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DISSERTATION

Selected Topics in Numerics of Stochastic Differential Equations

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Kurzfassung der Dissertation

Das Thema dieser Dissertation kann als "Numerische Methoden für stochastische Differentialgleichungen" im weitesten Sinne wiedergegeben werden. Tatsächlich handelt es sich um eine Zusammenstellung von Arbeiten in vier verschiedenen Forschungsgebieten, bei denen jeweils sowohl Numerik als auch Stochastik eine Rolle spielen. Bei allen vorgestellten Problemen handelt es sich entweder direkt um numerische Probleme, oder sie stehen in einer engen Beziehung zu solchen. Die Berufung auf Stochastik ist hingegen so zu verstehen, dass diese Fragestellungen stochastische Methoden verwenden, sofern sie sie nicht direkt auf stochastische Probleme beziehen. Genauer gesagt ist hier unter Stochastik das weit kleinere Gebiet der stochastischen Analysis zu verstehen, das heißt wir betrachten die Lösungen stochastischer Differentialgleichung. Eine weitere Verbindung der verschiedenen Probleme, welcher im folgenden sehr verkürzt vorgestellt werden sollen, besteht in der großen Betonung ihrer jeweiligen Geometrie. Tatsächlich spielen geometrische Beobachtungen in allen hier behandelten Fragestellungen eine wesentliche Rolle. Schließlich soll noch bemerkt werden, dass Anwendungen in der Finanzmathematik in allen vorgestellten Bereichen im Hintergrund stehen. In Kapitel 2 und Kapitel 3 ist dieser Zusammenhang sehr naheliegend und direkt, aber auch in Kapitel 4 und Kapitel 5 lässt sich insofern eine Verbindung zur Finanzmathematik herstellen, als dass die dort behandelten Verfahren in finanzmathematischen Anwendungen (in naheliegender Art und Weise) Verwendung finden können.

Kapitel 1 besteht aus einer kurzen Einführung in stochastische Analysis, hauptsächlich zur Fixierung einer einheitlichen Schreibweise, sowie Einführungen in die Theorie stochastischer partieller Differentialgleichungen, das heißt stochastischer Differentialgleichungen auf unendlichdimensionalen separablen Hilberträumen, und in die Numerik stochastischer Differentialgleichungen. Kapitel 2 behandelt zunächst die Geometrie der iterierten Itô-Stratonovich Integrale der Brown'schen Bewegung. Als erste Anwendung dieser Betrachtungen stellen wir die "Cubature on Wiener space" Methode von Terry Lyons und Nicolas Victoir vor, eine Methode zur schwachen Approximation von Lösungen stochastischer Differentialgleichungen. Während die bisherigen Teile von Kapitel 2 hauptsächlich, aber nicht ausschließlich, Zusammenstellungen schon bekannter Ergebnisse beinhaltet, sind die weit-

eren Abschnitte des Kapitels neu. Darin stellen wir eine explizite Formel für die Berechnung der Momente der iterierten Itô-Stratonovich Integrale vor, sowie einen Algorithmus zur Berechnung der Momente der zugehörigen (Lévy) Flächen (areas) basierend auf der Darstellungstheorie der Strukturen, welche die Geometrie der iterierten Itô-Stratonovich Integrale beschreiben.

Das Kubaturverfahren am Wienerraum wird schließlich in Kapitel 3 auf den unendlichdimensionalen Fall verallgemeinert, das heißt auf stochastische partielle Differentialgleichungen, die bestimmte Regularitätsbedingungen erfüllen. Es ist vielleicht erwähnenswert, dass dies das erste, auf Kubatur am Wienerraum beruhende, Resultat für unbeschränkte Koeffizienten ist. Außerdem stellen wir eine Erweiterung für stochastische partielle Differentialgleichungen vor, welche durch Sprungprozesse (mit endlicher Aktivität) angetrieben werden. Neben den theoretischen Resultaten wird die Methode auch anhand zweier numerischer Beispiele illustriert. Die neuen Resultate in Kapitel 2 und Kapitel 3 sind in Zusammenarbeit mit Josef Teichmann entstanden.

Während die Themen der Kapitel 2 und 3 eng miteinander verbunden sind, behandeln die beiden folgenden Kapitel jeweils für sich ein separates Thema. Im Falle von Kapitel 4 handelt es sich um schwache numerische Approximation von reflektierten Diffusionen, das heißt von Lösungen stochastischer Differentialgleichungen, welche an den Grenzen eines bestimmten Gebietes reflektiert werden. Die Bedeutung dieser Prozesse liegt in der stochastischen Repräsentation der zugehörigen parabolischen partiellen Differentialgleichungen mit Neumann Randwertbedingungen. Aus numerischer Sicht sind reflektierte Diffusionen unangenehm, da die üblichen schwachen Eulerverfahren nur mit schwacher Ordnung $1/2$ konvergieren. Wir präsentieren zwei neue Approximationsverfahren. Das erste Verfahren nutzt einen Korrekturterm, der aus der Fehlerentwicklung des Eulerverfahrens konstruiert werden kann, und liefert Konvergenzordnung 1. Allerdings lässt es sich im Allgemeinen nur in Dimension eins anwenden. Das zweite Verfahren ist ein adaptives Verfahren, welches in jeder Dimension angewendet werden kann, auch bei Problemen, welche die Regularitätsvoraussetzungen üblicher Verfahren mit höherer Ordnung als $1/2$ nicht erfüllen. Empirische Tests weisen auf eine Verbesserung der Konvergenzrate über $1/2$ hin, aber Rate 1 konnte nicht erreicht werden. Kapitel 4 basiert auf Zusammenarbeit mit Anders Szepessy und Raul Tempone.

Kapitel 5 beinhaltet eine Implementierung eines neuen "Simuliertes Annealing" Verfahrens von Fabrice Baudoin, Martin Hairer und Josef Teichmann. "Simuliertes Annealing" ist ein bedeutendes Verfahren zum Auffinden globaler Minima nicht-konvexer Funktionen durch stochastischer Störung eines Gradientenflusses. Baudoin, Hairer und Teichmann konnten das Verfahren auf kompakte homogene Räume von Liegruppen ausdehnen. Angewendet auf Optimierungsaufgaben im $\mathbb{R}^n$ bedeutet das, dass hypoelliptische, also nicht-elliptische stochastische Störungen verwendet werden kön-

nen. Die Ergebnisse dieses Kapitels entstanden in Zusammenarbeit mit Josef Teichmann und Richard Warnung.

Abstract

The present thesis addresses four different topics which can be broadly subsumed under "Numerics of stochastic differential equations". More precisely, all the treated problems are concerned with or related to questions of numerical analysis or approximation. Moreover, all these numerical problems are either stochastic in nature, i. e. can be formulated in terms of stochastic differential equations, or are approached using stochastic methods, viz. methods involving stochastic differential equations. The problems are treated in a geometric way in the sense that special emphasis is placed on the geometry of the problem at hand and geometric methods are often employed. Moreover, several of the problems are motivated by mathematical finance. This is at least true for Chapter 2 and Chapter 3, but also the other two chapters can naturally find applications to financial mathematics. Thus, we have identified the four main threads of the present thesis: numerics, stochastic analysis, geometry and financial mathematics.

After a brief introduction into stochastic analysis in finite dimensions (here mainly to fix notations) and infinite dimensions, and to numerical methods for stochastic differential equations given in Chapter 1, Chapter 2 starts with a discussion on the geometry of iterated Itô-Stratonovich integrals of Brownian motion, which is the starting point for the subsequent sections and also for Chapter 3. Then a major application is presented, namely the method of "Cubature on Wiener space" by Terry Lyons and Nicolas Victoir, a method for weak approximation of solutions of stochastic differential equations. It should be stressed here that these parts are mainly collections of known results, albeit maybe taken into a new perspective. Then we switch to the problem of computing higher moments of the iterated Itô-Stratonovich integrals and the corresponding areas. We provide one explicit formula for the moments of the iterated Itô-Stratonovich integrals and one algorithm for the calculation of the moments of the Itô-Stratonovich areas using representation theory.

In Chapter 3, we extend the "Cubature on Wiener space" method to an appropriate class of stochastic partial differential equations, i. e. stochastic differential equations on separable Hilbert spaces. Notice that this is the first variant of the "Cubature on Wiener space" method that allows for unbounded driving vector fields, even in finite dimensions. Moreover, a "hy-

brid" extension to stochastic partial differential equations driven by jump diffusions (with finite activity) is presented. All the new results in Chapter 2 and Chapter 3 are based on joint work with Josef Teichmann.

Chapter 4 proposes two new algorithms for weak approximation of reflected diffusions, i. e. stochastic differential equations reflected at the boundary of a given domain. One algorithm uses an error expansion of the usual Euler method for reflected diffusions in order to construct a correction term which allows to improve the asymptotic order of convergence from 1/2 for the Euler method to 1. The algorithm, however, is often only applicable for dimension one. Furthermore, an adaptive algorithm for general dimensions is constructed, which is also suitable for problems, where the regularity conditions of usual higher order methods fail. Chapter 4 is based on joint work with Anders Szepessy and Raul Tempone.

Simulated annealing is a well-known stochastic method for global optimization of non-convex functions. Chapter 5 contains an implementation of the algorithm presented by Fabrice Baudoin, Martin Hairer and Josef Teichmann [4], which extends simulated annealing to homogenous spaces of Lie groups. In the context of global optimization on $\mathbb{R}^n$, this methods allows hypo-elliptic implementations of simulated annealing. Chapter 5 is based on joint work with Josef Teichmann and Richard Warnung.

Acknowledgments

Brain: an apparatus with which we think we think.
Ambrose Bierce, *The Devil's Dictionary*

The past four years, during which I have worked for and on the completion of this thesis, have been happy and exciting times. Therefore, I would like to take the opportunity to thank those people, who are largely responsible for that.

First and foremost, I would like to thank my supervisor Josef Teichmann. His contribution is threefold: On the purely mathematical level, he has always impressed me with his enormous creativity, which has fueled our joint thinking to an extent, which cannot be overrated. Furthermore, he has helped a lot in keeping my motivation up. Last but not least, I have always enjoyed our controversial conversations on topics such as politics and history.

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Contents

Chapter 1

Introduction

1.1 Prerequisites from stochastic analysis

In this section we collect the basic concepts, notations and results from the theory of stochastic analysis which we are going to routinely use in the subsequent parts of the text. The main aim of this part is to fix notations. The reader is referred to excellent books like Revuz and Yor [68], Karatzas and Shreve [40], Protter [64], Ikeda and Watanabe [38] and Øksendal [62] for more information on this subject and, in particular, on all the properties mentioned in this section.

Let $B = (B_t)_{t\in[0,\infty[} = (B_t^1, \dots, B_t^d)_{t\in[0,\infty[}$ denote a d-dimensional *Brownian motion* defined on the filtered probability space $\big(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\in[0,\infty[}, P\big)$, which is assumed to satisfy the usual conditions of right continuity and completeness. Frequently, we will only consider equations up to some fixed, finite time horizon $T > 0$. In this case, we will consider Brownian motions only defined on $[0, T]$ without special notice.

We are mainly interested in the Brownian motion as the driving noise for *stochastic differential equations* (SDEs). Given a collection of vector fields, i. e. smooth maps, $V, V_1, \dots, V_d : \mathbb{R}^n \to \mathbb{R}^n$, we consider the corresponding SDE

$$dX_t^x = V(X_t^x)dt + \sum_{i=1}^{d} V_i(X_t^x)dB_t^i, \quad t \in [0, T], \tag{1.1}$$

with initial value $X_0^x = x \in \mathbb{R}^n$.

Definition 1.1.1. A *(strong) solution* to the SDE (1.1) is an $(\mathcal{F}_t)_{t\in[0,T]}$-adapted stochastic process $(X_t^x)_{t\in[0,T]}$ with continuous paths such that

$$X_t^x = x + \int_0^t V(X_s^x)ds + \sum_{i=1}^{d} \int_0^t V_i(X_s^x)dB_s^i$$

for all $t \in [0,T]$. In particular, the Lebesgue and Itô integrals in the above equation have to be well-defined, e. g. we may require the (strong) L^2-condition that

$$E\Big(\int_0^t \Big(\|V(X_s^x)\| + \sum_{i=1}^d \|V_i(X_s^x)\|^2\Big)ds\Big) < \infty$$

for all $t \in [0,T]$.

By a solution to an SDE we will always understand a strong solution.

Even though we have formulated the definition of an SDE in terms of the Itô stochastic integral, it is often more convenient to work in terms of the *Stratonovich integral*. To this end, introduce a vector field $V_0 : \mathbb{R}^n \to \mathbb{R}^n$ defined by

$$V_0(x) = V(x) - \frac{1}{2}\sum_{i=1}^d DV_i(x) \cdot V_i(x), \tag{1.2}$$

where $Df(x) \cdot h$ denotes the directional derivative of the function f in direction h at the point x, where $x, h \in \mathbb{R}^n$. A (strong) solution of the SDE in Stratonovich form

$$dX_t^x = V_0(X_t^x)dt + \sum_{i=1}^d V_i(X_t^x) \circ dB_t^i, \quad t \in [0,T], \tag{1.3}$$

is the process X^x as defined in Definition 1.1.1.

Remark 1.1.2. Of course, the solution X^x of the Stratonovich SDE (1.3) satisfies the integral equation

$$X_t^x = x + \int_0^t V_0(X_s^x)ds + \sum_{i=1}^d \int_0^t V_i(X_s^x) \circ dB_s^i,$$

where "$\circ dB_s^i$" denotes the Stratonovich differential with respect to the Brownian motion.

Remark 1.1.3. Recall that vector fields $V : \mathbb{R}^n \to \mathbb{R}^n$ can be identified with first order differential operators via

$$Vf(x) = Df(x) \cdot V(x).$$

For convenience, we will usually assume that our vector fields are C^∞-*bounded*, i. e. they are infinitely often differentiable and the derivatives of order ≥ 1 are bounded – in particular, the vector fields themselves do not need to be bounded. Most of what follows will, of course, also hold under much weaker assumptions, namely linear growth and Lipschitz conditions.

We cite the classical *existence and uniqueness theorem* for SDEs.

Proposition 1.1.4. *Assume that the vector fields $V, V_1, \dots, V_d$ are C^∞-bounded. Then for all $x \in \mathbb{R}^n$ there is a unique strong solution $X^x = (X_t^x)_{t\in[0,T]}$ of equation (1.1) with initial value x. Moreover, X^x has moments of every order.*

At one point we will need to know whether the solution of a particular SDE stays in a certain submanifold of the space. This leads to the *invariance problem* for SDEs.

Definition 1.1.5. Given a submanifold $M \subset \mathbb{R}^n$. M is called *locally invariant* under (1.1) if for all $x \in M$ there is a strictly positive stopping time τ^x such that

$$X_t^x \in M, \quad \text{for all } 0 \le t \le \tau^x, \text{ a. s.}$$

Proposition 1.1.6. *A submanifold $M \subset \mathbb{R}^n$ is locally invariant with respect to the SDE (1.1) if and only if*

$$V_i(x) \in T_x M, \quad \textit{for all } x \in M,\ i = 0, \dots, d.$$

For a proof of this classical theorem see Appendix A.1.1.

We end this section by pointing out the connection between SDEs and partial differential equations (PDEs). Using the interpretation of vector fields as differential operator, we introduce the second order differential operator

$$Lf(x) = V_0 f(x) + \frac{1}{2}\sum_{i=1}^{d} \underbrace{V_i^2 f(x)}_{=V_i(V_i f)(x)}, \quad x \in \mathbb{R}^n, \tag{1.4}$$

and consider the heat equation

$$\begin{cases} \dfrac{\partial}{\partial t}u(t,x) = Lu(t,x), & (t,x) \in [0,T]\times\mathbb{R}^n, \\ u(0,x) = f(x), & x \in \mathbb{R}^n, \end{cases} \tag{1.5}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ and L is understood to act on the x-variable of u only.

Proposition 1.1.7 (Feynman-Kac Formula)**.** *Under appropriate regularity conditions on the vector fields and on f, the solution of the heat equation (1.5) is given by*

$$u(t,x) = E(f(X_t^x)).$$

We will sometimes assume that the stochastic processes under considerations have smooth transition densities. Recall that the transition density $p_t(x,y)$ of the n-dimensional stochastic process X^x with initial value $x \in \mathbb{R}^n$ at time $t > 0$ and $y \in \mathbb{R}^n$ is defined by

$$E(f(X_t^x)) = \int_{\mathbb{R}^n} f(y)p_t(x,y)dy$$

for all bounded measurable functions $f : \mathbb{R}^n \to \mathbb{R}$. Of course, this definition only makes sense if the law $(X_t^x)_*P$ of X_t^x is absolutely continuous with respect to the Lebesgue measure.

Definition 1.1.8. A stochastic process X^x with initial value x is called *hypo-elliptic* if its transitional density is smooth in (t, x, y).

It is not surprising that hypo-ellipticity is usually very hard to check. There is, however, a very simple sufficient condition found by Hörmander [36] and Malliavin [54], see also Nualart [61].

Definition 1.1.9. The SDE (1.1) satisfies *Hörmander's condition* if the Lie algebra generated by

$$\{V_1, \dots, V_d, [V_0, V_1], \dots, [V_0, V_d]\} \tag{1.6}$$

spans the whole space $\mathbb{R}^n$ at each point $x \in \mathbb{R}^n$, where V_0 denotes the Stratonovich corrected drift vector field (1.2).

Indeed, X^x is hypo-elliptic if its governing SDE satisfies Hörmander's condition. Actually, for smoothness of $(y, t) \mapsto p_t(x, y)$ it is already sufficient that (1.6) is satisfied at the initial value x.

1.2 Stochastic analysis in Hilbert spaces

We recapitulate the concepts and results of stochastic analysis on infinite dimensional Hilbert spaces which are most relevant to us. The interested reader is referred to da Prato and Zabczyk [18] for more information on this subject, see also Carmona and Tehranchi [11]. Furthermore, we discuss the restriction of SDEs in a Hilbert space to a subspace, which is only a Fréchet space. For background information on functional analysis see, for instance, Yosida [89] or Werner [87].

1.2.1 The abstract Cauchy problem in Hilbert spaces

Once and for all, let H be a real, *separable* Hilbert space with norm $\|\cdot\|_H$ and inner product $\langle \cdot, \cdot \rangle_H$. As a preparation for the stochastic case, we would like to take a short look at the deterministic, linear *abstract Cauchy problem*

$$\begin{cases} \dfrac{d}{dt}u(t) = Au(t) + f(t), \quad t \in [0, T], \\ u(0) = x, \end{cases} \tag{1.7}$$

where $x \in H$ and A is a linear, but (possibly) unbounded operator, $A : \mathcal{D}(A) \subset H \to H$, and $f : [0, T] \to H$ is measurable. The obvious problem which we are facing when trying to make sense of problem (1.7) is that we somehow need to make sure that $u(t) \in \mathcal{D}(A)$, for all $t \in [0, T]$. In general, this endeavor fails and we cannot solve (1.7). Therefore, we need to restrict our setting.

Remark 1.2.1. Usually, H will be a Hilbert space of functions and A a partial (integro-) differential operator defined on a subspace of (weakly) differentiable elements of H. Then equation (1.7) naturally corresponds to a PDE or PIDE (partial integro-differential equation).

Definition 1.2.2. A family $S = (S_t)_{t\in[0,\infty[}$ of bounded linear operators $H \to H$ is called *C_0-semigroup* if

(i) $S_t S_s = S_{t+s}$, for all $s, t \in [0, \infty[$,

(ii) $S_0 = \mathrm{id}_H$, the identity operator on H,

(iii) $\lim_{t\searrow 0} \|S_t x - x\|_H = 0$, for all $x \in H$.

The *(infinitesimal) generator* A of the C_0-semigroup S is the linear operator A defined by

$$Ax = \lim_{t\searrow 0} \frac{S_t x - x}{t}, \quad x \in \mathcal{D}(A),$$

where $\mathcal{D}(A) \subset H$ is the set of all $x \in H$ such that the above limit exists.

In the next Proposition 1.2.3 we collect some well-known facts about C_0-semigroups and their generators for future reference. The proofs of these results are standard and can be found in most text books on functional analysis.

Proposition 1.2.3. *Let $S = (S_t)_{t\in[0,\infty[}$ denote a C_0-semigroup on H with generator A.*

(1) A is a closed, densely defined linear operator on H.

(2) $x \in \mathcal{D}(A)$ implies $S_t x \in \mathcal{D}(A)$, for all $t \geq 0$.

(3) $\frac{d}{dt} S_t x = A S_t x = S_t A x$ for $x \in \mathcal{D}(A)$ and $t \geq 0$.

(4) There is a constant $c \in \mathbb{R}$ such that the resolvent set *$\rho(A)$ contains the interval $]c, \infty[$ and, moreover, $\|S_t\|_{L(H)} \leq M e^{ct}$, for all $t \in [0, \infty[$, where $M > 0$ is another constant and $\|\cdot\|_{L(H)}$ denotes the operator norm on the space $L(H)$ of bounded operators on H.*

(5) The map $t \mapsto S_t$ is continuous in the uniform norm in $L(H)$ if and only if A is a bounded operator. In that case, we have

$$S_t = e^{tA} = \sum_{k=0}^{\infty} \frac{1}{k!} t^k A^k$$

for $t \geq 0$.

Later on, we will also need the *Yosida approximation* of the unbounded operator A.

Definition 1.2.4. Let A be the generator of a C_0-semigroup. For $\lambda \in \rho(A)$, the Yosida approximation $A_\lambda \in L(H)$ is defined by

$$A_\lambda x = \lambda A(\lambda - A)^{-1} x, \quad x \in H.$$

Since the Yosida approximation is a bounded linear operator, the corresponding C_0-semigroup is denoted by $(e^{tA_\lambda})_{t\in[0,\infty[}$.

The Yosida approximations approximate the generator in the sense that

$$\lim_{n\to\infty} A_n x = Ax, \quad x \in \mathcal{D}(A), \tag{1.8}$$

$$\lim_{n\to\infty} e^{tA_n} x = S_t x, \quad x \in H, \tag{1.9}$$

where the convergence is uniform in t on compact subsets of $[0,\infty[$. Note that the limits in equations (1.8) and (1.9) make sense because we know that $n \in \rho(A)$ for all $n \in \mathbb{N}$ sufficiently large by Proposition 1.2.3 (1).

Coming back to the ordinary differential equation (ODE) (1.7), we now impose the condition that A is the generator of a C_0-semigroup S.[1] We distinguish between three types of solutions. $u : [0,T] \to H$ is called *strict solution* if u is differentiable, $u(t) \in \mathcal{D}(A)$, $t \in [0,T]$ and (1.7) holds for $t \in]0,T]$. We cannot expect to find strict solutions for each $x \in H$. Indeed, even in the homogeneous case, i. e. for $f \equiv 0$, it is easy to see that a strict solution for $x \in \mathcal{D}(A)$ is given by

$$u(t) = S_t x, \quad t \in [0,T],$$

which fails to be strict for $x \in H \setminus \mathcal{D}(A)$ in general.

As usual in functional analysis, we can arrive at a more general concept of a solution by testing with linear functionals. An H-valued function u is called *weak solution* of (1.7) if, for all $t \in [0,T]$,

$$\langle u(t), y\rangle_H = \langle x, y\rangle_H + \int_0^t \langle u(s), A^* y\rangle_H \, ds + \int_0^t \langle f(s), y\rangle_H \, ds, \quad \forall y \in \mathcal{D}(A^*),$$

where A^* denotes the adjoint operator of A.

The third concept comes from the variation of constants formula for ODEs in finite dimensions. $u : [0,T] \to H$ is called *mild solution* of equation (1.7) if

$$u(t) = S_t x + \int_0^t S_{t-s} f(s) ds, \quad \forall t \in [0,T].$$

Note that the above equation actually could serve as definition of u provided that the integral exists. While it is obvious that any strict solution u is also both a weak and a mild solution, it is not so simple to see that the latter two concepts are basically equivalent.[2]

[1] Note that the Hille-Yosida theorem, see Werner [87, Theorem VII.4.13] gives a criterion for the existence of a semigroup with generator A.

[2] If f is absolutely integrable, then there is a unique weak and mild solution u given by the variation of constants formula. See da Prato and Zabczyk [18, Proposition A.4].

1.2.2 Stochastic partial differential equations

Next we want to introduce stochastic differential equations in H, i. e. stochastic perturbations of (1.7). Since Hilbert spaces are usually function spaces and the operators are usually differential operators, SDEs in infinite dimensions are often called *stochastic partial differential equations* (SPDEs).

As before, let B denote a d-dimensional Brownian motion for some finite $d \in \mathbb{N}$. Consider the equation

$$\begin{cases} dX_t^x = \big(AX_t^x + \alpha(X_t^x)\big)dt + \sum_{i=1}^{d} \beta_i(X_t^x)dB_t^i, \quad t \in [0,T], \\ X_0^x = x \in H. \end{cases} \tag{1.10}$$

If $\alpha, \beta_1, \ldots, \beta_d : H \to H$ are vector fields, this is the direct infinite dimensional analogue to (1.1).

Remark 1.2.5. Equation (1.10) is an SDE with infinite dimensional state space but only driven by a finite number of Brownian motions. The theory of the corresponding equations with infinitely many Brownian motions is well-established and basically works completely analogous. There are, however, some technical points to observe due to the following observation: assume that $B = (B_t^i)_{i\in\mathbb{N}, t\in[0,\infty[}$ is an infinite collection of independent Brownian motions. Given a Hilbert space U with orthonormal basis (ONB) $(e_i)_{i\in\mathbb{N}}$, we cannot define a process

$$X_t = \sum_{i=1}^{\infty} B_t^i e_i$$

taking values in U because the above sum diverges (in L^2), since

$$E\Big(\|X_t\|_U^2\Big) = \sum_{i=1}^{\infty} E\big((B_t^i)^2\big) = \infty.$$

Consequently, one needs to work with *cylindrical Brownian motions* and the "(infinite dimensional) volatility matrix" needs to be a Hilbert-Schmidt type operator. We refer to da Prato and Zabczyk [18] for a full treatment of the general case.

We are content to stay in the framework with a finite number of Brownian motions because

- we believe that the main difficulties generally have to do with the infinite dimensionality of the state space and the unboundedness of the generator, not with the number of Brownian motions,
- we are mainly motivated by examples from finance, where a finite number of sources of randomness is usually already satisfactory, and

- numerical simulation anyhow requires to restrict one-self to finitely many Brownian motions.

Remark 1.2.6. In the literature, SPDEs are often defined as equations of the form

$$\frac{\partial}{\partial t}u(t,x) = Au(t,x) + F(u(t,x))\dot{W}(t,x), \tag{1.11}$$

where $t \in [0,T]$, $x \in \mathbb{R}^n$ and $\dot{W}$ is a space-time white noise on $[0,T] \times \mathbb{R}^n$. This approach is roughly equivalent to the da Prato-Zabczyk approach of (1.10), but always uses an infinite number of Brownian motions. The reader is referred to Nualart [61] and Walsh [86] for more information about this point of view.

Coming back to the SPDE (1.10), we may report the first benefit of our restriction to a finite number of Brownian motions: the theory of stochastic integration works exactly as in the finite dimensional case! In particular, Itô's isometry and Itô's formula look just as usual. Nevertheless, we have to consider several concepts of solutions to (1.10), just as in the infinite dimensional deterministic case (1.7). Before doing so, let us impose some conditions on the coefficients of the equation.

Assumption 1.2.7. A is the generator of a C_0-semigroup $S = (S_t)_{t\in[0,\infty[}$ on H and the vector fields $\alpha, \beta_1, \dots, \beta_d : H \to H$ are C^∞-*bounded*, i. e. they are C^∞ in the sense of Fréchet derivatives and all their derivatives – but not necessarily the vector fields themselves – are bounded (as maps from H to the respective space of multi-linear functions on H).

The above assumption in particular implies that the coefficients are globally Lipschitz and have linear growth.

Definition 1.2.8. Fix $x \in H$ and consider a continuous, predictable process $X^x = (X_t^x)_{t\in[0,T]}$ with values in H.

(1) X^x is called *strong solution* of the SPDE (1.10) if $X_t^x \in \mathcal{D}(A)$ a. s. and

$$X_t^x = x + \int_0^t \big(AX_s^x + \alpha(X_s^x)\big)ds + \sum_{i=1}^d \int_0^t \beta_i(X_s^x)dB_s^i, \tag{1.12a}$$

for $t \in [0,T]$.

(2) X^x is called *weak solution* of (1.10) if for all $y \in \mathcal{D}(A^*)$ we have

$$\langle X_t^x, y\rangle_H = \langle x, y\rangle_H + \int_0^t \big(\langle X_s^x, A^*y\rangle_H + \langle \alpha(X_s^x), y\rangle_H\big)ds + \sum_{i=1}^d \int_0^t \langle \beta_i(X_s^x), y\rangle_H \, dB_s^i, \quad t \in [0,T]. \tag{1.12b}$$

(3) Finally, X^x is a *mild solution* of the SPDE (1.10) if it satisfies the variation of constants formula

$$X_t^x = S_t x + \int_0^t S_{t-s}\alpha(X_s^x)ds + \sum_{i=1}^d \int_0^t S_{t-s}\beta_i(X_s^x)dB_s^i, \tag{1.12c}$$

$t \in [0,T]$.

Note that we implicitly require all the integrals in (1.12) to exist.

Remark 1.2.9. Mild or weak solutions of an SPDE are, in general, no semimartingales. Indeed, if a, say, mild solution X^x had a Doob-Meyer decomposition, Itô's formula reveals that it would have the form (1.12a). But this decomposition only exists if X^x actually also was a strong solution. Consequently, we cannot pass to Stratonovich formulations of SPDEs. In particular, there is no Itô formula for mild solutions of SPDEs! However, see [63] and [72], where Itô formulas for $f(X_t^x)$ are provided under additional smoothness assumptions on the functional f.

Under minimal assumptions, any strong solution of an SPDE is also a weak solution and any weak solution is a mild solution, but usually weak and mild solutions coincide. We concentrate on the concept of mild solutions which is most suitable for our purposes.

Proposition 1.2.10. *Given Assumption 1.2.7, the SPDE (1.10) has a mild solution X^x for any $x \in H$ which is unique among all processes Y satisfying*

$$P\left(\int_0^T \|Y_s\|_H^2 \, ds < \infty\right) = 1.$$

Moreover, the solution has bounded moments in the sense that

$$\sup_{t\in[0,T]} E(\|X_t^x\|_H^p) \leq C_{p,T}(1 + \|x\|_H^p)$$

for any $p \geq 2$.

Proof. The result is stated, under weaker conditions, in da Prato and Zabczyk [18, Theorem 7.4]. □

An important approach in the context of SPDEs is to use the Yosida approximations A_n of the generator A, see Definition 1.2.4, solve the corresponding SPDE and try to infer properties of the solution of the original problem from the solutions of the "approximate problems". More precisely, consider the solution $X^{x,n}$ of the SDE

$$dX_t^{x,n} = \big(A_n X_t^{x,n} + \alpha(X_t^{x,n})\big)dt + \sum_{i=1}^d \beta_i(X_t^{x,n})dB_t^i, \quad t \in [0,T], \tag{1.13}$$

with $X_0^{x,n} = x \in H$. Since A_n is a bounded operator, any mild solution of (1.13) is also a strong solution, so all the concepts of solutions coincide.

Proposition 1.2.11. *Let X be the mild solution of (1.10) and let $X^{x,n}$ be the solution of (1.13), provided that $n \in \mathbb{N}$ is large enough such that the Yosida approximation A_n of A exists. Then*

$$\lim_{n\to\infty} \sup_{t\in[0,T]} E\big(\|X_t^x - X_t^{x,n}\|_H^2\big) = 0$$

for any $x \in H$.

Proof. Once again, we refer to da Prato and Zabczyk [18, Proposition 7.5]. □

The preceeding discussion remains virtually unchanged if the SPDE is driven by Lévy processes of *finite activity*, i. e. the jump parts of the Lévy processes are compound Poisson processes. In the general Lévy setting, Filipović and Tappe [23] provide the existence and uniqueness theorem, but have to impose a contractivity assumption on the generator A. In the finite activity case, we would also like to mention the decomposition theorem of Forster, Lütkebohmert and Teichmann [25].

Let $L_t = (L_t^1, \dots, L_t^e)$, $t \in [0, \infty[$, be a vector of e independent compound Poisson processes with jump rates $\mu_j > 0$ and jump distribution ν_j, i. e. ν_j is a probability measure on $\mathbb{R}$, $j = 1, \dots, e$. This means that

$$L_t^j = \sum_{k=1}^{N_t^j} Z_k^j, \quad t \in [0, \infty[, \tag{1.14}$$

where N_t^j is a Poisson process with intensity μ_j and $(Z_k^j)_{k\in\mathbb{N}}$ is a sequence of independent, identically distributed random variables with distribution ν_j, $j = 1, \dots, e$. We assume that the jump distribution ν_j admits all moments, $j = 1, \dots, e$. See Protter [64] for more information on Poisson and Lévy processes. Furthermore, let $\delta_1, \dots, \delta_e : H \to H$ be C^∞-bounded vector fields. Similar to (1.10), consider the jump driven SPDE

(1.15)
$$\begin{cases} dX_t^x = \big(AX_{t^-}^x + \alpha(X_{t^-}^x)\big)dt + \sum_{i=1}^d \beta_i(X_{t^-}^x)dB_t^i + \sum_{j=1}^e \delta_j(X_{t^-}^x)dL_t^j, \quad t \in [0,T], \\ X_0^x = x \in H. \end{cases}$$

Then, in analogy to Definition 1.2.8, a *strong solution* X^x of (1.15) is a càdlàg process satisfying

$$X_t^x = x + \int_0^t (AX_{s^-}^x + \alpha(X_{s^-}^x))ds + \sum_{i=1}^d \int_0^t \beta_i(X_{s^-}^x)dB_s^i + \sum_{j=1}^e \int_0^t \delta_j(X_{s^-}^x)dL_s^j, \tag{1.16a}$$

$t \in [0, \infty[$, whereas a *mild solution* X^x is a càdlàg process satisfying

$$X_t^x = S_t x + \int_0^t S_{t-s}\alpha(X_{s-}^x)ds + \sum_{i=1}^{d}\int_0^t S_{t-s}\beta_i(X_{s-}^x)dB_s^i + \sum_{j=1}^{e}\int_0^t S_{t-s}\delta_j(X_{s-}^x)dL_s^j, \tag{1.16b}$$

$t \in [0, \infty[$. (We shall not need the concept of a weak solution in this case.)

1.2.3 Stochastic differential equations in $\mathcal{D}(A^\infty)$

Analysis of stochastic partial differential equations is severly restricted by the fact that some of the most important tools of finite dimensional stochastic analysis, like the Itô formula, are only available for strong solutions of SPDEs, but not for mild or weak ones, see Remark 1.2.9. The general existence and uniqueness theorem, however, only guarantees the existence of mild solutions, and a quick glance at the deterministic, homogeneous case reveals that there cannot be strong solutions for all initial data in H even for simple problems. Indeed, the solution $X_t^x = S_t x$ of the deterministic, homogeneous abstract Cauchy problem is only a strong solution if $x \in \mathcal{D}(A)$. If we restrict ourselves to the space $\mathcal{D}(A)$ instead, we immediately face the same problem: $S_t x$ is in the domain of the (unbounded) operator $A : \mathcal{D}(A) \to \mathcal{D}(A)$ if x lies in the subspace $\{\, y \in \mathcal{D}(A) \mid Ay \in \mathcal{D}(A) \,\} \subset \mathcal{D}(A)$. If we iterate this procedure until we arrive at the "infinitely often differentiable" elements in H, then we might have a chance to actually succeed. In this section, we want to carry out that program. The more general concepts can be found in Nagel [1], whereas the applications to SPDEs are given in Filipović and Teichmann [24].

For the rest of the section let $(A, \mathcal{D}(A))$ be the generator of a C_0-semigroup $(S_t)_{t\in[0,\infty[}$ on the Hilbert space H. Consider the space $\mathcal{D}(A)$ and define the *graph norm* thereon, i. e.

$$\|x\|_{\mathcal{D}(A)}^2 = \|x\|_H^2 + \|Ax\|_H^2 \,. \tag{1.17}$$

Since A is a closed operator, $(\mathcal{D}(A), \|\cdot\|_{\mathcal{D}(A)})$ is a Hilbert space – the inner product is, of course, given by polarization. Actually, the domain of an operator endowed with the graph norm is a Hilbert space if and only if the operator is closed. By recursion, we also define spaces $\mathcal{D}(A^n)$ for all $n \in \mathbb{N}$ by

$$\mathcal{D}(A^{n+1}) = \{\, x \in \mathcal{D}(A^n) \mid Ax \in \mathcal{D}(A^n) \,\}\,, \quad n \in \mathbb{N}. \tag{1.18}$$

Furthermore, we set

$$\mathcal{D}(A^\infty) = \bigcap_{n\in\mathbb{N}} \mathcal{D}(A^n). \tag{1.19}$$

Note that each $\mathcal{D}(A^n)$ and also $\mathcal{D}(A^\infty)$ are dense subspaces of H. The following example taken from Nagel [1, Example A-I 1.10] shows that this is not true for general closed operators.

