jk}(\underline{X}_n)\xi^j\xi^k .$$

which is obtained from (3–85) by making the substitutions (3–91). In the below we show that the local error (or one-step error) of the scheme (3-96) is of order h^3 in the weak sense.

For clarity, let $\underline{Y}_{n+1}$, $\underline{Z}_{n+1}$ denote the numerical solutions in (3-85) and (3-96) at t_{n+1} with the exact value $\underline{Y}_n = \underline{Z}_n = \underline{x}(t_n)$ imposed at t_n. Consider

$$\underline{x}(t_n) = \underline{Y}_n + \underline{R}_n .$$

By a argument similar to that in the derivation of (3-90), we have

$$\begin{aligned}\varphi(\underline{x}(t_n)) &= \varphi(\underline{Y}_n + \underline{R}_n)\\ &= E[\varphi(\underline{Y}_n) + \varphi_{,j}(\underline{Y}_n)R_n^j] + O(h^5)\\ &= E[\varphi(\underline{Y}_n)] + O(h^3),\end{aligned}$$

that is,

$$|E\varphi(\underline{x}(t_{n+1})) - E\varphi(\underline{Y}_{n+1})| \approx h^3 \tag{3-97}$$

for a sufficiently smooth functional φ satisfying the Lipshitz condition (3–82). Combining the results in (3-95) and (3-97), we obtain

$$\begin{aligned}|E\varphi(\underline{x}(t_{n+1}) - E\varphi(\underline{Z}_{n+1})| &\le |E\varphi(\underline{x}(t_{n+1})) - E\varphi(\underline{Y}_{n+1})|\\ &+ |E\varphi(\underline{Y}_{n+1}) - E\varphi(\underline{Z}_{n+1})| \approx h^3 + h^3 \approx h^3 .\end{aligned} \tag{3-98}$$

which means exactly that the local error of the scheme (3–96) is of order h^3 in the weak sense. A class of Runge-Kutta methods with the same accuracy as (3-96) can be designed as follows:

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + k\sqrt{h}\,\underline{\xi} \tag{3-99}$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + l\sqrt{h}\,\underline{\xi}$$

$$\underline{X}_{n+1} = \underline{X}_n + \sqrt{h}\,\underline{\xi} + h[\, a\cdot\underline{f}(\underline{Q}_n) + b\cdot\underline{f}(\underline{Q}_n')\,]$$

where

$$a + b = 1, \quad a\cdot k + b\cdot l = \frac{1}{2}, \quad a\cdot k^2 + b\cdot l^2 = \frac{1}{2}. \tag{3-100}$$

On the other hand, one may notice that the conditions (i) and (ii) following (3-90) are also satisfied by the scheme (3-60), as can be seen from (3-64) if in (3-85) we make the following substitution:

$$\left\{\vartheta^{jk}\right\} \longrightarrow \left\{\frac{3}{2}h^2\beta^{\cdot j}\beta^{\cdot k}\right\}. \tag{3-101}$$

Since we have shown that one-step error of the scheme (3–96) is of order h^3 in the weak sense, we make the following

Conjecture. Under the assumptions of theorem 3.1, the family of schemes (3-59) and the family (3-99) are of order h^2 in the weak sense defined in (0-14) or (3-83), provided that the initial error is of order h^2 in the L_2 sense.

Remark. The difficulty in proving this conjecture lies in the fact that there is no obvious way to 'link' the errors at successive time steps. Since we have proved that the family of schemes (3-59) are of order $1\frac{1}{2}$, it seems conceivable that they are of order 2 in the weak sense. Indeed, computational results (in Chapter 5) show that these two families have about the same order accuracy in the weak sense.

In particular, if we choose a rational solution of (3–100) : $a = b = \frac{1}{2}$, $k = 0$, $l = 1$, we have:

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) \tag{3-102}$$

$$\underline{Q}_n{}' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + \sqrt{h}\,\underline{\xi}$$

$$\underline{X}_{n+1} = \underline{X}_n + \sqrt{h}\,\underline{\xi} + \frac{1}{2}h[\,\underline{f}(\underline{Q}_n) + \underline{f}(\underline{Q}_n{}')\,]\,.$$

Furthermore, if we replace the substitutions in (3-91) by

$$\left\{\beta^j\right\} \longrightarrow \left\{\frac{1}{2}h^{\frac{3}{2}}\xi^j + \frac{1}{2\sqrt{3}}h^{\frac{3}{2}}\eta^j\right\},\quad \left\{\vartheta^{jk}\right\} \longrightarrow \left\{\frac{1}{3}h^2\xi^j\xi^k + \frac{1}{6}h^2\eta^j\eta^k\right\}$$

where, again, $\underline{\eta} = \{\eta^j\}$ is a set of d independent Gaussian random variables with mean 0 and variance 1; and define

$$\underline{S}_n'' = \sqrt{h}\,\underline{\xi} + \frac{1}{2}h^{\frac{3}{2}}\underline{f}_{,j}(\underline{B}_n)[\xi^j + \frac{1}{\sqrt{3}}\eta^j] + \frac{1}{12}h^2\underline{f}_{,jk}(\underline{B}_n)[2\cdot\xi^j\xi^k + \eta^j\eta^k]\,, \tag{3-104}$$

$$\underline{X}_{n+1}'' = \underline{B}_n + \underline{S}_n''$$

then the the difference between $E[\varphi(\underline{X}_{n+1})]$ (in (3-90)) and $E[\varphi(\underline{X}_{n+1}'')]$ is only of order h^4. But then we have to sample two R^d-valued random variables $\{\underline{\xi}\}$ and $\{\underline{\eta}\}$.

Chapter 4

Variance Reduction Techniques

In this chapter we consider variance reduction techniques for evaluating the expectations of functionals of solutions of stochastic differential equations. Intrinsically, the numerical evaluation of these expectations involves a sampling process, i.e., Monte-Carlo computation. Being a finite process, Monte-Carlo computation creates statistical errors due to imperfect sampling. The errors depends heavily on how one chooses the estimators for the expectations.

Our goal is to construct estimators with a small variance. In the first section we consider Chorin's variance reduction technique for evaluating expectations of functionals of Gaussian random variables. This technique exploits specific properties of the Hermite polynomials. In section 2 we introduce the concept of partial variance reduction and show how to implement Chorin's techniques for functionals of solutions of stochastic differential equations.

4.1 Variance Reduction Using Hermite Polynomials--Chorin's Estimator

Consider a random function $g(\underline{\xi}) = g(\xi^1,\cdots,\xi^d)$ where $\underline{\xi} = (\xi^1,\cdots,\xi^d)$ is an R^d-valued Gaussian random variable with distribution $N(\underline{0}, I_d)$ (see (1–40)). The expectation of $g(\underline{\xi})$ is

$$E[g(\underline{\xi})] = E[g(\xi^1,\cdots,\xi^d)] = (2\pi)^{-\frac{d}{2}} \int g(\underline{u})\, e^{-\frac{1}{2}|\underline{u}|^2}\, d\underline{u} \qquad (4\text{-}1)$$

where $\underline{u} = (u^1,\cdots, u^d)$, $d\underline{u} = du^1\cdots du^d$ and we recall that $|\underline{u}|$ is the 2-norm of $\underline{u}$ in the R^d space. The Gaussian random variable $\underline{\xi}$ can be readily sampled (see chapter 5). The usual Monte-Carlo estimate of $E[g(\xi)]$ is given by

$$E[g(\xi)] = N^{-1}\sum_{j=1}^{N} g(\xi_j) = N^{-1}\sum_{j=1}^{N} g(\xi_j^1, \cdots, \xi_j^d) \tag{4-2}$$

where $\{ \xi_j^k \}$ are drawn from the Gaussian distribution with mean 0 and variance 1. The standard deviation of this estimate, which yields the order of magnitude of error, is

$$N^{-\frac{1}{2}}\Big(E[g^2(\xi)] - [Eg(\xi)]^2 \Big)^{\frac{1}{2}} \tag{4-3}$$

which is proportional to $N^{-\frac{1}{2}}$, thus may not be acceptable for reasonable size N. Hence, an estimate of $E[g(\xi)]$ with smaller standard deviation is needed to achieve more accuracy of Monte-Carlo computation.