Example 1.2.12. Consider the Banach space $H = C([0,1])$ and the closed operator B with $\mathcal{D}(B) = C^1([0,1])$ defined by

$$Bx(u) = f(u)\frac{d}{du}x(u), \quad u \in [0,1],$$

for some nowhere differentiable function f. Then $\mathcal{D}(B^2) = \{0\}$.

The next proposition is also taken from Nagel [1]. Since it might not be familiar to the reader, we repeat the proof here.

Proposition 1.2.13. *Let us endow each of the spaces $\mathcal{D}(A^n)$, $n \in \mathbb{N}$, with a norm*

$$\|x\|^2_{\mathcal{D}(A^n)} = \|x\|^2_H + \sum_{k=1}^{n} \left\|A^k x\right\|^2_H.$$

Then each space $(\mathcal{D}(A^n), \|\cdot\|_{\mathcal{D}(A^n)})$ is a Hilbert space. Moreover, the restriction $(S_t\big|_{\mathcal{D}(A^n)})_{t\in[0,\infty[}$ of S to $\mathcal{D}(A^n)$ is a C_0-semigroup on the Hilbert space $\mathcal{D}(A^n)$ with generator $(A, \mathcal{D}(A^{n+1}))$.

Proof. We start with $n = 1$. Note that $\mathcal{D}(A)$ is invariant under S_t, $t \in [0,\infty[$, therefore we can restrict S_t to $\mathcal{D}(A)$. By definition of $\|\cdot\|_{\mathcal{D}(A)}$ and boundedness of S_t on H, the restriction of S_t to $\mathcal{D}(A)$ is bounded thereon. Analogously one shows that

$$\lim_{t\searrow 0} \|S_t x - x\|_{\mathcal{D}(A)} = 0, \quad x \in \mathcal{D}(A),$$

establishing that the restriction of (S_t) to $\mathcal{D}(A)$ defines a C_0-semigroup. We claim that the generator $(A', \mathcal{D}(A'))$ of that semigroup is given by $(A, \mathcal{D}(A^2))$. To this end, let $x \in \mathcal{D}(A')$. Consequently,

$$A'x = \lim_{t\searrow 0} \frac{S_t x - x}{t} \text{ in } \mathcal{D}(A),$$

where the limit is understood in the topology of the Hilbert space $(\mathcal{D}(A), \|\cdot\|_{\mathcal{D}(A)})$. By construction of $\|\cdot\|_{\mathcal{D}(A)}$, this implies that

$$A'x = \lim_{t\searrow} \frac{S_t x - x}{t} = Ax \text{ in } H,$$

since $x \in \mathcal{D}(A)$. Thus,$(A', \mathcal{D}(A')) \subset (A, \mathcal{D}(A^2))$. For the reverse direction, let $x \in \mathcal{D}(A^2)$, i. e. $x \in \mathcal{D}(A)$ and $Ax \in \mathcal{D}(A)$. Therefore, we have

$$\exists \lim_{t\searrow 0} \frac{S_t x - x}{t} = Ax \text{ in } H,$$
$$\exists \lim_{t\searrow 0} \frac{S_t Ax - Ax}{t} = A^2 x \text{ in } H,$$

implying that $\frac{S_t x - x}{t}$ converges to Ax in $\mathcal{D}(A)$. Consequently, $\mathcal{D}(A^2) \subset \mathcal{D}(A')$.

We have now established that $(A, \mathcal{D}(A^2))$ is again the generator of a strongly continuous semigroup on the Hilbert space $\mathcal{D}(A)$. Since the domains of generators of C_0-semigroups endowed with the graph norm are again Hilbert spaces, this shows that $(\mathcal{D}(A^2), \|\cdot\|_{\mathcal{D}(A^2)})$ is a Hilbert space and the proposition follows by induction. □

Definition 1.2.14. $(\mathcal{D}(A^n), \|\cdot\|_{\mathcal{D}(A^n)})$ is called *n-th Sobolev space* and the restriction of S to it is called the *n-th Sobolev semigroup*, $n \in \mathbb{N}$.

Let $\lambda \in \rho(A)$, then the resolvent $R(\lambda, A) = (\lambda - A)^{-1} : H \to \mathcal{D}(A)$ is an isomorphism from the Hilbert space H to the Hilbert space $\mathcal{D}(A)$ with inverse $(\lambda - A) : \mathcal{D}(A) \to H$. Since the analogous statements hold true for the Hilbert spaces $\mathcal{D}(A^n)$ and $\mathcal{D}(A^{n+1})$, we get the following commutating diagram (the *hierarchy of Sobolev spaces*):

(1.20)

$$\begin{array}{ccc}
H & \xrightarrow{S_t} & H \\
\downarrow{\scriptstyle R(\lambda,A)} & & \uparrow{\scriptstyle \lambda - A} \\
\mathcal{D}(A) & \xrightarrow{S_t} & \mathcal{D}(A) \\
\downarrow{\scriptstyle R(\lambda,A)} & & \uparrow{\scriptstyle \lambda - A} \\
\mathcal{D}(A^2) & \xrightarrow{S_t} & \mathcal{D}(A^2) \\
\vdots & & \vdots \\
\mathcal{D}(A^n) & \xrightarrow{S_t} & \mathcal{D}(A^n) \\
\downarrow{\scriptstyle R(\lambda,A)} & & \uparrow{\scriptstyle \lambda - A} \\
\mathcal{D}(A^{n+1}) & \xrightarrow{S_t} & \mathcal{D}(A^{n+1}) \\
\vdots & & \vdots
\end{array}$$

We still need to endow $\mathcal{D}(A^\infty)$ with a topology.

Definition 1.2.15. $\mathcal{D}(A^\infty)$ is endowed with the initial topology of the canonical injections $\mathcal{D}(A^\infty) \hookrightarrow \mathcal{D}(A^n)$.

Proposition 1.2.16. $\mathcal{D}(A^\infty)$ *is a* Fréchet space*, i. e. a complete, metrizable locally convex vector space.*

Proof. Obviously, the topology on $\mathcal{D}(A^\infty)$ is the locally convex topology generated by the family of (semi-)norms

$$p_n(x) = \|x\|_{\mathcal{D}(A^n)}, \quad x \in \mathcal{D}(A^\infty),\ n \in \mathbb{N}.$$

Since it is generated by a countable family of semi-norms, the topology can be metrized, e. g., by

$$d(x,y) = \sum_{n=0}^{\infty} \frac{1}{2^n} \frac{p_n(x-y)}{\max(1, p_n(x-y))}, \quad x, y \in \mathcal{D}(A^\infty),$$

and only completeness is left to be shown. Given a Cauchy sequence $(x_n)_{n\in\mathbb{N}}$, then the sequence is also a Cauchy-sequence for each norm p_k, $k \in \mathbb{N}$. By completeness of $\mathcal{D}(A^k)$,

$$\exists \lim_{n\to\infty} x_n = x^{(k)} \in \mathcal{D}(A^k)$$

and $x^{(k)} = x^{(l)}$ for $l \leq k$. Consequently, all these limits coincide and define an element $x \in \mathcal{D}(A^\infty)$. Naturally, $x = \lim_{n\to\infty} x_n$ also in the topology of $\mathcal{D}(A^\infty)$. □

It is still true that S restricted to $\mathcal{D}(A^\infty)$ defines a semi-group with generator A, so we can include $\mathcal{D}(A^\infty)$ in the Sobolev-hierarchy. We shall see that this is an exceptional situation in the sense that differential equations in Fréchet spaces usually do not even have local solutions. We will impose quite strict assumptions on the coefficients of the SPDE in order to get a solution of the SPDE in $\mathcal{D}(A^\infty)$ using the hierarchy of Sobolev spaces (1.20). For a good introduction to analysis on Fréchet spaces see Hamilton [32] and the following considerations are closely based on that article.

We begin with the definition of a derivative of maps. Unlike in the case of Banach spaces, we can only use the notion of *Gateaux derivatives*.

Definition 1.2.17. Given two Fréchet spaces F and G and a continuous map $f : F \to G$, the derivative of f at the point $x \in F$ in direction $h \in F$ is defined as

$$Df(x) \cdot h = \lim_{t\to\infty} \frac{f(x+th) - f(x)}{t},$$

provided that the limit exists, in which case f is called *differentiable at x in direction h*. We say that f is *continuously differentiable* if it is differentiable for all $x \in F$ in all directions $h \in F$ and the function

$$Df : F \times F \to G$$

is continuous.

Remark 1.2.18. It is important to understand Df as a function $F \times F \to G$, and not as a function with values in the space of (bounded) linear operators, since the latter space has an even worse topology. Indeed, one can show that the dual space of a Fréchet space F is a Fréchet space if and only if F is a Banach space.

Higher derivatives are defined analogously, e. g. the second derivative is defined by

$$D^2 f(x) \cdot (h,k) = \lim_{t \to 0} \frac{Df(x+tk) \cdot h - Df(x) \cdot h}{t},$$

and a function is two times continuously differentiable if $Df \in C^1(F \times F; G)$. Many of the standard results of calculus still hold in principle, but sometimes they have to be stated in a different way.

The *inverse function theorem* does, however, not hold for Fréchet spaces, see Hamilton [32] for counterexamples and much background information. Moreover, Fréchet spaces are bad places for ODEs, as the following example shows.

Example 1.2.19 (Hamilton [32], Counterexample I.5.6.1)**.** Define the Fréchet space

$$F = \{ f \in C^\infty(\mathbb{R}; \mathbb{R}) \mid \forall x \notin [0,1] : f(x) = 0 \}.$$

The derivative operator $\frac{d}{dx} : F \to F$ is obviously smooth since it is a continuous linear operator. Consider the ODE

$$\frac{d}{dt} f_t = \frac{d}{dx} f_t, \quad f_0 = f \in F. \tag{1.21}$$

A (local) solution $(f_t)_{0 \le t < \epsilon}$ of (1.21) necessarily satisfies

$$f_t(x) = f(t+x), \quad 0 \le t < \epsilon,\ x \in \mathbb{R}.$$

Note, however, that $x \mapsto f(t+x) \in F$ if and only if $f(y) = 0$, $\forall y \in [0,t[$. In particular, if we choose f such that $f(x) \neq 0$, $\forall x \in]0,1[$, then the equation (1.21) is not locally solvable for this initial value.

Remark 1.2.20. The operator $\frac{d}{dx}$ of Example 1.2.19 is continuous, the semigroup $e^{t\frac{d}{dx}}$, however, does not even exist locally on F. Similar examples show that also uniqueness may fail if local solutions exist.

The Fréchet space $\mathcal{D}(A^\infty)$ has a particular structure, since it is a projective limit of the Hilbert spaces $\mathcal{D}(A^n)$, $n \in \mathbb{N}$, so we might hope that things, after all, work out nicely in $\mathcal{D}(A^\infty)$. Note, however, that any Fréchet space can be written as projective limit of a sequence of Banach spaces, see Schaefer [73].

Fortunately, we can avoid all problems caused by the topology on $\mathcal{D}(A^\infty)$ by imposing stricter conditions on the coefficients of the SPDE, following Baudoin and Teichmann [5].

Assumption 1.2.21. Additionally to Assumption 1.2.7, let $\alpha, \beta_1, \ldots, \beta_d : H \to \mathcal{D}(A^\infty)$ such that they are C^∞-bounded when understood as maps $\alpha, \beta_1, \ldots, \beta_d : (\mathcal{D}(A^n), \|\cdot\|_{\mathcal{D}(A^n)}) \to (\mathcal{D}(A^n), \|\cdot\|_{\mathcal{D}(A^n)})$, for all $n \in \mathbb{N}$.

Proposition 1.2.22. *Given vector fields satisfying Assumption 1.2.21. (1) Fix $n \in \mathbb{N}$ and $x \in \mathcal{D}(A^n)$ and interpret the SPDE (1.10) as an SDE in the Hilbert space $\mathcal{D}(A^n)$. Then there is a unique mild solution in $\mathcal{D}(A^n)$, which is a strong solution if the initial value lies in the dense subspace $\mathcal{D}(A^{n+1}) \subset \mathcal{D}(A^n)$. Moreover, the solution X^x coincides with the solution of the equation in $\mathcal{D}(A^{n-1})$ with the same initial value $x \in \mathcal{D}(A^n) \subset \mathcal{D}(A^{n-1})$. (2) For given $x \in \mathcal{D}(A^\infty)$ there is a solution of (1.10) with continuous trajectories in $\mathcal{D}(A^\infty)$.*

Proof. Fix $x \in \mathcal{D}(A^n)$. By a direct application of Proposition 1.2.10 for the Hilbert space $\mathcal{D}(A^n)$, we find that there is a mild solution $X^{x,n} = (X_t^{x,n})_{t\in[0,T]}$ for any $x \in \mathcal{D}(A^n)$. This solution is unique in the sense that each solution is a version of $X^{x,n}$. The C_0-semigroup S^n generated by $(A, \mathcal{D}(A^{n+1}))$ is nothing but the restriction of S to $\mathcal{D}(A^n)$, see Proposition 1.2.13. Therefore, since the restriction of S^n to $\mathcal{D}(A^{n+1})$ coincides with S^{n+1}, it is clear that $X^{x,n} = X^{x,n+1}$ provided that $x \in \mathcal{D}(A^{n+1})$, again in the sense of being versions of each other. Consequently, we may omit the superscript n.

Moreover, if $x \in \mathcal{D}(A^{n+1})$, then X^x is a semi-martingale in $\mathcal{D}(A^n)$ and Itô's formula applied to

$$X_t^x = S_t x + \int_0^t S_{t-s}\alpha(X_s^x)ds + \sum_{i=1}^d \int_0^t S_{t-s}\beta_i(X_s^x)dB_s^i$$

gives

$$X_t^x = x + \int_0^t \big(AX_s^x + \alpha(X_s^x)\big)ds + \sum_{i=1}^d \int_0^t \beta_i(X_s^x)dB_s^i,$$

implying that X^x is a strong solution (of the equation in $\mathcal{D}(A^n)$). This shows (1).

For $x \in \mathcal{D}(A^\infty)$ let X^x be the mild (and strong) solution of (1.10) in any (and therefore all) $\mathcal{D}(A^n)$, $n \in \mathbb{N}$. More precisely, not that $X^{x,n}$ is a version of $X^{x,1}$, for any $n \in \mathbb{N}$. Consequently, $X^x = X^{x,1}$ is unique in that sense. X^x is continuous in all the Sobolev spaces $\mathcal{D}(A^n)$, therefore $X_t^x \in \mathcal{D}(A^\infty)$ and the process is continuous there. □

Under Assumption 1.2.21, X^x is a strong solution of equation (1.10) in $\mathcal{D}(A^n)$ for any $x \in \mathcal{D}(A^{n+1})$ – and therefore a semi-martingale. Thus, it makes sense to consider its *Stratonovich formulation*, cf. (1.3) in the finite-dimensional setting. To this end, introduce a (densely defined) vector field $\beta_0 : \mathcal{D}(A^{n+1}) \subset \mathcal{D}(A^n) \to \mathcal{D}(A^n)$ defined by

$$\beta_0(x) = Ax + \alpha(x) - \frac{1}{2}\sum_{i=1}^d D\beta_i(x)\cdot\beta_i(x), \quad x \in \mathcal{D}(A^{n+1}). \tag{1.22}$$

Of course, β_0 corresponds to the vector field V_0 defined in (1.2). For $x \in \mathcal{D}(A^{n+1}) \cap \mathcal{D}(A^{m+1})$, $n, m \in \mathbb{N}$, the derivatives of $\beta_i : \mathcal{D}(A^n) \to \mathcal{D}(A^n)$ and $\beta_i : \mathcal{D}(A^m) \to \mathcal{D}(A^m)$ coincide for $i = 1, \ldots, d$ by definition of the graph norms. Consequently, we get the *Stratonovich drift vector field* β_0 on $\mathcal{D}(A^{n+1}) \subset \mathcal{D}(A^n)$ simply by restricting $\beta_0 : \mathcal{D}(A) \to H$ to $\mathcal{D}(A^{n+1})$. For $x \in \mathcal{D}(A^{n+1})$, the solution X^x of (1.10) on $\mathcal{D}(A^n)$ satisfies the *Stratonovich SDE*

$$dX_t^x = \beta_0(X_t^x)dt + \sum_{i=1}^{d} \beta_i(X_t^x) \circ dB_t^i, \quad t \in [0, T] \tag{1.23}$$

with initial value $X_0^x = x$. Equation (1.23) is an immediate consequence of the fact that X^x is a semi-martingale on $\mathcal{D}(A^n)$ for $x \in \mathcal{D}(A^{n+1})$ and the Itô Formula.

1.3 Approximation of SDEs

Back to the finite dimensional setting, consider once again the stochastic differential equation (1.1). In many situations, the solution X^x of the SDE is not directly needed but the true quantities of interest are of the form

$$E(f(X_T^x))$$

for some function $f : \mathbb{R}^n \to \mathbb{R}$. For instance, f might be the (discounted) payoff function of a (European) option. Then $E(f(X_T^x))$ corresponds to an arbitrage-free price of the option, provided that (1.1) describes the dynamics of the underlying under a martingale measure. Or we need to solve the heat equation

$$\frac{\partial}{\partial t} u(t, x) = Lu(t, x)$$

with initial condition $u(0, x) = f(x)$, where L is the partial differential operator defined in (1.4). By the Feynman-Kac formula, Proposition 1.1.7, we have $u(t, x) = E(f(X_t^x))$.

In most situations we are not able to solve (1.1) explicitly: we cannot give a formula expressing X_T^x as a function of B and we cannot give a direct way to sample from the distribution $(X_T^x)_* P$ of X_T^x. Therefore, we need to approximate the solution X^x or its law. We will introduce some notations and give some remarks on the basis of the *Euler scheme*, which is the most simple numerical approximation scheme for SDEs. The standard reference for approximation of SDEs is Kloeden and Platen [42].

Given a fixed partition $0 = t_0 < t_1 < \cdots < t_N = T$ of $[0, T]$ with size N and a fixed initial value $x \in \mathbb{R}^n$, introduce a discrete-time stochastic process $(\overline{X}_k^N)_{k=0}^N$ by recursively defining $\overline{X}_0^N = x$ and

$$\overline{X}_{k+1}^N = \overline{X}_k^N + V(\overline{X}_k^N)\Delta t_k + \sum_{i=1}^{d} V_i(\overline{X}_k^N)\Delta \overline{B}_k^i, \quad k = 0, \ldots, N-1. \tag{1.24}$$

Since $\overline{X}_k^N$ is regarded as an approximation of $X_{t_k}^x$, we have to choose $\Delta t_k = t_{k+1} - t_k$, $k = 0, \dots, N-1$. The choice of $\Delta\overline{B}_k$, however, is not so simple. We shall distinguish between two cases.

Case A. $\Delta\overline{B}_k^i = B_{t_{k+1}}^i - B_{t_k}^i$, $k = 0, \dots, N-1$, $i = 1, \dots, d$. More sloppily, we shall write $\Delta\overline{B}_k = \Delta B_k$.

This choice seems natural having the Euler method for ODEs in mind, and it is feasible for numerical implementations, since $\Delta B_k \sim \sqrt{\Delta t_k} Y$, if Y is a d-dimensional standard normal random variable, symbolically we write $Y \sim \mathcal{N}(0, I_d)$. Moreover, all the increments of B are independent. Of course, standard normal random variables can be sampled fairly easily, and therefore $\overline{X}_k^N$ can be sampled in Case A.

Remark 1.3.1. Notice, however, that sampling the random increments in higher order schemes is, in general, a difficult task.

Case B. Let $(\epsilon_k)_{k=0}^{N-1}$ be *any* family of independent, identically distributed d-dimensional random variables such that the moments of ϵ_0 of order up to 3 – and, consequently, of any ϵ_k – coincide with the corresponding moments of a d-dimensional standard normal random variable. Then set

$$\Delta\overline{B}_k = \sqrt{\Delta t_k}\epsilon_k, \quad k = 0, \dots, N-1.$$

The only condition on $\Delta\overline{B}_k$ in Case B is that it has the same moments as ΔB_k. Therefore, it makes sense to choose ϵ_k as simple as possible among all random variables with this condition. Especially for computational purposes, this leads to

$$\epsilon_k^i = \begin{cases} +1 & \text{with probability } 1/2 \\ -1 & \text{with probability } 1/2 \end{cases}, \quad i = 1, \dots, d, \ k = 0, \dots, N-1, \tag{1.25}$$

which we understand in the sense that all ϵ_k^i, $i = 1, \dots, d$, $k = 0, \dots, N-1$ are independent of each other.

Remark 1.3.2. $(\Delta\overline{B}_k)_{k=0}^{N-1}$ of Case A trivially satisfies the above moment condition of Case B. Therefore, Case A is a special case of Case B.

There is a big probabilistic difference between Case A and Case B: while ΔB is, by construction, defined on the same probability space $(\Omega, \mathcal{F}, P)$ as B, this is not necessarily true for $\Delta\overline{B}$ chosen according to Case B. In fact, the requirements of Case B are only formulated in terms of the distribution of $\Delta\overline{B}$, so these random variables could be defined on any probability space. Especially if we work with the discrete choice (1.25), there is no need to use such a complicated probability space as Ω – which essentially encompasses the Wiener space. Therefore, in Case B, X_T^x and $\overline{X}_N^N$, the discrete approximation, are random variables defined on different probability spaces, so there is no direct way to compare them.

Definition 1.3.3. The Euler scheme with choice of $\Delta\overline{B}$ according to Case A is called *strong Euler scheme* and the resulting random variables $\overline{X}^N$ are called *strong (Euler) approximations* of X^x. Conversely, in Case B, the scheme is called *weak Euler scheme* and the approximating random variables $\overline{X}^N$ are called *weak (Euler) approximations* of X^x.

As already anticipated above, two types of convergences of the approximations to the exact random variables can be studied. For the definitions, let $\overline{X}_N^N$ be the approximation of X_T^x given by any numerical scheme based on a time-partition $(t_k^N)_{k=0}^N$ with

$$\Delta(t^N) = \max_{k=0,\dots,N-1} \Delta t_k^N$$

converging to 0 for $N \to \infty$.

Definition 1.3.4. The family of random variables $(\overline{X}_N^N)_{N\in\mathbb{N}}$ *converges strongly* to X_T^x if

$$\lim_{N\to\infty} E\Big(\Big|X_T^x - \overline{X}_N^N\Big|\Big) = 0.$$

The scheme has *strong order* $\gamma > 0$ if there is a constant $C > 0$ such that

$$E\Big(\Big|X_T^x - \overline{X}_N^N\Big|\Big) \le C\Delta(t^N)^\gamma.$$

Of course, the notion of strong convergence does only make sense for strong schemes, because the approximation needs to be defined on the same probability space as the exact solution.

Definition 1.3.5. Let $\mathcal{G}$ be a (sufficiently large) family of functions $\mathbb{R}^n \to \mathbb{R}$. The family of random variables $(\overline{X}_N^N)_{N\in\mathbb{N}}$ *converges weakly* to X_T^x if

$$\lim_{N\to\infty} E\big(f\big(\overline{X}_N^N\big)\big) = E(f(X_T^x)), \quad \text{for all } f \in \mathcal{G}.$$

The scheme has *weak order* $\gamma > 0$ if for all $f \in \mathcal{G}$ there is a constant $C = C(f) > 0$ such that

$$\Big|E(f(X_T^x)) - E\big(f\big(\overline{X}_N^N\big)\big)\Big| \le C\Delta(t^N)^\gamma, \quad \text{for all } N \in \mathbb{N}.$$

Classically, weak convergence is defined in terms of $\mathcal{G} = C_b(\mathbb{R}^n)$, the family of bounded continuous functions, but no order of convergence can be obtained in that case. For getting a rate of convergence, more regularity is necessary. Moreover, in practical applications one is often interested in the moments of a random variable. Therefore, $\mathcal{G}$ is often chosen to include polynomials up to some degree.

Of course, it is a basic result of numerics of SDEs that the strong Euler scheme converges strongly to the true solution with strong order 1/2 and

that the weak Euler scheme converges weakly with weak order 1. For the strong approximation result one only needs the standard (uniform) Lipschitz and linear growth condition, the situation for the weak convergence is a little bit more complicated. Essentially, Kloeden and Platen [42, Theorem 14.1.5] show that a weak order 1 holds for "$C^{4+\epsilon}$-bounded" test functions provided that the coefficients of the SDE are "$C^{2+\epsilon}$-bounded", where $(k+\epsilon)$-times differentiable means k times differentiable with ϵ-Hölder continuous kth derivative.

Note that the strong differentiability conditions on the test functions cannot be relaxed in general. This reveals a certain gap between strong and weak approximation: in fact, given a uniformly Lipschitz test function f – which is not C^2 – and let $\overline{X}_N^N$ be a *strong* approximation of X_T^x. If the coefficients of (1.1) satisfy mild regularity conditions, then $\overline{X}_N^N$ converges strongly with order $1/2$ and we may conclude that

$$\left|E(f(X_T^x)) - E\big(f\big(\overline{X}_N^N\big)\big)\right| \leq \|\nabla f\|_\infty E\Big(\Big|X_T^x - \overline{X}_N^N\Big|\Big) \leq \|\nabla f\|_\infty \Delta(t^N)^{\frac{1}{2}}.$$

Consequently, we get a weak order of convergence $1/2$ for a family of functions f, for which the usual theory does not give convergence at all. While it is perfectly possible to use strong schemes, i. e. schemes based on Case A, for weak approximation of random variables, and study their weak rate of convergence, it is, of course, not possible to use weak schemes, i. e. schemes based on Case B, for strong approximation, simply because they do not need to be defined on the same probability space as the random variable, which needs to be approximated.

In fact, the weak convergence of strong schemes can be extended to much larger classes of test functions, as was shown by Bally and Talay [2].

Proposition 1.3.6. *Assume that the driving vector fields of (1.1) are C^∞-bounded and satisfy a uniform Hörmander condition. Then the strong Euler scheme converges weakly with weak order* 1 *for all bounded measurable functions f.*

Remark 1.3.7. Bally and Talay [2] even prove the existence of an error expansion for the strong approximation for bounded measurable functions in the sense of Talay and Tubaro [80].

Chapter 2

Iterated Stratonovich integrals

This chapter is concerned with a study of the iterated Itô-Stratonovich integrals of the d-dimensional Brownian motion. Of course, the analysis of these processes, and in particular of the corresponding "areas" like the Lévy area, have a long tradition, going back to the calculation of an explicit formula for the Laplace transform of the Lévy area by P. Lévy.

We are interested in the iterated integrals because of two reasons. Firstly, they appear prominently in the stochastic Taylor expansion, i. e. an expansion of the solution of an SDE similar to the Taylor expansion in the deterministic case, see Subsection 2.1.1 below. As a consequence, iterated integrals play an important rôle in the numerical analysis of SDEs, in particular for the construction of higher order Taylor methods. Moreover, the more recent theory of T. Lyons [52] has impressively shown the central position of the iterated integrals in the theory of stochastic differential equations well beyond of the stochastic Taylor expansion.

On the other hand, iterated integrals of Brownian motions can be understood as natural Brownian motions on certain important nilpotent Lie groups, see Section 2.1. In some sense, we have turned this relationship around by considering these Lie groups as the natural geometry of the iterated Itô-Stratonovich integrals of the Brownian motion. This is the content of the first Section 2.1. Afterwards, we present the "Cubature on Wiener space" method by T. Lyons and N. Victoir [51] as an important application of this geometric analysis. (Both Section 2.1 and Section 2.2 strongly rely on the above mentioned paper.)

Finally, we consider the question of moments of iterated integrals. In Section 2.3 we present an explicit formula for all moments of the iterated integrals of the Brownian motion, again strongly using their geometry, while in the last Section 2.4 we present an algorithm for efficient computation of the moments of the corresponding area processes using the representation theory of the geometry of the iterated integrals.

2.1 Geometry of iterated Stratonovich integrals

2.1.1 Stochastic Taylor expansion

Although iterated Stratonovich integrals of Brownian motion are interesting objects per se, our motivation for studying them stems from the *stochastic Taylor expansion*, where they play a similar rôle as polynomials do in the deterministic Taylor expansion.

Let $B_t = (B_t^1, \dots, B_t^d)$, $t \geq 0$, denote a d-dimensional Brownian motion on the filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t), P)$ satisfying the usual conditions. We introduce a notation which will help us to write down many formulas in the following sections in a more concise way.

Definition 2.1.1. Let $f : [0,T] \to \mathbb{R}^d$ or $f : [0,\infty[\to \mathbb{R}^d$, $f(t) = (f^1(t), \dots, f^d(t))$. Then we define a 0th component of f by setting

$$f^0(t) = t, \quad t \in [0,T] \text{ or } t \in [0,\infty[,$$

respectively. In particular, we set $B_t^0 = t$ for the Brownian motion.

As usual, let $V_0, \dots, V_d : \mathbb{R}^n \to \mathbb{R}^n$ be C^∞-*bounded* vector fields on $\mathbb{R}^n$. We also require the vector fields themselves to be bounded. Recalling Remark 1.1.3, we understand that V^2 is a second order differential operator for any vector field V, i. e.

$$V^2 f(x) = D^2 f(x) \cdot (V(x), V(x)) + Df(x) \cdot DV(x) \cdot V(x), \quad x \in \mathbb{R}^n.$$

Let $X^x = (X_t^x)_{t \in [0,T]}$ denote the strong solution of the Stratonovich SDE (1.3) driven by the vector fields $V_0, V_1, \dots, V_d$ with initial value $x \in \mathbb{R}^n$.

Definition 2.1.2. Let $\mathcal{A}$ denote the set of all *multi-indices* with values in $\{0, 1, \dots, d\}$, i. e.

$$\mathcal{A} = \bigcup_{k=0}^{\infty} \{0, 1, \dots, d\}^k ,$$

which contains the empty multi-index $\emptyset$. The generic element of $\mathcal{A}$ will be denoted by $I = (i_1, \dots, i_k)$. A *degree* deg is defined on $\mathcal{A}$ by

$$\deg(I) = \deg((i_1, \dots, i_k)) = k + \#\{\, j \in \{1, \dots, k\} \mid i_j = 0 \,\},$$

i. e. the degree function counts zeros twice. We will also use

$$\mathcal{A}_m = \{\, I \in \mathcal{A} \mid \deg(I) \leq m \,\}, \quad m \in \mathbb{N}.$$

Definition 2.1.3. Let $f : [0,T] \to \mathbb{R}^d$ or $f : [0,\infty[\to \mathbb{R}^d$ be *either* a deterministic function of bounded variation *or* a d-dimensional Brownian motion.

For $I \in \mathcal{A} \setminus \{\emptyset\}$ we define the *iterated integral* of f by

$$f^I(t) = f^{(i_1,\dots,i_k)}(t) = \int_{0<t_1<\cdots<t_k<t} df^{i_1}(t_1)\cdots df^{i_k}(t_k) = \int_0^t \int_0^{t_k} \cdots \int_0^{t_1} df^{i_1}(t_1)\cdots df^{i_k}(t_k).$$

Moreover, $f^\emptyset(t) \equiv 1$. In the case of of a f being a Brownian motion, the above integrals are understood in the sense of *Stratonovich stochastic integrals* and we accordingly call them *iterated Itô-Stratonovich integrals*.

Notice that the iterated Itô-Stratonovich integral is not defined pathwise, but only up to a set of measure zero. According to Definition 2.1.1, also dt-integrals may show up in iterated integrals. The unusual choice of the degree function can now be clarified by considering iterated Stratonovich integrals. Indeed, for any multi-index I and any $t \geq 0$ we have the equality-in-law

$$B_t^I \sim t^{\deg(I)/2} B_1^I, \tag{2.1}$$

which is a generalization of the fact $B_t \sim \sqrt{t} B_1$ for Brownian motion.

Proposition 2.1.4 (Stochastic Taylor expansion)**.** *For fixed $m \in \mathbb{N}$ let $f \in C_b^{m+1}(\mathbb{R}^n)$. Consider the solution X^x of the SDE* (1.1)*. Then*

$$f(X_t^x) = \sum_{\substack{I=(i_1,\dots,i_k)\in\mathcal{A} \\ \deg(I)\leq m,\, k\in\mathbb{N}}} V_{i_1}\cdots V_{i_k} f(x) B_t^I + R_m(t,x,f). \tag{2.2}$$

The remainder term satisfies

$$\sup_{x\in\mathbb{R}^n} \sqrt{E\big(R_m(t,x,f)^2\big)} \leq C t^{\frac{m+1+\mathbf{1}_{\{t>1\}}}{2}} \sup_{I\in\mathcal{A}_{m+2}\setminus\mathcal{A}_m} \|V_{i_1}\cdots V_{i_k} f\|_\infty, \tag{2.3}$$

i. e. the remainder is of order $\mathcal{O}\big(t^{\frac{m+1}{2}}\big)$ for $t \to 0$.

Proof. The key idea of the proof of Proposition 2.1.4 is iterated application of the Itô formula. Indeed, for $f \in C_b^{m+1}(\mathbb{R}^n)$ and $x \in \mathbb{R}^n$, Itô's formula in the Stratonovich formulation reads

$$f(X_t^x) = f(x) + \sum_{i=0}^d \int_0^t (V_i f)(X_s^x) \circ dB_s^i. \tag{2.4}$$

Each of the functions $V_i f : \mathbb{R}^n \to \mathbb{R}$ satisfies the conditions of Itô's formula and by applying it again to the integrands in (2.4) we get

$$f(X_t^x) = f(x) + \sum_{i=0}^d (V_i f)(x) B_t^i + \sum_{i,j=0}^d \int_0^t \int_0^s (V_j V_i f)(X_u^x) \circ dB_u^j \circ dB_s^i.$$

By iterating this procedure further and collecting all terms of deg $\leq m$ we arrive at (2.2), where the remainder term is a linear combination of iterated Stratonovich integrals of functions of X^x. Then, the estimate (2.3) follows by rewriting those Stratonovich integrals in Itô integrals and applying the Itô isometry repeatedly. For details, see Kloeden and Platen [42] and Lyons and Victoir [51]. □

The stochastic Taylor expansion is the starting point of stochastic numerical analysis, see Kloeden and Platen [42] for details on stochastic Taylor expansions and many methods originating from it.

Ignoring the remainder term, the only stochastic ingredients of the stochastic Taylor expansion are the iterated Stratonovich integrals of Brownian motion and a better understanding of them can give ideas for interesting new methods for numerical treatment of SDEs. In the stochastic Taylor expansion, the iterated integrals of Brownian motion play the rôle of polynomials in the classical, deterministic Taylor expansion.

Indeed, assume that $n = 1$ and consider the constant vector fields $V(y) = y$, $y \in \mathbb{R}$. Let $x = 0$, then $X_t^x = t$, and (2.2) reads

$$f(t) = f(0) + f'(0)t + \frac{1}{2}f'')(0)t^2 + \cdots + \frac{1}{\lfloor m/2 \rfloor !} f^{(\lfloor m/2 \rfloor)}(0)t^{\lfloor m/2 \rfloor} + R_m(t, 0, f),$$

where $\lfloor y \rfloor$ denotes the biggest integer smaller than y. We have used

$$B_t^{(0,0,\ldots,0)} = \frac{1}{|(0,0,\ldots,0)|!} t^{|(0,0,\ldots,0)|},$$

where $|\cdot|$ denotes the usual length of a multi-index. Thus, we can see the correspondence between iterated Itô-Stratonovich integrals in the stochastic Taylor formula and polynomials in the classical Taylor formula.

As a first step, we "encode" the iterated Stratonovich integrals of order up to m as a random variable with values in an appropriate algebra. Before we go back to iterated Stratonovich integrals, we need to study this algebra in some detail, in order to exploit its properties later on.

2.1.2 Free nilpotent Lie groups

Let $\mathbb{A}_{d,1}$ denote the space of all non-commutative polynomials in $d+1$ variables $e_0, \ldots, e_d$ including the constant polynomials. $\mathbb{A}_{d,1}$ is the *free associative algebra with unit* generated by $e_0, \ldots, e_d$ over the field of real numbers. We follow this definition with a series of remarks.

Remark 2.1.5. In this text, we shall only consider associative algebras over the field $\mathbb{R}$ of real numbers which have a unit. Therefore, we will usually omit the full specification – even in definitions – and only call them "algebras".

Remark 2.1.6. $\mathbb{A}_{d,1}$ satisfies the *universal property* of free algebras in $d+1$ generators, i. e. for any algebra C and any function $f : \{e_0, e_1, \dots, e_d\} \to C$ there is a unique algebra homomorphism $\tilde{f} : \mathbb{A}_{d+1} \to C$ extending f. In the following, all our "free" structures are actually free in the sense of universal algebra, i. e. they will also satisfy the respective universal properties. We will, however, not go into details here. For the simple proof of the above fact and much more information on the algebra needed in this text, see Serre [75]. A very useful monograph focusing on free Lie algebras is Reutenauer [67].

Remark 2.1.7. Obviously, the monomials in $\mathbb{A}_{d,1}$ correspond to the multi-indices in $\{0, \dots, d\}$ by $\mathcal{A} \to \mathbb{A}_{d,1}$, $I = (i_1, \dots, i_k) \mapsto e_I := e_{i_1} \cdots e_{i_k}$ (and $e_\emptyset = 1$, the unit element in $\mathbb{A}_{d,1}$). In order to give algebraic meaning to this map, one can equip $\mathcal{A}$ with a multiplication $*$ defined by concatenation of multi-indices. Then $(\mathcal{A}, *)$ is a monoid and the map is a monoid-homomorphism into the monoid of monomials.

Following Remark 2.1.7, we extend the degree function from $\mathcal{A}$ to $\mathbb{A}_{d,1}$ by

$$\deg(e_{i_1} \cdots e_{i_k}) = \deg((i_1, \dots, i_k)), \tag{2.5}$$

i. e. e_0 has twice the weight of the other generators. As usual, the degree of a polynomial – i. e. of an element of $\mathbb{A}_{d,1}$ – is defined as the maximum of the degrees of the respective monomials.

Remark 2.1.8. The definition of the degree on $\mathbb{A}_{d,1}$ now gives e_0 a special rôle among the generators of $\mathbb{A}_{d,1}$, and this justifies the peculiar notation for the algebra. In the end, as already prepared in Definition 2.1.1, e_0 will be associated to t, whereas the other generators will be associated to the components of Brownian motion. In particular, if we are not interested in a drift component at all, then we may omit e_0 and we simply write $\mathbb{A}_d$ for the corresponding free algebra and, analogously, for all the other algebraic constructs below.

Definition 2.1.9. Fix $m \in \mathbb{N}$. The *free step-m nilpotent associative real algebra with unit in d generators of degree* 1 *and one generator of degree* 2 is the space of all non-commutative polynomials in $e_0, \dots, e_d$ of degree less or equal m. We denote it by $\mathbb{A}_{d,1}^m$.

Remark 2.1.10. $\mathbb{A}_{d,1}^m$ is isomorphic to $\mathbb{A}_{d,1}$ factorized by the ideal generated by the monomials of degree greater than m. Thus, it also has the structure of an algebra, with the relations $e_I e_J = 0$ for $\deg(I * J) > m$. Therefore, the algebra is really nilpotent.

Remark 2.1.11. As mentioned in Remark 2.1.6, the free step-m nilpotent algebra $\mathbb{A}_{d,1}^m$ satisfies the universal property of free step-m nilpotent algebras, i. e. for any step-m nilpotent algebra C and any map $f : \{e_0, \dots, e_d\} \to C$ there is a unique extension $\tilde{f} : \mathbb{A}_{d,1}^m \to C$ of f as a homomorphism of step-m nilpotent algebras.

The degree function deg induces a grading on the algebra: if W_k denotes the linear span of all monomials of degree k, then

$$\mathbb{A}_{d,1}^m = \mathbb{R} \oplus W_1 \oplus \cdots \oplus W_m, \tag{2.6}$$

where $\mathbb{R} \simeq W_0 = \langle \{1\} \rangle_{\mathbb{R}}$ and 1 refers to the unit element of the algebra. Here, $\langle A \rangle_{\mathbb{R}}$ denotes the linear span of a set A over $\mathbb{R}$. Indeed, $W_k \cdot W_l \subset W_{k+l}$, $k, l \in \mathbb{N}$, keeping in mind that $W_k = \{0\}$ for $k > m$. According to the grading, we will write $x = x_0 + \cdots + x_m$ for $x \in \mathbb{A}_{d,1}^m$, where $x_i \in W_i$ is the projection of x onto W_i, $i = 0, \ldots, m$. For $t \in \mathbb{R}$, we define the *canonical dilatation* $\Delta_t : \mathbb{A}_{d,1}^m \to \mathbb{A}_{d,1}^m$ by

$$\Delta_t(x) = x_0 + tx_1 + t^2 x_2 + \cdots + t^m x_m, \quad x \in \mathbb{A}_{d,1}^m. \tag{2.7}$$

Note that Δ_t is an algebra-homomorphism.

We define the exponential function on $\mathbb{A}_{d,1}^m$ using the usual power series expansion, i. e.

$$\exp(x) = \sum_{k=0}^{\infty} \frac{x^k}{k!}. \tag{2.8}$$

Remark 2.1.12. Note that $\mathbb{A}_{d,1}^m$ is a finite-dimensional vector space, thus the exponential function is well defined – and smooth – using the natural topology on $\mathbb{A}_{d,1}^m$. If we used the same definition in the non-truncated algebra $\mathbb{A}_{d,1}$, as in Lyons and Victoir [51], we would get convergence problems and would need to work in the completion of $\mathbb{A}_{d,1}$ with respect to some non-elementary topology. Finite dimensionality of all the spaces involved is one of the benefits of working in the nilpotent setting from the beginning.

The logarithm is defined for $x \in \mathbb{A}_{d,1}^m$ with $x_0 > 0$ by

$$\log(x) = \log(x_0) + \sum_{k=1}^{m} \frac{(-1)^{k-1}}{k} \Big(\frac{x - x_0}{x_0} \Big)^k, \tag{2.9}$$

with $\log(x_0)$ being the logarithm of x_0 interpreted as a real number. Note that we may truncate the power series of the logarithm due to nil-potency: $(x - x_0)^{m+1} = 0$. Thus, the logarithm is a polynomial (for fixed x_0).

Recall that any algebra carries the structure of a Lie algebra with respect to the commutator $[x, y] = xy - yx$. We now consider the Lie algebra generated by $e_0, \ldots, e_d$.

Definition 2.1.13. The *free step-m nilpotent Lie algebra* with d generators of degree 1 and one generator of degree 2 is denoted by $\mathfrak{g}_{d,1}^m$. The *free step-m nilpotent Lie group* $G_{d,1}^m$ is defined as the exponential image of the Lie algebra $\mathfrak{g}_{d,1}^m$.

Definition 2.1.13 needs some clarification. One should think of $\mathfrak{g}_{d,1}^m$ as the sub-Lie algebra of the Lie algebra $\mathbb{A}_{d,1}^m$ generated by $\{e_0, \dots, e_d\} \subset \mathbb{A}_{d,1}^m$. For a direct construction of $\mathfrak{g}_{d,1}^m$, define a map $e_{[\cdot]} : \mathcal{A} \to \mathbb{A}_{d,1}$ recursively by $e_{[\emptyset]} = 0$, $e_{[(i)]} = e_i$, $i \in \{0, \dots, d\}$, and

$$e_{[(i_1,i_2,\dots,i_k)]} = [e_{i_1}, e_{[(i_2,\dots,i_k)]}], \tag{2.10}$$

$(i_1, \dots, i_k) \in \mathcal{A}$, $k > 1$. Then

$$\mathfrak{g}_{d,1}^m = \left\langle \left\{ e_{[I]} \;\middle|\; I \in \mathcal{A}_m \right\} \right\rangle_{\mathbb{R}}. \tag{2.11}$$

Notice that $\{ e_I \mid I \in \mathcal{A}_m \}$ gives a basis of $\mathbb{A}_{d,1}^m$, whereas $\left\{ e_{[I]} \;\middle|\; I \in \mathcal{A}_m \right\}$ is not a linearly independent set, e. g. $e_{[(1,2)]} = [e_1, e_2] = -[e_2, e_1] = -e_{[(2,1)]}$. Similarly, $G_{d,1}^m = \exp(\mathfrak{g}_{d,1}^m) \subset \mathbb{A}_{d,1}^m$.

By the *Baker-Campbell-Hausdorff formula*

$$\exp(y)\exp(z) = \exp\Big(y+z+\frac{1}{2}[y,z]+\frac{1}{12}([y,[y,z]]-[z,[z,y]])+\cdots\Big), \tag{2.12}$$

for $y, z \in \mathfrak{g}_{d,1}^m$, $G_{d,1}^m$ is a subgroup of the Lie group $1 \oplus W_1 \oplus \cdots \oplus W_m$. Furthermore, by continuity of the logarithm, $G_{d,1}^m$ is even a closed subgroup, consequently it is a Lie group in its own right and $\mathfrak{g}_{d,1}^m$ is its Lie algebra. The tangent spaces are given by

$$T_x G_{d,1}^m = \left\{ xw \;\middle|\; w \in \mathfrak{g}_{d,1}^m \right\}, \quad x \in G_{d,1}^m. \tag{2.13}$$

$\mathfrak{g}_{d,1}^m$ inherits the grading of the algebra via $U_k = \mathfrak{g}_{d,1}^m \cap W_k$, $k = 1, \dots, m$, hence,

$$\mathfrak{g}_{d,1}^m = U_1 \oplus \cdots \oplus U_m.$$

By definition, $z_0 = 0$ for $z \in \mathfrak{g}_{d,1}^m$ and $x_0 = 1$ for $x \in G_{d,1}^m$. Note that

$$\exp : \mathfrak{g}_{d,1}^m \to G_{d,1}^m$$

is smooth and bijective and, hence, the logarithm – being its inverse – is a global chart for the manifold $G_{d,1}^m$. (For more information on differential geometry see, e. g., Jänich [39].)

Example 2.1.14. The simplest non-trivial example is the case $d = 2$ and $m = 2$ without drift. That is, we set $e_0 = 0$ and consider $\mathbb{A}_2^2$, the space spanned by 1, e_1, e_2 and e_1^2, e_1e_2, e_2e_1, e_2^2. The corresponding Lie algebra $\mathfrak{g}_2^2$ is spanned by e_1, e_2 and $[e_1, e_2]$. The Lie group G_2^2 is called *Heisenberg group*.

The Heisenberg group has the following faithful representation as a matrix group:

$$G_2^2 \simeq \left\{ \begin{pmatrix} 1 & a & c \\ 0 & 1 & b \\ 0 & 0 & 1 \end{pmatrix} \;\middle|\; a, b, c \in \mathbb{R} \right\}$$

with the usual matrix multiplication as group operation. The corresponding Lie algebra – i. e. the tangent space at the unit element $I_3 = \left(\begin{smallmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{smallmatrix}\right)$ – is then given by

$$\mathfrak{g}_2^2 \simeq \left\{ \begin{pmatrix} 0 & x & z \\ 0 & 0 & y \\ 0 & 0 & 0 \end{pmatrix} \;\middle|\; x, y, z \in \mathbb{R} \right\}$$

and is a representation of $\mathfrak{g}_2^2$. The Lie bracket of two matrices is defined as the usual commutator of matrices. We can think of the Heisenberg group as $\mathbb{R}^3$ with the (non-commutative) multiplication $(x_1, x_2, x_3) \star (y_1, y_2, y_3) = (x_1 + y_1, x_2 + y_2, x_3 + y_3 + x_1 y_2)$.

If we identify e_1 and e_2 with $E_1 = \left(\begin{smallmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{smallmatrix}\right)$ and $E_2 = \left(\begin{smallmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{smallmatrix}\right)$, respectively, then we have $[E_1, E_2] = \left(\begin{smallmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{smallmatrix}\right)$, which verifies that the Lie algebra is spanned by E_1, E_2 and $[E_1, E_2]$. We will come back to this example later on.

Notice that similar representations exist for general Heisenberg groups G_d^2.

2.1.3 Iterated Stratonovich integrals in $G_{d,1}^m$

Let $Y^y = (Y_t^y)_{t \in [0,\infty[}$, $y \in \mathbb{A}_{d,1}^m$, denote the stochastic process

$$Y_t^y = y \sum_{I \in \mathcal{A}_m} B_t^I e_I. \tag{2.14}$$

As long as y is invertible, e. g. for $y = 1$, Y^y encodes the iterated Stratonovich integrals of degree up to m as a stochastic process in $\mathbb{A}_{d,1}^m$, since the collection of all e_Is forms a linear basis of $\mathbb{A}_{d,1}^m$. Y^y is the solution of an $\mathbb{A}_{d,1}^m$-valued SDE. Indeed,

$$\begin{aligned} dY_t^y &= y \left(\sum_{\substack{I \in \mathcal{A} \\ \deg(I) \le m-2}} B_t^I \, dt \, e_I \, e_0 + \sum_{i=1}^{d} \sum_{\substack{I \in \mathcal{A} \\ \deg(I) \le m-1}} B_t^I \circ dB_t^i \, e_I \, e_i \right) \\ &= y \sum_{\substack{I \in \mathcal{A} \\ \deg(I) \le m}} B_t^I e_I e_0 \, dt + y \sum_{i=1}^{d} \sum_{\substack{I \in \mathcal{A} \\ \deg(I) \le m}} B_t^I e_I e_i \circ dB_t^i, \end{aligned}$$

where we used freeness of the algebra $\mathbb{A}_{d,1}^m$ in the first line and its nil-potency in the second line. Consequently, Y^y is the unique solution of the SDE

$$\begin{cases} dY_t^y = Y_t^y e_0 dt + \sum_{i=1}^{d} Y_t^y e_i \circ dB_t^i, \\ Y_0^y = y \in \mathbb{A}_{d,1}^m. \end{cases} \tag{2.15}$$

Defining vector fields $D_i(y) = ye_i$, $i = 0, \dots, d$, on $\mathbb{A}_{d,1}^m$, we immediately recognize that equation (2.15) is of the general form (1.3) of an SDE in Stratonovich formulation for the vector fields $D_0, \dots, D_d$. If we restrict D_i to $G_{d,1}^m$, then we get a left-invariant vector field D_i on $G_{d,1}^m$ – not surprisingly coinciding with the element $e_i \in \mathfrak{g}_{d,1}^m$ under the identification of left-invariant vector fields on a Lie group with elements of its Lie algebra. We will freely switch between the perceptions of D_i as vector fields on $G_{d,1}^m$ and on $\mathbb{A}_{d,1}^m$, depending on convenience.

Remark 2.1.15. The canonical dilatation Δ allows us to express the equality in law $B_t^I \sim \sqrt{t}^{\deg(I)}$, see (2.1), in a particularly nice form, namely

$$Y_t^1 \sim \Delta_{\sqrt{t}}(Y_1^1).$$

Now we are finally in the position to reveal the connection between iterated Stratonovich integrals of Brownian motion and certain Lie groups: it turns out that $G_{d,1}^m$ precisely gives us the geometry of the iterated integrals.

Proposition 2.1.16. *Given an initial value $y \in G_{d,1}^m$, $Y_t^y \in G_{d,1}^m$ a. s. for all $t \geq 0$. In particular, $Y_t^1 \in G_{d,1}^m$ almost surely.*

Proof. Since $Y_t^y = yY_t^1$, we only need to consider the initial value $y = 1 \in G_{d,1}^m$. By (2.15), Y^1 solves the Stratonovich-SDE driven by the vector fields $D_i(y) = ye_i$, $i = 0, 1, \dots, d$. This already implies that $G_{d,1}^m$ is locally invariant with respect to the SDE (2.15), i. e. for all $y \in G_{d,1}^m$ there is a strictly positive stopping time τ_y such that $Y_t^y \in G_{d,1}^m$ for all $t \leq \tau_y$ a. s., compare Definition 1.1.5 and Proposition 1.1.6.

$G_{d,1}^m$ is a closed subset of $\mathbb{A}_{d,1}^m$, since it is the pre-image of the closed set $\mathfrak{g}_{d,1}^m \subset \mathbb{A}_{d,1}^m$ under the continuous map log. Let τ be the first hitting time of $\mathbb{A}_{d,1}^m \setminus G_{d,1}^m$. Then $Y_\tau^1 \in G_{d,1}^m$ on $\{\tau < \infty\}$ and, consequently, local invariance implies existence of a positive stopping time $\tilde{\tau}$ such that Y_t^1 remains in $G_{d,1}^m$ up to time $\tau + \tilde{\tau}$, showing that $P(\tau < \infty) = 0$. □

Hence, Y_t^y, $y \in G_{d,1}^m$, really takes its values in the Lie group $G_{d,1}^m$, which is a much smaller dimensional manifold – e. g. $\dim \mathfrak{g}_{2,1}^3 = 8$ whereas $\dim \mathbb{A}_{2,1}^3 = 20$, i. e. the iterated integrals of two Brownian motions up to order 3 evolve on an 8-dimensional submanifold of the 20-dimensional space $\mathbb{A}_{2,1}^3$. Put differently, collecting the iterated Stratonovich integrals of Brownian motion in the process Y^1 is a concise way of expressing the well-known relations between the iterated integrals.

On the other hand, $G_{d,1}^m$ is not a linear space and it is often desirable to work in a vector space instead of a manifold. Therefore, we use the global chart and define a stochastic process

$$Z_t = \log(Y_t^1), \quad t \geq 0, \tag{2.16}$$

on $\mathfrak{g}_{d,1}^m$, which contains all the information of Y^1.

Proposition 2.1.17 (Chen-Strichartz formula)**.** *Let $\mathfrak{S}_k$ denote the symmetric group in k elements. For $\sigma \in \mathfrak{S}_k$ let*

$$e(\sigma) = \#\{\, j \in \{1, \dots, k-1\} \mid \sigma(j) > \sigma(j+1) \,\}$$

be the number of inversions of σ. Then

$$Z_t = \log(Y_t^1) = \sum_{I \in \mathcal{A}_m \setminus \{\emptyset\}} \Lambda_t^I e_{[I]},$$

where, for a multi-index $I = (i_1, \dots, i_k) \in \mathcal{A} \setminus \{\emptyset\}$,

$$\Lambda_t^I = \sum_{\sigma \in \mathfrak{S}_k} \frac{(-1)^{e(\sigma)}}{k^2 \binom{k-1}{e(\sigma)}} B_t^{\sigma^{-1}(I)}$$

with $\sigma((i_1, \dots, i_k)) = (i_{\sigma(1)}, \dots, i_{\sigma(k)})$ for $\sigma \in \mathfrak{S}_k$.

Proof. Apply Proposition A.1.2 in the Appendix to the $(d+1)$-dimensional semi-martingale $(t, B_t^1, \dots, B_t^d)_{t \in [0,\infty[}$ and project the formal Lie series down to $\mathfrak{g}_{d,1}^m$. □

Remark 2.1.18. The Chen-Strichartz formula roughly says that Z_t is a linear function of Y_t^1. Recall, however, that the set $\{e_{[I]} \mid I \in \mathcal{A} \setminus \{\emptyset\}\}$ is not a basis of $\mathfrak{g}_{d,1}^m$. Thus, in a second step one would need to expand the Chen-Strichartz formula with respect to a basis of $\mathfrak{g}_{d,1}^m$.

Example 2.1.19 (Continuation of Example 2.1.14)**.** In the case of the Heisenberg group, a basis of $\mathfrak{g}_2^2$ is given by $\{e_1, e_2, [e_1, e_2]\}$ and we have $Z_t = B_t^1 e_1 + B_t^2 e_2 + A_t [e_1, e_2]$, where

$$A_t = \frac{1}{2} \int_0^t B_s^1 \circ dB_s^2 - \frac{1}{2} \int_0^t B_s^2 \circ dB_s^1 = \frac{1}{2} \int_0^t B_s^1 dB_s^2 - \frac{1}{2} \int_0^t B_s^2 dB_s^1$$

denotes *Lévy's area*.

The setting $\mathbb{A}_{d,1}^m$ provides a nice way to write the expected value of iterated Stratonovich integrals.

Proposition 2.1.20. *For $t \geq 0$ and $y \in \mathbb{A}_{d,1}^m$ we have*

$$E\big(Y_t^y\big) = y \exp\Big(t e_0 + \frac{t}{2} \sum_{i=1}^d e_i^2\Big).$$

Proof. Proposition 2.1.20 is not surprising considering the SDE (2.15) for Y^y. Indeed, the infinitesimal generator of Y_t^y is given by $L = D_0 + \frac{1}{2} \sum_{i=1}^d D_i^2$, again interpreting the vector fields $D_i(y) = y e_i$ as first-order differential

operators. Thus, $u(t,y) = E(\lambda(Y_t^y))$ satisfies the Kolmogorov backward equation

$$\frac{\partial}{\partial t}u(t,y) = Lu(t,y)$$

with initial condition $u(0,y) = \lambda(y)$ for any linear functional $\lambda : \mathbb{A}_{d,1}^m \to \mathbb{R}$. Formally, this can be expressed by $u(t,y) = e^{tL}(\lambda)(y)$.

Now denote

$$v(t,y) = \lambda\Big(y\exp\Big(te_0 + \frac{t}{2}\sum_{i=1}^d e_i^2\Big)\Big).$$

$v(t,y)$ solves the equation

$$\frac{\partial v}{\partial t}(t,y) = \lambda\Big(y\exp\Big(te_0 + \frac{t}{2}\sum_{i=1}^d e_i^2\Big)\Big(e_0 + \frac{1}{2}\sum_{i=1}^d e_i^2\Big)\Big) = Lv(t,y)$$

and the result follows by uniqueness of the solution of the Kolmogorov backward equation. □

Remark 2.1.21. $E(Y_t^y) \notin G_{d,1}^m$ since its logarithm is not in the Lie algebra.

Of course, Proposition 2.1.20 is not an interesting result in its own right, it is rather a convenient way of writing the easily obtained recursive formulas for the expected value of an iterated Stratonovich integral. Nevertheless, it is the starting point to the applications presented in the next two sections.

2.2 Cubature on Wiener space

"Cubature on Wiener space" is a weak approximation scheme in the sense of Definition 1.3.3 for solutions of standard SDEs of the type (1.3). Just like most other weak schemes, it is a deterministic scheme with deterministic a-priori error bounds in terms of the function f and the vector fields $V_0, \dots, V_d$ – we use the Stratonovich formulation – provided that one is able to do the integration step explicitly. Usually, this is not possible and one has to revert to (Quasi) Monte Carlo routines, notice, however, that Schmeiser, Soreff, and Teichmann [74] allow for very high dimensional integration by using inherent recombination possibilities in the cubature on Wiener space method. The method was introduced by Lyons and Victoir [51]. A similar method has been studied by Kusuoka [43], [44]. Mathematically, the method is very attractive because it combines results from different areas like numerical analysis (classical cubature formulas), algebra (nilpotent Lie groups as in Section 2.1) and differential geometry (Chow's theorem) together with stochastic analysis. We start our presentation of the method with a short look onto classical cubature formulas.

2.2.1 Classical cubature formulas

Cubature (also known as quadrature) formulas are a classical technique for numerical integration, see Stroud [78] and Überhuber [83]. Before giving a definition of the notion of a cubature formula, let us recall that the *support* $\operatorname{supp}\mu$ of the Borel measure μ on $\mathbb{R}^n$, i. e. μ is a measure defined on the Borel σ-algebra of $\mathbb{R}^n$, is the complement of the biggest open set $O \subset \mathbb{R}^n$ with $\mu(O) = 0$.

Definition 2.2.1. Given a positive Borel measure μ on $\mathbb{R}^n$ and $m \in \mathbb{N}$ such that all moments up to order m exist, i. e.

$$\int_{\mathbb{R}^n} \|x\|^k \, \mu(dx) < \infty, \quad k = 0, \dots, m.$$

A finite sequence of points $x_1, \dots, x_N \in \operatorname{supp}\mu$ and weights $\lambda_1, \dots, \lambda_N > 0$ is called *cubature formula* of degree m if

$$\int_{\mathbb{R}^n} p(x)\mu(dx) = \sum_{i=1}^{N} \lambda_i p(x_i)$$

for all polynomials p of degree less or equal to m on $\mathbb{R}^n$.

Given a cubature formula as in Definition 2.2.1 and a function $f : \mathbb{R}^n \to \mathbb{R}$, then we can approximate

$$\int_{\mathbb{R}^n} f(x)\mu(dx) \approx \sum_{i=1}^{N} \lambda_i f(x_i).$$

The approximation is good if f can be approximated by polynomials of degree less or equal m sufficiently well. Note that f only needs to be defined on $\operatorname{supp}\mu$ for the integral $\int f d\mu$ to make sense, therefore we require that all the points of a cubature formula lie in $\operatorname{supp}\mu$, see Stroud [78] for more information on this point.

Even though construction of cubature formulas is a non-trivial task, especially in higher dimensions, and especially if one wants to avoid an unnecessarily large size N of the cubature formula, there is a very general existence result. Let $\mathbb{A}^m_{n,\mathrm{com}}$ denote the *free, commutative, step m nilpotent algebra* in n generators $e_1, \dots, e_n$, where the convention of Remark 2.1.5 is still used.

Remark 2.2.2. Obviously, we get $\mathbb{A}^m_{n,\mathrm{com}}$ by factorizing the algebra $\mathbb{A}^m_n$ of Definition 2.1.9 with respect to the ideal generated by $\{ e_i e_j - e_j e_i \mid 1 \le i, j \le n \}$. Moreover, we may identify $\mathbb{A}^m_{n,\mathrm{com}}$ with the space of polynomials on $\mathbb{R}^n$ with degree less or equal m.

Theorem 2.2.3. *Given a finite, positive Borel measure μ on $\mathbb{R}^n$ and $m \in \mathbb{N}$ such that μ has finite moments of order up to m. Then there is an integer $1 \le N \le \dim \mathbb{A}^m_{n,\mathrm{com}}$ such that a cubature formula of degree m with size N exists for μ.*

Theorem 2.2.3 is known as *Chakalov's theorem*, since it was first proved by Chakalov [12] in the case of compactly supported Borel measures. Later on, it was extended by Putinar [65] and Curto and Fialkow [17] to non-compactly supported measures with finite $(m+1)$-st moments. Theorem 2.2.3 was finally proved by Bayer and Teichmann [7], and the presentation here is based on the latter paper.

Let us recall some basic notions and results from convex analysis, for more details see Rockafellar [70]. For any set $A \subset \mathbb{R}^n$, let $\operatorname{conv} A$ denote its convex hull and $\overline{\operatorname{conv}} A$ the (topological) closure of $\operatorname{conv} A$. Note that $\overline{A}$ is convex for any convex set A, but the converse is not necessarily true: the convex hull of a closed set A is, in general, not closed unless A is compact. Similarly, the convex cone generated by $A \subset \mathbb{R}^n$ is denoted by $\operatorname{cone} A$ and its closure by $\overline{\operatorname{cone}} A$.

Convex sets can be characterized by their *supporting hyperplanes* and *supporting half-spaces*. Given a convex set $C \subset \mathbb{R}^n$ and a point $x \in \partial C$, then there is a vector n_x such that C is touched by the hyperplane

$$\{n_x = n_x(x)\} = \{\, y \in \mathbb{R}^n \mid \langle n_x\,, y\rangle = \langle n_x\,, x\rangle \,\}$$

at x and contained in the corresponding half-space

$$\{n_x \le n_x(x)\} = \{\, y \in \mathbb{R}^n \mid \langle n_x\,, y\rangle \le \langle n_x\,, x\rangle \,\}\,.$$

$\overline{C}$ is the intersection of all supporting half-spaces of C. Moreover, assuming that C is not contained in a hyperplane of $\mathbb{R}^n$, i. e. $\operatorname{int} C \neq \varnothing$, then $x \in C$ is a boundary point if and only if x is contained in at least one supporting hyperplane of C. In the case of a convex cone C, all the supporting hyperplanes are homogeneous, i. e. contain the origin 0.

A point $x \in C$ lies in the *relative interior* of the convex set C if

$$\forall y \in C\, \exists \epsilon > 0 : x - \epsilon(y - x) \in C.$$

The relative interior of C is denoted by $\operatorname{ri} C$. Note that $\operatorname{int} C \subset \operatorname{ri} C$, where $\operatorname{int} C$ denotes the interior of C. If C is contained in a proper hyperplane of $\mathbb{R}^n$, then $\operatorname{ri} C$ contains the interior of C with respect to the topology of the hyperplane.

Let us first prove a special case of Theorem 2.2.3, namely the case $m = 1$.

Theorem 2.2.4. *Let μ be a positive Borel measure with $\int_{\mathbb{R}^n} \|x\|\,\mu(dx) < \infty$ and let $A \subset \mathbb{R}^n$ be a measurable set such that μ is concentrated on A, i. e. $\mu(\mathbb{R}^n \setminus A) = 0$. Then the barycenter of μ,*

$$\operatorname{bary}(\mu) = \int_{\mathbb{R}^n} x\mu(dx) \in \mathbb{R}^n,$$

is contained in $\operatorname{cone} A$.

Proof. Without loss of generality, we may assume that A is not contained in a proper hyperplane of $\mathbb{R}^n$, more precisely, that there is no $B \subset A$ such that $\mu(A \setminus B) = 0$ and B is contained in a proper hyperplane of $\mathbb{R}^n$, since otherwise we may reduce the dimension of the space and proceed with B instead of A.

For $x \in \partial(\operatorname{cone} A)$, consider any supporting half-space $\{n_x \leq 0\}$ of $\operatorname{cone} A$ at x. Obviously, the linear functional $y \mapsto \langle n_x \, , y \rangle$ is absolutely integrable and we get

$$\langle n_x \, , \operatorname{bary}(\mu) \rangle = \int_{\mathbb{R}^n} \langle n_x \, , y \rangle \, \mu(dy) \leq 0,$$

since $\langle n_x \, , y \rangle \leq 0$ for all $y \in A$. Consequently, $\operatorname{bary}(\mu)$ lies in the intersection of all the supporting half-spaces of $\operatorname{cone} A$, i. e. $\operatorname{bary}(\mu) \in \overline{\operatorname{cone}} \, A$.

In order to show that $\operatorname{bary}(\mu) \in \operatorname{cone} A$, we will refine the above argument and actually show that $\langle n_x \, , \operatorname{bary}(\mu) \rangle < 0$ for any $x \in A$ and any supporting half-space n_x. First note that

$$\mu \left(\{ \, y \in A \mid \langle n_x \, , y \rangle < 0 \, \} \right) > 0,$$

since otherwise $\mu(A \setminus (A \cap \{n_x = 0\})) = 0$, in contradiction to the assumption in the beginning of this proof. On the other hand, the existence of the first moment implies that $\mu(B(0, \epsilon)^c) < \infty$ for any $\epsilon > 0$. Combining these two facts, we find the existence of $\epsilon = \epsilon(x, n_x) > 0$ such that

$$0 < \mu \left(\{ \, y \in A \mid \langle n_x \, , y \rangle \leq -\epsilon \, \} \right) < \infty.$$

Consequently, we get a bound

$$\langle n_x \, , \operatorname{bary}(\mu) \rangle \leq -\epsilon \mu \left(\{ \, y \in A \mid \langle n_x \, , y \rangle \leq -\epsilon \, \} \right) < 0, \tag{2.17}$$

showing that $\operatorname{bary}(\mu) \in \operatorname{int} \overline{\operatorname{cone}} \, A \subset \operatorname{cone} A$. □

Notice that the proof actually shows that $\operatorname{bary}(\mu) \in \operatorname{ri}(\operatorname{cone} A)$.

Corollary 2.2.5. *Let μ be a positive Borel measure concentrated on $A \subset \mathbb{R}^n$ with finite first moment. Then there exists $1 \leq N \leq n$, points $x_1, \ldots, x_N \in A$ and weights $\lambda_1, \ldots, \lambda_N > 0$ such that for any polynomial p of degree 1*

$$\int_{\mathbb{R}^n} p(x) \mu(dx) = \sum_{i=1}^{N} \lambda_i p(x_i).$$

Proof. By Theorem 2.2.4 and Carathéodory's theorem for cones, see Rockafellar [70, Theorem 17.1, Corollary 17.2], there are points and weights as in Corollary 2.2.5 such that

$$\operatorname{bary}(\mu) = \sum_{i=1}^{N} \lambda_i x_i,$$

which immediately implies the corollary. □

Corollary 2.2.6. *Given a positive measure μ on the measurable space $(\Omega, \mathcal{F})$ concentrated on $A \in \mathcal{F}$. For any Borel-measurable map $\phi : \Omega \to \mathbb{R}^n$ such that*

$$\int_\Omega \|\phi(\omega)\| \, \mu(d\omega) < \infty$$

there are an integer $1 \leq N \leq n$, points $\omega_1, \ldots, \omega_N \in \Omega$ and weights $\lambda_1, \ldots, \lambda_N > 0$ such that

$$\int_\Omega p(\phi(\omega))\mu(d\omega) = \sum_{i=1}^N \lambda_i \phi(\omega_i)$$

for any polynomial $p : \mathbb{R}^n \to \mathbb{R}$ of order 1.

Proof. We repeat the idea of the proof of Theorem 2.2.4 in the current setting, i. e. we prove the statement by induction on n. For $n = 1$, we distinguish between two situations: either ϕ is constant μ-almost everywhere, or it is not. In any case, the statement follows immediately.

Now assume that the statement holds for $n - 1$. If there is $B \in \mathcal{F}$, $B \subset A$, such that $\phi(B)$ is contained in a proper hyperplane of $\mathbb{R}^n$ and $\mu(A \setminus B) = 0$, then we may reduce the problem to the $(n-1)$-dimensional case by replacing A by B. Therefore, we may suppose that this is not the case. Choose $x \in \partial(\operatorname{cone} A)$ and a corresponding supporting hyperplane given by n_x. Then

$$\langle n_x \, , \operatorname{bary}(\phi_* \mu) \rangle = \int_\Omega \langle n_x \, , \phi(\omega) \rangle \, \mu(d\omega) \leq 0,$$

which implies that $\operatorname{bary}(\phi_*\mu) \in \overline{\operatorname{cone}}\, \phi(A)$.

If $\operatorname{bary}(\phi_*\mu) \in \partial(\overline{\operatorname{cone}}\, \phi(A))$, then, with $x = \operatorname{bary}(\phi_*\mu)$, any corresponding hyperplane n_x satisfies

$$0 = \langle n_x \, , x \rangle = \langle n_x \, , \operatorname{bary}(\phi_* \mu) \rangle = \int_A \langle n_x \, , \phi(\omega) \rangle \, \mu(d\omega).$$

Since the integrand on the right hand side is non-negative, we may conclude that $\mathbf{1}_A \langle n_x \, , \phi \rangle = 0$ μ-almost everywhere, i. e.

$$\mu \left(A \setminus \{ \, \omega \in \Omega \mid \langle n_x \, , \phi(\omega) \rangle = 0 \, \} \right) = 0.$$

Consequently, $\operatorname{bary}(\phi_*\mu) \in \partial(\overline{\operatorname{cone}}\, \phi(A))$ would imply that ϕ takes its values inside the proper hyperplane $\{n_{\operatorname{bary}(\phi_*\mu)} = 0\}$ outside a set of μ-measure 0, in contradiction to our assumption. Thus, $\operatorname{bary}(\phi_*\mu) \in \operatorname{int}(\overline{\operatorname{cone}}\, \phi(A)) \subset \operatorname{cone} \phi(A)$, and the statement follows again by appealing to Carathéodory's theorem. □

Remark 2.2.7. Notice that $\phi(A)$ is not necessarily Borel measurable. If it were Borel measurable, or more precisely, if it were measurable with respect to the completion of the Borel σ-algebra under the measure $\phi_*\mu$, then Corollary 2.2.6 would immediately follow from Corollary 2.2.5 by replacing A by $\phi(A)$ and μ by $\phi_*\mu$, respectively. The proof in Bayer and Teichmann [7] is incorrect by omitting this implicit assumption.

Remark 2.2.8. Theorem 2.2.4 and its corollaries do not require μ to have finite mass, because only finite first moments are necessary.

Remark 2.2.9. If μ has finite mass, then we can add $\phi_0(\omega) \equiv 1$ in Corollary 2.2.6 and get $1 \leq N' \leq n+1$, points $\omega_1, \ldots, \omega_{N'}$, weights $\lambda_1, \ldots, \lambda_{N'} > 0$ with $\lambda_1 + \cdots + \lambda_{N'} = \mu(\Omega)$ – and likewise for the setting of Theorem 2.2.4.