In [6] Chorin proposed a method to obtain an estimator for $E[g(\xi)]$ with substantial reduction in standard deviation. The main idea is to use finite Hermite series of the goal function g to design an estimator of control variate type for $E[g(\xi)]$. The set of Hermite polynomials

$$H_n(z) = \frac{(-1)^n}{\sqrt{n!}} e^{\frac{z^2}{2}} \frac{d^n}{dz^n} e^{-\frac{z^2}{2}}, \quad n = 1, 2, \cdots, \tag{4-4}$$

form a family of orthonormal functions in the space $L_2(R)$ of square integrable functions defined on R with respect to the weight $\frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}}$. That is,

$$(2\pi)^{-\frac{1}{2}} \int H_n(z) H_m(z) e^{-\frac{z^2}{2}} dz = \delta_{nm} \tag{4-5}$$

The first few of them are $H_0(z) = 1$, $H_1(z) = z$, $H_2 = \frac{1}{\sqrt{2}}(z^2 - 1)$, $H_3(z) = \frac{1}{\sqrt{6}}(z^3 - 3z)$. In fact, Hermite polynomials satisfy the recursive relation:

$$H_{n+1}(z) = \frac{1}{\sqrt{n+1}} z H_n(z) - \sqrt{\frac{n}{n+1}} H_{n-1}(z) \tag{4-6}$$

In general, let $\underline{m} = (m^1, \cdots, m^d)$ with m^j nonnegative integers and denote $|\underline{m}| = m^1 + \cdots + m^d$. We define the product polynomials:

$$H_{\mathbf{m}} = H_{(m^1, \cdots, m^d)}(\underline{u}) = H_{m^1}(u^1) \cdots H_{m^d}(u^d) \,. \tag{4-7}$$

Then the family of functions

$$H_{\mathbf{m}}(\underline{u}) \cdot e^{-\frac{1}{2}|u|^2}, \quad 0 \le |\underline{m}| < \infty \tag{4-8}$$

form a complete orthonormal set in the space $L_2(R^d)$ of all square integrable functions defined on R^d with respect to the weight $(2\pi)^{-\frac{1}{d}} e^{-\frac{1}{2}|u|^2}$. For a more detailed analysis of the family of Hermite polynomials $H_{\mathbf{m}}$, see Chorin [6], Hitzl and Maltz [19]. Assuming that the function $g(\underline{u})\, e^{-\frac{1}{2}|u|^2}$ lies in the space $L_2(R^d)$ we can expand it in terms of the orthonormal functions in (4-8):

$$g(\underline{u})\, e^{-\frac{1}{2}|u|^2} = \sum_{\mathbf{m}} a_{\mathbf{m}}\, H_{\mathbf{m}}(\underline{u})\, e^{-\frac{1}{2}|u|^2} \tag{4-9}$$

,i.e.,

$$g(\underline{u}) = \sum_{\mathbf{m}} a_{\mathbf{m}}\, H_{\mathbf{m}}(\underline{u})$$

where

$$a_{\mathbf{m}} = E[H_{\mathbf{m}}(\underline{\xi}) g(\underline{\xi})] = (2\pi)^{-\frac{d}{2}} \int H_{\mathbf{m}}(\underline{u}) g(\underline{u})\, e^{-\frac{1}{2}\|u\|^2}\, d\underline{u} \tag{4-10}$$

because of the orthonormality:

$$E[H_{\mathbf{n}}(\underline{\xi}) H_{\mathbf{m}}(\underline{\xi})] = E[H_{n^1, \cdots, n^d}(\underline{\xi}) H_{m^1, \cdots, m^d}(\underline{\xi})] = \delta^{\mathbf{n}, \mathbf{m}} = \delta^{n^1 m^1, \cdots, n^d m^d}$$

We also notice that (i): $a_{\underline{0}} = E[g(\underline{\xi})]$, and recall that (ii): $E[H_{\mathbf{m}}(\underline{\xi})] = 0$. Consider

$$E[g(\underline{\xi})] = b_{\underline{0}} + E\Big[g(\underline{\xi}) - \sum_{|\mathbf{m}| \le |\underline{p}|} b_{\mathbf{m}} H_{\mathbf{m}}(\underline{\xi}) \Big] \tag{4-11}$$

which is valid for any set of numbers $\{ b_{\mathbf{m}} \}$. In actual computation, we will take $\{ b_{\mathbf{m}} \}$ to be $\{ a_{\mathbf{m}}^* \}$. The success of Chorin's variance reduction lies in the fact that the identity does not imply that Monte-Carlo estimatiors on the both sides of it will have the same amount of standard deviation.

Chorin's idea is to make a first sampling to determine the coefficients $b_{\mathbf{m}}$ in (4-11) according to the formula (4-10), then a second sampling to simulate the Gaussian variables that appear in the argument of g and the polynomials $H_{\mathbf{m}} = H_{m^1,\dots,m^d}$ on the right hand side of (4−11). Specifically, we have

$$a_{\mathbf{m}}^* = \frac{1}{N}\sum_{j=1}^{N} \left\{ H_{\mathbf{m}}(\underline{\xi}_j)\, g(\underline{\xi}_j) \right\} \tag{4-12}$$

and

$$E[g(\underline{\xi})] = a_{\mathbf{n}}^* + \frac{1}{N}\sum_j \left\{ g(\underline{\hat{\xi}}_j) - \sum_{|\mathbf{m}| \le |\mathbf{p}|} a_{\mathbf{m}}^* H_{\mathbf{m}}(\underline{\hat{\xi}}^j) \right\} \tag{4-13}$$

where $\underline{\xi}_j = \{ \xi_j^i \}$ and $\underline{\hat{\xi}}_j = \{ \hat{\xi}_j^i \}$ are two sets of independent samples drawn from the Gaussian distribution with mean 0 and variance 1. The formulae (4-12) and (4-13) are called **Chorin's estimator** for $E[g(\underline{\xi})]$. In order to see the standard deviation of Chorin's estimator, let us define the remainder

$$r_{\mathbf{p}}(\underline{u}) = g(\underline{u}) - \sum_{|\mathbf{m}| \le |\mathbf{p}|} a_{\mathbf{m}} H_{\mathbf{m}}(\underline{u}) \tag{4-14}$$

the L_2 norm of which is given by $[E\|r_{\mathbf{p}}\|^2]^{\frac{1}{2}}$. Then Chorin's estimator has the following standard deviation:

$$N^{-\frac{1}{2}}\left[E\|r_{\mathbf{p}}\|^2\right]^{\frac{1}{2}} + N^{-1}O(C|\underline{\mathbf{p}}|) \tag{4-15}$$

where C is constant depending on the function g. For sufficiently smooth g and $|\underline{\mathbf{p}}| = O(N^{\varepsilon})$, $\varepsilon>0$; (4-15) is of order $O(N^{-(1-\varepsilon)})$ since $[E\|r_{\mathbf{p}}\|^2]^{\frac{1}{2}}$ is relatively small. Indeed, Maltz and Hitzl [19] showed that Chorin estimator has the exact standard deviation:

$$N^{-\frac{1}{2}}\left[E\|r_{\underline{p}}\|^2 + N^{-1}\sum_{|\underline{m}|\le|\underline{p}|}\sigma_{\underline{m}}^{\ 2}\right]^{\frac{1}{2}} \tag{4-16}$$

where $\sigma_{\underline{m}}^2$ is the variance of $a_{\underline{m}}^*$ in (4-12) with $N = 1$, i.e., the single sample variance in the Monte-Carlo estimate of $a_{\underline{m}}$.