Remark 2.2.10. In particular, if μ is a probability measure on $\mathbb{R}^n$, then $\mathrm{bary}(\mu) \in \operatorname{conv} A$. This result is well-known and goes back to Riesz [69] for compactly supported measures.

Proof of Theorem 2.2.3. Define a map $\phi : \mathbb{R}^n \to \mathbb{A}^m_{n,\mathrm{com}}$ by

$$\phi(x_1, \ldots, x_n) = \sum_{k=0}^{m} \sum_{(i_1,\ldots,i_k)\in\{1,\ldots,n\}^k} x_{i_1} \cdots x_{i_k} e_{i_1} \cdots e_{i_k}. \tag{2.18}$$

The significance of ϕ is that it linearizes the problem: polynomials are now simply linear functionals in ϕ. $\mathbb{A}^m_{n,\mathrm{com}}$ is a finite dimensional vector space, therefore the notion of the Borel σ-algebra is well-defined on $\mathbb{A}^m_{n,\mathrm{com}}$ and ϕ – being continuous – is measurable. By assumption, the conditions of Corollary 2.2.6 are satisfied with $\Omega = \mathbb{R}^n$ and $A = \operatorname{supp}\mu$ and we get the statement of the theorem, see also Remark 2.2.9. □

Remark 2.2.11. Theorem 2.2.3 has a relation to the *truncated moment problem*, cf. Curto and Fialkow [17]. Given a non-empty, closed set $A \subset \mathbb{R}^n$ and a finite sequence of real numbers $c_{i_1,\ldots,i_k}$, $(i_1, \ldots, i_k) \in \{1, \ldots, n\}^k$ with $k \leq m$. The sequence represents the sequence of moments up to order m of a probability measure with support $\operatorname{supp}\mu \subset A$ if and only if

$$\sum_{k=0}^{m} \sum_{(i_1,\ldots,i_k)\in\{1,\ldots,n\}^k} c_{i_1,\ldots,i_k} e_{i_1} \cdots e_{i_k} \in \operatorname{conv} \phi(K). \tag{2.19}$$

Indeed, if there is a probability measure supported in A with the prescribed moments, then the moments satisfy (2.19) by Chakalov's theorem. On the other hand, any member of $\operatorname{conv}\phi(A)$ can be written as a convex combination of elements of $\phi(A)$, and thus corresponds to the moments of the underlying finitely supported measure.

Theorem 2.2.3 is an essentially unconstructive theorem, since it relies on Carathéodory's theorem. Indeed, the construction of cubature formulas

is usually a highly non-trivial task, especially if the size should be close to the optimal size for the particular measure. See Victoir [85] for ideas about construction of cubature formulas avoiding "unnecessary" symmetries.

2.2.2 Cubature on Wiener space

Most of the problems addressed in this text are motivated by the calculation of functionals of solutions of SDEs. As usual, let $X^x = (X_t^x)_{t\in[0,T]}$ denote the solution of the Stratonovich SDE (1.3) with initial value $X_0^x = x$ driven by the vector fields $V_0, \dots, V_d$ on $\mathbb{R}^n$. For a given and fixed, say, bounded measurable function $f : \mathbb{R}^n \to \mathbb{R}$, we want to compute

$$E(f(X_T^x)) = \int_\Omega f \circ X_T^x(\omega) P(d\omega). \tag{2.20}$$

Without loss of generality, we may assume that the probability space $(\Omega, \mathcal{F}, P)$ is the canonical probability space of Brownian motion, i. e. *Wiener space* $C_0([0,T];\mathbb{R}^d)$ of continuous functions starting at 0 equipped with its Borel σ-algebra with respect to $\|\cdot\|_\infty$ and with the *Wiener measure* P. Consequently, the problem to calculate (2.20) is actually a numerical integration problem on a high dimensional space, namely on $C_0([0,T];\mathbb{R}^d)$. Therefore, it is natural to ask one-selves whether cubature can help integrating (2.20).

Considering Definition 2.2.1, we first have to choose a suitable class of "polynomials" on the Wiener space. It is easy to see that the class of proper polynomials – i. e. polynomials in linear functionals on $C_0([0,T];\mathbb{R}^d)$ – is not adequate regarding cubature. First, there are too many polynomials on Wiener space, but more importantly, there are extremely important functionals on $C_0([0,T];\mathbb{R}^d)$ that cannot be described well by polynomials. For instance, Lévy's area – introduced in Example 2.1.19 for $d = 2$ – is a measurable function on Wiener space, but it is not continuous, not even on subspaces of functions regular enough such that the stochastic integrals make sense path-wise as Riemann-Stieltjes integrals. This problem is treated in much detail by Lyons [52].

Motivated by the stochastic Taylor expansion, see Proposition 2.1.4, Lyons and Victoir [51] choose the iterated Stratonovich integrals as analogues to the polynomials in finite dimensions.

Definition 2.2.12. Fix $T > 0$ and $m \in \mathbb{N}$. A finite sequence of weights $\lambda_1, \dots, \lambda_N > 0$ and paths $\omega_1, \dots, \omega_N \in C_0([0,T];\mathbb{R}^d)$ forms a *cubature formula on Wiener space* of degree m if the paths $\omega_1, \dots, \omega_N$ are of *bounded variation* and

$$E(B_T^I) = \sum_{i=1}^N \lambda_i \omega_i^I(T), \quad \forall I \in \mathcal{A}_m, \tag{2.21}$$

where we use Definition 2.1.3 for iterated integrals of Brownian motion and for paths of bounded variation.

Remark 2.2.13. By the scaling property (2.1) of iterated Stratonovich integrals, cubature formulas for any $T > 0$ can be constructed from a cubature formula for $T = 1$ by rescaling. Note, however, that the paths are getting rougher with smaller T.

Remark 2.2.14. The integrals on the right hand side are well-defined because the cubature paths are required to have bounded variation on $[0, T]$. Note that $\omega^I(T)$ may be interpreted as evaluation of the random variable $B_T^I(\omega)$ for a path $\omega \in C_0([0,T];\mathbb{R}^d)$ of bounded variation. Then the formula (2.21) in Definition 2.2.12 can be written as

$$E(B_T^I) = \sum_{i=1}^{N} \lambda_I B_T^I(\omega_i),$$

in more direct analogy to Definition 2.2.1.

Kusuoka [43], [44] introduces a similar concept. He calls a family $Z_I \in \bigcap_{1\le p<\infty} L^p(\Omega, \mathcal{F}, P)$, $I \in \mathcal{A}$, *m-moment similar* if $Z_\emptyset = 1$ and

$$E(Z_{I_1} \cdots Z_{I_k}) = E(B_T^{I_1} \cdots B_T^{I_k}), \tag{2.22}$$

for $k \in \mathbb{N}$ and $I_1, \dots, I_k \in \mathcal{A}$ with $\deg(I_1)+\cdots+\deg(I_k) \le m$. Note that any cubature formula on Wiener space of degree m gives an m-moment similar family of random variables by setting

$$Z_I = \begin{cases} B_T^I(\omega_i) \text{ with prob. } \lambda_i,\ i = 1, \dots, N, & \deg(I) \le m, \\ 0, & \deg(I) > m. \end{cases} \tag{2.23}$$

Indeed, the family of random variables defined by (2.23) trivially satisfies (2.22) for $k = 1$. The Chen-Strichartz formula implies that $B_T^{I_1} \cdots B_T^{I_k}$ can be expressed as linear combination – with deterministic weights – of iterated Stratonovich integrals of degree smaller than m provided that $\deg(I_1) + \cdots + \deg(I_k) \le m$, $k \ge 1$. (In particular, see (A.5) for an explicit formula.) Consequently, (2.22) holds for any k. On the other hand, moment similar families of random variables do not need to respect the geometry of iterated integrals in the sense that the support of the random vector $(Z_I : I \in \mathcal{A}_m)$ does not need to be contained in the support of $(B_T^I : I \in \mathcal{A}_m)$, which is isomorphic to $G_{d,1}^m$. Moreover, even though the class of moment similar random variables is larger than the class of cubature formulas on Wiener space, it does not seem to be easier to construct moment similar families of random variables.

The proof of existence of cubature formulas on Wiener space is taken from Teichmann [81] – which is an adaption of the original proof by Lyons and Victoir [51] – and relies on the algebraic setting introduced in Section 2.1. Therefore, we shall first translate Definition 2.2.12 into that setting. Recall that we denote the vector of all iterated Stratonovich integrals of order up

to m – understood as process taking values in $G^m_{d,1} \subset \mathbb{A}^m_{d,1}$ – by $(Y^1_t)_{t\in[0,\infty[}$, cf. (2.14). For any $\omega \in C_0([0,T];\mathbb{R}^d)$ of bounded variation, we define a function $t \mapsto \Phi(\omega)^1_t$ by the analogous formula

$$\Phi(\omega)^1_t = \sum_{I\in\mathcal{A}_m} \omega^I(t)e_I, \quad t \in [0,T]. \tag{2.24}$$

$y_t = \Phi(\omega)^1_t$ satisfies the ODE

$$\begin{cases} dy_t = \sum_{i=0}^{d} y_t e_i d\omega^i(t), \\ y_0 = 1, \end{cases} \tag{2.25}$$

cf. equation (2.15). Of course, $\Phi(\omega)^1_t \in G^m_{d,1}$ for any $t \in [0,T]$ and any path of bounded variation ω.

Now we may rephrase the defining equation (2.21) as

$$E(Y^1_T) = \sum_{i=1}^{N} \lambda_i \Phi(\omega_i)^1_T. \tag{2.26}$$

We shall show existence of paths of bounded variation ω_i and weights λ_i, $i = 1,\dots,N$, in two steps: First we show that the left hand side of (2.26) can be written as convex combination of elements of $G^m_{d,1}$, then we show that any element of $G^m_{d,1}$ is the endpoint of the solution of an ODE (2.25) starting at the neutral element 1 for some path of bounded variation ω.

Lemma 2.2.15. *For any $T > 0$ we can find $N \in \mathbb{N}$, points $y_1,\dots,y_N \in G^m_{d,1}$ and positive weights $\lambda_1,\dots,\lambda_N$ such that*

$$E(Y^1_T) = \exp\Big(Te_0 + \frac{T}{2}\sum_{j=1}^{d} e_j^2\Big) = \sum_{i=1}^{N} \lambda_i y_i.$$

Proof. The law $(Y^1_T)_*P$ of Y^1_T is a Borel probability measure on the finite dimensional vector space $\mathbb{A}^m_{d,1}$ with

$$\operatorname{supp}((Y^1_T)_*P) = G^m_{d,1} \subset \mathbb{A}^m_{d,1}.$$

Therefore, the statement of the lemma is implied by Chakalov's theorem, see Corollary 2.2.5. □

For the second step, we need a version of *Chow's theorem* from sub-Riemannian geometry given in Lemma 2.2.16 below. For a proof we refer to Montgomery [59].

Lemma 2.2.16. *Let M be an n-dimensional smooth manifold. Assume that there are $d < n$ vector fields denoted by $D_1, \dots, D_d$ such that the tangent space T_xM at $x \in M$ is spanned by $D_1(x), \dots, D_d(x)$ together with all the iterated Lie brackets $[D_i, D_j](x)$, $[D_i, [D_j, D_k]](x)$, $\dots$, $i, j, k = 1, \dots, d$ at any $x \in M$. Then for any two points $x, y \in M$ and any $T > 0$ there is a function $\omega : [0, T] \to \mathbb{R}^d$ of bounded variation such that the solution z of the ODE*

$$\begin{cases} dz_t = \sum_{i=1}^{d} D_i(z_t) d\omega^i(t), \quad t \in [0, T], \\ z_0 = x, \end{cases}$$

satisfies $z_T = y$. In other words, any two points of M can be joined by a horizontal *path, i. e. a path tangent to the distribution spanned by $D_1, \dots, D_d$.*

Proposition 2.2.17. *Cubature formulas on Wiener space exist for any time T and all positive integers m and d.*

Proof. By Lemma 2.2.15, we need to show that the points $y_i \in G^m_{d,1}$ can be represented as

$$y_i = \Phi(\omega_i)^1_T$$

for paths ω_i of bounded variation, $i = 1, \dots, N$. Note that the Lie group $G^m_{d,1}$ satisfies the assumption of Lemma 2.2.16 for the vector fields $D_j(y) = ye_j$, $j = 0, \dots, d$. Consequently, we can find paths of bounded variation $\omega_i : [0, T] \to \mathbb{R}^{d+1}$, $i = 1, \dots, N$, joining 1 to x_i. A closer look to the construction reveals that these paths of bounded variation can actually by chosen such that, by abuse of notation, $\omega^0_i(t) = t$. Hence, they can be regarded as paths of bounded variation with values in $\mathbb{R}^d$ *and* added 0-th component t, which shows (2.26) and concludes the proof. □

The existence proof of cubature formulas on Wiener space includes two separate constructions, both of which are difficult to perform explicitly, namely the construction of a classical cubature formula on the (typically high-dimensional) space $\mathbb{A}^m_{d,1}$, cf. Lemma 2.2.15, followed by the construction of paths of bounded variation joining 1 to the cubature points, cf. Lemma 2.2.16. Therefore, it is not surprising that the actual construction of cubature paths is a difficult task.

Example 2.2.18. For $m = 3$, let the positive weights $\lambda_1, \dots, \lambda_N$ and the points $x_1, \dots, x_N \in \mathbb{R}^d$ form a classical cubature formula of degree 3 for the standard Gaussian measure on $\mathbb{R}^d$, e. g. $N = 2^d$, $\{x_1, \dots, x_N\} = \{+1, -1\}^d$ and $\lambda_i = 2^{-d}$, $i = 1, \dots, N$. (Of course, the size of this cubature formula is far away from being optimal.) Then a cubature formula on Wiener space of degree $m = 3$ for d Brownian motions is given by $\omega_i(t) = tz_i$, $t \in [0, 1]$, and λ_i as before, $i = 1, \dots, N$.

For degree $m = 5$ and $d = 2$ Brownian motions, Lyons and Victoir [51] construct piecewise linear cubature paths. They also show how to do this for $m = 5$ and arbitrary d.

2.2.3 Weak approximation using cubature formulas

For the convenience of the reader, we provide a very short resumé of finite-dimensional numerical approximation schemes based on cubature formulas on Wiener space. Naturally, the prime reference is once again Lyons and Victoir [51]. While they are dealing with many questions regarding cubature on Wiener space, Kusuoka [43], [44] is almost exclusively interested in weak approximation based on the more general framework of m-moment similar families of random variables, see Subsection 2.2.2. Note, however, that Kusuoka gave the first convergence proof for Lipschitz claims for schemes based on m-moment similar families of random variables, which is, a-fortiori, also a convergence proof for the cubature scheme.

As we shall see, the general weak approximation scheme based on cubature formulas is, from a numerical point of view, prohibitively costly in some situations. Schmeiser, Soreff, and Teichmann [74] try to remedy this in full generality by introducing recombination techniques, see also Soreff [76]. A related numerical approach was introduced by Ninomiya and Victoir [60].

As usual, the weak approximation scheme is based on the stochastic Taylor expansion, Proposition 2.1.4. Let us introduce yet another shorthand notation: for $f \in C^m(\mathbb{R}^n)$ and a multi-index $I = (i_1, \dots, i_k) \in \mathcal{A}_m$, let

$$V_I f(x) = V_{(i_1,\dots,i_k)} f(x) = V_{i_1} \cdots V_{i_k} f(x), \quad x \in \mathbb{R}^n, \tag{2.27}$$

and

$$V_{[I]} f(x) = V_{[(i_1,\dots,i_k)]} f(x) = [V_{i_1}, [V_{i_2}, \dots, [V_{i_{k-1}}, V_{i_k}] \cdots]] f(x), \tag{2.28}$$

where $V_0, \dots, V_d$ are the driving vector fields of the Stratonovich-SDE (1.3) under consideration. As usual, its solution is denoted by $X^x = (X_t^x)_{t \in [0,T]}$ for initial values $x \in \mathbb{R}^n$. For the sake of simplicity, let us assume that $T < 1$, since we are only interested at the asymptotic analysis at this stage. This allows us to get rid of the "$\mathbf{1}_{\{T>1\}}$"-terms.

Let $\lambda_1, \dots, \lambda_N > 0$ and $\omega_1 = \omega_1^{(T)}, \dots, \omega_N = \omega_N^{(T)} : [0,T] \to \mathbb{R}^d$, denote a cubature formula on Wiener space for the interval $[0,T]$ and fixed degree m. We emphasize the (simple) dependence of the cubature paths on the horizon T because we shall later change T and, consequently, also the cubature paths by rescaling to the new T. By definition of cubature formulas on Wiener

space, the stochastic Taylor expansion implies

$$\begin{aligned} E(f(X_T^x)) &= \sum_{I\in\mathcal{A}_m} V_I f(x) E(B_T^I) + \mathcal{O}(T^{\frac{m+1}{2}}) \\ &= \sum_{j=1}^{N} \lambda_j \sum_{I\in\mathcal{A}_m} V_I f(x) \omega_j^I(T) + \mathcal{O}(T^{\frac{m+1}{2}}) \end{aligned} \tag{2.29}$$

for $f \in C^{m+1}(\mathbb{R}^n;\mathbb{R})$. By a slight abuse of notation, see Remark 2.2.14, let $X_T^x(\omega)$ denote the solution x_T of the ODE

$$\begin{cases} dx_t = \sum_{i=0}^{d} V_i(x_t) d\omega^i(t), \quad t \in [0,T], \\ x_0 = x \in \mathbb{R}^n, \end{cases} \tag{2.30}$$

where $\omega : [0,T] \to \mathbb{R}^d$ is a path of bounded variation. Taylor expansion of $f(X_T^x(\omega))$ up to degree m in the sense of deg yields

$$f(X_T^x(\omega)) = \sum_{I\in\mathcal{A}_m} V_I f(x) \omega^I(T) + \mathcal{O}(T^{\frac{m+1}{2}}) \tag{2.31}$$

provided that $\omega = \omega^{(T)}$ has the correct scaling

$$\omega_T^{(T),I} = \sqrt{T}^{\deg(I)} \omega_1^{(1),I}.$$

Combining equation (2.29) and equation (2.31) for the cubature paths $\omega_1, \dots, \omega_N$, we immediately get

$$E(f(X_T^x)) = \sum_{i=1}^{N} \lambda_i f(X_T^x(\omega_i)) + \mathcal{O}(T^{\frac{m+1}{2}}). \tag{2.32}$$

The quantity of interest on the left hand side of equation (2.32) is approximated by a weighted sum of *solutions of ODEs* on the right hand side. Therefore, the task of solving an SDE is replaced by the task of solving N ordinary differential equations. Furthermore, note that the error term on the right hand side is deterministic and can be computed a-priori. Moreover, (2.32) respects the geometry of the SDE in the sense that the solutions $X^x(\omega_i)$, $i = 1, \dots, N$, of the ODEs stay on invariant manifolds of the solution X^x to the SDE. Once again, this is a remarkable difference to the usual Euler scheme. Of course, this property is only preserved in actual computations, if the ODE-solver used to solve (2.30) respects invariant manifolds of the ODE as good as possible.

Formula (2.32) represents the one-step version of the cubature on Wiener space scheme. In the computation process, the original interval $[0,T]$ is divided into sufficiently many smaller intervals and the one-step scheme is

iteratively applied to all the smaller intervals. More precisely, fix a (possibly non-uniform) partition $0 = t_0 < t_1 < \cdots < t_M = T$ of $[0,T]$. We denote the time increments by $\Delta t_i = t_{i+1} - t_i$, $i = 0, \ldots, M-1$. Next we construct cubature paths on $[0,T]$ by concatenating cubature paths on the smaller sub-intervals: fix $(i_1, \ldots, i_M) \in \{1, \ldots, N\}^M$ and define a path $\omega_{(i_1,\ldots,i_M)} : [0,T] \to \mathbb{R}^d$ of bounded variation by setting $\omega_{(i_1,\ldots,i_M)}(t) = \omega_{i_1}^{(\Delta t_0)}(t)$ for $t \in [0, t_1]$ and, recursively,

$$\omega_{(i_1,\ldots,i_M)}(t) = \omega_{(i_1,\ldots,i_M)}(t_k) + \omega_{i_{k+1}}^{(\Delta t_k)}(t - t_k), \quad t \in]t_k, t_{k+1}],$$

$k = 1, \ldots, M-1$. We associate the weight $\lambda_{i_1} \cdots \lambda_{i_M}$ to the path $\omega_{(i_1,\ldots,i_M)}$ and approximate

$$E(f(X_T^x)) = \sum_{(i_1,\ldots,i_M)\in\{1,\ldots,N\}^M} \lambda_{i_1} \cdots \lambda_{i_M} f(X_T^x(\omega_{(i_1,\ldots,i_M)})) + CT \max_{k=0,\ldots,M-1} (\Delta t_k)^{\frac{m-1}{2}}. \tag{2.33}$$

Note that the order of the rest term is reduced from $\frac{m+1}{2}$ to $\frac{m-1}{2}$ by the iteration procedure: in each step we have an error of order $\frac{m+1}{2}$ and summing up these local errors gives a total error of order $\frac{m-1}{2}$.

Remark 2.2.19. Repeating an observation already made in Remark 2.2.13, we note that the cubature path $\omega_{(i_1,\ldots,i_M)}$ is getting rougher and rougher with higher M.

Proposition 2.2.20. *Let $f \in C_b^{m+1}(\mathbb{R}^n; \mathbb{R})$ and let the vector fields $V_0, \ldots, V_d$ be C^∞-bounded. Then (2.33) holds with a constant C which is independent of x and the partition.*

Proof. This is Lyons and Victoir [51, Theorem 10]. □

$X_T^x(\omega_{(i_1,\ldots,i_M)})$ is the solution of the following problem: start at x and follow the ODE (2.30) driven by $\omega_{i_1}^{(\Delta t_1)}$ until time t_1. Then, from time t_1 to time t_2, follow the ODE driven by $\omega_{i_2}^{(\Delta t_2)}$ and so on until time T. Once again, the task of computing a solution of the SDE (1.3) is replaced by the task of computing solutions of the corresponding ODEs (2.29), but this time we have to solve N^M ODEs. Indeed, in general there is a difference between following a path ω_i first and a different path ω_j afterwards and following ω_j first and ω_i thereafter. Obviously, the number of ODEs gets too large even for efficient ODE solvers and only moderate partition sizes M.

One way out of the exponential decrease of the numerical expense of the cubature method is by doing Monte-Carlo simulation on the tree. Note that

$$\sum_{(i_1,\ldots,i_M)\in\{1,\ldots,N\}^M} \lambda_{i_1} \cdots \lambda_{i_M} = 1,$$

therefore we can regard the right hand side of (2.33) as the expected value of a discrete random variable taking value $f(X_T^x(\omega_{(i_1,\dots,i_M)}))$ with probability $\lambda_{i_1}\cdots\lambda_{i_M}$, $(i_1,\dots,i_M)\in\{1,\dots,N\}^M$. We stress that this is completely analogous to the usual weak Euler-Maruyama scheme: precise integration of the corresponding discrete random variable is not possible, therefore one uses Monte-Carlo simulation for the integration.

A completely different approach is presented in a still unpublished work by Schmeiser, Soreff, and Teichmann [74].

Unfortunately, the smoothness conditions of Proposition 2.2.20 on the function f are unrealistically strong. Indeed, using the prime motivating example of mathematical finance, not even one of the simplest possible payoff function f, the one corresponding to the European put option, is continuously differentiable. The results of Kusuoka [43], [44] allow us to extend the method to more realistic scenarios, where the payoff function f is only assumed to be Lipschitz continuous.

Theorem 2.2.21. *Additional to the usual assumption of C^∞-boundedness, let the vector fields $V_0,\dots,V_d$ satisfy the* UFG condition*: there is $l\in\mathbb{N}$ such that*

$$\forall I\in\mathcal{A}\setminus\{\emptyset,(0)\}\,:\,V_{[I]}\in\left\langle\left\{V_{[J]}|J\in\mathcal{A}_l\setminus\{\emptyset,(0)\}\right\}\right\rangle_{C_b^\infty(\mathbb{R}^n)}, \tag{2.34}$$

where $\langle A\rangle_{C_b^\infty(\mathbb{R}^n)}$ denotes the $C_b^\infty(\mathbb{R}^n)$-module generated by the set A. Furthermore, fix a cubature formula of degree m and $\gamma>m-1$. Then there is a constant $C>0$ such that

$$E(f(X_T^x))=\sum_{(i_1,\dots,i_M)\in\{1,\dots,N\}^M}\lambda_{i_1}\cdots\lambda_{i_M}f(X_T^x(\omega_{(i_1,\dots,i_M)}))+C\frac{\|\nabla f\|_\infty}{M^{(m-1)/2}}$$

for any function f satisfying a uniform Lipschitz condition provided *that the time mesh is given by*

$$t_i=\frac{i^\gamma T}{M^\gamma},\quad i=0,\dots,M.$$

Proof. See Kusuoka [44, Theorem 4]. □

2.3 Moments of iterated integrals

In the course of our considerations of the geometry of iterated Stratonovich integrals, we have encountered the remarkable formula

$$E(Y_t^1)=\exp\Big(te_0+\frac{t}{2}\sum_{i=1}^d e_i^2\Big), \tag{2.35}$$

see Proposition 2.1.20. Recall that Y^1 is the $G^m_{d,1}$-valued process of all iterated Stratonovich integrals of Brownian motion up to degree m, in the sense of the degree deg defined in Definition 2.1.2. As we have remarked earlier, the above equation encodes the steps of iterative applications of Itô's formula to compute the first moment of iterated Stratonovich integrals. The goal of this section is to derive a similar representation for higher moments of iterated Stratonovich integrals, which can be used to calculate them in an efficient way.

In fact, we will follow two approaches: first we will derive an explicit formula, similar to the one above. Then, in Section 2.4, we will use representation theory in order to get an algorithm for computation of moments.

The theoretical background for the derivation of the explicit formula is rather simple. Given k vector spaces $W_1, \dots, W_k$, $k \in \mathbb{N}$, let us consider their tensor product $W_1 \otimes \cdots \otimes W_k$. Recall the universal property of the tensor product: Let

$$\varphi : W_1 \times \cdots \times W_k \to W_1 \otimes \cdots \otimes W_k, \quad (w_1, \dots, w_k) \mapsto w_1 \otimes \cdots \otimes w_k$$

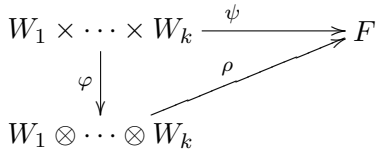
be the natural embedding of $W_1 \times \cdots \times W_k$ into the tensor product $W_1 \otimes \cdots \otimes W_k$. Furthermore, let F be a vector space and let

$$\psi : W_1 \times \cdots \times W_k \to F$$

be a k-multi-linear map. Then there is a unique linear map

$$\rho : W_1 \otimes \cdots \otimes W_k \to F$$

such that $\psi = \rho \circ \varphi$.



In our setting, we will use

$$\mathbb{A}^{m,\otimes k}_{d,1} = \mathbb{A}^m_{d,1} \otimes \cdots \otimes \mathbb{A}^m_{d,1},$$

the k-fold tensor product of $\mathbb{A}^m_{d,1}$ with itself, and $Y_t = Y^1_t \in \mathbb{A}^m_{d,1}$, the vector of iterated Stratonovich integrals as introduced in (2.14).

Lemma 2.3.1. *Given a homogenous polynomial $p : \mathbb{A}^m_{d,1} \to \mathbb{R}$ of degree k. Then we can find a linear functional $\widetilde{p} : \mathbb{A}^{m,\otimes k}_{d,1} \to \mathbb{R}$ such that*

$$p(y) = \widetilde{p}(y^{\otimes k}), \quad y \in \mathbb{A}^m_{d,1},$$

where we used the notation

$$y^{\otimes k} = \varphi(y, \dots, y) = y \otimes \cdots \otimes y \in \mathbb{A}^{m,\otimes k}_{d,1}.$$

Proof. By homogeneity of p, there are $l \in \mathbb{N}$, linear functionals $\lambda_1^j, \dots, \lambda_k^j : \mathbb{A}_{d,1}^m \to \mathbb{R}$ and real numbers a^j, $j = 1, \dots, l$, such that

$$p(y) = \sum_{j=1}^{l} a^j \lambda_1^j(y) \cdots \lambda_k^j(y)$$

for all $y \in \mathbb{A}_{d,1}^m$. We can, therefore, extend p to a k-multi-linear functional

$$\overline{p} : \mathbb{A}_{d,1}^m \times \cdots \times \mathbb{A}_{d,1}^m \to \mathbb{R},$$

e. g. by setting

$$\overline{p}(y_1, \dots, y_k) = \sum_{j=1}^{l} a^j \lambda_1^j(y_1) \cdots \lambda_k^j(y_k).$$

Obviously, $p(y) = \overline{p}(y, \dots, y)$, notice, however, that the extension is by no means unique.

The existence of $\widetilde{p}$ directly follows from the universal property of the tensor product $\mathbb{A}_{d,1}^{m,\otimes k}$ (with $F = \mathbb{R}$) now. □

By Lemma 2.3.1, an explicit formula for

$$E\big(Y_t^{\otimes k}\big) = E\big(Y_t \otimes \cdots \otimes Y_t\big)$$

corresponds to an explicit formula for the kth moments of Y_t. Therefore, Theorem 2.3.2 below is the natural generalization of equation (2.35). Before formulating the theorem, we need to define the appropriate exponential function. Let us define a multiplication on $\mathbb{A}_{d,1}^{m,\otimes k}$ by specifying

$$(y_1 \otimes \cdots \otimes y_k)\ (z_1 \otimes \cdots \otimes z_k) = (y_1 z_1) \otimes \cdots \otimes (y_k z_k) \tag{2.36}$$

for $y_1, \dots, y_k, z_1, \dots, z_k \in \mathbb{A}_{d,1}^m$ and extending it to $\mathbb{A}_{d,1}^{m,\otimes k} \times \mathbb{A}_{d,1}^{m,\otimes k}$ as a bi-linear map. We define an exponential function

$$\exp : \mathbb{A}_{d,1}^{m,\otimes k} \to \mathbb{A}_{d,1}^{m,\otimes k}$$

using the multiplication (2.36), i. e. by

$$\exp(y) = \sum_{k=0}^{\infty} \frac{y^k}{k!}, \quad y \in \mathbb{A}_{d,1}^{m,\otimes k},$$

with $y^0 = 1 \otimes \cdots \otimes 1$, the neutral element of the multiplication. Notice that the above series is, in fact, a polynomial by nil-potency of $\mathbb{A}_{d,1}^m$, provided that at least one factor of each summand of $y \in \mathbb{A}_{d,1}^{m,\otimes k}$ is of degree larger than 0.

Theorem 2.3.2. *Given the process $Y_t^1 = Y_t$ of iterated Stratonovich integrals defined in (2.14) with initial value $y = 1 \in \mathbb{A}_{d,1}^m$. Then*

$$\begin{aligned} E\big(Y_t^{\otimes k}\big) = \exp\Big(& t(e_0 \otimes 1 \otimes \cdots \otimes 1 + \cdots + 1 \otimes \cdots \otimes 1 \otimes e_0) \\ & + \frac{t}{2} \sum_{i=1}^{d} (e_i^2 \otimes 1 \otimes \cdots \otimes 1 + \cdots + 1 \otimes \cdots 1 \otimes e_i^2) \\ & + t \sum_{i=1}^{d} (e_i \otimes e_i \otimes 1 \otimes \cdots \otimes 1 + e_i \otimes 1 \otimes e_i \otimes 1 \otimes \cdots \otimes 1 + \cdots \\ & + 1 \otimes \cdots \otimes 1 \otimes e_i \otimes e_i) \Big). \end{aligned}$$

In particular, let p denote a homogenous polynomial of degree k on $\mathbb{A}_{d,1}^m$ and let $\widetilde{p}$ be the corresponding linear functional on $\mathbb{A}_{d,1}^{m,\otimes k}$. Then

$$E(p(Y_t)) = \widetilde{p}(\exp(H_t)),$$

where H_t denotes the logarithm of the right hand side in the above formula.

Proof. We use the same strategy as in the proof of Proposition 2.1.20. First we compute the SDE solved by $Y_t^{\otimes k}$. By multi-linearity of the tensor product, i. e. of the map φ, we have

$$\begin{aligned} dY_t^{\otimes k} = & \Big(Y_t \sum_{i=0}^{d} e_i \circ dB_t^i \Big) \otimes Y_t \otimes \cdots \otimes Y_t \\ & + Y_t \otimes \Big(Y_t \sum_{i=0}^{d} e_i \circ dB_t^i \Big) \otimes \cdots \otimes Y_t + \cdots \\ & + Y_t \otimes Y_t \otimes \cdots \otimes \Big(Y_t \sum_{i=0}^{d} e_i \circ dB_t^i \Big) \\ = & \sum_{i=0}^{d} \Big(\big(Y_t e_i\big) \otimes Y_t \otimes \cdots \otimes Y_t \\ & + Y_t \otimes \big(Y_t e_i\big) \otimes \cdots \otimes Y_t + \cdots \\ & + Y_t \otimes Y_t \otimes \cdots \otimes \big(Y_t e_i\big) \Big) \circ dB_t^i. \end{aligned}$$

Define linear vector fields $D_i^{\otimes k} : \mathbb{A}_{d,1}^{m,\otimes k} \to \mathbb{A}_{d,1}^{m,\otimes k}$ by

$$\begin{aligned} D_i^{\otimes k}(y_1 \otimes \cdots \otimes y_k) = & (y_1 e_i) \otimes y_2 \otimes \cdots \otimes y_k \\ & + y_1 \otimes (y_2 e_i) \otimes \cdots \otimes y_k + \cdots \\ & + y_1 \otimes y_2 \otimes \cdots \otimes (y_k e_i), \end{aligned}$$

$i = 0, \dots, d$, then we have

$$dY_t^{\otimes k} = \sum_{i=0}^{d} D_i^{\otimes k}\big(Y_t^{\otimes k}\big) \circ dB_t^i, \tag{2.37}$$

corresponding to equation (2.15) for Y_t. Indeed, notice that $D_i^{\otimes k}$ is the push-forward of the vector field D_i under the map

$$y \mapsto y^{\otimes k},$$

$i = 0, \dots, d$.

Let $L^{\otimes k}$ denote the infinitesimal generator of the Markov process $Y_t^{\otimes k}$, i. e.

$$L^{\otimes k} = D_0^{\otimes k} + \frac{1}{2}\sum_{i=1}^{d}\big(D_i^{\otimes k}\big)^2.$$

Fix a linear functional $\widetilde{p} : \mathbb{A}_{d,1}^{m,\otimes k} \to \mathbb{R}$. In order to emulate the proof of Proposition 2.1.20, we need to compute $L^{\otimes k}\widetilde{p}(y^{\otimes k})$, $y \in \mathbb{A}_{d,1}^{m,\otimes k}$. Note that $D_i^{\otimes k}\widetilde{p}$ is the linear functional defined by

$$\begin{aligned} D_i^{\otimes k}\widetilde{p}(y_1 \otimes \cdots \otimes y_k) &= \frac{\partial}{\partial \epsilon}\bigg|_{\epsilon=0} \widetilde{p}\big(y_1 \otimes \cdots \otimes y_k + \epsilon D_i^{\otimes k}(y_1 \otimes \cdots \otimes y_k)\big) \\ &= \widetilde{p}\big(D_i^{\otimes k}(y_1 \otimes \cdots \otimes y_k)\big), \end{aligned}$$

$i = 0, \dots, d$, $y_1, \dots, y_k \in \mathbb{A}_{d,1}^m$. Moreover, $\big(D_i^{\otimes k}\big)^2\widetilde{p}$ is the linear functional on $\mathbb{A}_{d,1}^{m,\otimes k}$ defined by

$$\big(D_i^{\otimes k}\big)^2\widetilde{p}(y_1 \otimes \cdots \otimes y_k) = \widetilde{p}\big(\big(D_i^{\otimes k}\big)^2(y_1 \otimes \cdots \otimes y_k)\big),$$

again for $i = 0, \dots, d$ and $y_1, \dots, y_k \in \mathbb{A}_{d,1}^m$. In order to obtain a concise notation, let us introduce

$$\begin{aligned} \kappa(r; y) &= 1 \otimes \cdots \otimes \underbrace{y}_{r} \otimes \cdots \otimes 1, \\ \kappa(r, r; y) &= 1 \otimes \cdots \otimes \underbrace{y^2}_{r} \otimes \cdots \otimes 1, \\ \kappa(r, s; y) &= 1 \otimes \cdots \otimes \underbrace{y}_{r} \otimes \cdots \otimes \underbrace{y}_{s} \otimes \cdots \otimes 1, \end{aligned}$$

for $y \in \mathbb{A}_{d,1}^m$ and $r \in \{1, \dots, k\}$, $s \in \{1, \dots, k\}$ with $r < s$ in case both r and s appear in the formula. Then

$$D_i^{\otimes k}(y_1 \otimes \cdots \otimes y_k) = y_1 \otimes \cdots \otimes y_k \ \Big(\sum_{r=1}^{k} \kappa(r; e_i)\Big),$$

with the multiplication defined in (2.36), and

$$\big(D_i^{\otimes k}\big)^2(y_1\otimes\cdots\otimes y_k) = y_1\otimes\cdots\otimes y_k\,\Big(\sum_{r=1}^{k}\kappa(r,r;e_i)+2\sum_{r<s\in\{1,\dots,k\}}\kappa(r,s;e_i)\Big),$$

$i=0,\dots,d$.

Let, for $z\in\mathbb{A}_{d,1}^{m,\otimes k}$,

$$u(t,z)=E\big(\widetilde{p}\big(zY_t^{\otimes k}\big)\big)=\widetilde{p}\big(E\big(zY_t^{\otimes k}\big)\big).$$

u solves the heat equation

$$\begin{cases}\dfrac{\partial}{\partial t}u(t,z)=L^{\otimes k}u(t,z),\\ \quad u(0,z)=\widetilde{p}(z).\end{cases}\tag{2.38}$$

Now let

$$v(t,z)=\widetilde{p}\bigg(z\exp\bigg(t\sum_{r=1}^{k}\kappa(r;e_0)+\frac{t}{2}\sum_{i=1}^{d}\sum_{r=1}^{k}\kappa(r,r;e_i)+t\sum_{i=1}^{d}\sum_{r<s\in\{1,\dots,k\}}\kappa(r,s;e_i)\bigg)\bigg).$$

We claim that v solves (2.38), too, which implies the theorem by uniqueness of the solution of the Kolmogorov backward equation. Indeed, $v(0,z)=\widetilde{p}(z)$

and

$$\begin{aligned}
\frac{\partial}{\partial t}v(t,z) &= \widetilde{p}\Big(z\frac{\partial}{\partial t}\exp\Big(t\sum_{r=1}^{k}\kappa(r;e_0)+\frac{t}{2}\sum_{i=1}^{d}\sum_{r=1}^{k}\kappa(r,r;e_i)\\
&\qquad +t\sum_{i=1}^{d}\sum_{r<s\in\{1,\dots,k\}}\kappa(r,s;e_i)\Big)\Big)\\
&= \widetilde{p}\Big(z\exp\Big(t\sum_{r=1}^{k}\kappa(r;e_0)+\frac{t}{2}\sum_{i=1}^{d}\sum_{r=1}^{k}\kappa(r,r;e_i)\\
&\qquad +t\sum_{i=1}^{d}\sum_{r<s\in\{1,\dots,k\}}\kappa(r,s;e_i)\Big)\cdot\\
&\qquad \cdot\Big(\sum_{r=1}^{k}\kappa(r;e_0)+\frac{1}{2}\sum_{i=1}^{d}\sum_{r=1}^{k}\kappa(r,r;e_i)+\sum_{i=1}^{d}\sum_{r<s\in\{1,\dots,k\}}\kappa(r,s;e_i)\Big)\Big)\\
&= L^{\otimes k}\widetilde{p}\Big(z\exp\Big(t\sum_{r=1}^{k}\kappa(r;e_0)+\frac{t}{2}\sum_{i=1}^{d}\sum_{r=1}^{k}\kappa(r,r;e_i)\\
&\qquad +t\sum_{i=1}^{d}\sum_{r<s\in\{1,\dots,k\}}\kappa(r,s;e_i)\Big)\Big)\\
&= L^{\otimes k}v(t,z).
\end{aligned}$$

□

Remark 2.3.3. Notice that we have never used nil-potency of $\mathbb{A}_{d,1}^m$ in the proof of Theorem 2.3.2. Therefore, the theorem also holds true in the non-truncated situation, if the exponential is understood as a formal series, giving us *all* moments of *all* iterated Stratonovich integrals of Brownian motion.

Remark 2.3.4. Similar results hold for all Lévy processes on the group $G_{d,1}^m$.

Example 2.3.5. In order to calculate the second moments of Y_t, we need to compute $E(Y_t \otimes Y_t)$. Theorem 2.3.2 for $k = 2$ gives

$$\begin{aligned}
&E(Y_t\otimes Y_t) =\\
&\qquad \exp\Big(t(e_0\otimes 1+1\otimes e_0)+\frac{t}{2}\sum_{i=1}^{d}(e_i^2\otimes 1+1\otimes e_i^2)+t\sum_{i=1}^{d}e_i\otimes e_i\Big).
\end{aligned}$$

2.4 Calculation of moments of Z_t

The aim of this section is to construct a method to compute moments of the Stratonovich areas of B, i. e. of the process $Z_t = \log(Y_t^1)$ introduced in (2.16). The areas are important in numerical analysis of SDEs as well as in the theory of SDEs. In the former field, they are related to higher

order (weak and strong) methods for discretization of SDEs like the Milstein scheme, see Kloeden and Platen [42]. On the other hand, the rough paths theory of T. Lyons [52] has shown that Itô-Stratonovich areas lie at the heart of the theory of stochastic differential equations.

Of course, we could simply apply the Chen-Strichartz formula, see Proposition 2.1.17, to the explicit formula for the moments of Y_t^1 given in Theorem 2.3.2. Recall, however, that we cannot directly read out the moments of Z_t from the Chen-Strichartz formula since it does not give us an expansion of $\log(E(Y_t^1)$ in terms of a basis of $\mathfrak{g}_{d,1}^m$. Therefore, Theorem 2.3.2 in connection with Proposition 2.1.17 does not give us an explicit formula for the moments of Z_t, since we will have to perform a basis expansion first.

The second method, which we will present in the remainder of this section, does neither rely on the explicit formula for the moments of Y_t^1 given in Theorem 2.3.2 nor on the Chen-Strichartz formula. Instead, it uses representation theory, as sketched in (2.39).

(2.39)
$$\begin{array}{ccccc} \mathfrak{g}_{d,1}^m & & \xrightarrow{\rho\ (=\mathrm{id})} & & \mathfrak{h} = \mathfrak{g}_{d,1}^m \\ \Big\downarrow{\scriptstyle \exp} & & & & \Big\downarrow{\scriptstyle \exp_H} \qquad \Big\downarrow{\scriptstyle \exp_{\tilde{m}}} \\ \mathbb{A}_{d,1}^m \supset G_{d,1}^m & & \xrightarrow[R\ (=\mathrm{id})]{} & & H = \mathbb{A}_{d,1}^{m,\tilde{m}} \end{array}$$

R denotes a representation of the algebra $\mathbb{A}_{d,1}^m$ and ρ denotes the corresponding representation of $\mathfrak{g}_{d,1}^m$. More precisely, we will choose the spaces H and $\mathfrak{h}$ so that we may identify $\mathfrak{g}_{d,1}^m$ with $\mathfrak{h}$ such that H, however, covers objects of higher degree than $\mathbb{A}_{d,1}^m$. In fact, H will be chosen to be an appropriate factor algebra of $\mathbb{A}_{d,1}^{\tilde{m}}$ for some $\tilde{m} > m$ large enough. We will construct the moments of Z_t by combining two formulas: the first formula expresses $R(Y_t^1)$ in terms of Z_t, the second formula gives an expression of $E(R(Y_t^1))$ in terms of $\exp_H$. Both together will give an algorithm allowing the computation of moments of Z_t.

2.4.1 Algebra of iterated integrals

We need to go back to the algebraic setting of free nilpotent algebras, Lie algebras and Lie groups, see Subsection 2.1.2. Now we focus more on the algebraic properties of that framework, not on the geometric ones as before.

Recall the free step-m nilpotent Lie algebra $\mathfrak{g}_{d,1}^m$ generated by d generators $\{e_1, \dots, e_d\}$ of degree 1 and one generator e_0 of degree 2. We have remarked earlier that the linear generators in (2.11) do not form a basis of $\mathfrak{g}_{d,1}^m$. Now we want to perform calculations in $\mathfrak{g}_{d,1}^m$, therefore we cannot ignore this issue any more and need to specify a basis, namely the *Hall basis*, see Reutenauer [67].

We consider letters corresponding to the generators of $\mathfrak{g}_{d,1}^m$ and denote the *alphabet* by A, i. e.

$$A = \{e_0, e_1, \dots, e_d\}\,.$$

By a *word* we understand a monomial in the letters. On the set A^* of all words in A we define a product $*$ by concatenation, i. e.

$$(e_{i_1} \cdots e_{i_k}) * (e_{j_1} \cdots e_{j_r}) = e_{i_1} \cdots e_{i_k} e_{j_1} \cdots e_{j_r}.$$

Usually we will omit the symbol $*$ in the notation. Note that the set A^* of all words equipped with the concatenation product forms the *free monoid* generated by the letters $e_0, \ldots, e_d$ with the empty word as neutral element, see Remark 2.1.7. We specify a total order $<$ on the letters, e. g. $e_0 < e_1 < \cdots < e_d$, and follow the construction of the ordered set $(H, <)$, $H \subset A^*$, of *Hall words* as presented by Reutenauer [67]. Note the Hall set $(H, <)$ is not uniquely determined and that the definition of Hall sets is not canonical, i. e. other authors sometimes use other but essentially equivalent concepts under this name. Instead of giving a formal definition, we give the following constructive description of Hall words.

Lemma 2.4.1 (Properties of Hall words)**.** *(i) Each letter is a Hall word and each Hall word $h \in H$, which is not a letter, admits a* standard factorization *$h = h'h''$, $h', h'' \in H$ with $h' < h''$ and $h < h''$.*
(ii) Given two Hall words $h < k \in H$, hk is a Hall word with standard factorization hk, if and only if h is a letter or $h'' \geq k$, where $h = h'h''$ is the standard factorization of h.
(iii) Each word has a unique decreasing factorization into Hall words, i. e. given $w \in A^*$ there is a unique $k \in \mathbb{N}$ and there are unique $h_1 \geq h_2 \geq \cdots \geq h_k \in H$ such that $w = h_1 * \cdots * h_k = h_1 \cdots h_k$.

Proof. See Reutenauer [67], Corollary 4.7 and the paragraph below it. □

Definition 2.4.2. The *Hall polynomial* P_h corresponding to the Hall word $h \in H$ is defined recursively by

$$P_h = \begin{cases} h, & h \in A, \text{ i. e. } h = e_i \text{ for some } i \in \{0, \ldots, d\}, \\ [P_{h'}, P_{h''}], & \text{h has standard factorization } h = h'h''. \end{cases}$$

Note that there are only finitely many Hall polynomials $P_h \in \mathfrak{g}_{d,1}^m$ due to nil-potency in $\mathfrak{g}_{d,1}^m$.

Let $|w|$ denote the length of the word $w \in A^*$. For a letter $a \in A$ define the *partial length* of w with respect to a as the number of times a occurs in w. The partial length is denoted by $|w|_a$. A polynomial $\sum_{i=1}^n \lambda_i w_i$, $w_i \in A^*$, $\lambda_i \in \mathbb{R} \setminus \{0\}$, $i = 1, \ldots, n$, is called *finely homogeneous* if

$$\forall a \in \{e_0, \ldots, e_d\} : \ |w_1|_a = |w_2|_a = \cdots = |w_n|_a \,. \tag{2.40}$$

Fine homogeneity implies homogeneity of the polynomial with respect to the length $|\cdot|$ as well as with respect to the degree deg.

Lemma 2.4.3. *The set of all Hall polynomials forms a basis of the Lie algebra $\mathfrak{g}_{d,1}^m$. More precisely,*

$$P_H = \{P_h \mid h \in H,\ \deg(h) \leq m\}$$

is a basis of $\mathfrak{g}_{d,1}^m$ called Hall basis. *All Hall polynomials are finely homogenous.*

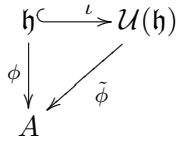
Proof. See Reutenauer [67, Theorem 4.9 (i)]. Fine homogeneity is given by construction, since taking Lie brackets does not destroy this property. □

We define an order on P_H by simply letting $P_h < P_k$ if $h < k$, $h, k \in H$. Let $N = \#P_H = \dim_{\mathbb{R}} \mathfrak{g}_{d,1}^m$ and write

$$P_H = \{f_1, \ldots, f_N\}, \quad f_1 < f_2 < \cdots < f_N. \tag{2.41}$$

The expectation formula (2.35) only covers the first moment. Of course, it also contains higher moments of iterated integrals of low degree. Nevertheless, in order to get information about higher moments of iterated integrals of high degree, this is not sufficient and we will have to embed $\mathfrak{g}_{d,1}^m$ into enveloping structures of higher degree. More precisely, we consider representations of $\mathfrak{g}_{d,1}^m$, where polynomials of higher order than m exist (in the sense that they are non-trivial).

Definition 2.4.4. Given a Lie algebra $\mathfrak{h}$, the *universal enveloping algebra* $\iota : \mathfrak{h} \to \mathcal{U}(\mathfrak{h})$ is an algebra[1] $\mathcal{U}(\mathfrak{h})$ together with a homomorphism ι of Lie algebras such that the universal property holds: for any algebra C and any Lie algebra homomorphism $\phi : \mathfrak{h} \to C$ there is a unique homomorphism $\tilde{\phi} : \mathcal{U}(\mathfrak{h}) \to C$ of algebras such that the following diagram commutes:



ι is injective by the Poincaré-Birkhoff-Witt theorem below.

Proposition 2.4.5 (Poincaré-Birkhoff-Witt theorem)**.** *Given an ordered basis $\{ f_i \mid i \in \mathbb{I} \}$ of the Lie algebra $\mathfrak{h}$, then*

$$\left\{ \iota(f_{i_1}) \cdots \iota(f_{i_k}) \;\middle|\; k \in \mathbb{N},\ (i_1, \ldots, i_k) \in \mathbb{I}^k,\ i_1 \geq i_2 \geq \cdots \geq i_k \right\}$$

gives a basis of the universal enveloping algebra $\mathcal{U}(\mathfrak{h})$.

Proof. See Serre [75, Theorem III.4.3 and Lemma III.4.5]. □

[1] Recall Remark 2.1.5.

Let $\iota : \mathfrak{g}_{d,1}^m \to \mathcal{U}(\mathfrak{g}_{d,1}^m)$ be the universal enveloping algebra of the free nilpotent Lie algebra $\mathfrak{g}_{d,1}^m$. By the above comment, ι is injective, therefore we may identify $\mathfrak{g}_{d,1}^m$ with $\iota(\mathfrak{g}_{d,1}^m) \subset \mathcal{U}(\mathfrak{g}_{d,1}^m)$. Consequently, given an element $f_i \in P_H$ of the Hall basis of $\mathfrak{g}_{d,1}^m$, f_i will also denote the corresponding element $\iota(f_i) \in \mathcal{U}(\mathfrak{g}_{d,1}^m)$, $i = 1, \dots, N$.

Lemma 2.4.6. *Given two Lie algebras with their respective universal enveloping algebras $\iota : \mathfrak{g} \hookrightarrow \mathcal{U}(\mathfrak{g})$ and $\varepsilon : \mathfrak{h} \hookrightarrow \mathcal{U}(\mathfrak{h})$ and a surjective homomorphism of Lie algebras $\pi : \mathfrak{g} \to \mathfrak{h}$. Define $\tilde{\pi} : \mathcal{U}(\mathfrak{g}) \to \mathcal{U}(\mathfrak{h})$ by $\tilde{\pi} \circ \iota = \varepsilon \circ \pi$.*

$$\begin{array}{ccc} \mathfrak{g} & \xrightarrow{\pi} & \mathfrak{h} \\ {\scriptstyle\iota}\downarrow & & \downarrow{\scriptstyle\varepsilon} \\ \mathcal{U}(\mathfrak{g}) & \xrightarrow{\tilde{\pi}} & \mathcal{U}(\mathfrak{h}) \end{array}$$

Then $\ker(\tilde{\pi}) \cap \mathfrak{g} = \ker(\pi)$, $\ker(\tilde{\pi}) = \langle \ker(\pi) \rangle$, *the ideal in* $\mathcal{U}(\mathfrak{g})$ *generated by* $\ker(\pi)$, *and*

$$\mathcal{U}(\mathfrak{h}) = \mathcal{U}(\mathfrak{g}) / \ker(\tilde{\pi}).$$

Proof. By the universal property of the enveloping algebra with $A = \mathcal{U}(\mathfrak{h})$ and $\phi = \varepsilon \circ \pi$, $\tilde{\pi}$ is a uniquely defined algebra homomorphism.

Choose a basis $\{ f_i \mid i \in \mathbb{I} \}$ of $\mathfrak{g}$, $\mathbb{I}$ being a totally ordered set, such that there is an $\mathbb{I}' \subset \mathbb{I}$ with the properties that $\{ \pi(f_i) \mid i \in \mathbb{I}' \}$ is a basis of $\mathfrak{h}$ and $\pi(f_i) = 0$ for $i \in \mathbb{I} \setminus \mathbb{I}'$. Then the products $\pi(f_{i_1}) \cdots \pi(f_{i_k}) = \tilde{\pi}(f_{i_1} \cdots f_{i_k})$, $i_1 \geq \cdots \geq i_k \in \mathbb{I}'$, form a basis of $\mathcal{U}(\mathfrak{h})$, implying surjectivity of $\tilde{\pi}$. Consequently, $\mathcal{U}(\mathfrak{h}) = \mathcal{U}(\mathfrak{g}) / \ker(\tilde{\pi})$. The equations for the kernels of π and $\tilde{\pi}$ follow immediately. Indeed,

$$\ker \pi = \left\langle \{ f_i \mid i \in \mathbb{I} \setminus \mathbb{I}' \} \right\rangle_{\mathbb{R}},$$
$$\ker \tilde{\pi} = \left\langle \left\{ f_{i_1} \cdots f_{i_k} \;\middle|\; k \in \mathbb{N},\ (i_1, \dots, i_k) \in \mathbb{I}^k,\ \exists\, 1 \leq l \leq k : i_l \in \mathbb{I} \setminus \mathbb{I}' \right\} \right\rangle_{\mathbb{R}}. \square$$

Lemma 2.4.6 gives an explicit representation of $\mathcal{U}(\mathfrak{g}_{d,1}^m)$ in terms of the universal enveloping algebra of $\mathfrak{g}_{d,1}$, the free Lie algebra generated by A. Let $\mathbb{A}_{d,1}$ be the free algebra[2] generated by A. By the universal property of the free algebra, $\mathbb{A}_{d,1}$ is a universal enveloping algebra of $\mathfrak{g}_{d,1}$ and we extend the definition of the degree function to $\mathbb{A}_{d,1}$, as well as the grading. That is, analogously to (2.6) and the corresponding decomposition of $\mathfrak{g}_{d,1}^m$,

$$\mathbb{A}_{d,1} = \bigoplus_{n=0}^{\infty} W_n,$$
$$\mathfrak{g}_{d,1} = \bigoplus_{n=0}^{\infty} U_n.$$

[2] Once again, recall Remark 2.1.5.

Note that it is not necessary to introduce different notations for $W_n \subset \mathbb{A}_{d,1}^m$ and $W_n \subset \mathbb{A}_{d,1}$ since both spaces W_n are isomorphic as long as $m \geq n$. The same is true for U_n.

Corollary 2.4.7. *Let $\tilde{\pi} : \mathcal{U}(\mathfrak{g}_{d,1}) \to \mathcal{U}(\mathfrak{g}_{d,1}^m)$ be the extension as in Lemma 2.4.6 of the canonical projection $\pi : \mathfrak{g}_{d,1} \to \mathfrak{g}_{d,1}^m$. Then*

$$\mathcal{U}(\mathfrak{g}_{d,1}^m) = \mathcal{U}(\mathfrak{g}_{d,1}) / \ker(\tilde{\pi})$$

and $\ker(\tilde{\pi}) = \big\langle \bigoplus_{k>m} U_k \big\rangle_{\mathcal{U}(\mathfrak{g}_{d,1})}$, the $\mathcal{U}(\mathfrak{g}_{d,1})$-ideal generated by the Lie polynomials of degree greater than m.

Proof. The corollary follows by Lemma 2.4.6 noting that $\ker \pi = \bigoplus_{k>m} U_k$. □

For $\tilde{m} \geq m$ consider the ideal $J_{m,\tilde{m}} = \big\langle \bigoplus_{n=m+1}^{\tilde{m}} U_n \big\rangle_{\mathbb{A}_{d,1}^{\tilde{m}}}$ generated by all Lie monomials of degree higher than m in the algebra $\mathbb{A}_{d,1}^{\tilde{m}}$. $J_{m,\tilde{m}}$ is isomorphic to $\big\langle \mathfrak{g}_{d,1}^{\tilde{m}} / \mathfrak{g}_{d,1}^m \big\rangle$ again in $\mathbb{A}_{d,1}^{\tilde{m}}$. Define

$$\mathbb{A}_{d,1}^{m,\tilde{m}} = \mathbb{A}_{d,1}^{\tilde{m}} / J_{m,\tilde{m}}. \tag{2.42}$$

Note that $\mathfrak{g}_{d,1}^{\tilde{m}}$ understood as subset of $\mathbb{A}_{d,1}^{\tilde{m}}$ is reduced to $\mathfrak{g}_{d,1}^m$ by factoring with respect to $J_{m,\tilde{m}}$. For $m \leq \mu \leq \nu$ define a projection $\mathrm{pr}_{\nu,\mu} : \mathbb{A}_{d,1}^{m,\nu} \to \mathbb{A}_{d,1}^{m,\mu}$ by cutting off all components of degree larger than μ. More precisely, let $x \in \mathbb{A}_{d,1}^{\nu}$ be a representative of the class $[x]_{m,\nu} = x + J_{m,\nu} \in \mathbb{A}_{d,1}^{m,\nu}$ and let

$$\Pi_{\nu,\mu} : \mathbb{A}_{d,1}^{\nu} = \bigoplus_{i=0}^{\nu} W_i \to \mathbb{A}_{d,1}^{\mu} = \bigoplus_{i=0}^{\mu} W_i \tag{2.43}$$

be the projection cutting off all terms of higher order than μ. Then we define

$$\mathrm{pr}_{\nu,\mu}\big([x]_{m,\nu}\big) = \big[\Pi_{\nu,\mu} x\big]_{m,\mu} \in \mathbb{A}_{d,1}^{m,\mu}. \tag{2.44}$$

$\mathrm{pr}_{\nu,\mu}$ is a well-defined algebra homomorphism, since $\Pi_{\nu,\mu}(J_{m,\nu}) \subset J_{m,\mu}$ and $\Pi_{\nu,\mu}$ is an algebra homomorphism. The family of projections $\mathrm{pr}_{\nu,\mu}$, $\nu \geq \mu \geq m$, is compatible in the sense that

$$\mathrm{pr}_{\mu,\kappa} \circ \mathrm{pr}_{\nu,\mu} = \mathrm{pr}_{\nu,\kappa}, \quad m \leq \kappa \leq \mu \leq \nu.$$

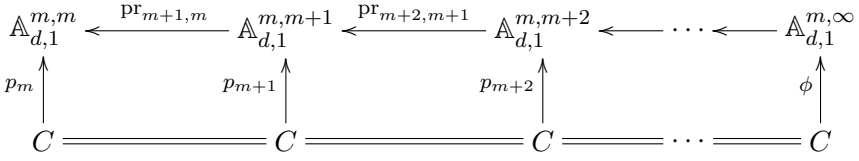
Thus, we can define the projective limit

$$\mathbb{A}_{d,1}^{m,\infty} = \operatorname*{proj\,lim}_{\tilde{m}\to\infty} \mathbb{A}_{d,1}^{m,\tilde{m}} \tag{2.45}$$

with the projections $\mathrm{pr}_{\tilde{m}} : \mathbb{A}_{d,1}^{m,\infty} \to \mathbb{A}_{d,1}^{m,\tilde{m}}$, $m \leq \tilde{m} < \infty$.

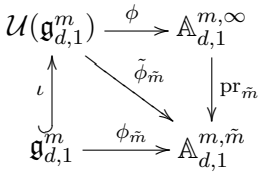
Lemma 2.4.8. *The universal enveloping algebra $\mathcal{U}(\mathfrak{g}_{d,1}^m)$ can be embedded into the algebra $\mathbb{A}_{d,1}^{m,\infty}$.*

Proof. Recall the universal property of the projective limit: for any algebra C and any family of algebra homomorphisms $p_{\tilde{m}} : C \to \mathbb{A}_{d,1}^{m,\tilde{m}}$ such that $p_\mu = \mathrm{pr}_{\nu,\mu} \circ p_\nu$ for $m \le \mu \le \nu$, there is a uniquely determined homomorphism of algebras $\phi : C \to \mathbb{A}_{d,1}^{m,\infty}$ such that $p_{\tilde{m}} = \mathrm{pr}_{\tilde{m}} \circ \phi$ for $m \le \tilde{m} < \infty$.



By the universal property of the universal enveloping algebra, see Definition 2.4.4, for any $\tilde{m} \ge m$ there is a uniquely determined $\tilde{\phi}_{\tilde{m}} : \mathcal{U}(\mathfrak{g}_{d,1}^m) \to \mathbb{A}_{d,1}^{m,\tilde{m}}$ with $\phi_{\tilde{m}} = \tilde{\phi}_{\tilde{m}} \circ \iota$, where $\phi_{\tilde{m}}$ denotes the embedding of $\mathfrak{g}_{d,1}^m$ in $\mathbb{A}_{d,1}^{m,\tilde{m}}$. Obviously, the family $\phi_{\tilde{m}}$ satisfies the compatibility condition. By the defining equation of $\tilde{\phi}_{\tilde{m}}$, compatibility extends to the family $\tilde{\phi}_{\tilde{m}}$, $\tilde{m} \ge m$. The universal property of the projective limit then yields the existence of an algebra homomorphism $\phi : \mathcal{U}(\mathfrak{g}_{d,1}^m) \to \mathbb{A}_{d,1}^{m,\infty}$ fulfilling $\tilde{\phi}_{\tilde{m}} = \mathrm{pr}_{\tilde{m}} \circ \phi$. This construction is visualized in (2.46).

(2.46)



We need to show injectivity of ϕ, i. e. that $\ker(\phi) = \{0\} \subset \mathcal{U}(\mathfrak{g}_{d,1}^m)$. An element $y \in \mathbb{A}_{d,1}^{m,\infty}$ is equal to 0, if and only if all its projections $\mathrm{pr}_{\tilde{m}}(y) = 0 \in \mathbb{A}_{d,1}^{m,\tilde{m}}$, see Lang [45]. We claim that for any fixed $x \in \mathcal{U}(\mathfrak{g}_{d,1}^m) \setminus \{0\}$ and all $\tilde{m}$ large enough, we have $\mathrm{pr}_{\tilde{m}}(\phi(x)) = \tilde{\phi}_{\tilde{m}}(x) \neq 0 \in \mathbb{A}_{d,1}^{m,\tilde{m}}$.

Fix a basis $\{ f_i \mid i \in \mathbb{I} \}$ of $\mathfrak{g}_{d,1}^m$ indexed by a totally ordered set $\mathbb{I}$. We may assume that all the Lie polynomials f_i, $i \in \mathbb{I}$, are sums of monomials of the same degree $\deg(f_i)$, e. g. by choosing the Hall basis P_H. Fix $\tilde{m} > m$ and consider

$$\langle \deg > \tilde{m} \rangle = \langle \{ f_{i_1} \cdots f_{i_k} \mid k \in \mathbb{N},\ i_1 \ge \cdots \ge i_k \in \mathbb{I},\ \deg(f_{i_1}) + \cdots + \deg(f_{i_k}) > \tilde{m} \} \rangle_{\mathbb{R}}$$

Actually, this subspace of $\mathcal{U}(\mathfrak{g}_{d,1}^m)$ is an ideal. By nil-potency of $\mathbb{A}_{d,1}^{\tilde{m}}$, we get that $\langle \deg > \tilde{m} \rangle \subset \ker(\tilde{\phi}_{\tilde{m}})$. Thus, we may regard $\tilde{\phi}_{\tilde{m}}$ as a homomorphism of algebras $\tilde{\phi}_{\tilde{m}} : \mathcal{U}(\mathfrak{g}_{d,1}^m) / \langle \deg > \tilde{m} \rangle \to \mathbb{A}_{d,1}^{m,\tilde{m}}$.

We show that this homomorphism is an isomorphism by constructing its inverse. Let ψ denote the embedding of the set of generators $A = \{e_0, e_1, \dots, e_d\}$ into $\mathfrak{g}_{d,1}^m \hookrightarrow \mathcal{U}(\mathfrak{g}_{d,1}^m)/\langle \deg > \tilde{m}\rangle$. Since $\mathbb{A}_{d,1}^{\tilde{m}}$ is free over A, the universal property of the free algebra implies the existence of a uniquely determined homomorphism of step $\tilde{m}$-nilpotent algebras $\tilde{\psi} : \mathbb{A}_{d,1}^{\tilde{m}} \to \mathcal{U}(\mathfrak{g}_{d,1}^m)/\langle \deg > \tilde{m}\rangle$ extending ψ.

$$\begin{array}{ccc} A & \xrightarrow{\psi} & \mathfrak{g}_{d,1}^m \\ \downarrow & & \downarrow \iota \\ \mathbb{A}_{d,1}^{\tilde{m}} & \xrightarrow[\tilde{\psi}]{} & \mathcal{U}(\mathfrak{g}_{d,1}^m)/\langle \deg > \tilde{m}\rangle \end{array}$$

$J_{m,\tilde{m}} \subset \ker(\tilde{\psi})$, since $\mathcal{U}(\mathfrak{g}_{d,1}^m)$ is isomorphic to the free algebra with generators $e_0, \dots, e_d$, where the ideal generated by the Lie polynomials of degree greater than m is factored out, see Corollary 2.4.7. By this factorization, $J_{m,\tilde{m}}$ understood as a subset of the free algebra is mapped to $0 \in \mathcal{U}(\mathfrak{g}_{d,1}^m)$. Thus, $\tilde{\psi}$ can be extended to a homomorphism of algebras from $\mathbb{A}_{d,1}^{m,\tilde{m}}$ to $\mathcal{U}(\mathfrak{g}_{d,1}^m)/\langle \deg > \tilde{m}\rangle$. The composition $\tilde{\phi}_{\tilde{m}} \circ \tilde{\psi} : \mathbb{A}_{d,1}^{m,\tilde{m}} \to \mathbb{A}_{d,1}^{m,\tilde{m}}$ is a homomorphism of algebras. $\psi(e_i) = e_i$ implies that

$$\tilde{\psi}\big([e_i]_{m,\tilde{m}}\big) = [e_i]_{\langle \deg > \tilde{m}\rangle},$$

where $[e_i]_{\langle \deg > \tilde{m}\rangle} = e_i + \langle \deg > \tilde{m}\rangle$ with $e_i \in \mathcal{U}(\mathfrak{g}_{d,1}^m)$. Consequently, since $\phi_{\tilde{m}}(e_i) = [e_i]_{m,\tilde{m}}$, we get

$$\tilde{\phi}_{\tilde{m}}\big(\tilde{\psi}\big([e_i]_{m,\tilde{m}}\big)\big) = \tilde{\phi}_{\tilde{m}}\big([e_i]_{\langle \deg > \tilde{m}\rangle}\big) = [e_i]_{m,\tilde{m}}$$

for each $i = 0, \dots, d$. Analogously, we get for the elements of the Poincaré-Birkhoff-Witt basis

$$\tilde{\psi} \circ \tilde{\phi}_{\tilde{m}}\big([f_i]_{\langle \deg > \tilde{m}\rangle}\big) = \tilde{\psi}([f_i]_{m,\tilde{m}}) = [f_i]_{\langle \deg > \tilde{m}\rangle}.$$

Since these elements generate the algebras $\mathbb{A}_{d,1}^{m,\tilde{m}}$ and $\mathcal{U}(\mathfrak{g}_{d,1}^m)/\langle \deg > \tilde{m}\rangle$, respectively, we can conclude that

$$\tilde{\phi}_{\tilde{m}} \circ \tilde{\psi} = \mathrm{id}_{\mathbb{A}_{d,1}^{m,\tilde{m}}}, \quad \tilde{\psi} \circ \tilde{\phi}_{\tilde{m}} = \mathrm{id}_{\mathcal{U}(\mathfrak{g}_{d,1}^m)/\langle \deg > \tilde{m}\rangle},$$

showing that both $\tilde{\phi}_{\tilde{m}}$ and $\tilde{\psi}$ are bijective and the inverses of each other.

Now for some element $f_{i_1} \cdots f_{i_k}$ of the Poincaré-Birkhoff-Witt basis of the universal enveloping algebra, let $\tilde{m} = \deg(f_{i_1}) + \cdots + \deg(f_{i_k})$. Then $f_{i_1} \cdots f_{i_k} \neq 0 \in \mathcal{U}(\mathfrak{g}_{d,1}^m)/\langle \deg > \tilde{m}\rangle$ and thus by bijectivity,

$$\tilde{\phi}_{\tilde{m}}\big(f_{i_1} \cdots f_{i_k}\big) \neq 0 \in \mathbb{A}_{d,1}^{m,\tilde{m}},$$

which shows that

$$\phi\big(f_{i_1} \cdots f_{i_k}\big) \neq 0 \in \mathbb{A}_{d,1}^{m,\infty}. \qquad \square$$

Using (2.41), the above proof implies that

$$\{\, [f_{i_1}]_{m,\tilde{m}} \cdots [f_{i_k}]_{m,\tilde{m}} \mid k \in \mathbb{N},\ N \geq i_1 \geq \ldots \geq i_k \geq 1,\ \deg(f_{i_1}) + \cdots + \deg(f_{i_k}) \leq \tilde{m} \,\}$$

forms a basis of $\mathbb{A}_{d,1}^{m,\tilde{m}}$.

2.4.2 Calculation of moments

Now we have finished setting up the stage and we can return to the process Y^y of all iterated Stratonovich integrals of degree less or equal to m as defined in equation (2.14). Since we are no longer working with one fixed free nilpotent algebra $\mathbb{A}_{d,1}^m$ as before, we indicate the degree m by an additional superscript, i. e.

$$dY_t^{y,m} = \sum_{i=0}^{d} D_i(Y_t^{y,m}) \circ dB_t^i, \quad Y_0^{y,m} = y,$$

where $D_i(y) = ye_i$, $y \in \mathbb{A}_{d,1}^m$, as before, $i = 0, \ldots, d$. Furthermore, we recall the convention that "$dB_t^0 = dt$", see Definition 2.1.1, and the definition of the sets of multi-indices $\mathcal{A}$ and of multi-indices $\mathcal{A}_m$ of degree less or equal m. Following equation (2.16), let

$$Z_t^m = \log(Y_t^{1,m}) = \sum_{i=1}^{N} Z_t^{i,m} f_i \in \mathfrak{g}_{d,1}^m, \quad t \geq 0, \tag{2.47}$$

where $P_H = \{f_1, \ldots, f_N\}$ denotes the Hall basis of $\mathfrak{g}_{d,1}^m$ and the right hand side of (2.47) is the expansion of Z_t^m in terms of the Hall basis.

By the Chen-Strichartz formula, Proposition 2.1.17, we can calculate the coefficients $Z^{i,m}$, $i = 1, \ldots, N$ of Z^m by expanding $e_{[I]}$, $I \in \mathcal{A}_m$, in terms of the Hall basis.

For convenience in working with the Hall and the Poincaré-Birkhoff-Witt basis, we introduce another set of multi-indices. Let

$$\tilde{\mathcal{A}} = \bigcup_{r=0}^{\infty} \{1, \ldots, N\}^r \,. \tag{2.48}$$

The generic element of $\tilde{\mathcal{A}}$ will be denoted by $J = (j_1, \ldots, j_r)$, where we understand $j_1, \ldots, j_r \in \{1, \ldots, N\}$ and $r \in \mathbb{N}$. We define a degree function on $\tilde{\mathcal{A}}$ by $\widetilde{\deg}(\emptyset) = 0$ and

$$\widetilde{\deg}(J) = \widetilde{\deg}((j_1, \ldots, j_r)) = \deg(f_{j_1}) + \cdots + \deg(f_{j_r}), \quad J \in \tilde{\mathcal{A}} \setminus \{\emptyset\} \,. \tag{2.49}$$

Moreover, we again set

$$\tilde{\mathcal{A}}_m = \left\{ J \in \tilde{\mathcal{A}} \;\middle|\; \widetilde{\deg}(J) \leq m \right\}, \quad m \in \mathbb{N}.$$

Lemma 2.4.9. *For $m, \tilde{m} \in \mathbb{N}$ with $1 \leq m \leq \tilde{m}$ we have the following formula*

$$\left[Y_t^{1,\tilde{m}}\right]_{m,\tilde{m}} = \sum_{J \in \bar{\mathcal{A}}_{\tilde{m}}} \frac{1}{r!} Z_t^{j_1,m} \cdots Z_t^{j_r,m} [f_{j_1}]_{m,\tilde{m}} \cdots [f_{j_r}]_{m,\tilde{m}}.$$

For an element f of the Hall basis of $\mathfrak{g}_{d,1}^m$, $[f]_{m,\tilde{m}}$ is understood as the equivalence class of $f \in \mathbb{A}_{d,1}^{m,\tilde{m}}$.