4.2 Partial Variance Reduction in Numerical Simulation

Let φ be a sufficiently smooth functional; we consider how to implement Chorin's variance reduction technique to evaluate accurately the expectation $E[\varphi(\underline{X}_n)]$ where $\underline{X}_n$ is the numerical solution of equation (3-1) with some numerical method. To be specific, we consider the scheme (3–99):

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) \tag{4-17}$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + \sqrt{h}\,\underline{\xi}_n$$

$$\underline{X}_{n+1} = \underline{X}_n + \sqrt{h}\,\underline{\xi}_n + \frac{1}{2}h[\underline{f}(\underline{Q}_n) + \underline{f}(\underline{Q}_n')]\,.$$

We recall that the R^d-valued random variables $\{\underline{\xi}_n\}$ have the Gaussian distribution $N(\underline{0}, \underline{I}_d)$ and are independent of each other. For convenience in later discussion, we define

$$\underline{Y}_n = \frac{1}{2}[\underline{f}(\underline{Q}_n) + \underline{f}(\underline{Q}_n')] \quad , n = 0, 1, 2, \cdots. \tag{4-18}$$

We note that $\underline{X}_n$, thus $\varphi(\underline{X}_n)$ is a function of the n independent R^d-valued Gaussian random variables $\{\underline{\xi}\}$ since we implement the scheme (4-17) n times. That is, $\varphi(\underline{X}_n)$ is a function of $n \cdot d$ (scalar) Gaussian random variables.

Hence, it is not acceptable even if the variance technique considered in the previous section is applied only once to all these Gaussian variables to evaluate expectation $[\varphi(\underline{X}_n)]$. since then we need to apply Chorin's estimator with respect to $n \cdot d$ Gaussian random variables.

Therefore, we wish to do only partial variance reduction, i.e., to determine a proper expression for $E[\varphi(\underline{X}_{n+1})]$ so that we have some *distinguished* $\underline{\xi}$ in this expression and apply Chorin's variance reduction technique to them only.

Strategy A We observe that, in terms of the definition in (4-18)

$$\varphi(\underline{X}_n) = \varphi(\underline{X}_{n-1} + \sqrt{h}\,\underline{\xi}_n + h\underline{V}_n) \tag{4-19}$$
$$= \cdots$$
$$= \varphi(\underline{X}_0 + \sqrt{h}\,[\underline{\xi}_0 + \cdots + \underline{\xi}_{n-1}] + h[\underline{V}_0 + \cdots + \underline{V}_{n-1}])$$

from which we see that the accumulating random variable $\underline{\xi}_0 + \cdots + \underline{\xi}_{n-1}$ play a major role in determing $\varphi(\underline{X}_n)$ while the individual $\underline{\xi}_k$, $0 \le k \le n-1$ plays only minor role. Hence, our first strategy is to apply Chorin's estimator to evaluate $E[\varphi(\underline{X}_n)]$ at each time step with respect to $\underline{\xi}_0 + \cdots + \underline{\xi}_{n-1}$ only.

The main drawbacks with strategy A are (i): variance reduction is only done with respect to $\underline{\xi}_0 + \cdots + \underline{\xi}_{n-1}$ and (ii): there is no connection between any two successive evaluations $E[\varphi(\underline{X}_n)]$ and $E[\varphi(\underline{X}_n)]$ for any fixed n. To improve variance reduction technique and '*link*' $E[\varphi(\underline{X}_n)]$ at each time step, we write first

$$\varphi(\underline{X}_{n+1}) = [\varphi(\underline{X}_{n+1}) - \varphi(\underline{X}_n)] + \cdots + [\varphi(\underline{X}_{k+1}) - \varphi(\underline{X}_k)] + \cdots + \varphi(\underline{X}_0) \,. \tag{4-20}$$

For each piece of $\varphi(\underline{X}_{k+1}) - \varphi(\underline{X}_k)$, we carry out the Taylor expansion of $\varphi(\underline{X}_{k+1})$ about $\underline{X}_k$ by using the definition in (4-18):

$$\varphi(\underline{X}_{k+1}) - \varphi(\underline{X}_k) = \varphi_{,j}(\underline{X}_k)[\sqrt{h}\,\underline{\xi}_k + h\underline{V}_k]^j \tag{4-21}$$
$$+ \frac{1}{2}h\ \varphi_{,jl}(\underline{X}_k)\ \xi_k^j\ \xi_k^l + O(h^{\frac{3}{2}})$$

where $\underline{\xi}_k = \{\ \xi_k^j\ \}$ is the random variable sampled at the k^{th} time step. Removing the first term on the right hand side to the left and denoting the resultant expression by Φ_k, we have

$$\Phi_k = \varphi(\underline{X}_{k+1}) - \varphi(\underline{X}_k) - \sqrt{h}\,\varphi_{,j}(\underline{X}_k)\,\xi_k^j \qquad (4\text{-}22)$$

$$= h\varphi_{,j}(\underline{X}_k)\,\underline{V}_k^j + \frac{1}{2}h\varphi_{,jl}(\underline{X}_k)\,\xi_k^j\,\xi_k^l + O(h^{\frac{3}{2}})\,.$$

Note the independence of $\underline{X}_k$ from $\underline{\xi}_k$. Taking expectations on both sides of the first equality in (4-22) and summing the results over k from 0 to $n-1$, we have

$$E[\varphi(\underline{X}_n)] = E[\Phi_{n-1}] + \cdots + E[\Phi_1] + E[\varphi(\underline{X}_0)] \qquad (4\text{-}23)$$

which is equivalent to

$$E[\varphi(\underline{X}_n)] = E[\varphi(\underline{X}_{n-1})] + E[\Phi_{n-1}]\,. \qquad (4\text{-}24)$$

Thus we obtain a recursive relation between $E[\varphi(\underline{X}_n)]$ and $E[\varphi(\underline{X}_{n+1})]$. From the second equality of (4–22), we see that, for each fixed k, $\underline{\xi}_k$ play a leading role in determing Φ_k. And the same argument as in **A** shows that $\underline{\xi}_0 + \cdots + \underline{\xi}_{k-1}$ play a major role in determing $\varphi_{,j}(\underline{X}_k)$ and $\varphi_{,jk}(\underline{X}_k)$. Hence we have

Strategy B We evaluate the expectation $E[\varphi(\underline{X}_n)]$ by applying Chorin's estimator to evaluate $E[\Phi_{n-1}]$ in (4-24) with respect to $\underline{\xi}_n$ and $\frac{1}{\sqrt{n}}(\underline{\xi}_0 + \cdots + \underline{\xi}_{n-1})$ (nomalized) where Φ_{n-1} is computed according to first equality in (4-22), and adding the result to $E[\varphi(\underline{X}_{n-1})]$ which is obtained from the previous (the $(n-1)^{th}$) time step.