Proof. Starting with the same (infinite) set of Hall words $(H, <)$ as in Lemma 2.4.1, we construct the Hall basis $\{g_1 < \cdots < g_M\}$ of $\mathfrak{g}_{d,1}^{\tilde{m}}$, $M = \dim_{\mathbb{R}} \mathfrak{g}_{d,1}^{\tilde{m}}$. Note that $\{f_1, \ldots, f_N\} \subset \{g_1, \ldots, g_M\}$ in a natural way such that the order in $\{f_1, \ldots, f_N\}$ is preserved. This is true, because the order on both sets of Hall polynomials comes from the (same) order on the Hall words. For $j \in \{1, \ldots, N\}$, let $k(j)$ be the unique $k \in \{1, \ldots, M\}$ such that $f_j = g_k$.

By definition,

$$Y_t^{1,\tilde{m}} = \exp\left(\sum_{k=1}^{M} Z_t^{k,\tilde{m}} g_k\right) = 1 + \sum_{i=1}^{\tilde{m}} \frac{1}{i!} \left(\sum_{k=1}^{M} Z_t^{k,\tilde{m}} g_k\right)^i.$$

Applying the algebra-homomorphism $\Pi_{\tilde{m},m}$ and using $Y_t^{1,m} = \Pi_{\tilde{m},m}(Y_t^{1,\tilde{m}})$, we get

$$Y_t^{1,m} = 1 + \sum_{i=1}^{\tilde{m}} \frac{1}{i!} \left(\sum_{k=1}^{M} Z_t^{k,\tilde{m}} \Pi_{\tilde{m},m}(g_k)\right)^i = 1 + \sum_{i=1}^{m} \frac{1}{i!} \left(\sum_{j=1}^{N} Z_t^{k(j),\tilde{m}} f_j\right)^i,$$

since $\Pi_{\tilde{m},m}(g_k) = 0$ for $g_k \in \{g_1, \ldots, g_M\} \setminus \{f_1, \ldots, f_N\}$. Thus,

$$\sum_{j=1}^{N} Z_t^{k(j),\tilde{m}} f_j = \log(Y_t^{1,m}) = Z_t^m = \sum_{j=1}^{N} Z_t^{j,m} f_j,$$

implying that $Z_t^{k(j),\tilde{m}} = Z_t^{j,m}$, $\forall j \in \{1, \ldots, N\}$.

By the proof of Lemma 2.4.8, we see that $[g]_{m,\tilde{m}} = 0$ if $g \in \{g_1, \ldots, g_M\} \setminus \{f_1, \ldots, f_N\}$. As above, we get

$$\begin{aligned} \left[Y_t^{1,\tilde{m}}\right]_{m,\tilde{m}} &= 1 + \sum_{i=1}^{\tilde{m}} \frac{1}{i!} \left(\sum_{j=1}^{N} Z_t^{j,m} [f_j]_{m,\tilde{m}}\right)^i \\ &= \sum_{J \in \bar{\mathcal{A}}_{\tilde{m}}} \frac{1}{r!} Z_t^{j_1,m} \cdots Z_t^{j_r,m} [f_{j_1}]_{m,\tilde{m}} \cdots [f_{j_r}]_{m,\tilde{m}}. \end{aligned}$$

□

For the next definition, let us specify an embedding of $\mathbb{A}_{d,1}^m$ into $\mathbb{A}_{d,1}^{\tilde{m}}$, $\tilde{m} \geq m$, as follows. Write $y \in \mathbb{A}_{d,1}^m$ as $y = y_0 + y_1 + \cdots + y_m$ according to (2.6). Define a corresponding element $y' \in \mathbb{A}_{d,1}^{\tilde{m}}$ by its decomposition $y' = y_0 + y_1 + \cdots + y_m + y_{m+1} + \cdots + y_{\tilde{m}}$ with $y_{m+1} = 0 \in W_{m+1}, \ldots, y_{\tilde{m}} = 0 \in W_{\tilde{m}}$. Note that $\Pi_{\tilde{m},m}(y') = y$, but y' is certainly not the only element of $\mathbb{A}_{d,1}^{\tilde{m}}$ with this property. Put differently, the projection $\Pi_{\tilde{m},m} : \mathbb{A}_{d,1}^{\tilde{m}} \to \mathbb{A}_{d,1}^m$ is canonical, but the embedding $y \mapsto y'$ is not. We define an exponential function $\exp_{\tilde{m}} : W_1 \oplus \cdots \oplus W_m \subset \mathbb{A}_{d,1}^m \to \mathbb{A}_{d,1}^{m,\tilde{m}}$ by setting

$$\exp_{\tilde{m}}(y) = [1]_{m,\tilde{m}} + \sum_{k=1}^{\tilde{m}} \frac{1}{k!}[y']_{m,\tilde{m}}^k, \quad y \in W_1 \oplus \cdots \oplus W_m \subset \mathbb{A}_{d,1}^m. \tag{2.50}$$

Now we can formulate the analogue of Proposition 2.1.20 for the exponential function defined above.

Theorem 2.4.10. *For fixed $m, \tilde{m} \in \mathbb{N}$, $\tilde{m} \geq m \geq 2$ and fixed $t > 0$ we have*

$$E\Big(\big[Y_t^{1,\tilde{m}}\big]_{m,\tilde{m}}\Big) = \exp_{\tilde{m}}\Big(te_0 + \frac{t}{2}\sum_{i=1}^d e_i^2\Big).$$

Proof. By linearity of the factorization map $\mathbb{A}_{d,1}^{\tilde{m}} \to \mathbb{A}_{d,1}^{m,\tilde{m}}$, we have

$$\begin{aligned} E\Big(\big[Y_t^{1,\tilde{m}}\big]_{m,\tilde{m}}\Big) &= \Big[E\big(Y_t^{1,\tilde{m}}\big)\Big]_{m,\tilde{m}} \\ &= \Big[\exp\Big(te_0' + \frac{t}{2}\sum_{i=1}^d (e_i^2)'\Big)\Big]_{m,\tilde{m}} \\ &= \exp_{\tilde{m}}\Big(te_0 + \frac{t}{2}\sum_{i=1}^d e_i^2\Big), \end{aligned}$$

where the exponential in the second line is to be computed in $\mathbb{A}_{d,1}^{\tilde{m}}$, as indicated by the "$'$". Note that we used the equality $\exp_{\tilde{m}}(y) = [\exp(y')]_{m,\tilde{m}}$ for $y \in \mathbb{A}_{d,1}^m$ with $y = te_0 + \frac{t}{2}\sum_{i=1}^d e_i^2 \in \mathbb{A}_{d,1}^m$ in order to pass from the second to the third line. □

The moments of Z_t, or more precisely of $Z_t^{1,m}, \ldots, Z_t^{N,m}$ are contained in the expected value of $\big[Y_t^{1,\tilde{m}}\big]_{m,\tilde{m}}$ for $\tilde{m}$ large enough. Since this expected value is given by Theorem 2.4.10, we need to extract the moments of Z^m out of the expected of $\big[Y_t^{1,\tilde{m}}\big]_{m,\tilde{m}}$, which amounts to solving a system of linear equation (A.11) with a triangular matrix with diagonal entries equal to 1, see Theorem A.1.11. Because the construction is rather technical, we have moved it to the appendix, Subsection A.1.3.

Chapter 3

Cubature on Wiener space in infinite dimension

This chapter is based on the joint article [6] with Josef Teichmann.

3.1 Theoretical results

We want to construct a weak approximation scheme in the sense of Definition 1.3.3 for stochastic partial differential equations. Before going into details, let us briefly review the setting as given in Section 1.2.2.

Let H be a separable, real Hilbert space. We consider the stochastic (partial) differential equation (1.10) for a diffusion process X^x with values in H with dynamics

$$dX_t^x = (AX_t^x + \alpha(X^x t))dt + \sum_{i=1}^{d} \beta_i(X_t^x)dB_t^i$$

or – in the presence of jumps – the stochastic differential equation (1.15) for a jump-diffusion process X^x with values in H with dynamics

$$dX_t^x = (AX_{t^-}^x + \alpha(X_{t^-}^x))dt + \sum_{i=1}^{d} \beta_i(X_{t^-}^x)dB_t^i + \sum_{j=1}^{e} \delta_j(X_{t^-}^x)dL_t^j.$$

$A : \mathcal{D}(A) \subset H \to H$ denotes an, in general, unbounded linear operator, $\alpha, \beta_1, \ldots, \beta_d, \delta_1, \ldots, \delta_e : H \to H$ denote C^∞-bounded vector fields, i. e. smooth vector fields with bounded derivatives (of degree ≥ 1). $(B_t)_{t\geq 0} = (B_t^1, \ldots, B_t^d)_{t\geq 0}$ denotes a finite dimensional Brownian motion on the Wiener space $(\Omega, \mathcal{F}, P)$, and $(L_t^j)_{t\geq 0}$ a compound Poisson process with jump-rate μ_j for $j = 1, \ldots, e$, see equation (1.14). The Brownian motion and the compound Poisson process are assumed to be independent and together generate the filtration $(\mathcal{F}_t)_{t\in[0,\infty[}$. A is the generator of a C_0-semigroup denoted by $(S_t)_{t\geq 0}$.

Recall the notions of strong and mild solutions of the above SPDEs, cf. Definition 1.2.8 and equation (1.16). Notice that mild solutions, in general, are no semi-martingales, which is problematic in light of the cubature on Wiener space method, see Proposition 2.2.20, which is based on the Stratonovich formulation of the underlying finite dimensional SDE.

Of course, neither strong nor mild solutions can usually be given explicitly, which makes numerical approximation necessary. We are interested in *weak approximation* of the solution in the sense that we want to approximate the value

$$P_t f(x) = E(f(X_t^x))$$

for a suitable class of test functions $f : H \to \mathbb{R}$ at points $x \in H$. As in the finite dimensional setting, the function $(t, x) \mapsto P_t f(x)$ solves the Kolmogorov equation in the weak sense, see for instance da Prato and Zabczyk [18] in the diffusion case.

Let us assume for a moment that there are no jump-components: usually, infinite dimensional SDEs are numerically solved by finite element or finite difference schemes, see, for instance, Hausenblas [33], Yan [88], Gyöngy [29] and [30]. This means that the original equation is projected onto some finite dimensional subspace $H_h \subset H$ and A is approximated by some operator A_h defined thereon. This procedure, which corresponds to a space discretization of the stochastic PDE, is followed by a conversion of the stochastic differential equation on H_h to a stochastic difference equation by discretizing in time, using an Euler method or a related scheme. Finally, the stochastic difference equation is solved by Monte-Carlo simulation, which may be interpreted as a discretization on the Wiener space. For general information about approximation of finite dimensional SDEs see Kloeden and Platen [42].

We want to tackle the problem in the reverse order: we want to do the discretization on the Wiener space Ω first, reducing the problem to a deterministic problem. Then, the deterministic problem can be solved by standard methods for numerical treatment of deterministic PDEs, e. g. by standard finite element or finite difference methods. The benefit of this order is that once the discretization on the Wiener space has been done, we can use the well-established theory of the corresponding deterministic problems, without complications from stochasticity. Our method of choice for discretization on Ω is cubature on Wiener space, as amply introduced in the preceeding Chapter 2. In the spirit of these methods we shall obtain weak approximation schemes of any prescribed order.

Before going into details, let us motivate the use of cubature formulas in this context. Recall the notation introduced in (2.30) and adopt it to the current situation, i. e. let $X_t^x(\omega)$ denote the solution of (1.10), formally

rewritten in Stratonovich form, if each "dB_t^i" is replaced by "$d\omega^i(t)$", i. e.

$$dX_t^x(\omega) = (AX_t^x(\omega) + \alpha(X_t^x(\omega)) - \frac{1}{2}\sum_{i=1}^{d} D\beta_i(X_t^x(\omega)) \cdot \beta_i(X_t^x(\omega)))dt + \sum_{i=1}^{d} \beta_i(X_t^x(\omega))d\omega^i(t) \tag{3.1}$$

for a curve function $\omega = (\omega^1, \dots, \omega^d) : \mathbb{R}_{\geq 0} \to \mathbb{R}^d$ of bounded variation. Notice that $X_t^x(\omega)$ is the weak solution of a partial differential equation (or partial integro-differential equation). Then, as in the finite dimensional situation, we would like to approximate $P_t f(x)$ for fixed $t > 0$ and $x \in H$ by a weighted sum of $f(X_t^x(\omega))$ for paths ω of bounded variation chosen according to a cubature formula on Wiener space, see Proposition 2.2.20 for finite dimensional cubature on Wiener space and Definition 1.3.3 for general weak approximation. As we have just seen, the cubature on Wiener space method for weak approximation of SDEs can be easily generalized to an infinite dimensional setting, at least on a conceptual level.

Here also the main advantage of cubature methods in contrast to Taylor methods gets visible. The time-discretization in the realm of cubature methods always leads to reasonable expressions, namely to equations of type (3.1). If we wanted to apply the usual discretization methods in time like the Euler-Maruyama-Monte-Carlo method, we might run into problems. Indeed, the naive Euler scheme is well-suited for the differential formulation (1.10) of the problem,

$$X_0 = x \text{ and } X_n = (AX_{n-1} + \alpha(X_{n-1}))\frac{t}{n} + \sum_{i=1}^{d} \beta_i(X_{n-1})\Delta_n B^i,$$

for $n \geq 1$, but this might immediately lead to some $X_n \notin \mathcal{D}(A)$. Even in the case of an existing strong solution, there is no reason why the discrete approximation should always stay in $\mathcal{D}(A)$. Hence the naive implementation does not work.

Only the mild formulation (1.12c) seems to be suitable for using an Euler-like method. If one understands the semigroup S well, one can approximate X_t^x by expressing the integrals in (1.12c) as Riemannian sums, involving evaluations of S_{t-s}, which yields a sort of strong Euler method (see for instance the book of Prévôt and Röckner [63] for strong convergence theorems in this direction).

We do not discretize the integral in formulation (1.12c), but (weakly) approximate the Brownian paths so well by paths of bounded variation, that those paths can be used to obtain a weak approximation of the integrals and finally of X_t^x.

In the presence of jumps, things do not get more complicated, since the short time asymptotics of a jump-diffusion can be easily derived from a diffusion's short-time asymptotics by conditioning on the jumps. The arising picture is the following. Discretizing the equation (1.15) means to allow a certain number of jumps between to consecutive points in the time grid. Between two jumps we apply a diffusion cubature formula to express the short-time asymptotics. Finally, we integrate with respect to jump times and sizes using Monte-Carlo simulation. Therefore, we have a kind of hybrid method between cubature and Monte-Carlo simulation in mind.

3.1.1 Cubature for equations without jumps

In this subsection we shall assume that there are no jumps, i. e. we consider equation (1.10). Recall the hierarchy of Sobolev spaces as introduced in Definition 1.2.14 and Definition 1.2.15. In addition to our standard Assumption 1.2.7 of C^∞-boundedness of the vector fields, we impose the following assumption, which is slightly weaker than Assumption 1.2.21.

Assumption 3.1.1. The diffusion vector fields $\alpha, \beta_1, \dots, \beta_d$ map $\mathcal{D}(A^n) \to \mathcal{D}(A^n)$ for each $n \geq 0$ and are C^∞-bounded thereon, i. e. as maps from the Hilbert space $(\mathcal{D}(A^n), \|\cdot\|_{\mathcal{D}(A^n)})$ into itself.

Note that Proposition 1.2.22 still holds true under Assumption 3.1.1, as a short look at the proof reveals. There are subtle phenomena of explosion, which can occur in this setting: for instance it might be that the law of a strong solution process X^x solving equation (1.10) is bounded in H but unbounded in $\mathcal{D}(A)$, where it is a mild solution. Due to such phenomena the discussion after Theorem 3.1.5 is in fact quite subtle.

Moreover, we assume that we always take a fixed cubature formula, which we rescale properly for the interval under consideration.

Assumption 3.1.2. Once and for all, we fix one cubature formula on Wiener space in the sense of Definition 2.2.12 of degree $m \geq 1$ on the interval $[0, 1]$. Denoting the paths of this cubature formula with $\widetilde{\omega}_1, \dots, \widetilde{\omega_N}$, we will, by abuse of notation, denote by $\omega_l(s) = \widetilde{\omega}_l(s/\sqrt{t})$, $s \in [0, t]$, $l = 1, \dots, N$, the corresponding cubature formula for $[0, t]$.

Recall the definition of the vector field β_0 given in (1.22), i. e.

$$\beta_0 = Ax + \alpha(x) - \frac{1}{2} \sum_{i=1}^{d} D\beta_i(x) \cdot \beta_i(x). \tag{3.2}$$

β_0 is defined for $x \in \mathcal{D}(A)$. As a vector field taking values in $\mathcal{D}(A^n)$, it is only well-defined on $\mathcal{D}(A^{n+1})$. Consequently, for $x \in \mathcal{D}(A^{n+1})$, we may reformulate the SDE (1.10) – understood as equation in $\mathcal{D}(A^n)$ – in Stratonovich form, see (1.23).

Now we formulate the stochastic Taylor expansion in some $\mathcal{D}(A^{r(m)})$ with a degree of regularity $r(m) \geq 0$ depending on $m \geq 1$, cf. Proposition 2.1.4 for the finite dimensional version. For the estimation of the error term, we will use the *extended support* $\operatorname{esupp}(X_t^x; \omega_1, \ldots, \omega_r)$ defined by

$$\operatorname{esupp}(X_t^x; \omega_1, \ldots, \omega_r) = \operatorname{supp}(X_t^x) \cup \{X_t^x(\omega_1), \ldots, X_t^x(\omega_r)\}, \tag{3.3}$$

where $t > 0$, $x \in H$, and $\omega_1, \ldots, \omega_r$ are paths of bounded variation. Despite Assumption 3.1.2, let us, for one moment, enter the dependence of the cubature formula on the interval $[0, t]$ explicitly into the notation, in the sense that $\omega_1^{(t)}, \ldots, \omega_N^{(t)}$ are the paths of bounded variation scaled in such a way that they, together with the weights, form a cubature formula on $[0, t]$. Then we denote

$$\mathfrak{S}_T(x) = \bigcup_{0 \leq s \leq t \leq T} \operatorname{esupp}(X_s^x; \omega_1^{(t)}, \ldots, \omega_r^{(t)}).$$

Remark 3.1.3. If the support theorem holds in infinite dimensions, we can replace the extended support by the ordinary support of X_t^x, since the solution of the corresponding ODE driven by paths of bounded variation lie in the support of the solution of the SDE according to that theorem. However, up to our knowledge, the support theorem has not been established for our setting so far. Furthermore, notice that it does not matter, in which topology the support is understood, because we only need that $P(X_t^x \notin \operatorname{supp}(X_t^x)) = 0$.

Theorem 3.1.4. *Let $m \geq 1$ be fixed, then there is $r(m) \geq 0$ such that for any $f \in C^\infty(H; \mathbb{R})$, $x \in \mathcal{D}(A^{r(m)})$, and $0 < t < 1$ we have*

$$f(X_t^x) = \sum_{\substack{k \leq m, (i_1, \ldots, i_k) \in \mathcal{A} \\ \deg(i_1, \ldots, i_k) \leq m}} (\beta_{i_1} \cdots \beta_{i_k} f)(x) B_t^{(i_1, \ldots, i_k)} + R_m(t, f, x), \quad x \in \mathcal{D}(A^{r(m)}),$$

with

$$\begin{aligned} \sqrt{E(R_m(t, f, x)^2)} &\leq C t^{\frac{m+1}{2}} \max_{m < \deg(i_1, \ldots, i_k) \leq m+2} \sup_{0 \leq s \leq t} |E(\beta_{i_1} \cdots \beta_{i_k} f(X_s^x))| \\ &\leq C t^{\frac{m+1}{2}} \max_{m < \deg(i_1, \ldots, i_k) \leq m+2} \sup_{y \in \mathfrak{S}_t(x)} |\beta_{i_1} \cdots \beta_{i_k} f(y)| . \end{aligned}$$

We can choose $r(m) = \lfloor \frac{m}{2} \rfloor + 1$, where $\lfloor \frac{m}{2} \rfloor$ denotes the largest integer smaller than $\frac{m}{2}$.

Proof. The proof is the same as in the finite dimensional situation, but one has to switch between different spaces on the way.

Fix m and f as above and $x \in \mathcal{D}(A^{\lfloor \frac{m}{2} \rfloor + 1})$. We interpret the equation in $\mathcal{D}(A^{\lfloor \frac{m}{2} \rfloor + 1})$. By the above remarks, we can express the SDE in its Stratonovich form (1.23). By Itô's formula,

$$f(X_t^x) = f(x) + \int_0^t (\beta_0 f)(X_s^x) ds + \sum_{i=1}^d \int_0^t (\beta_i f)(X_s^x) \circ dB_s^i. \tag{3.4}$$

The idea is to express $(\beta_i f)(X_s^x)$ again by Itô's formula and insert it in equation (3.4). This is completely unproblematic for $i \in \{1, \dots, d\}$. For $i = 0$, recall that

$$(\beta_0 f)(x) = Df(x) \cdot Ax + Df(x) \cdot \Big(\alpha(x) - \frac{1}{2} \sum_{i=1}^{d} D\beta_i(x) \cdot \beta_i(x)\Big).$$

By re-expressing (3.4) in Itô formulation, applying Itô's formula, and re-expressing it back to Stratonovich formulation, we see that

$$(\beta_0 f)(X_s^x) = (\beta_0 f)(x) + \int_0^s (\beta_0^2 f)(X_u^x) du + \sum_{i=1}^{d} \int_0^s (\beta_i \beta_0 f)(X_u^x) \circ dB_u^i,$$

where

$$(3.5) \quad (\beta_0^2 f)(x) = D^2 f(x)(Ax, Ax) + Df(x) \cdot (A^2 x + A\alpha(x) + \cdots) + \cdots,$$

provided that all the new vector-fields are well-defined and the processes $(\beta_i \beta_0 f)(X_u^x)$ are still semi-martingales. Both conditions are satisfied if $x \in \mathcal{D}(A^2)$ – notice that the maps $\mathcal{D}(A^{k+1}) \to \mathcal{D}(A^k)$, $x \mapsto Ax$ are C^∞, $k \in \mathbb{N}$. By induction, we finally get

$$f(X_t^x) = \sum_{\substack{(i_1,\dots,i_k) \in \mathcal{A} \\ \deg(i_1,\dots,i_k) \le m}} (\beta_{i_1} \cdots \beta_{i_k} f)(x) B_t^{(i_1,\dots,i_k)} + R_m(t, f, x)$$

with

$$R_m(t, x, f) = \sum_{\substack{(i_1,\dots,i_k) \in \mathcal{A},\, i_0 \in \{0,\dots,d\} \\ \deg(i_1,\dots,i_k) \le m < \deg(i_0,i_1,\dots,i_k)}} \int_{0<t_0<\cdots<t_k<t} (\beta_{i_0} \cdots \beta_{i_k} f)(X_{t_0}^x) \circ dB_{t_0}^{i_0} \cdots \circ dB_{t_k}^{i_k}.$$

Note that R_m is well-defined for $x \in \mathcal{D}(A^{\lfloor \frac{m}{2} \rfloor + 1})$ because integration of non-semi-martingales with respect to dt is possible, which corresponds to the index $i_0 = 0$.

As in the finite dimensional case, we re-express R_m in terms of Itô integrals and use the (one-dimensional) Itô isometry several times, until we arrive at the desired estimate. Notice that we refine the estimate of the values of $y \mapsto \beta_{i_1} \cdots \beta_{i_k} f(y)$ on the support of the process X_s^x for $0 \le s \le t$. □

We recall the notation $P_t f(x) = E(f(X_t^x))$ for bounded measurable functions $f : H \to \mathbb{R}$. Analogously to Proposition 2.2.20 in finite dimensions, we get

Theorem 3.1.5. *Fix $T > 0$, $m \geq 1$, $r(m)$, $x \in \mathcal{D}(A^{r(m)})$ as in Theorem 3.1.4, a cubature formula on Wiener space of degree m as in Definition 2.2.12 and a partition $0 = t_0 < t_1 < \cdots < t_p = T$. Under Assumption 3.1.1, for any $f \in C^\infty(H;\mathbb{R})$ with*

$$\sup_{0\leq t\leq T} \sup_{y\in \mathfrak{S}_T(x)} |\beta_{i_1} \cdots \beta_{i_k} P_t f(y)| < \infty$$

for all $(i_1, \ldots, i_k) \in \mathcal{A}$ with $m < \deg(i_1, \ldots, i_k) \leq m + 2$, $k \in \mathbb{N}$, there is a constant D independent of the partition such that

$$\left| E(f(X_T^x)) - \sum_{(l_1,\ldots,l_p)\in\{1,\ldots,N\}^p} \lambda_{l_1} \cdots \lambda_{l_p} f(X_T^x(\omega_{l_1,\ldots,l_p})) \right| \leq DT \max_{r=1,\ldots,p} (t_r - t_{r-1})^{(m-1)/2},$$

where the ODE defining $X_T^x(\omega)$ is, again, understood as the mild solution to an ODE in $\mathcal{D}(A^{r(m)})$ for any path ω of bounded variation.

Proof. The proof follows Kusuoka [43], [44], see also Kloeden and Platen [42]. For $f : H \to \mathbb{R}$ and $x \in H$ let

$$Q_{(t)} f(x) = \sum_{l=1}^N \lambda_l f(X_t^x(\omega_l)),$$

where $\omega_1, \ldots, \omega_l$ are scaled to form a cubature formula on $[0, t]$. Denote $\Delta t_r = t_r - t_{r-1}$, $r = 1, \ldots, p$, the increments of the time partition given in the statement of the theorem. By iterating the operators $Q_{(\Delta t_r)}$ (and the semigroup property of ODEs), we immediately obtain

$$\sum_{(l_1,\ldots,l_p)\in\{1,\ldots,N\}^p} \lambda_{l_1} \cdots \lambda_{l_p} f(X_T^x(\omega_{l_1,\ldots,l_p})) = Q_{(\Delta t_p)} \circ \cdots \circ Q_{(\Delta t_1)} f(x). \tag{3.6}$$

By ordinary Taylor expansion, keeping in mind the degree function deg, we note that

$$Q_{(t)} f(x) = \sum_{l=1}^N \lambda_l \sum_{\substack{k\leq m,\,(i_1,\ldots,i_k)\in\mathcal{A} \\ \deg(i_1,\ldots,i_k)\leq m}} (\beta_{i_1} \cdots \beta_{i_k} f)(x) \omega_l^{(i_1,\ldots,i_k)}(t) + \widetilde{R}_m(t, x, f),$$

where $x \in \mathcal{D}(A^{r(m)})$ and

$$\widetilde{R}_m(t, x, f) = \sum_{l=1}^N \lambda_l \sum_{\substack{(i_1,\ldots,i_k)\in\mathcal{A},\, i_0\in\{0,\ldots,d\} \\ \deg(i_1,\ldots,i_k)\leq m<\deg(i_0,\ldots,i_k)}} \int_{0\leq t_0\leq\cdots\leq t_k\leq t} (\beta_{i_0} \cdots \beta_{i_k} f)(X_{t_0}^x(\omega_l)) d\omega_l^{i_0}(t_0) \cdots d\omega_l^{i_k}(t_k).$$

In the following, C denotes a constant independent of the partition and x which may change from line to line. We can estimate the approximation error by

$$\left|\widetilde{R}_m(t,x,f)\right| \leq C \sup_{0\leq s\leq t,\, l=1,\dots,N} \max_{m\leq \deg(i_0,\dots,i_k)\leq m+2} |\beta_{i_0}\cdots\beta_{i_k} f(X_s^x(\omega_l))|\, t^{\frac{m+1}{2}}.$$

Combining this result with Theorem 3.1.4, we may conclude that

$$\left|P_t f(x) - Q_{(t)} f(x)\right| \leq C \sup_{y\in \mathfrak{S}_t(x)} |\beta_{i_0}\cdots\beta_{i_k} f(y)|\, t^{\frac{m+1}{2}}. \tag{3.7}$$

By telescopic sums,

$$P_T f(x) - Q_{(\Delta t_p)}\circ\cdots\circ Q_{(\Delta t_1)} f(x) = \sum_{r=1}^{p} Q_{(\Delta t_p)}\circ\cdots\circ Q_{(\Delta t_{r+1})}(P_{t_r} f(x) - Q_{(\Delta t_r)} P_{t_{r-1}} f(x)).$$

For the estimation of the rear term

$$P_{t_r} f(x) - Q_{(\Delta t_r)} P_{t_{r-1}} f(x) = (P_{\Delta t_r} - Q_{(\Delta t_r)}) P_{t_{r-1}} f(x),$$

we may use (3.7) with $f(x)$ being replaced by $P_{t_{r-1}} f(x)$, giving us

$$\begin{aligned}
|P_T f(x) - Q_{(\Delta t_p)}\circ\cdots\circ Q_{(\Delta t_1)} f(x)| &\leq \sum_{r=1}^{p} \left|P_{t_r} f(x) - Q_{(\Delta t_r)} P_{t_{r-1}} f(x)\right| \\
&\leq C \sum_{r=1}^{p} \sup_{\substack{y\in \mathfrak{S}_{\Delta t_r}(x) \\ m\leq \deg(i_0,\dots,i_k)\leq m+2}} \left|\beta_{i_0}\cdots\beta_{i_k} P_{t_{r-1}} f(y)\right| (\Delta t_r)^{\frac{m+1}{2}} \\
&\leq C \sup_{\substack{y\in \mathfrak{S}_T(x),\, 0\leq t\leq T \\ m\leq \deg(i_0,\dots,i_k)\leq m+2}} |\beta_{i_0}\cdots\beta_{i_k} P_t f(y)| \sum_{r=1}^{p} (\Delta t_r)^{\frac{m+1}{2}},
\end{aligned}$$

from which we may easily conclude the theorem. □

Remark 3.1.6. Gyöngy and Shmatkov [31] show a strong Wong-Zakai-type approximation result, where they also need to impose smoothness assumptions on the initial value x. Otherwise, the assumptions in [31] are different from ours, they allow densely defined vector fields and general adapted coefficients, on the other hand, the generator A needs to be elliptic.

Remark 3.1.7. Under the previous assumptions we can also prove a Donsker-type result on the weak convergence of the "cubature tree" to the diffusion. This result will be proved elsewhere.

Remark 3.1.8. If f is smooth then we can show by (first and higher) variation processes, as introduced for instance in Baudoin and Teichmann [5], that $x \mapsto P_t f(x)$ is smooth on $\mathcal{D}(A^n)$.

Fix $n \geq 0$. Let $J_{0\to t}(x) \cdot h$ denote the first variation process of X_t^x in direction $h \in \mathcal{D}(A^n)$, i. e.

$$J_{0\to t}(x) \cdot h = \frac{\partial}{\partial \epsilon}\bigg|_{\epsilon=0} X_t^{x+\epsilon h} \in \mathcal{D}(A^k).$$

Recall that $J_{0\to t}(x)\cdot h$ is defined as mild solution of the stochastic differential equation

$$\begin{cases} dJ_{0\to t}(x) \cdot h = \big(A(J_{0\to t}(x) \cdot h) + D\alpha\big(X_t^x\big) \cdot J_{0\to t}(x) \cdot h\big)dt \\ \qquad\qquad\qquad + \sum_{i=1}^{d} D\beta_i\big(X_t^x\big) \cdot J_{0\to t}(x) \cdot h \; dB_t^i, \\ J_{0\to 0}(x) \cdot h = h, \end{cases}$$

for $h \in H$, $x \in H$, $t \geq 0$. Notice that the above equation depends explicitly on X^x, i. e. it is a stochastic differential equation with stochastic coefficients. Therefore, it is often more convenient to think of the pair $\big(X_t^x, J_{0\to t}(x) \cdot h\big)$ as solution of an SDE in H^2.

Since $J_{0\to t}(x) \cdot h$ is the mild solution to an SDE of the type (1.10), it is bounded in $L^2(\Omega, \mathcal{F}, P; \mathcal{D}(A^n))$ and we may conclude that

$$\frac{\partial}{\partial \epsilon}\bigg|_{\epsilon=0} P_t f(x + \epsilon h) = E\Big(Df(X_t^x) \cdot J_{0\to t}(x) \cdot h\Big)$$

exists and is bounded by boundedness of Df and integrability of the first variation. Similarly, we get existence and continuity of higher order derivatives on $\mathcal{D}(A^n)$.

Example 3.1.9. We shall provide examples, where the previous conditions are satisfied, i. e. where we obtain high-order convergence of the respective cubature methods. Indeed, the following conditions allow us to conclude that the requirements of Theorem 3.1.5 are satisfied.

Assume that there are smooth vector fields $\widetilde{\alpha}, \widetilde{\beta}_1, \ldots, \widetilde{\beta}_d$ such that

$$\alpha = \widetilde{\alpha} \circ R(\lambda, A)^{r(m)}, \quad \beta_i = \widetilde{\beta}_i \circ R(\lambda, A)^{r(m)},$$

for $i = 1, \ldots, d$ and some $\lambda \in \rho(A)$. Furthermore, we assume that

- $\widetilde{\alpha}, \widetilde{\beta}_1, \ldots, \widetilde{\beta}_d$ map $\mathcal{D}(A^{k+r(m)})$ to $\mathcal{D}(A^{k+2r(m)})$ for any $k \in \mathbb{N}$,
- the restrictions of $\widetilde{\alpha}, \widetilde{\beta}_1, \ldots, \widetilde{\beta}_d$ to the Hilbert space $\mathcal{D}(A^{r(m)})$ have bounded support, and

- the function f is of the type $f = g \circ (R(\lambda, A)^{r(m)})$ for bounded, C^∞-bounded functions $g : H \to \mathbb{R}$.

Under these assumptions we can readily check that the law of the mild solution X_t^x starting at the initial value $x \in \mathcal{D}(A^{r(m)})$ has bounded support in H: outside a ball of radius $R > 0$ in H the solution process is deterministic, $X_t^x = S_t x$ on some interval, hence by the uniform boundedness theorem there is a large R such that the image of the ball with radius $R > 0$ under the maps S_t lies in a ball with radius $R' > 0$ on $[0, T]$.

For smooth functions f of the stated type we have

$$\sup_{0 \le t \le T} \sup_{y \in H, \|y\| \le R'} |\beta_{i_0} \cdots \beta_{i_k} P_t f(y)| < \infty,$$

since we only take the supremum over bounded sets, namely the extended support of X_t^x for $0 \le s \le t$, $\deg(i_0, \ldots, i_k) \le m + 2$.

Remark 3.1.10. The previous assumptions in Example 3.1.9 on the vector fields are not too restrictive since we can always obtain them by a linear isomorphism and (smoothly) cutting off outside a ball in $\mathcal{D}(A^{r(m)})$. Both operations are numerically innocent. Under Assumption 3.1.1 we can apply the following isomorphism to the solution of our stochastic differential equation (1.10):

$$R(\lambda, A)^{-r(m)} : \mathcal{D}(A^{r(m)}) \to H.$$

This isomorphism transforms the solutions X_t^x on $\mathcal{D}(A^{r(m)})$ to a H-valued process

$$Y_t^y = R(\lambda, A)^{-r(m)} X_t^{R(\lambda, A)^{r(m)} y}$$

satisfying an SDE, where the transformed vector fields (if well defined) factor over $R(\lambda, A)^{r(m)}$ such as previously assumed in Example 3.1.9, namely

$$\begin{aligned} (3.8) \quad dY_t^y = (AY_t^y + ((R(\lambda, A)^{-r(m)} \circ \alpha \circ R(\lambda, A)^{r(m)})(Y^y t))dt \\ + \sum_{i=1}^{d} (R(\lambda, A)^{-r(m)} \circ \beta_i \circ R(\lambda, A)^{r(m)})(Y_t^y) dB_t^i, \end{aligned}$$

In order to obtain the conditions in Example 3.1.9, we must (smoothly) cut off the vector fields $\alpha, \beta_1, \ldots, \beta_d$ outside sets of large norm $||.||_{\mathcal{D}(A^r(m))}$, which is an event – under Assumption 3.1.1 – of small probability (recall that the vector fields are Lipschitz on $\mathcal{D}(A^{r(m)})$ and, therefore, second moments with respect to the norm $||.||_{\mathcal{D}(A^r(m))}$ exist). Notice that the cut-off vector fields do not have an extension to H since continuous functions with bounded support on $\mathcal{D}(A^{r(m)})$ do generically not have a continuous extension on H. For $(Y_t^y)_{t \ge 0}$ we can take initial values $y \in H$, however, those initial values correspond to quite regular initial values $x = R(\lambda, A)^{r(m)} y \in \mathcal{D}(A^{r(m)})$ for the original process $(X_t^x)_{t \ge 0}$.