Intuitively, we would expect that strategy **B** give a better result than strategy **A** in the evaluation of $E[\varphi(\underline{X}_n)]$ since we apply Chorin's estimator to more Gaussian random variables in the former case. However, it is not clear how the standard deviation, at each time step, of the estimate in strategy **B** will accumulate and whether this accumulation will destroy the accuracy of the variance reduction. These questions are answered in theorem 1 in the below.

Lemma 4.1. Let $z_1, z_2, \cdots, z_n$ be n random variables, then their variances satisfy the following relation

$$\sigma^2_{z_1+\cdots+z_n} \le [\sigma_{z_1} + \cdots + \cdots + \sigma_{z_n}]^2 \qquad (4\text{-}25)$$

By applying the Cauchy-Schwartz inequality to the right hand side of the above inequality, we find

$$\sigma^2_{z_1+\cdots+z_n} \le n\ [\ \sigma^2_{z_1} + \cdots + \sigma^2_{z_n}\ ] \qquad (4\text{-}26)$$

From the second equality in (4-22), we may write $\Phi_k = h\ g_k$ for each fixed k, where g_k is of order h^0. Then from formula (4–16) we see that the standard deviation SD_k of Chorin's estimator for each $E[\Phi_k]$ is of order

$$h \cdot SD_k = h \cdot N^{-\frac{1}{2}} \left[E|\underline{r}_{\underline{p}}|^2 + N^{-1} \sum_{|\underline{m}| \le |\underline{p}|} \sigma^2_{\underline{m}} \right]^{\frac{1}{2}} \qquad (4\text{-}27)$$

for some finite $\underline{m}$'s, where $\underline{r}_{\underline{p}}$ is defined similar as in (4–14) with $g = g_k$ and we suppress the dependence of $\underline{r}_{\underline{m}}$ on k. Let the maximum of (4-27) over k be SD_{k_0} for some k_0, then by lemma 1, we have the bound $n \cdot hSD_{k_0} = t_n \cdot SD_{k_0}$ for the estimate in strategy **B** Hence we have

Theorem 4.1. The standard deviations of the estimates in strategy **B** with N samplings are of the form in (4-16) which is proportional to t_n at the n^{th} step, i.e., the piecewise application of Chorin's variance reduction technique to each summand in (4-23) produces a standard deviation as in (4-16).

This theorem tells us that, for short time, t_n is small and the strategy **B** produces a very small standard deviation which is proportional to t_n and SD_{k_0}. This is consistent with computed results as we shall see in next chapter. Of course, the main disadvantage of strategy B is that we need to evaluate the first order partial derivatives of φ as can be seen in (4-22) and (4-23).

Chapter 5

Nunmerical Implementation

In order to compare the accuracy between various numerical schemes and support the conjecture made in section 4 of Chapter 3, in this chapter, we present computational results for the following schemes:

Euler's Method

$$\underline{X}_{n+1} = \underline{X}_n + \Delta_n \underline{w} + h\underline{f}(\underline{X}_n)$$

Method A (3-102)

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n)$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + \sqrt{h}\,\underline{\xi}$$

$$\underline{X}_{n+1} = \underline{X}_n + \sqrt{h}\,\underline{\xi} + \frac{1}{2}h[\,\underline{f}(\underline{Q}_n) + \underline{f}(\underline{Q}_n')\,]$$

Method B (3-60)

$$\underline{Q}_n = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n)$$

$$\underline{Q}_n' = \underline{X}_n + \frac{1}{2}h\underline{f}(\underline{X}_n) + \frac{3}{2}\sqrt{h}\,\underline{\beta}'$$

$$\underline{X}_{n+1} = \underline{X}_n + \Delta_n \underline{w} + \frac{1}{3}h[\,\underline{f}(\underline{Q}_n) + 2\cdot\underline{f}(\underline{Q}_n')\,]$$

To simulate the Gaussian random variables $\Delta_n \underline{w}$ and $\underline{\beta}'$ in Euler's method and Method B, we write

$$\Delta_n \underline{w} = \sqrt{h}\,\underline{\xi}, \quad \underline{\beta}' = \frac{1}{2}\underline{\xi} + \frac{\sqrt{3}}{6}\underline{\eta}$$

where $\underline{\xi}$ (as in Method B) and $\underline{\eta}$ are two independent R^d-valued Gaussian variables with distribution $N(0, I_d)$. These expressions give the exact correlation between $\Delta_n \underline{w}$ and $\underline{\beta}'$. Then $\underline{\xi}$ and $\underline{\eta}$ are sampled according to the Box-Muller formula

$$\xi^i = \cos(2\pi u^i)\left[-2\log(v^i)\right]^{\frac{1}{2}}$$

$$\eta^i = \sin(2\pi u^i)\left[-2\log(v^i)\right]^{\frac{1}{2}}$$

where $\underline{u}$ and $\underline{v}$ are two independent R^d-valued uniform distribution over $[0, 1]^d$.

The first computational example which we present here is the 2×2 system of linear equations:

$$dx_1 = -x_2dt + dw_1$$

$$dx_2 = -x_1dt + dw_2$$

with zero initial data $x_1(0) = x_2(0) = 0$. Adding these two equations together and by a simple calculation, we find

$$x_1(t) + x_2(t) = \int_{t_n}^{t_n+h} e^{-(t-s)}\, d(w_1(s) + w_2(s))$$

which is a Gaussian random variable with mean 0 and variance $1 - \exp(-2t)$. We consider the expectation: $E[\cos(x_1(t) + x_2(t))]$ which has the exact value:

$$\exp(-\frac{1}{2}(1 - e^{-2t}))$$

The second computational example is the 2×2 system of nonlinear equations:

$$dx_1 = e^{-(x_1 + x_2)}dt + dw_1$$

$$dx_2 = e^{-(x_1 + x_2)}dt + dw_2$$

with the zero initial data $x_1 = x_2(0) = 0$. By a calculation, we can find

$$e^{(x_1(t) + x_2(t))} = 1 + \int_{t_n}^{t_n+h} e^{-(w_1(s) + w_2(s))}\, ds$$

We consider the expectation: $E[e^{(x_1(t) + x_2(t))}]$ which has the exact value

$$3\exp(t) - 2$$

For each scheme we compute the expectations in two ways: (i): the usual Monte-Carlo estimator and (ii): Chorin's estimator in **Strategy B** of Chapter 4. The errors depend on the stepsize (Δt) and the number of simulation (N). The situation is shown in table 5.1-6. In each table, we list the results at three different time: 0.2, 0.4 and 0.8.

For each scheme, in the first subcolumn, we list the errors of computed solution obtained by using usual Monte-Carlo estimators and the second column for Chorin's estimators. Especially, in table 5.2 and 5.5, we also list the standard deviations of the computed solutions.

From these tables, we can see that Chorin's estimators can precisely show that Euler's method is a first order method. For methods B and C, Chorin's estimators can roughly show that they are second order method. But, to effect variance reduction for many step runs, we must increase the number of simulations N.