From the point of view of the process Y we have hence proved that

$$f(Y_T^y) = g \circ (R(\lambda, A)^{r(m)}) \circ (R(\lambda, A)^{-r(m)})(X_T^x) = g(X_T^x)$$

is weakly approximated by evaluating f on the cubature tree for Y. This is equivalent to evaluating g on the cubature tree for X for approximating $E(g(X_T^x))$.

3.1.2 The cubature method in the presence of jumps

The extension of cubature formulas to jump diffusions seems to be new even in the finite dimensional case. We shall heavily use the fact that only finitely many jumps occur in compact time intervals almost surely.

We shall first prove an asymptotic result on jump-diffusions. In the whole Subsection 3.1.2, X^x denotes a mild solution of (1.15).

Lemma 3.1.11. *Let $f : H \to \mathbb{R}$ be a bounded measurable function, then we obtain*

$$E(f(X_t^x)) = \sum_{n_1,\ldots,n_e \geq 0} \frac{\mu_1^{n_1} \cdots \mu_e^{n_e}}{n_1! \cdots n_e!} e^{-t\mu_1 n_1 - \ldots - t\mu_e n_e} t^{n_1+\ldots+n_e} \times \times E(f(X_t^x) \mid N_t^j = n_j \text{ for } j = 1, \ldots, e) \tag{3.9}$$

for $t \geq 0$.

Proof. We condition on the jump times (but not on the jump sizes) and read off the results by inserting the probabilities for a Poisson process with intensity μ_j to reach level n_j at time t. □

This result gives the time-asymptotics with respect to the jump-structure of the process X^x. This can now be combined with the original cubature result for the diffusion between the jumps, in order to obtain a result for jump-diffusions. We denote by τ_n^j the jump-time of the Poisson process N^j for the n-th jump. We know that for each Poisson process the vector $(\tau_1^j, \ldots, \tau_k^j - \tau_{k-1}^j, t - \tau_k^j)$ is uniformly distributed if conditioned on the event that $N_t^j = k \geq 1$. The uniform distribution is on the k-simplex $t\Delta^k \subset \mathbb{R}^{k+1}$. This allows us to apply an original cubature formula between two jumps of order $m - 2n_1 - \ldots 2n_e$, since we gain, for each jump, one order of time-asymptotics from the jump structure.

Assume now that the jump distributions ν_j are concentrated at one point $z_j \neq 0$, i. e. $\Delta L^j_{\tau_k^j} = z_j$ for $j = 1, \ldots, e$ and $k \geq 1$. If we want to consider a general jump-structure this amounts to additional integration with respect to the jump distribution ν_j.

We define an approximation due to cubature on Wiener space for the conditional expectations.

$$E(f(X_t^x) \mid N_t^j = n_j \text{ for } j = 1, \ldots, e)$$

of order $m-2n_1-\dots 2n_e$ with $n_1+\dots+n_e \leq \frac{m+1}{2}$. Expressed in words, we are going to do the following: from the initial value $x \in \mathcal{D}(A^{r(m)})$ on we solve the stochastic differential equation (1.15) along the cubature paths ω_l with probability $\lambda_l > 0$ until the first jump appears. We collect the end-points of the trajectories, add the jump size at this point and start a new cubature method from the resulting point on. Notice that we can take a cubature method of considerably lower degree since every jump increases the local order of time-asymptotics by t. The jump times are chosen independent and uniformly distributed on simplices of certain dimension n_j such that $n_1+\dots+n_e = n$. We denote the cubature trajectory between jump τ^j_{q-1} and τ^j_q for $1 \leq q \leq n_j$ with $\omega_{l,j,q}$. If $n_j = 0$ no trajectories are associated. Hence we obtain the following theorem:

Theorem 3.1.12. *Fix $m \geq 1$. Consider the stochastic differential equation* (1.15) *under the condition $N^j_t = n_j$ for $j = 1,\dots,m$ with $n_1+\dots+n_e = n$ along concatenated trajectories of type $\omega_{l,j,q}$. Choose a cubature method of degree*

$$m' = m - 2n \geq 1.$$

Concatenation is only performed with increasing q-index and a typical concatenated trajectory is denoted by $\omega_{l_1,\dots,l_n}$, where we have in mind that the intervals, where the chosen path is $\omega_{l_r,j,q}$, come from an N^j-jump and have length $\tau^j_q - \tau^j_{q-1}$.

Then there is $r(m') \geq 0$ such that

$$\begin{aligned}
&\big|E(f(X^x_t) \mid N^j_t = n_j) \\
&\qquad - \sum_{l_1,\dots,l_n=1}^{N} \lambda_{l_1}\dots\lambda_{l_n} E(f(X^x_t(\omega_{l_1,\dots,l_n})) \mid N^j_t = n_j)\big| \\
&\leq Ct^{\frac{m'+1}{2}} \max_{\substack{(i_1,\dots,i_k)\in\mathcal{A}\\ \deg(i_1,\dots,i_k)\leq m+2}} \sup_{\substack{y\in\mathrm{supp}(X^x_s),\\ 0\leq s\leq t}} |\beta_{i_1}\cdots\beta_{i_k} E(f(X^y_{\tau_q,t}(\omega_{l_{q+1},\dots,l_n}))\,|\,N^j_t = n_j)|,
\end{aligned}$$

where $X^x_t(\omega)$ denotes the solution of the stochastic differential equation (1.15) *in Stratonovich form*

$$dX^x_t(\omega) = \beta_0(X^x_{t^-}(\omega))dt + \sum_{i=1}^{d} \beta_i(X^x_{t^-}(\omega)) \circ dB^i_t + \sum_{j=1}^{e} \delta_j(X^x_{t^-})dL^j_t,$$

along trajectory ω.

Proof. By our main Assumption 3.1.1 we know that the linkage operators $x \mapsto \delta^j(x)$ are C^∞-bounded on each $\mathcal{D}(A^k)$, hence, through concatenation the errors, which appear on each subinterval $[t_{n-q}, t[$, are of the type $y \mapsto E(X^y_{\tau_q,t}(\omega_{l_{q+1}q,\dots,l_n}))$ for some $1 \leq q \leq n$. Taking the supremum yields the result. □

Combining the previous result with Lemma 3.1.11 yields, under certain conditions on the vector fields (see the discussion after Theorem 3.1.4 in the previous subsection), by the triangle inequality that there is a constant $D > 0$ such that

$$\begin{aligned}(3.10)\quad \Big|E(f(X_t^x)) - \sum_{2(n_1+\ldots+n_e)\leq m} \sum_{l_1,\ldots,l_n=1}^{N} \frac{\mu_1^{n_1}\cdots\mu_m^{n_e}}{n_1!\cdots n_e!} e^{-t\mu_1 n_1-\ldots-t\mu_e n_e} \times \\ \times \lambda_{l_1}\ldots\lambda_{l_n} E(f(X_t^x(\omega_{l_1,\ldots,l_n})) \mid N_t^j = n_j)\Big| \leq D t^{\frac{m+1}{2}},\end{aligned}$$

By iteration of the previous result, we obtain in precisely the same manner as in Subsection 3.1.1 a cubature method of order m by applying several cubature methods of order $m' \leq m$ between the jumps.

For the implementation, one has to simulate the uniform distributions on the simplices $t\Delta^k$ and the jump distribution. Since the integrals on the simplices $t\Delta^k$ are with respect to jumping-times, we cannot expect more regularity than continuity for those integrands, and hence one has to be careful to implement other methods than a Monte-Carlo simulation. For instance, classical cubature methods will not work due to increasing derivatives of higher order with respect to the time variable.

3.2 Numerical experiments

We test the cubature method for two concrete examples: one toy example, where explicit solutions of the SPDE are readily available, and another, more interesting example. Since cubature on Wiener space is a weak method, we calculate the expected value of a functional of the solution to the SPDE in both cases, i. e. the outputs of our computations are real numbers. Notice, however, that the cubature method will be implemented for a class of infinite dimensional Heath-Jarrow-Morton models in the financial numerics package Premia.

The results presented here are calculated in MATLAB using the built-in PDE-solver `pdepe` for solving the deterministic PDEs given by inserting the cubature paths into the SPDE under consideration. This PDE solver depends on a space grid given by the user as well as on a time grid, which is not very critical because it is adaptively refined by the program.

We do not use recombination techniques for cubature on Wiener space as in Schmeiser, Soreff and Teichmann [74] and use the simplest possible cubature formula for $d = 1$ Brownian motions:

$$\omega_1^{(T)}(t) = -\frac{t}{\sqrt{T}},\ \omega_2^{(T)} = \frac{t}{\sqrt{T}}, \quad t \in [0,T]$$

with weights $\lambda_1 = \lambda_2 = \frac{1}{2}$ define a cubature formula of degree $m = 3$ on $[0,T]$. Consequently, solving an SDE on a Hilbert space with cubature on

Wiener space for the above cubature formula and p iterations means solving 2^p PDEs. This starts to get restrictive even for a very simple problem for, say, $p = 10$ – where one already has to solve more than one thousand PDEs. One possibility to overcome these tight limitations is to use "a Monte-Carlo simulation on the tree". Recall that a p-step cubature method approximates

$$E(f(X_T^x)) \approx \sum_{(j_1,\dots,j_p)\in\{1,\dots,N\}^p} \lambda_{j_1}\cdots\lambda_{j_p} f(X_T^x(\omega_{j_1,\dots,j_p})).$$

Since $\sum \lambda_{j_1}\cdots\lambda_{j_p} = 1$, we can interpret the right hand side as the expectation of a random variable $f(X_T^x(\omega.))$ on the tree $\{1,\dots,N\}^p$. Therefore, we can approximate the right hand side by picking tuples $(j_1,\dots,j_p) \in \{1,\dots,N\}^p$ at random – according to their probabilities $\lambda_{j_1}\cdots\lambda_{j_p}$ – and calculating the average of the corresponding outcomes $f(X_T^x(\omega_{j_1,\dots,j_p}))$. Of course, by following this strategy we have to replace the deterministic error estimates by a stochastic one, which heavily depends on the standard deviation of $f(X_T^x(\omega.))$ understood as a random variable on the tree.

Consider the Ornstein-Uhlenbeck process X_t^x defined as solution to the equation

$$dX_t^x = \Delta X_t^x dt + \phi dB_t \tag{3.11}$$

on the Hilbert space $H = L^2(]0,1[)$. Δ denotes the Dirichlet Laplacian on $]0,1[$, i. e. Δ is a negative definite self-adjoint operator on H with $\mathcal{D}(\Delta) = H_0^1(]0,1[) \cap H^2(]0,1[)$ extending the classical Laplace operator defined on $C_c^\infty(]0,1[)$. It is easy to see that Δ is dissipative and therefore, by the Lumer-Phillips theorem, it is the generator of a C_0 contraction semigroup $(S_t)_{t\geq 0}$ on H. $\phi \in H$ is some fixed vector.

In this case, the definition of a mild solution

$$X_t^x = S_t x + \int_0^t S_{t-s}\phi dB_s \tag{3.12}$$

already gives a representation of the solution provided that the heat-semigroup S_t applied to the starting vector x and to ϕ is available. We choose $x(u) = \sin(\pi u)$, $u \in]0,1[$, and may conclude that

$$S_t x = e^{-\pi^2 t} x$$

because x is an eigenvector of Δ with eigenvalue $-\pi^2$. Consider the linear functional $\Phi : H \to \mathbb{R}$ given by

$$\Phi(y) = \int_0^1 y(u)du, \quad y \in H. \tag{3.13}$$

We want to compute

$$E(\Phi(X_1^x)) = E\Big(\int_0^1 e^{-\pi^2}\sin(\pi u)du + \int_0^1\int_0^1 S_{1-s}\phi(u)dB_s du\Big)$$
$$= \int_0^1 e^{-\pi^2}\sin(\pi u)du = 0.3293\times 10^{-4}.$$

p	Error
1	-0.3601×10^{-4}
2	-0.2192×10^{-4}
3	-0.1226×10^{-4}
4	-0.0652×10^{-4}
5	-0.0334×10^{-4}
6	-0.0172×10^{-4}
7	-0.0084×10^{-4}
8	-0.0031×10^{-4}
9	-0.0002×10^{-4}
10	-0.0013×10^{-4}

Table 3.1: Error for the cubature method in the OU-case (absolute error)

In Table 3.1, the error, i. e. the output of the method minus the true value given above, are presented. p is the number of cubature steps, i. e. the number of iterations of the one-step cubature method. We use a uniform grid with respect to the cubature formula. The discretization in space, i. e. of $]0,1[$, used by the PDE solver contains 50 uniform points, the discretization of the time-interval – additional to the one induced by the cubature method – contains 500 points. The stochastic perturbation factor ϕ is chosen to be $\phi(u) = \sin(\pi u)$, i. e. $\phi \in \mathcal{D}(\Delta^\infty)$ even. We see a very fast decrease of the error in this simple situation. On the other hand, the variance of the random variable on the tree considered before is clearly too high for the Monte-Carlo simulation on the tree to work. Indeed, $\Phi(X_1^x)$ has true standard deviation of

$$\mathrm{sd}(\Phi(X_1^x)) = \sqrt{\frac{2}{\pi^4}(1-e^{-2\pi^2})} = 0.1433. \tag{3.14}$$

Assuming that the central limit theorem applies, confidence intervals around the solution given by a Monte-Carlo method are proportional to the standard deviation divided by the square root of the number of trajectories. Consequently, we would roughly need to calculate 10^{12} paths on the tree in order to achieve a similar level of exactness as in Table 3.1! Indeed, note that the standard deviation of the solution is of order 10^{-1}, while the error in the last

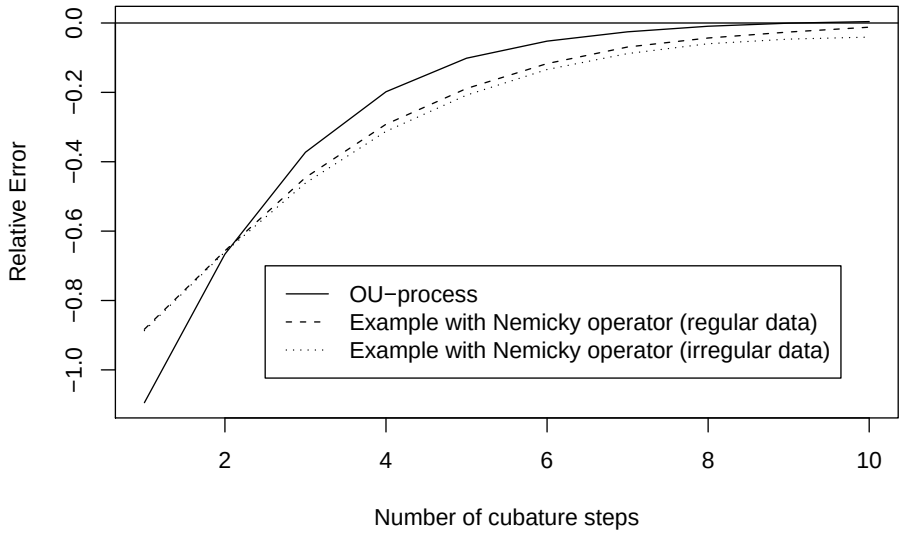


Figure 3.1: Relative errors for the OU-process (equation (3.11)) and the process with nonlinear volatility (equation (3.15)). In the latter case, both initial values $x(u) = \sin(\pi u)$ – referred to as "regular case" – and x given by (3.18) – referred to as "irregular case" – are used.

row of Table 3.1 is of order 10^{-7}. The equation

$$\frac{10^{-1}}{\sqrt{m}} \approx 10^{-7}$$

then gives $m \approx 10^{12}$. Note that this heuristics is also confirmed by our experiments, where Monte-Carlo simulation on the tree clearly fails. The data are also shown in Figure 3.1 and Figure 3.2, where the failure of the Monte-Carlo simulation on the cubature tree can be seen.

Remark 3.2.1. The failure of Monte-Carlo simulation on the tree also applies to any other (naive) Monte-Carlo approach to problem (3.11), including the usual finite element or finite difference approaches.

As a more realistic example we consider the heat equation with a stochastic perturbation involving a Nemicky operator. More precisely, consider

$$dX_t^x = \Delta X_t^x dt + \sin \circ X_t^x dB_t, \tag{3.15}$$

with $x(u) = \sin(\pi u)$. Even though we do not know the law of the solution X_1^x of (3.15), we are still able to calculate $E(\Phi(X_1^x))$ explicitly because Φ is

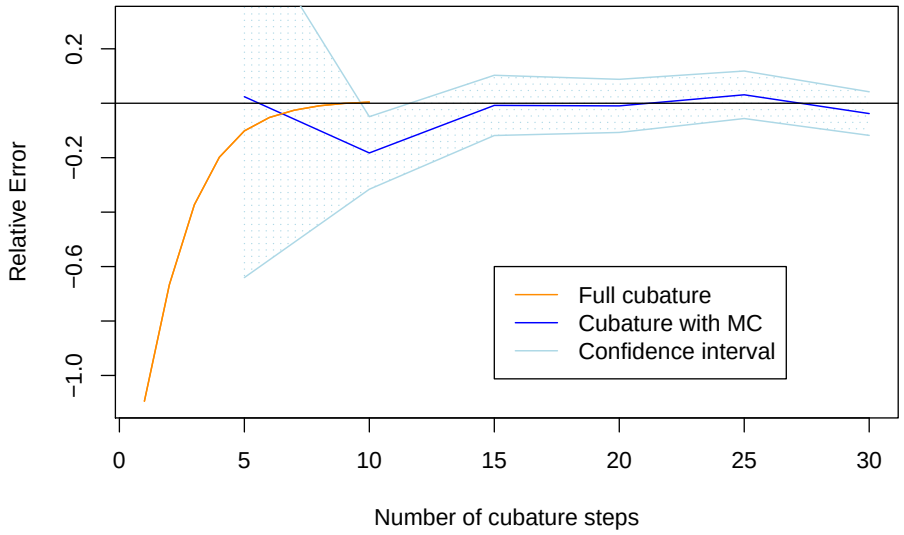


Figure 3.2: Relative errors for the OU-process (equation (3.11)) using the cubature method and the Monte-Carlo simulation on the cubature tree

a linear functional. Indeed, X_1^x is given by

$$X_1^x = S_1 x + \int_0^1 S_{1-s} \sin \circ X_s^x dB_s \tag{3.16}$$

and, consequently,

$$\Phi(X_1^x) = \Phi(S_1 x) + \int_0^1 \Phi(S_{1-s} \sin \circ X_s^x) dB_s.$$

The expectation of the (one-dimensional) Itô-integral is 0 and we get the same result as before, i. e.

$$E(\Phi(X_1^x)) = \Phi(S_1 x) = 0.3293 \times 10^{-4}$$

for $x(u) = \sin(\pi u)$. Nevertheless, we believe that this example is already quite difficult, especially since the cubature method actually has to work with the Stratonovich formulation

$$dX_t^x = \big(\Delta X_t^x - \frac{1}{2} \cos \circ X_t^x \sin \circ X_t^x\big) dt + \sin \circ X_t^x dB_t. \tag{3.17}$$

In particular, the equation (in Stratonovich form) has a non-linear drift and a non-linear volatility.

l	Error
1	-0.2907×10^{-4}
2	-0.2163×10^{-4}
3	-0.1467×10^{-4}
4	-0.0961×10^{-4}
5	-0.0622×10^{-4}
6	-0.0385×10^{-4}
7	-0.0228×10^{-4}
8	-0.0142×10^{-4}
9	-0.0086×10^{-4}
10	-0.0040×10^{-4}

Table 3.2: Results of the cubature method for (3.15) (absolute error)

Note that we expect the standard deviation of the solution of the above equation to be smaller than before, because $(\sin \circ X_t^x)^2$ decreases as X_t^x decreases in t. The space discretization used by the PDE-solver has size 50, which already seems to be sufficient, because using a finer discretization (100 grid points) does not change the results significantly. Table 3.3 shows the

l	m	Error	Stat. Error
5	32	0.0567×10^{-4}	0.1498×10^{-4}
10	1000	-0.0325×10^{-4}	0.0179×10^{-4}
15	1500	-0.0184×10^{-4}	0.0172×10^{-4}
20	2000	0.0128×10^{-4}	0.0170×10^{-4}
25	2500	0.0179×10^{-4}	0.0145×10^{-4}
30	3000	0.0596×10^{-4}	0.0167×10^{-4}

Table 3.3: Results of the cubature method with Monte-Carlo simulation on the tree for (3.15) (absolute error)

results using Monte-Carlo simulation on the tree. m denotes the number of trajectories followed, while the "Statistical Error" in the table is an indicator for the error of the Monte-Carlo simulation. More precisely, the values in the last column are the empirical standard deviations of the result divided by the square root of the number of trajectories. Comparable to the Ornstein-Uhlenbeck process, the convergence of the pure cubature method is very fast, see Table 3.2. The (empirical) variance is, however, quite large such that the Monte-Carlo aided method does not work at all. Note that the statistical error in Table 3.3 is of the order of the total computational error, which can be almost completely attributed to the Monte Carlo simulation.

To test the method further we also try more irregular data. Let

$$x(u) = \frac{1}{2}\sqrt{\frac{1-2\left|u-\frac{1}{2}\right|}{\sqrt{\left|u-\frac{1}{2}\right|}}}. \tag{3.18}$$

The exact value of the quantity of interest $E(\Phi(X_1^x)) = \Phi(S_1 x)$ is calculated by solving the corresponding heat equation numerically. This gives the value $E(\Phi(X_1^x)) = 0.3002 \times 10^{-4}$. x given in (3.18) is in $L^2(]0,1[)$ but its derivative is no longer square-integrable. Consequently, $x \notin \mathcal{D}(A)$ and the theory does not provide an order of approximation. Nevertheless, probably due to the smoothing-properties of the Laplace operator, numerical results show the same behavior as before, see Figure 3.1.

If we replace the heat equation (3.11) by an evolution equation of the form

$$dX_t^x = \frac{d}{du}X_t^x dt + \sin \circ X_t^x dB_t, \tag{3.19}$$

then we still see the same kind of behavior if we fix the space-discretization for the PDE-solver. This time, the PDEs require a much finer space resolution in order to give reliable numbers.

Chapter 4

Reflected diffusions

In this chapter, algorithms for approximations of reflected diffusions, i. e. of SDEs which are defined in a certain domain such that the solution is reflected at the boundary of the said domain in a certain, well-specified sense. From a numerical point of view, these stochastic differential equations are interesting because they provide stochastic representations for (suitable) parabolic PDEs with Neumann boundary conditions. Moreover, certain applications in financial mathematics also exist, e. g. in the context of look-back options. Unfortunately, the speed of convergence of standard numerical methods is unsatisfactory slow, therefore we have constructed an adaptive Euler scheme for reflected diffusion. Furthermore, we give a second scheme, which, however, can only be applied in certain circumstances.

This chapter is based on joint work with Anders Szepessy and Raùl Tempone. Since this is still work in progress, even though in already rather advanced shape, a more detailed and polished presentation of this work shall appear later in an article.

4.1 Introduction

4.1.1 Theory of reflected diffusions

Let $B = (B_t)_{t\in[0,\infty[}$ be a Brownian motion defined on $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\in[0,\infty[}, P)$. Informally, a reflected diffusion will be the solution of a stochastic differential equation "reflected" at the boundary of a domain D, i. e. the reflected diffusions

- (locally) solves the governing SDE in the interior $\operatorname{int} D$,
- stays in $\overline{D}$ almost surely and
- satisfies "some boundary behavior" at the boundary ∂D of the domain.

In stochastic analysis, properties of a process at the boundary of a domain are closely linked with the so-called *local time* of the process. Consequently,

we will first briefly recall the definition of local times, for more information see Revuz and Yor [68]. For simplicity, we only consider the one dimensional situation. The following Definition 4.1.1 uses [68, Corollary VI.1.9].

Definition 4.1.1. Given a continuous semi-martingale $X = (X_t)_{t\in[0,\infty[}$ with values in $\mathbb{R}$ and a fixed number $a \in \mathbb{R}$. The *local time* of X at a is the stochastic process defined by

$$L_t^a(X) = \lim_{\epsilon\to 0+} \frac{1}{\epsilon} \int_0^t \mathbf{1}_{[a,a+\epsilon[}(X_s) d\left\langle X\,, X\right\rangle_s,$$

where $\langle X\,, X\rangle$ denotes the quadratic variation of X. If X is a continuous locale martingale, we may equivalently write

$$L_t^a(X) = \lim_{\epsilon\to 0+} \frac{1}{2\epsilon} \int_0^t \mathbf{1}_{]a-\epsilon,a+\epsilon[}(X_s) d\left\langle X\,, X\right\rangle_s.$$

The process $L^a = (L_t^a(X))_{t\in[0,\infty[}$ is a continuous increasing stochastic process, and the corresponding random measure is a. s. supported by $\{\, t \mid X_t = a \,\}$. Moreover, we have *Tanaka's formula*

$$|X_t - a| = |X_0 - a| + \int_0^t \operatorname{sign}(X_s - a) dX_s + L_t^a. \tag{4.1}$$

Let us now specialize to the case of a Brownian motion. In the sequel, let $L_t = L_t^0(B)$ be the local time of the Brownian motion at 0. By Tanaka's formula,

$$|B_t| = \int_0^t \operatorname{sign}(B_s) dB_s + L_t,$$

where

$$\beta_t = \int_0^t \operatorname{sign}(B_s) dB_s$$

is, again, a standard Brownian motion. β is known as *Lévy transformation* of the Brownian motion B. Its natural filtration coincides with the filtration generated by the process $|B|$, which is called Brownian motion reflected at 0. In this case, we have a rather simple formula for the local time by

$$L_t = \sup_{0\le s\le t} (-\beta_s). \tag{4.2}$$

Now we give a formal definition of a reflected diffusion and an existence and uniqueness result based on Saisho [71]. First we have to impose some regularity conditions on the domain. Let $D \subset \mathbb{R}^d$ be an open set and consider, for $x \in \partial D = \overline{D} \setminus \operatorname{int} D$, the set of *inward normal unit vectors* $\mathcal{N}_x$ defined by

$$\mathcal{N}_x = \bigcup_{r>0} \mathcal{N}_{x,r}, \quad \mathcal{N}_{x,r} = \left\{ y \in \mathbb{R}^d \;\middle|\; \|y\| = 1,\ B(x - ry, r) \cap D = \varnothing \right\},$$

where $B(x, r)$ denotes the sphere with radius r centered at x. We impose the following uniform condition on D.

Assumption 4.1.2. There exists a constant $r > 0$ such that $\mathcal{N}_x = \mathcal{N}_{x,r} \neq \varnothing$ for every $x \in \partial D$.

Remark 4.1.3. Note that Assumption 4.1.2 does not require uniqueness of the inward normal unit vector, in particular, non-differentiable domains are not excluded. In [71], an alternative local assumption is provided. We choose the above uniform condition because it will be satisfied by our numerical examples.

Let B be a d-dimensional Brownian motion and consider a drift vector field $V : \overline{D} \to \mathbb{R}^d$ and diffusion vector fields $V_1, \ldots, V_d : \overline{D} \to \mathbb{R}^d$, which are assumed to be bounded and Lipschitz continuous. We consider the Skorohod equation

$$dX_t^x = V(X_t^x)dt + \sum_{i=1}^{d} V_i(X_t^x)dB_t^i + n(t)dZ_t^x, \tag{4.3}$$

with initial value $X_0^x = x \in D$, $Z_0^x = 0 \in \mathbb{R}$, and an adapted process $n(t)$ satisfying $n(t) \in \mathcal{N}_{X_t^x}$ provided that $X_t^x \in \partial D$.

Remark 4.1.4. The theory and the numerical analysis of reflected diffusions works just as well in the non-autonomous case, i. e. if the above vector fields $V, V_1, \ldots, V_d$ are time-dependent – sometimes with obvious modifications. For simplicity, we formulate our results only in the autonomous situation.

Definition 4.1.5. A pair $(X^x, Z^x) = (X_t^x, Z_t^x)_{t\in[0,\infty[}$ of continuous adapted processes with values in $\overline{D}$ and $[0, \infty[$, respectively, are strong solutions of the Skorohod equation (4.3) if $X_0^x = x$, $Z_0^x = 0$, Z^x is an increasing process satisfying

$$Z_t^x = \int_0^t \mathbf{1}_{\partial D}(X_s^x)dZ_s^x \tag{4.4}$$

for all $t \in [0, \infty[$ and the integrated version of equation (4.3) holds true, where $n(t)$ is a given adapted process such that $n(s) \in \mathcal{N}_{X_s^x}$ provided that $X_s^x \in \partial D$.

Remark 4.1.6. For general domains as in Assumption 4.1.2, the solution of (4.3) depends on the choice of the process n. In most situations, however, the boundary of D will be regular enough such that there is almost always a unique inward pointing normal vector. Then $n(t) = n(X_t^x)$ is a function of the position for t such that $X_t^x \in \partial D$.

Remark 4.1.7. Equation (4.3) defines a reflected diffusion with normal reflection. It is also possible to consider oblique reflections. The existence and uniqueness result requires, however, that the oblique reflection is uniformly non-parallel to the boundary.

Remark 4.1.8. Equation (4.4) means that the random measure induced by the increasing process Z^x is concentrated on $\{ t \mid X_t^x \in \partial D \}$. Therefore, we informally call Z^x *local time*. Notice, however, that this practice is incorrect because Z_t^x is not the local time in the sense of Definition 4.1.1. Indeed, let $d = 1$ and consider $V \equiv 0$ and $V_1 \equiv 1$ and the domain $D =]0, \infty[$. If we start at $x = 0$, we have

$$X_t = B_t + Z_t,$$

noting that the inward pointing normal vector is given by $n \equiv 1$. Given a Brownian motion W and its Lévy transform $\beta_t = \int_0^t \operatorname{sign}(W_s) dW_s$, the reflected Brownian motion satisfies

$$|W_t| = \beta_t + L_t$$

by Tanaka's formula, where L_t denotes the local time of W_t at 0. Comparing these two equations, we see that Z_t is not the local time of B, but it is the local time of a Brownian motion W such that

$$B_t = \int_0^t \operatorname{sign}(W_s) dW_s,$$

i. e. $Z_t = L_t(W)$. Moreover, $X_t = |W_t|$. Of course, we have the equalities in law

$$X_t \sim |B_t| \text{ and } Z_t \sim L_t(B).$$

Proposition 4.1.9. *Under the above assumptions, the Skorohod equation* (4.3) *has a unique strong solution.*

Proof. This is [71, Theorem 5.1]. □

Reflected diffusions give stochastic representations of parabolic PDEs with Neumann boundary conditions. We refer to Freidlin [26] for more details. Recall the definition of the infinitesimal generator L in (1.4). For simplicity, we confine ourselves to the Neumann problem with normal Neumann condition.

$$\text{(4.5)} \qquad \begin{cases} \dfrac{\partial}{\partial t} u(t,x) = Lu(t,x), & (t,x) \in [0,T] \times D, \\ u(0,x) = f(x), & x \in D, \\ \dfrac{\partial}{\partial n} u(t,x) = h(x), & x \in \partial D, \end{cases}$$

where $f : \overline{D} \to \mathbb{R}$ and $h : \partial D \to \mathbb{R}$ are sufficiently regular functions, $n(x)$ is assumed to be the unique inward normal vector at $x \in \partial D$ and we denote

$$\frac{\partial}{\partial n} u(t,x) = \langle \nabla u(t,x), n(x) \rangle,$$

the normal derivative of $u(t,x)$ at $x \in \partial D$. By a solution of (4.5) we understand a function $u \in C^{1,2}([0,T] \times \overline{D})$ satisfying the above PDE.

Proposition 4.1.10. *Assume that the solution u of problem (4.5) has bounded time-derivative, gradient and Hessian matrix for all $(t,x) \in [0,T] \times \overline{D}$. Then we have the stochastic representation*

$$u(t,x) = E\Big(f(X_t^x) - \int_0^t h(X_s^x) dZ_s^x\Big).$$

Proof. The proposition is a special case of [26, Theorem II.5.1]. Nevertheless, we repeat the simple and instructive proof.

Fixing $T > 0$ and applying Itô's formula to $u(T-t, X_t^x)$ gives

$$\begin{aligned} u(0, X_T^x) = u(T,x) &+ \int_0^T \Big(Lu(T-t,x) - (\frac{\partial}{\partial t}u)(T-t, X_t^x)\Big) dt \\ &+ \sum_{i=1}^n \int_0^T \langle \nabla u(T-t, X_t^x), V_i(X_t^x)\rangle \, dB_t^i \\ &+ \int_0^T \langle \nabla u(T-t, X_t^x), n(X_t^x)\rangle \, dZ_t^x. \end{aligned}$$

Note that dZ_t^x is concentrated on $\{X_t^x \in \partial D\}$, consequently we may replace the integrand in the last term by $\frac{\partial}{\partial n} u(T-t, X_t^x) = h(X_t^x)$. Furthermore, the $Lu - \frac{\partial}{\partial t} u = 0$ by the PDE. Taking expectations concludes the proof. □

4.1.2 Approximation of reflected diffusions

We give a review of the some approximation methods for reflected diffusions as introduced above. We first present the standard Euler approach, see Costantini, Pacchiarotti and Sartoretto [16]. This approach yields a method with weak order of convergence $\frac{1}{2}$ – in particular, they give a simple example, where this convergence rate is precise. Note that their algorithm allows for mixed Neumann and Dirichlet (corresponding to stopped diffusions) boundary conditions, as in our second example. On the other hand, they only consider normal reflection. Gobet [28] has constructed an algorithm based on a half-space approximation of the the boundary of the domain. In certain cases, he can prove a convergence with rate 1. Finally, Bossy, Gobet and Talay [10] have found a method with order one based on symmetrization, provided that the boundary condition satisfies $h \equiv 0$ (also for oblique reflections).

Since the algorithm in [16] is the basis of our algorithms, as well as of the two other algorithms mentioned above, we shall give a rather detailed description. For simplicity, assume that $\#\mathcal{N}_x = 1$ for each $x \in \partial D$. Furthermore, assume that we can find a unique projection $\Pi(x) \in \partial D$ for each $x \notin \overline{D}$. Fix $T > 0$ and an initial condition $x \in \overline{D}$. Algorithm 4.1.11 is, in fact, a straight-forward discretization of the Skorohod equation (4.3). Indeed, we

have

$$X^x_{t_{i+1}} \approx X^x_{t_i} + V\big(X^x_{t_i}\big)\Delta t_i + \sum_{j=1}^{d} V_j\big(X^x_{t_i}\big)\Delta B^j_i + n\big(X^x_{t_i}\big)\Delta Z_{t_i}.$$

Setting

$$\hat{X}_{i+1} = X^x_{t_i} + V\big(X^x_{t_i}\big)\Delta t_i + \sum_{j=1}^{d} V_j\big(X^x_{t_i}\big)\Delta B^j_i,$$

we get

$$X^x_{t_{i+1}} - \hat{X}_{i+1} \approx n\big(X^x_{t_i}\big)\Delta Z_{i+1},$$

or

$$\Delta Z_{i+1} \approx \left\| X^x_{t_{i+1}} - \hat{X}_{i+1} \right\|.$$

This motivates the following algorithm.

Algorithm 4.1.11. *Fix a uniform time discretization $0 = t_0 < t_1 < \cdots < t_N = T$, i. e. $\Delta t_i = t_{i+1} - t_i = \frac{T}{N}$, $i = 0, \ldots, N-1$. Moreover, fix an i. i. d. sequence of random variables $(\Delta\overline{B}_i)_{i=0}^{N-1}$ such that the moments of order up to three of $\Delta\overline{B}_0$ (and hence of all $\Delta\overline{B}_i$) coincide with those of an n-dimensional normal random variable with covariance matrix $\frac{T}{N}\,\mathrm{id}_n$, cf. Case B in Section 1.3.*

(1) Set $\overline{X}^N_0 = x$, $\overline{Z}^N_0 = 0$, and $i = 0$.