Ex.A: t = 0.2 N = 2,500 T = 0.8480						
Δt	Euler		Sch. A		Sch. B	
0.2000	-3.16-2	-2.92-2	5.50-4	2.55-3	2.15-4	2.21-3
0.1000	-1.94-2	-1.36-2	-4.82-3	1.02-3	-4.94-3	2.95-4
0.0500	-1.40-2	-6.80-3	-6.97-3	3.02-4	-7.12-3	-2.20-4
0.0250	-1.07-2	-3.23-3	-7.31-3	9.88-4	-7.34-3	-5.02-5
0.0125	-3.47-2	-1.85-3	1.24-3	3.01-4	-1.22-3	-2.62-4

Ex.A: t = 0.4 N = 2,500 T = 0.7593						
Δt	Euler		Sch. A		Sch. B	
0.2000	-4.76-2	-3.92-2	-4.35-3	4.50-3	-5.15-3	1.87-3
0.1000	-2.95-2	-1.89-2	9.74-3	-1.41-3	-1.03-2	-2.16-4
0.0500	-1.98-2	-9.11-3	-1.04-2	2.92-3	-1.05-2	-2.92-4
0.0250	-9.79-4	-6.06-3	3.34-3	2.28-4	3.29-3	-1.17-3
0.0125	5.91-4	-3.41-3	2.74-3	5.81-4	2.78-3	-1.25-3

Ex.A: t = 0.8 N = 2,500 T = 0.6710						
Δt	Euler		Sch. A		Sch. B	
0.2000	-5.54-2	-4.23-2	-9.30-3	5.56-3	-1.15-2	1.38-3
0.1000	-3.22-2	-2.08-2	-1.12-2	7.13-3	-1.16-2	-1.04-3
0.0500	-2.87-3	-1.68-2	6.64-3	-1.53-3	6.49-3	-7.07-3
0.0250	7.57-4	-9.62-3	5.44-3	-1.36-3	5.55-3	-4.89-3
0.0125	3.02-3	-8.37-3	5.35-3	-2.82-3	5.37-3	-6.15-3

Table 5.1

Ex.A: t = 0.2 N = 10,000 T = 0.8480						
Δt	Euler		Sch. A		Sch. B	
0.2000	-2.85-2 ±2.33-3	-2.92-2 ±2.16-4	3.07-3 ±1.97-3	2.50-3 ±1.80-4	2.77-3 ±1.96-3	2.31-3 ±1.67-4
0.1000	-1.50-2 ±2.14-3	-1.36-2 ±5.15-4	-6.87-4 ±2.01-3	6.50-4 ±3.79-4	-7.32-4 ±1.97-3	5.26-4 ±3.86-4
0.0500	-8.46-3 ±2.09-3	-6.66-3 ±2.21-4	-1.70-3 ±2.11-3	4.42-4 ±1.33-4	-1.70-3 ±2.01-3	3.28-5 ±1.89-4
0.0250	-3.87-3 ±2.05-3	-3.07-3 ±1.73-4	-6.03-4 ±1.98-3	5.76-4 ±2.23-4	-5.74-4 ±2.01-3	1.83-4 ±1.80-4
0.0125	6.15-4 ±2.00-3	-1.56-3 ±2.25-4	2.20-3 ±2.02-3	-6.12-5 ±1.99-4	2.22-3 ±1.98-3	4.46-5 ±2.28-4

Ex.A: t = 0.4 N = 10,000 T = 0.7593						
Δt	Euler		Sch. A		Sch. B	
0.2000	-4.14-2 ±3.39-3	-3.88-2 ±1.55-3	1.26-3 ±2.07-2	3.76-3 ±4.86-3	6.83-4 ±1.18-2	2.88-3 ±2.24-3
0.1000	-2.10-2 ±3.22-3	-1.87-2 ±7.56-4	-1.73-3 ±2.93-3	-1.70-3 ±1.16-3	-1.85-3 ±2.96-3	3.05-4 ±1.17-3
0.0500	-9.16-3 ±3.14-3	-8.52-3 ±5.00-4	-1.20-4 ±2.08-3	1.78-3 ±3.97-4	-6.40-5 ±3.04-3	4.80-4 ±5.48-4
0.0250	-7.54-4 ±3.03-3	-4.52-3 ±7.08-4	3.61-3 ±2.03-3	-3.03-4 ±7.02-4	3.67-3 ±2.98-3	-6.60-5 ±7.07-4
0.0125	5.67-4 ±3.01-3	-2.22-3 ±7.62-4	2.73-3 ±2.63-3	-1.20-3 ±7.18-4	2.71-3 ±2.98-3	-2.87-5 ±7.58-4

Ex.A: t = 0.8 N = 10,000 T = 0.6710						
Δt	Euler		Sch. A		Sch. B	
0.2000	-4.40-2 ±4.26-3	-4.20-2 ±2.29-3	1.14-3 ±3.68-3	5.97-3 ±1.08-3	1.96-2 ±3.88-3	1.80-2 ±1.79-3
0.1000	-1.79-2 ±4.13-3	-1.88-2 ±1.07-3	2.29-1 ±3.70-3	4.87-3 ±1.21-3	2.29-3 ±3.94-4	1.25-3 ±1.21-3
0.0500	-4.57-3 ±3.91-3	-1.08-2 ±1.92-3	5.13-3 ±3.68-3	-1.03-3 ±1.18-3	5.26-3 ±3.86-3	-9.18-4 ±1.89-3
0.0250	-1.00-3 ±3.91-3	-5.24-3 ±2.44-3	3.75-3 ±3.59-3	2.92-3 ±2.00-3	3.69-3 ±3.87-3	-3.57-4 ±2.11-3
0.0125	1.57-3 ±3.87-3	-2.36-3 ±2.20-3	3.94-3 ±3.75-3	-5.90-3 ±2.17-3	3.94-3 ±3.85-3	5.74-5 ±2.18-3

Table 5.2

Ex.A: t = 0.2 N = 40,000 T = 0.8480						
Δ t	Euler		Sch. A		Sch. B	
0.2000	-2.92-2	-2.93-2	5.08-3	2.38-3	2.02-3	1.85-3
0.1000	-1.25-2	-1.35-2	1.60-3	6.65-4	1.51-3	5.96-4
0.0500	-5.31-3	-6.59-3	1.34-2	-6.90-6	1.31-3	9.76-5
0.0250	-2.55-3	-3.30-3	6.86-4	-2.03-5	6.67-4	-6.21-5
0.0125	1.17-3	1.67-3	2.75-3	-2.64-4	2.74-3	6.53-5

Ex.A: t = 0.4 N = 40,000 T = 0.7593						
Δ t	Euler		Sch. A		Sch. B	
0.2000	-3.70-2	-3.86-2	5.08-3	3.64-3	4.40-3	2.99-3
0.1000	-1.63-2	-1.85-2	2.65-3	2.76-4	2.47-5	5.18-4
0.0500	-7.73-3	-9.28-3	1.31-3	-1.51-4	1.23-3	-2.65-4
0.0250	-2.66-4	-4.68-3	4.11-3	-8.19-4	4.10-3	-2.40-4
0.0125	-3.59-3	-1.94-3	-1.39-3	-2.44-4	-1.40-3	2.36-4

Ex.A: t = 0.8 N = 40,000 T = 0.6710						
Δ t	Euler		Sch. A		Sch. B	
0.2000	-3.86-2	-4.18-2	6.11-3	2.30-3	5.11-3	2.46-3
0.1000	-1.80-2	-2.13-2	2.42-3	-5.88-4	2.13-3	-8.37-4
0.0500	-4.47-3	-1.07-2	5.27-3	-2.20-3	5.13-3	-7.99-4
0.0250	-7.33-3	-3.72-3	-2.48-3	-2.27-4	-2.53-3	1.06-3
0.0125	-3.02-3	-1.73-3	-6.39-4	-1.46-4	-6.34-4	6.47-4

Table 5.3

Ex.B: t = 0.2 N = 2,500 T = 1.6640						
Δt	Euler		Sch. A		Sch. B	
0.2000	1.83-1	1.62-1	8.01-3	-8.46-3	7.50-3	-8.66-3
0.1000	8.03-2	7.40-2	6.36-3	4.57-4	6.85-3	1.03-3
0.0500	3.73-2	2.95-2	1.68-2	-5.98-4	3.27-3	-3.79-3
0.0250	6.47-3	-1.32-2	-9.54-3	-6.41-4	-9.51-3	-1.77-3
0.0125	-1.10-2	5.78-3	-1.87-2	1.46-4	-1.86-2	-3.96-4

Ex.B: t = 0.4 N = 2,500 T = 2.4750						
Δt	Euler		Sch. A		Sch. B	
0.2000	3.72-1	3.52-1	9.77-3	-7.01-3	1.21-2	-4.94-3
0.1000	1.92-1	1.44-1	3.52-2	-6.00-3	3.61-2	-6.96-3
0.0500	9.30-2	5.96-2	-2.40-2	-4.74-3	-5.80-2	-5.81-3
0.0250	-4.92-2	2.53-2	-3.38-2	2.61-3	-3.35-2	-2.02-3
0.0125	-1.61-2	9.28-3	-3.23-2	-5.75-4	-3.23-2	-2.22-3

Ex.B: t = 0.8 N = 2,500 T = 4.6770						
Δt	Euler		Sch. A		Sch. B	
0.2000	8.92-2	7.29-1	7.20-2	-5.14-2	8.12-2	-5.24-2
0.1000	2.30-1	2.63-1	-1.07-1	-3.64-2	-1.05-1	-5.76-2
0.0500	9.37-2	1.16-1	-6.50-2	-4.04-3	-6.26-2	-1.40-2
0.0250	1.23-2	4.80-2	-6.40-2	1.20-3	-6.35-2	-7.31-3
0.0125	-2.26-2	1.42-2	-6.01-2	-1.51-3	-5.98-2	-8.76-3

Table 5.4

Ex.B: t = 0.2 N = 10,000 T = 1.6640						
Δt	Euler		Sch. A		Sch. B	
0.2000	1.68-1 ±1.30-2	1.58-1 ±3.24-4	-3.27-3 ±9.89-3	-1.10-2 ±8.79-3	-3.13-3 ±1.00-2	-1.08-2 ±9.49-4
0.1000	7.72-3 ±1.13-2	6.96-2 ±1.19-3	3.45-3 ±1.00-2	-3.45-3 ±1.01-3	3.14-3 ±1.01-2	-3.63-3 ±8.35-4
0.0500	3.97-2 ±1.07-2	3.29-2 ±9.63-4	8.01-3 ±9.97-3	-7.43-4 ±8.36-4	5.37-3 ±1.02-2	-1.16-3 ±2.20-4
0.0250	2.12-2 ±1.04-2	1.62-2 ±1.17-3	4.90-3 ±9.87-3	-1.46-3 ±9.46-4	4.77-3 ±1.01-2	-2.36-4 ±1.12-3
0.0125	1.73-2 ±1.03-2	7.91-3 ±1.22-3	9.25-3 ±9.82-3	-3.35-4 ±9.33-4	9.17-3 ±1.02-2	3.14-4 ±1.20-3

Ex.B: t = 0.4 N = 10,000 T = 2.4750						
Δt	Euler		Sch. A		Sch. B	
0.2000	3.52-1 ±2.76-2	3.34-1 ±7.51-3	-7.70-3 ±2.11-2	-2.30-2 ±4.83-3	-7.94-3 ±2.18-2	-2.23-2 ±5.84-3
0.1000	1.67-1 ±2.44-2	1.45-1 ±3.90-2	1.23-2 ±1.47-2	-5.61-3 ±1.33-3	1.17-2 ±1.86-2	-7.97-3 ±3.32-3
0.0500	7.80-2 ±2.26-2	6.99-2 ±4.71-3	7.18:3 ±1.87-3	1.02-3 ±4.33-3	6.79-3 ±2.16-2	-1.41-3 ±4.44-3
0.0250	5.12-2 ±2.25-2	3.39-2 ±4.85-3	1.70-2 ±1.86-2	-1.36-3 ±3.13-3	1.66-2 ±2.20-2	-1.06-3 ±4.72-3
0.0125	6.97-3 ±2.21-2	1.61-2 ±4.79-3	-9.50-3 ±2.02-2	-2.03-3 ±4.17-3	9.46-3 ±2.19-2	-8.97-4 ±4.73-3

Ex.B: t = 0.8 N = 10,000 T = 4.6770						
Δt	Euler		Sch. A		Sch. B	
0.2000	8.16-1 ±6.34-2	7.45-1 ±2.65-2	6.83-3 ±5.16-2	-3.95-2 ±2.11-2	4.90-3 ±6.70-2	-5.24-2 ±2.12-2
0.1000	3.46-2 ±6.76-2	3.37-1 ±2.66-2	1.01-3 ±5.20-2	-3.41-3 ±2.01-2	-1.04-3 ±6.33-2	1.17-2 ±2.41-2
0.0500	1.98-1 ±6.92-2	1.62-1 ±2.65-2	3.79-2 ±5.83-2	-6.96-3 ±2.07-2	3.61-2 ±6.61-2	-4.15-3 ±2.47-2
0.0250	5.12-2 ±6.88-2	7.38-2 ±2.53-2	-2.56-2 ±5.83-2	-1.19-2 ±2.13-2	-2.54-2 ±6.74-2	-4.86-3 ±2.47-2
0.0125	-6.27-3 ±6.11-2	3.28-2 ±2.53-2	-4.36-2 ±5.56-2	-1.07-2 ±2.03-2	-4.37-2 ±6.44-2	2.01-3 ±2.50-2

Table 5.5

Ex.B: t = 0.2 N = 40,000 T = 1.6640						
Δ t	Euler		Sch. A		Sch. B	
0.2000	1.52-1	1.57-1	-1.56-2	-1.21-2	-1.35-2	-1.01-2
0.1000	6.38-2	7.08-2	8.73-3	-2.27-3	-8.30-3	-1.80-3
0.0500	2.88-2	3.28-2	-4.74-3	-6.21-4	-4.60-3	-4.42-3
0.0250	5.62-3	1.56-2	-1.03-2	1.05-4	-1.03-2	1.07-4
0.0125	-8.06-3	7.46-3	-1.58-2	2.23-4	-1.58-2	3.90-4

Ex.B: t = 0.4 N = 40,000 T = 2.4750						
Δ t	Euler		Sch. A		Sch. B	
0.2000	3.21-1	3.38-1	-3.28-2	-1.87-2	-2.95-2	-1.51-2
0.1000	1.37-1	1.46-1	-1.43-2	-5.26-3	-1.34-2	-4.11-3
0.0500	4.96-2	6.81-2	-2.00-2	3.01-4	-1.98-2	3.61-4
0.0250	-2.48-3	3.20-2	-3.56-2	3.36-4	-3.54-2	1.18-3
0.0125	-7.12-3	1.46-2	-1.65-2	5.70-4	-1.65-2	1.01-3

Ex.B: t = 0.8 N = 40,000 T = 4.6770						
Δ t	Euler		Sch. A		Sch. B	
0.2000	7.24-1	7.50-1	-6.60-2	-3.96-2	-6.00-2	-3.14-2
0.1000	3.05-1	3.40-1	-3.77-2	6.35-3	-3.61-2	6.81-3
0.0500	4.88-2	1.51-1	-1.07-1	6.87-4	-1.06-1	4.80-3
0.0250	3.75-2	6.83-2	-3.90-2	1.54-3	-3.89-2	4.06-3
0.0125	-1.95-2	2.30-2	-5.68-2	-5.85-4	-5.67-2	5.34-4

Table 5.6

Appendix A

In this appendix, we will carry out the two calculations that leads to (2–74) and (2-77) respectively. To do this, we need the following lemma.

Lemma A.1. Let ξ and η are two Gaussian random variables with mean 0 and variance 1 and have the correlation coefficient ρ. Then the random variable $\zeta = \frac{1}{\sqrt{1-\rho^2}}(\eta - \rho\xi)$ is Gaussian with mean 0 and variance 1, independent of ξ.

Proof. From the given condition, we know that the joint probability density of ξ and η is given by

$$f_{\xi,\eta}(u,v) = \frac{1}{2\pi\sqrt{1-\rho^2}}\exp[-\frac{1}{2(1-\rho^2)}(u^2 - 2\rho uv + v^2)] \qquad \text{(a-1)}$$

Let $z = \frac{1}{\sqrt{1-\rho^2}}(v - \rho u)$. We see that the Jacobian of the transformation $(u, v) \longrightarrow (u, z)$ is $|J| = \sqrt{1-\rho^2}$. Hence, the exponential part of the density (a-1) becomes

$$-\frac{1}{2(1-\rho^2)}(u^2 - 2\rho uv + v^2)$$

$$= -\frac{1}{2(1-\rho^2)}[u^2 - 2\rho u(\rho u + \sqrt{1-\rho^2}z) + (\rho u + \sqrt{1-\rho^2}z)^2]$$

$$= -\frac{1}{2}(u^2 + z^2)$$

Therefore, the joint probability density of ξ and ζ is:

$$f_{\xi,\zeta}(u,z) = |J|\, f_{\xi,\eta}(u,v) = \frac{1}{2\pi}\exp[-\frac{1}{2}(u^2 + z^2)]$$

which implies that ζ is Gaussian with mean 0 and variance 1 and is independent from ξ. This completes the proof.

Corollary 1. Under the assumption of the theorem 1 but that ξ and η have variances σ_1^2 and σ_2^2 respectively, we have $E[\xi^2\eta] = E[\xi\eta^2] = 0$ and $E[\xi^2\eta^2] = \sigma_1^2 \cdot \sigma_2^2 \cdot (1 + 2\rho^2)$.

Lemma A.2. The random variables β', γ', δ' have Gaussian distributions with mean 0. Their variances are $\frac{1}{3}$, $\frac{2}{15}$ and $\frac{1}{20}$ respectively.

Proof. Since these random variables are nothing but linear combination of independent increments of the Wiener process, they are Gaussian with mean 0. By the definition of β, we have

$$E[\beta^2] = \int_{t_n}^{t_n+h} \int_{t_n}^{t_n+h} \Delta w_r \Delta w_s \, drds$$

$$= 2 \cdot \int_{t_n}^{t_n+h} \int_{t_n}^{s} E[\Delta w_r \Delta w_s] \, drds$$

$$= 2 \cdot \int_0^h \int_0^s r \, drds = 2 \cdot \frac{1}{6} h^3 = \frac{1}{3} h^3$$

which is equivalent to saying that the variance of β' is $\frac{1}{3}$. Note that we changed the domain of integration in the last integral. The second variance can be found in a similar way. The evaluation of the third variance is a little more complicated. We have

$$E[\delta^2] = E\left\{ \int_{t_n}^{t_n+h} \int_{t_n}^{t_n+h} \int_{t_n}^{s_1} \int_{t_n}^{s_2} \Delta w_{r_1} \Delta w_{r_2} dr_1 dr_2 ds_1 ds_2 \right\}$$

$$= \int_{t_n}^{t_n+h} \int_{t_n}^{t_n+h} \int_{t_n}^{s_1} \int_{t_n}^{s_2} \min(r_1 - t_n, r_2 - t_n) \, dr_1 dr_2 ds_1 ds_2$$

$$= 2\cdot \int_{t_n}^{t_n+h} \int_{t_n}^{s_1}\int_{t_n}^{s_1}\int_{t_n}^{s_2} \min(r_1-t_n, r_2-t_n)\, dr_2 dr_1 ds_2 ds_1$$

$$= 2\cdot \int_0^h\int_0^{s_1} \left\{ \int_0^{s_2}\int_{r_2}^{s_1} r_2\, dr_1 dr_2 + \int_0^{s_2}\int_0^{r_2} r_1\, dr_1 dr_2 \right\} ds_2 ds_1$$

$$= 2\cdot \int_0^h\int_0^{s_1} \left\{ \int_0^{s_2} (s_1 r_2 - r_2^2) dr_2 + \int_0^{s_2} \frac{1}{2} r_2^2\, dr_2 \right\} ds_2 ds_1$$

$$= 2\cdot \int_0^h\int_0^{s_1} \left\{ \left\{ \frac{1}{2} s_1 s_2^2 - \frac{1}{3} s_2^3 \right\} + \frac{1}{6} s_2^3 \right\} ds_2 ds_1 = \frac{1}{20} h^5$$

which says that the variance of $\delta^{'}$ is $\frac{1}{20}$. This completes the proof of the lemma 2.

Now we begin to carry out the details of (2–74) and (2-77). A careful look at the calculation in (2–31) and of V_n of (2–24) shows that everything is straightforward except the expectation of $\beta^{'2}\vartheta^{'}$. Remember that $\beta^{'}$ is a Gaussian variable; we can employ the technique of the lemma 1, since

$$E[\beta^2\vartheta] = \int_{t_n}^{t_n+h} E[\beta^2 \Delta w_s^{\,2}]\, ds \, . \tag{a-2}$$

Let σ_1 and $\sigma_2(s)$ denote the standard deviations of β and Δw_s respectively. Then the correlation coefficient $\rho(s)$ of β and Δw_s can be calculated in

$$\sigma_1 \cdot \sigma_2(s) \cdot \rho(s) = E[\beta \Delta w_s] = \int_{t_n}^{t_n+h} E[\Delta w_s \Delta w_r]\, dr$$

$$= \int_{t_n}^{s} (r - t_n)\, dr + \int_{s}^{t_n+h} (s - t_n)\, ds = (s-t_n)h - \frac{1}{2}(s-t_n)^2 \, .$$

Then by corollary 1 of lemma 1, from (a-2), we have

$$E[\beta^2\vartheta] = \int_{t_n}^{t_n+h} \left\{ \frac{1}{3}h^3 \cdot (s-t_n)[1+2\rho(s)^2] \right\} ds \tag{a-3}$$

$$= \int_0^h \left\{ \frac{1}{3}sh^3 + 2\cdot\left\{s^2h^2 - s^3h + \frac{1}{4}s^4\right\} \right\} ds = \frac{13}{30}h^5$$

which is equivalent to saying that $E[\beta'^2\vartheta'] = \frac{13}{30}$. In the same way, we have $E[\vartheta'^2] = \frac{7}{12}$, thus we arrive at

Lemma A.3. $E[\beta'^2\vartheta'] = \frac{13}{30}$ and $E[\vartheta'^2] = \frac{7}{12}$

Now we come to carry out the calculation in (2-53). The techniques are quite similar to those used in the above. By using lemma 1, 2 and corollary 1 of lemma 1 and noting dependences between random variables, one is able to show that

$$E[(2\gamma' - \beta')^2] = E[4\gamma'^2 - 4\gamma'\beta' + \beta'^2] = 4\cdot\frac{2}{15} - 4\cdot\frac{5}{24} + \frac{1}{3} = \frac{1}{30} \tag{a-4}$$

Now we evaluate the expectation of $(\tau' - 3\beta'\vartheta' + 2\beta'^3)^2$. There is no substantial difference from the above in the calculation except that more work is needed. The result is

$$E[\,(\tau' - 3\beta'\vartheta' + 2\beta'^3)^2\,]$$

$$= E[\tau'^2] + 9E[\beta'^2\beta'^2] + 4E[\beta'^6] - 6E[\tau'\beta'\vartheta'] + 4E[\tau'\beta'^3] - 12E[\beta'^4\vartheta']$$

$$= \frac{9}{5} + 9\cdot\frac{25}{28} + 4\cdot\frac{5}{9} - 6\cdot\frac{301}{240} + 4\cdot\frac{271}{280} - 12\cdot\frac{7}{10} = \frac{11}{2520} \tag{a-5}$$

We collect the results from (a-3) to (a-5) in the following

Lemma A.4. $E[2\gamma' - \beta']^2 = \frac{1}{30}$ and $E[\tau' - 3\beta'\vartheta' + 2\beta'^3]^2 = \frac{11}{2520}$.

Finally, to illustrate the role that independence play in the calculation, we evaluate the expectation $E[\tau'^2]$ in (a-5). For convenience, we will calculate

$E[\tau^2]$. Recall the definition of $\tau = \int_{t_n}^{t_n+h} \Delta w_s^{\,3}\, ds$. We have

$$E[\tau^2] = \int_{t_n}^{t_n+h} \int_{t_n}^{t_n+h} E[\, \Delta w_{s_1}^{\,3} \Delta w_{s_2}^{\,3}\,]\, ds_1 ds_2 \qquad \text{(a-6)}$$

$$= 2\cdot \int_{t_n}^{t_n+h} \int_{t_n}^{s_2} E[\, \Delta w_{s_1}^{\,3} \Delta w_{s_2}^{\,3}\,]\, ds_1 ds_2\,,$$

in which we rewrite

$$\Delta w_{s_1}^{\,3} \Delta w_{s_2}^{\,3} = [\, (\Delta w_{s_2} - \Delta w_{s_1}) + \Delta w_{s_1}\,]^3 \Delta w_{s_1}^{\,3}$$

$$= (\Delta w_{s_2} - \Delta w_{s_1})^3 \Delta w_{s_1}^3 + 3\cdot(\Delta w_{s_2} - \Delta w_{s_1})^2 \Delta w_{s_1}^4 + 3\cdot(\Delta w_{s_2} - \Delta w_{s_1}) \Delta w_{s_1}^5 + \Delta w_{s_1}^6$$

Then the independence between Δw_{s_1} and $\Delta w_{s_2} - \Delta w_{s_1}$ shows that expectations of the first and third terms on the right hand side of the above identity are zero. Thus from (a-6), we are led to

$$E[\tau^2] = 2\cdot \int_{t_n}^{t_n+h} \int_{t_n}^{s_2} [3\cdot E[(\Delta w_{s_2} - \Delta w_{s_1})^2 \Delta w_{s_1}^4\,] + E[\Delta w_{s_1}^{\,6}]\, ds_1 ds_2$$

$$= 2\cdot \int_0^h \int_0^{s_2} [\, 9(s_2 - s_1)s_1^2 + 15 s_1^3\,]\, ds_1 ds_2 = 2\cdot \int_0^h \left\{ 3s_2^4 + \frac{3}{2} s_1^4 \right\} ds_2 = \frac{9}{5} h^5\,.$$

References

[1] V.I. Arnold, ' Stochastic Differential Equations: Theory and Applications, ' John Wiley & Sons, Inc., 1974

[2] S.W. Benson, ' The Foundations of Chemical Kinetics, ' McGraw-Hill, New York, 1960

[3] R.H. Cameron, " A Simpson's rule for the numerical evaluation of Wiener's integrals in function space, " Duke Math. J., v.18, pp. 111-130, 1951

[4] S. Chandraseskhar, " Stochastic Problems in Physics and Astronomy, " Noise and Stochastic Processes (N. Wax, Ed.), Dover, New York, 1954

[5] A.J. Chorin, " Accurate Evaluation of Wiener Integrals ", Mathematics of Computation, v. 27, pp. 1-15, 1973

[6] A.J. Chorin, " Hermite expansions in Monte-Carlo computation, " J. Computational Phys. v. 8, pp. 472-482, 1971

[7] A.J. Chorin, ' Lectures on Turbulence Theory, ' Publish or Perish, Inc., Boston, 1975

[8] A.J. Chorin, " Numerical study of slightly viscous flow, " J. Fluid Mech. v. 57, pp. 785-796, 1973

[9] A.J. Chorin, T.J.R. Hughes, M.F. McCracken, and J.E. Marsden, " Product formula and numerical algorithms, " Comm. Pure Appl. Math. v. 31, 1978, pp. 205-256

[10] R.P. Feynman & A.R. Hibbs, ' Quantum Mechanics and Path Integrals, ' McGraw-Hill, New York, 1965

[11] A.L. Fogelson, " A Mathematical Model and Numerical Method for Studying Platelet Adhesion and Aggregation during Blood Clotting, " Journal of Computational Physics, v. 50, pp. 111-134, 1984

[12] J.N. Franklin, " Difference methods for stochastic ordinary differential equations, " Math. Comp. v. 19, pp. 552-561, 1965

[13] C.W. Gear, " Numerical Initial Value Problems in Ordinary Differential Equations, " Prentice Hall, New Jersey, 1971

[14] J. Glimm & A. Jaffe, ' Quantum Physics: a functional integral point of view, ' Springer-Verlag, New York, 1981

[15] A.H. Jazwinski, " Stochastic Processes and Filtering Theory, " Academic Press, New York, 1970

[16] P. Levy, " Wiener's random function and other Laplacian random functions, " Proc. 2th Berkeley Symp. Math. Stat. Probability, Univ. of Calif. Press, v.1, 1951, pp. 171-187 pp.

[17] E.J. McShane, " Stochastic differential equations and models of random processes, " Proc. 6th Berkeley Symp. Math. Stat. Probability, Univ. of Calif. Press, v. 1, 1966, pp. 263-294

[18] E.J. McShane, ' Stochastic Calculus and Stochastic Models, ' Academic Press, New York, 1974

[19] F.H. Maltz & D.L. Hitzl, ' Variance Reduction in Monte-Carlo Computations using Multi-Dimensional Hermite Polynomials, ' J. Computational Physics, v. 32, pp. 345-376, 1979

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