(2) Set

$$\hat{X}^N_{i+1} = \overline{X}^N_i + V\big(\overline{X}^N_i\big)\Delta t_i + \sum_{j=1}^{n} V_j\big(\overline{X}^N_i\big)\Delta\overline{B}^j_i.$$

(3) Set

$$\overline{X}^N_{i+1} = \begin{cases} \hat{X}^N_{i+1}, & \hat{X}^N_{i+1} \in \overline{D}, \\ \Pi(\hat{X}^N_{i+1}), & \hat{X}^N_{i+1} \notin \overline{D}, \end{cases}$$

$$\overline{Z}^N_{i+1} = \begin{cases} \overline{Z}^N_i, & \hat{X}^N_{i+1} \in \overline{D}, \\ \overline{Z}^N_i + \left\| \Pi(\hat{X}^N_{i+1}) - \hat{X}^N_{i+1} \right\|, & \hat{X}^N_{i+1} \notin \overline{D}. \end{cases}$$

(4) Increase i by one. If $i < N$, go back to (2).

(5) Calculate

$$\overline{F}^N = f\big(\overline{X}^N_N\big) - \sum_{i=0}^{N-1} h\big(\overline{X}^N_{i+1}\big)\Delta\overline{Z}^N_i.$$

The solution $u(T,x) \approx E\big(\overline{F}^N\big)$ is then calculated by Monte Carlo simulation from the distribution $\overline{F}^N$ given in Algorithm 4.1.11 above.

If u is sufficiently regular (e. g. $u \in C_b^3([0,T] \times \overline{D})$ and the random variables $\Delta\overline{B}_i$ are either bounded or Gaussian, then we have

$$\left|u(T,x) - E\Big(\overline{F}^N\Big)\right| \leq \frac{C}{N^{1/2}}, \tag{4.6}$$

where $\Delta\overline{Z}_i^N = \overline{Z}_{i+1}^N - \overline{Z}_i^N$, $i = 0, \ldots, N-1$. This result is [16, Theorem 3.4, Theorem 3.6], together with a remark in [28].

The basic idea of the half-space approach of [28] is that the solution of the Skorohod equation (4.3) with constant coefficients can be given explicitly, if D is a half-space, compare the one-dimensional version (4.2) given above, noting that the rôle of β is now played by B.

More precisely, assume that we have already constructed $\overline{X}_l^N$ and $\overline{Z}_l^N$, $l = 0, \ldots, i$. In order to construct $\overline{X}_{i+1}^N$ and $\overline{Z}_{i+1}^N$, we project $\overline{X}_i^N$ to the boundary (along the normal direction), finding the point $\widetilde{X}$. Now we calculate the exact solution $(\hat{X}_{i+1}^N, \hat{Z}_{i+1}^N)$ at time t_{i+1} of the reflected diffusion problem with constant coefficients $V\big(\overline{X}_i^N\big)$ and $V_1\big(\overline{X}_i^N\big), \ldots, V_n\big(\overline{X}_i^N\big)$ and for the domain given by the half-space bounded by the tangent hyperplane on D at $\widetilde{X}$. If the new point $\hat{X}_{i+1}^N \in \overline{D}$, then we set $\overline{X}_{i+1}^N = \hat{X}_{i+1}^N$ and $\overline{Z}_{i+1}^N = \overline{Z}_i^N + \hat{Z}_{i+1}^N$. Otherwise, we project $\hat{X}_{i+1}^N$ back to $\overline{D}$, $\overline{X}_{i+1}^N = \Pi(\hat{X}_{i+1}^N)$, and add an additional increment to the local time. The quantity of interest $u(T,x)$ is now similarly approximated as in (4.6), with one difference: now the approximation of the local time may increase in a subinterval $[t_i, t_{i+1}]$, i. e. $\Delta\overline{Z}_i^N > 0$, even though $\overline{X}_{i+1}^N \in \operatorname{int} D$. Consequently, we need to replace the term $h\big(\overline{X}_{i+1}^N\big)$ by $h\big(\Pi\big(\overline{X}_{i+1}^N\big)\big)$ this time.

Under some regularity conditions, Gobet [28] proves weak convergence of this method to the solution of the Neumann boundary problem (4.5). The rate of convergence is $\frac{1}{2}$, but it is 1 in case of *co-normal reflection*, i. e. if the reflection is along the (normalized) direction

$$\gamma(x) = \langle V_1(x), n(x)\rangle V_1(x) + \cdots + \langle V_d(x), n(x)\rangle V_n(x).$$

However, Gobet conjectures that this order of convergence holds for more general situations.

Finally, Bossy, Gobet and Talay [10] have constructed a symmetrized Euler scheme. But for one difference, the scheme is equal to Algorithm 4.1.11. This difference is the calculation of $\overline{X}_{i+1}^N$ from $\hat{X}_{i+1}^N$ in the case $\hat{X}_{i+1}^N \notin \overline{D}$: instead of merely projecting $\hat{X}_{i+1}^N$ to ∂D as in Algorithm 4.1.11, the new point $\overline{X}_{i+1}^N \in \operatorname{int} D$ is found by projecting onto ∂D and then following the direction γ of reflection further into the interior of the domain, such that $\overline{X}_{i+1}^N$ and $\hat{X}_{i+1}^N$ have the same distance to ∂D along the direction γ. The

algorithm converges with order 1 provided that $h \equiv 0$, but in that case also for oblique reflection.

4.2 New algorithms for reflected diffusions

Both our algorithms are based on the Algorithm 4.1.11 of Costantini et al. [16]. Let us first give an error expansion for this method, which is a slight variation of the proof of Proposition 4.1.10.

Definition 4.2.1. Let $\overline{X}_i^N$, $\overline{Z}_i^N$, $i = 0, \dots, N$, be the approximations of X^x and Z^x based on the grid $0 = t_0 < \cdots < t_N = T$ and Gaussian increments $\Delta\overline{B}_i^N = B_{t_{i+1}} - B_{t_i}$. We define a continuous process in continuous time by $\overline{X}_t^N = \overline{X}_i^N$ for $t = t_i$, $i = 0, \dots, N$, and

$$\overline{X}_t^N = \overline{X}_i^N + V\big(\overline{X}_i^N\big)(t - t_i) + \sum_{j=1}^{d} V_i\big(\overline{X}_i^N\big)(B_t^j - B_{t_i}^j),$$

for $t_i < t < t_{i+1}$, $i = 0, \dots, N-1$.

Of course, $\overline{X}_t^N$ is only defined for theoretical purposes. As in the proof of Proposition 4.1.10, we consider the function $v(t,x) = u(T-t,x)$. Obviously, v solves the Neumann problem

$$\begin{cases} \dfrac{\partial}{\partial t} v(t,x) + Lv(t,x) = 0, \\ v(T,x) = f(x), \\ \dfrac{\partial}{\partial n} v(t,x) = h(x), \end{cases} \tag{4.7}$$

where $t \in [0,T[$ and x needs to be chosen appropriately, cf. equation (4.5) for the Neumann problem solved by u. Moreover, v has the stochastic representation

$$v(t,x) = E\bigg(f(X_T) - \int_t^T h(X_s)\,dZ_s \;\bigg|\; X_t = x\bigg). \tag{4.8}$$

In order to get an error representation, we first rewrite $v(T,x) - v(0,x)$ using telescopic sum as

$$\begin{aligned} E\big(f\big(\overline{X}_N^N\big)\big) - v(0,x) &= \sum_{i=0}^{N-1} E\big(v(t_{i+1}, \overline{X}_{i+1}^N) - v\big(t_i, \overline{X}_i^N\big)\big) \\ &= \sum_{i=0}^{N-1} \underbrace{E\big(v(t_{i+1}, \overline{X}_{i+1}^N) - v\big(t_{i+1}, \hat{X}_{i+1}^N\big)\big)}_{(I)} \\ &\quad + \sum_{i=0}^{N-1} \underbrace{E\big(v\big(t_{i+1}, \hat{X}_{i+1}^N\big) - v\big(t_i, \overline{X}_i^N\big)\big)}_{(II)}. \end{aligned} \tag{4.9}$$

Here we implicitly assume that v also makes sense on $\overline{D}^c$, since $\hat{X}^N_{i+1} \notin \overline{D}$ is possible. We will come back to this point later.

For the expansion of (II), note that

$$\hat{X}^N_{i+1} - \overline{X}^N_i = \int_{t_i}^{t_{i+1}} d\overline{X}^N_s ,$$

by Definition 4.2.1 above. Consequently, Itô's formula yields

$$\begin{aligned} v\big(t_{i+1}, \hat{X}^N_{i+1}\big) - v\big(t_i, \overline{X}^N_i\big) &= \int_{t_i}^{t_{i+1}} \big(\frac{\partial}{\partial t} v\big)\big(s, \overline{X}^N_s\big) ds + \int_{t_i}^{t_{i+1}} \overline{L}_{\overline{X}^N_i} v\big(s, \overline{X}^N_s\big) ds + \cdots \\ &= \int_{t_i}^{t_{i+1}} \big(\overline{L}_{\overline{X}^N_i} - L\big) v\big(s, \overline{X}^N_s\big) ds + \cdots , \end{aligned}$$

where we used the PDE to re-express $\frac{\partial}{\partial t} v = -Lv$. Moreover, "$\cdots$" denotes a martingale term with expectation 0 and the differential operator $\overline{L}_y$, $y \in \mathbb{R}^n$ fixed, is the infinitesimal generator of the SDE with constant vector fields $V(y), V_1(y), \ldots, V_d(y)$, i. e.

$$\overline{L}_y g(x) = \sum_{j=1}^{d} V^j(y) \frac{\partial}{\partial x_j} g(x) + \frac{1}{2} \sum_{i,j=1}^{d} a_{ij}(y) \frac{\partial^2}{\partial x_i \partial x_j} g(x),$$

where $a(y) = \sigma(y)\sigma(y)^T$ and $\sigma(y) = (\sigma_{ij}(y))_{i,j=1}^d$ with $\sigma_{ij}(y) = V^i_j(y)$. Taking expectations, we get

$$(II) = \int_{t_i}^{t_{i+1}} E\Big(\big(\overline{L}_{\overline{X}^N_i} - L\big) v\big) s, \overline{X}^N_s \big)\Big) ds.$$

On the other hand, (I) is expanded by ordinary, path-wise Taylor expansion. Indeed, notice that

$$\overline{X}^N_{i+1} = \hat{X}^N_{i+1} + n\big(\overline{X}^N_{i+1}\big) \Delta \overline{Z}^N_i .$$

Thus,

$$\begin{aligned} (I) &= v\big(t_{i+1}, \overline{X}^N_{i+1}\big) - v\big(t_{i+1}, \overline{X}^N_{i+1} - n\big(\overline{X}^N_{i+1}\big) \Delta \overline{Z}^N_{i+1}\big) \\ &= \frac{\partial}{\partial n} v\big(t_{i+1}, \overline{X}^N_{i+1}\big) \Delta \overline{Z}^N_i \\ &\quad - \int_0^1 (1-\theta) \frac{\partial^2}{\partial n\big(\overline{X}^N_{i+1}\big)^2} v\big(t_{i+1}, \overline{X}^N_{i+1} - \theta \Delta \overline{Z}^N_i n\big(\overline{X}^N_{i+1}\big)\big) d\theta \big(\Delta \overline{Z}^N_i\big)^2, \end{aligned}$$

where $\frac{\partial^2}{\partial n}$ does not denote the second normal derivative in the sense of the normal derivative of the normal derivative, but

$$\frac{\partial^2}{\partial n(y)^2} g(x) = \frac{\partial^2}{\partial \epsilon^2}\Big|_{\epsilon=0} g(x + \epsilon n(y)) \tag{4.10}$$

$x, y \in \mathbb{R}^d$. By the boundary condition, $\frac{\partial}{\partial n} v\big(t_{i+1}, \overline{X}^N_{i+1}\big) = h\big(\overline{X}^N_{i+1}\big)$ at the boundary (otherwise, $\Delta \overline{Z}^N_i = 0$).

Re-inserting the changed terms (I) and (II), we get an error expansion for

$$\overline{v}(0,x) = E\bigg(f\big(\overline{X}^N_N\big) - \sum_{i=0}^{N-1} h\big(\overline{X}^N_{i+1}\big) \Delta \overline{Z}^N_i \bigg) \tag{4.11}$$

in the form

$$\begin{aligned} \overline{v}(0,x) - v(0,x) &= \int_0^T E\Big(\big(\overline{L}_{\overline{X}^N_{\lfloor t \rfloor}} - L\big) v\big(t, \overline{X}^N_t\big) \Big) dt \\ -E\bigg(\sum_{i=0}^{N-1} \big(\Delta \overline{Z}^N_i\big)^2 \int_0^1 (1-\theta) &\frac{\partial^2}{\partial n \big(\overline{X}^N_{i+1}\big)^2} v\big(t_{i+1}, \overline{X}^N_{i+1} - \theta \Delta \overline{Z}^N_i n\big(\overline{X}^N_{i+1}\big)\big) d\theta \bigg), \end{aligned} \tag{4.12}$$

where $\lfloor t \rfloor = \max\{\, t_i \mid i \in \{0, \dots, N\},\ t_i \le t \,\}$, $t \in [0,T]$. Naturally, this immediately gives an error expansion for $u(T,x) = v(0,x)$.

Remark 4.2.2. The error expansion (4.12) naturally splits into two parts. The first part, i. e.

$$\int_0^T E\Big(\big(\overline{L}_{\overline{X}^N_{\lfloor t \rfloor}} - L\big) v\big(t, \overline{X}^N_t\big) \Big) dt$$

is well understood since this is the first order term for the usual Euler-Maruyama method for (non-reflected) SDEs, provided that the equation can be extended outside of D. We will refer to this part as *interior error*, since its main contributions are discretization errors in the interior of the domain.

Much more interesting for our study is the second term in the error expansion,

$$E\bigg(\sum_{i=0}^{N-1} \big(\Delta \overline{Z}^N_i\big)^2 \int_0^1 (1-\theta) \frac{\partial^2}{\partial n \big(\overline{X}^N_{i+1}\big)^2} v\big(t_{i+1}, \overline{X}^N_{i+1} - \theta \Delta \overline{Z}^N_i n\big(\overline{X}^N_{i+1}\big)\big) d\theta \bigg), \tag{4.13}$$

which measure the contribution from the reflection. In order to assert the meaning of (4.13), let us take a first look at it. Assume that the equation is nice enough such that $\frac{\partial^2}{\partial n^2} v$ is uniformly bounded on $[0,T] \times \overline{D}$. Then the integral term can be bounded by some constant, and we are left with

$$CE\Big(\textstyle\sum_{i=0}^{N-1} \big(\Delta \overline{Z}^N_i\big)^2 \Big).$$

Heuristically, the number of hits at the boundary, i. e. the number of indices i such that $\Delta \overline{Z}^N_i \neq 0$, increases like $\sqrt{N}$ with the number of time-steps. On the other hand, given a hit takes place, then $\Delta \overline{Z}^N_i \approx \sqrt{\Delta t_i}$, since $\Delta \overline{Z}^N_i$

is, asymptotically, the modulus of the increment of a Brownian motion, or the increment of a Brownian motion conditioned to be positive. Combining these heuristic observations, we get

$$CE\Big(\sum\nolimits_{i=0}^{N-1}(\Delta\overline{Z}_i^N)^2\Big) \approx C\sqrt{N} \times \frac{1}{N} \approx \frac{C}{\sqrt{N}},$$

as it should be by the results of [16].

We present two new algorithms. The first algorithm is based on further analysis of the above error expansion and yields a convergence order $\frac{4}{5}$. The scope of this algorithm is, however, very limited, since it only works in dimension $d = 1$ or in dimensions $d > 1$ provided that we can extend the inward pointing normal vectors n to a vector field defined on $\overline{D}$ such that

$$[n, V](x) = [n, V_i](x) = 0, \quad x \in D,\ i = 1, \ldots, d.$$

The second algorithm is an adaptive algorithm, which is applicable in any dimension. Numerical experiments indicate that in convergence with a rate between $\frac{1}{2}$ and 1, but the rate is unknown to us. We believe that this algorithm is especially useful for domains with non-smooth boundaries and conflicting boundary conditions.

4.2.1 The algorithm with correction term

Since the error term (4.13) is of order $\sqrt{\Delta t}$, it seems to be a promising idea to carry the expansion one step further. If a calculation is still feasible, we may hope to get a better order of convergence for the reflection error. Indeed, the main idea of the algorithm presented in this subsection is to construct a correction term such that the error expansion of the Euler algorithm with correction starts with the term of order 1, instead of order 1/2 as in (4.12). Of course, the computation of the correction term will introduce additional complexity into the algorithm. It will turn out, however, that the resulting algorithm is still more efficient than the ordinary Euler scheme, Algorithm 4.1.11, since the computation of the correction term is comparably cheap in comparison to the approximation of the reflected diffusion.

Remark 4.2.3. It is well known that the interior error decreases with an order one of convergence in terms of Δt under mild conditions on the problem. Consequently, we can concentrate on the error from the reflection. Furthermore, for many considerations we may assume that the coefficients of the SDE in the interior $\operatorname{int} D$ are constant.

Remark 4.2.4. The arguments presented here will stay on the heuristic level as in Remark 4.2.2 above. Rigorous arguments are possible using the techniques of [16], but will only be presented in a subsequent article.

A second order Taylor expansion of the term A in the error expansion (4.9) gives

(4.14)

$$\begin{aligned}\overline{v}(0,x) - v(0,x) = \int_0^T E\Big(\big(\overline{L}_{\overline{X}^N_{\lfloor t \rfloor}} - L\big)v\big(t, \overline{X}^N_t\big)\Big)dt \\ - \frac{1}{2}E\bigg(\sum_{i=0}^{N-1}\big(\Delta\overline{Z}^N_i\big)^2 \frac{\partial^2}{\partial n\big(\overline{X}^N_{i+1}\big)^2} v\big(t_{i+1}, \overline{X}^N_{i+1}\big)\bigg) \\ + \frac{1}{2}E\bigg(\sum_{i=0}^{N-1}\big(\Delta\overline{Z}^N_i\big)^3 \times \\ \times \int_0^1 (1-\theta)^2 \frac{\partial^3}{\partial n\big(\overline{X}^N_{i+1}\big)^3} v\big(t_{i+1}, \overline{X}^N_{i+1} - \theta n\big(\overline{X}^N_{i+1}\big)\Delta\overline{Z}^N_i\big)d\theta\bigg).\end{aligned}$$

Consequently, let us define

(4.15)

$$\overline{\overline{v}}(0,x) = E\bigg(f\big(\overline{X}^N_N\big) - \sum_{i=0}^{N-1} h\big(\overline{X}^N_{i+1}\big)\Delta\overline{Z}^N_i + \frac{1}{2}\sum_{i=0}^{N-1}\big(\Delta\overline{Z}^N_i\big)^2 \overline{\partial^2_n v}(t_{i+1}, \overline{X}^N_{i+1})\bigg),$$

where $\overline{\partial^2_n v}(t_{i+1}, \overline{X}^N_{i+1})$ is a computable approximation

$$\overline{\partial^2_n v}(t_{i+1}, \overline{X}^N_{i+1}) \approx \frac{\partial^2}{\partial n\big(\overline{X}^N_{i+1}\big)^2} v\big(t_{i+1}, \overline{X}^N_{i+1}\big).$$

Remark 4.2.5. If we could work with the exact value for the second normal derivative, in the sense of equation (4.10), then equation (4.14) would give a precise error expansion for $\overline{\overline{v}}$. Indeed, with the same heuristics as before, this approximate error expansion indicates a convergence of order 1. Of course, this presupposes that the approximation $\overline{\partial^2_n v}$ can be calculated with sufficient accuracy and efficiency.

We present a scheme for efficient computation of $\overline{\partial^2_n v}$ applicable in *dimension one*. Unfortunately, we have not found sufficiently efficient methods to approximate the second normal derivative of v in more generality, but under special circumstances. For the remainder of the subsection, we assume $d = 1$. Consequently, all the normal derivatives are, in fact, ordinary derivatives with respect to the space variable x, possibly with a sign, and the domain is an interval $D =]a, b[$, where one of $a, b \in \mathbb{R} \cup \{\pm\infty\}$ may be $\pm\infty$. More precisely, the Neumann boundary condition reads

$$\frac{\partial}{\partial x} v(t,a) = h(a), \quad \frac{\partial}{\partial x} v(t,b) = -h(b), \tag{4.16}$$

provided that both a and b are real numbers. For simplicity, we will only consider the case $a = 0$ and $b = +\infty$, the extension to the general case is trivial.

$v_x = \frac{\partial}{\partial x} v$ solves the following PDE with Dirichlet boundary conditions

$$\text{(4.17)} \qquad \begin{cases} \dfrac{\partial}{\partial t} v_x(t,x) + \widetilde{L} v_x(t,x) = 0, \quad (t,x) \in [0,T[\times D, \\ v_x(T,x) = f'(x), \quad x \in \overline{D}, \\ v_x(t,x) = h(x), \quad (t,x) \in [0,T[\times \partial D. \end{cases}$$

In (4.17), the differential operator $\widetilde{L}$ is no longer of the same form as L, but it still allows for a stochastic representation using the Feynman-Kac formula. Indeed, if

$$Lg(x) = V(x)g'(x) + \frac{1}{2}(V_1(x))^2 g''(x),$$

then

$$\widetilde{L}g(x) = V'(x)g(x) + (V(x) + V_1'(x))g'(x) + \frac{1}{2}(V_1(x))^2 g''(x)$$

has the stochastic representation

$$\begin{aligned} \text{(4.18)} \quad v_x(t,x) = {} & E\left(f'(X_T) \exp\left(\int_t^T V'(X_s) ds \right) \mathbf{1}_{[T,\infty[}(\tau_{t,x}) \middle| X_t = x \right) \\ & + E\left(h(X_{\tau_{t,x}}) \exp\left(\int_t^{\tau_{t,x}} V'(X_s) ds \right) \mathbf{1}_{[t,T[}(\tau_{t,x}) \middle| X_t = x \right), \end{aligned}$$

where

$$\tau_{t,x} = \inf \left\{ \, s > t \, \middle| \, X_s^{t,x} \in \partial D \, \right\},$$

see (4.19). Consequently, in order to compute $v_x(t,x)$ one needs to solve a *stopped diffusion* following the well known SDE

$$\text{(4.19)} \qquad dX_s^{t,x} = V(X_s^{t,x})ds + V_1(X_s^{t,x})dB_s^1, \quad s > t,$$

started at time t and $X_t^{t,x} = x$ and stopped when hitting the boundary ∂D.

Remark 4.2.6. Notice that stopped diffusions are much simpler problems than reflected diffusions. As already indicated in the beginning of this subsection, the computation of the correction term amounts to additionally solving a number of simple problems (compared to the reflected diffusion), namely the stopped diffusions, in order to obtain a faster convergence rate for the reflected diffusion.

The idea for the approximation $\overline{\partial_n^2 v}$ is the following. First note that $\overline{\partial_n^2 v}(t,x)$ is only needed for $x \in \partial D$, i. e. $x = 0$, because otherwise $\Delta \overline{Z} = 0$ owing to the use of Algorithm 4.1.11, see (4.15). We approximate $v_{xx}(t,0) = \frac{\partial^2}{\partial x^2} v(t,x)$ by a finite difference quotient, i. e.

$$\begin{aligned} \text{(4.20)} \qquad v_{xx}(t,0) &= -\frac{v_x(t,0) - v_x(t,\Delta x)}{\Delta x} + \mathcal{O}(\Delta x) \\ &= -\frac{h(0) - v_x(t,\Delta x)}{\Delta x} + \mathcal{O}(\Delta x), \end{aligned}$$

for $\Delta x > 0$ sufficiently small. $v_x(t, \Delta x)$ is then approximated by a stopped diffusion. Notice that we do not need to perform an "inner" Monte Carlo simulation for this computation. Indeed, let $G(t,x)$ denote the random variable under the expectation in (4.18), i. e.

$$G(t,x) = f'(X_T^{t,x}) \exp\Big(\int_t^T V'(X_s^{t,x})ds\Big)\mathbf{1}_{[T,\infty[}(\tau_{t,x}) + h(X_{\tau_{t,x}}^{t,x}) \exp\Big(\int_t^{\tau_{t,x}} V'(X_s^{t,x})ds\Big)\mathbf{1}_{[t,T[}(\tau_{t,x}).$$

Notice that $G(t,x)$ is independent of $\mathcal{F}_t$. Consequently, we have

$$\begin{aligned} E\Big(\sum_{i=0}^{N-1} v_{xx}\big(t_{i+1}, \overline{X}_{i+1}^N\big)\big(\Delta\overline{Z}_i^N\big)^2\Big) &\approx E\Big(\sum_{i=0}^{N-1} \frac{v_x(t_{i+1},\Delta x) - h(0)}{\Delta x}\big(\Delta\overline{Z}_i^N\big)^2\Big) \\ &= E\Big(\sum_{i=0}^{N-1} \frac{E(G(t_{i+1},\Delta x)) - h(0)}{\Delta x}\big(\Delta\overline{Z}_i^N\big)^2\Big) \\ &= E\Big(\sum_{i=0}^{N-1} \frac{G(t_{i+1},\Delta x) - h(0)}{\Delta x}\big(\Delta\overline{Z}_i^N\big)^2\Big), \end{aligned}$$

by independence of $G(t_{i+1}, \Delta x)$ and $\Delta\overline{Z}_i^N$. In order to get a workable algorithm, we need to fix an approximation $\overline{G}(t,\Delta x)$ of $G(t,\Delta x)$. Then, we can finally set

$$\overline{\partial_n^2 v}\big(t_{I+1}, \overline{X}_{i+1}^N\big) = \frac{\overline{G}(t_{i+1},\Delta x) - h(0)}{\Delta x}. \tag{4.21}$$

Remark 4.2.7. Of course, $\overline{\partial_n^2 v}$ as in (4.21) is not a true approximation of v_{xx}, only its expected value is. Δx is a critical parameter for the algorithm and needs to be chosen depending on N and on the approximation method $\overline{G}$.

We use two different methods $\overline{G}$, namely the uniform Euler method, see Gobet [27], and an adaptive Euler scheme, see Dzougoutov et al. [21]. It is well known that the uniform Euler scheme converges with the rate $\frac{1}{2}$, whereas the adaptive scheme has the order 1.

Let us first consider the uniform scheme, i. e. let $(\overline{X}_j^{N,t_{i+1},\Delta x})_{j=i+1}^N$ be the Euler approximation of the SDE started at $\overline{X}_{i+1}^{N,t_{i+1},\Delta x} = \Delta x$ and calculated along the uniform grid $t_{i+1} < t_{i+2} < \ldots < t_N = T$. More precisely, we have

$$\overline{X}_{j+1}^{N,t_{i+1},\Delta x} = \overline{X}_j^{N,t_{i+1},\Delta x} + V\big(\overline{X}_j^{N,t_{i+1},\Delta x}\big)\Delta t_j + V_1\big(\overline{X}_j^{N,t_{i+1},\Delta x}\big)\Delta B_j^1,$$

$j = i+1, \ldots, N-1$. Moreover, let $\overline{\tau}^{N,t_{i+1},\Delta x}$ be the first hitting time of the discrete process $\overline{X}^{N,t_{i+1},\Delta x}$ at D^c – we set $\overline{\tau}^{N,t_{i+1},\Delta x} = \infty$ if no hitting

occurs. For $t = t_{k+1} \geq t_{i+1}$ let

$$I(t_{i+1}, t) = \exp\Big(\sum_{j=i+1}^{k} V'\big(\overline{X}_{j+1}^{N,t_{i+1},\Delta x}\big)\Delta t_j \Big)$$

and define the stopped diffusion started at Δx approximated by a uniform Euler scheme

$$\begin{aligned} \overline{G}^{un}(t_{i+1}, \Delta x) = \Big(& f'\big(\overline{X}_N^{N,t_{i+1},\Delta x}\big)\mathbf{1}_{\{T,\infty\}}\big(\overline{\tau}^{N,t_{i+1},\Delta x}\big) \\ & + h\big(\overline{X}_{\overline{\tau}^{N,t_{i+1},\Delta x}}^{N,t_{i+1},\Delta x}\big)\mathbf{1}_{\{t_{i+2},\ldots,t_{N-1}\}}\big(\overline{\tau}^{N,t_{i+1},\Delta x}\big)\Big) I\big(t_{i+1}, \overline{\tau}^{N,t_{i+1},\Delta x}\big). \end{aligned} \tag{4.22}$$

Of course, if the boundary has been hit before $j = N$, $\overline{G}^{un}$ can already be computed and the iteration does not need to be continued until time T.

Remark 4.2.8. Since we solve the stopped diffusion with the same grid as the outer reflected diffusion, we do not need to sample additional Brownian increments.

We still have to choose the parameter Δx. Notice that we approximate the second derivative v_{xx} with the error

$$v_{xx}(t,0) = \frac{E\big(\overline{G}(t,\Delta x)\big) - h(0)}{\Delta x} + \frac{\mathcal{O}(\sqrt{\Delta t})}{\Delta x} + \mathcal{O}(\Delta x),$$

where $\Delta t = T/N$. Optimizing the error with respect to Δx yields

$$\Delta x = \text{const} \times (\Delta t)^{1/4} = \text{const} \times \Big(\frac{T}{N}\Big)^{1/4}. \tag{4.23}$$

This gives an error from the approximation of the correction term of order

$$E\Big(\sum_{i=0}^{N-1} \mathcal{O}((\Delta t)^{1/4})\big(\Delta \overline{Z}_i^N\big)^2 \Big) = \mathcal{O}(\sqrt{N}) \times \mathcal{O}(N^{-1/4}) \times \mathcal{O}(N^{-1}) = \mathcal{O}(N^{-3/4}).$$

However, we have an additional complexity due to the simulation of $\overline{G}$. Indeed, since $E\big(\overline{\tau}^{N,t,\Delta x}\big) = \mathcal{O}(\Delta x)$, the additional work is of order $N \times \frac{\mathcal{O}(\Delta x)}{T} = \mathcal{O}(N^{3/4})$ per reflection at the boundary. Since these reflections take place $\mathcal{O}(\sqrt{N})$ times, the additional and, hence, the total work is $\mathcal{O}(N^{5/4})$. Therefore, the rate of convergence with respect to the total work $K \approx \text{const} \times N^{5/4}$ is expected to be $\mathcal{O}(K^{-3/5})$.

Remark 4.2.9. Of course, all the arguments in the preceeding paragraph are highly heuristic. For example, the number of hits at the boundary (of the reflected trajectory) and the time until stopping (of the stopped trajectory using the same Brownian increments) are certainly not independent. However, independence would hold if we sampled new, independent increments of Brownian motion for the stopped diffusion. Nevertheless, all the above observations seem to be consistent with the results of numerical experiments. Rigorous proofs need to be provided in a forthcoming paper.

Remark 4.2.10. $E\big(\overline{\tau}^{N,t,\Delta x}\big) = \mathcal{O}(\Delta x)$ is motivated by the following consideration. Let $B_t^{\Delta x}$ be a Brownian motion started at $B_0^{\Delta x} = \Delta x > 0$ and denote by $\tau^{\Delta x}$ the first hitting time of $B_t^{\Delta x}$ at 0, if $B_t^{\Delta x}$ hits 0 before time T, and $\tau^{\Delta x} = T$ otherwise. The distribution of $\tau^{\Delta x}$ is given by

$$P(\tau^{\Delta x} \in ds) = \frac{\Delta x}{\sqrt{2\pi s^3}} e^{-\frac{\Delta x^2}{2s}} ds, \quad s \in [0, T[,$$
$$P(\tau^{\Delta x} = T) = \frac{2}{2\pi} \int_0^{\Delta x/\sqrt{T}} e^{-\frac{s^2}{2}} ds,$$

see Karatzas and Shreve [40]. The first two moments of $\tau^{\Delta x}$ can be explicitly calculated and an expansion in Δx gives

$$E(\tau^{\Delta x}) = \frac{2\sqrt{2T}}{\sqrt{\pi}} \Delta x + \mathcal{O}(\Delta x^2),$$
$$E((\tau^{\Delta x})^2) = \frac{4\sqrt{2T^3}}{3\sqrt{\pi}} \Delta x + \mathcal{O}(\Delta x^3).$$

We do not give a detailed description of the adaptive algorithm for stopped diffusions. We just mention that the adaptive algorithm has an (empirical) rate of convergence 1 in the general case. If the coefficients of the equation are constant, i. e. if there is no error stemming from the discretization in the interior of the domain, then the adaptive algorithm for the stopped diffusion problem converges exponentially fast. Therefore, we can now approximate the second derivative v_{xx} with an error

$$v_{xx}(t,0) = \frac{E\big(\overline{G}^{ad}(t,\Delta x)\big) - h(0)}{\Delta x} + \frac{\mathcal{O}(\Delta t)}{\Delta x} + \mathcal{O}(\Delta x),$$

where $\overline{G}^{ad}(t,\Delta x)$ denotes the stopped diffusion started at Δx computed with the adaptive algorithm (noting that the discretization grid is random, too). Minimizing the error gives

$$\Delta x = \text{const} \times \sqrt{\Delta t} = \text{const} \times \sqrt{\frac{T}{N}}. \tag{4.24}$$

Consequently, the error from the approximation in the correction term is this time

$$E\bigg(\sum_{i=0}^{N-1} \mathcal{O}(\sqrt{\Delta t})\big(\Delta \overline{Z}_i^N\big)^2\bigg) = \mathcal{O}(\sqrt{N}) \times \mathcal{O}(1/\sqrt{N}) \times \mathcal{O}(1/N) = \mathcal{O}(1/N).$$

However, note that we still have an additional work of order $\mathcal{O}(N^{5/4})$, which leads to the total convergence rate $\mathcal{O}(K^{-4/5})$. Only in case of constant coefficients, the additional work is still of $\mathcal{O}(N)$, therefore giving us the desired order $\mathcal{O}(N^{-1})$.

Concluding, we propose the following algorithm for one dimensional problems.

Algorithm 4.2.11. *Fix a uniform time discretization* $0 = t_0 < t_1 < \cdots < t_N = T$, *i. e.* $\Delta t_i = t_{i+1} - t_i = \frac{T}{N}$, $i = 0, \ldots, N-1$. *Moreover, fix an i. i. d. sequence of random variables* $(\Delta\overline{B}_i)_{i=0}^{N-1}$ *such that the moments of order up to three of* $\Delta\overline{B}_0$ *(and hence of all* $\Delta\overline{B}_i$*) coincide with those of an one dimensional normal random variable with variance* $\frac{T}{N}$, *cf. Case B in Section 1.3.*

(1) Set $\overline{X}_0^N = x$, $\overline{Z}_0^N = 0$, *set* $i = 0$.

(2) Set

$$\hat{X}_{i+1}^N = \overline{X}_i^N + V\big(\overline{X}_i^N\big)\Delta t_i + \sum_{j=1}^{d} V_j\big(\overline{X}_i^N\big)\Delta\overline{B}_i^j.$$

(3) Set

$$\overline{X}_{i+1}^N = \begin{cases} \hat{X}_{i+1}^N, & \hat{X}_{i+1}^N \in \overline{D}, \\ \Pi(\hat{X}_{i+1}^N), & \hat{X}_{i+1}^N \notin \overline{D}, \end{cases}$$

$$\overline{Z}_{i+1}^N = \begin{cases} \overline{Z}_i^N, & \hat{X}_{i+1}^N \in \overline{D}, \\ \overline{Z}_i^N + \left\| \Pi(\hat{X}_{i+1}^N) - \hat{X}_{i+1}^N \right\|, & \hat{X}_{i+1}^N \notin \overline{D}. \end{cases}$$

(4) If $\Delta\overline{Z}_i^N > 0$, *calculate either* $\overline{G}^{un}(t_{i+1}, \Delta t^{1/4})$ *or* $\overline{G}^{ad}(t_{i+1}, \sqrt{\Delta t})$ *and compute the approximate second order normal derivative* $\overline{\partial_n^2 v}(t_{i+1}, 0)$ *according to* (4.21).

(5) Increase i *by one. If* $i < N$, *go back to (2).*

(6) Calculate

$$\overline{F}^N = f\big(\overline{X}_N^N\big) - \sum_{i=0}^{N-1} h\big(\overline{X}_{i+1}^N\big)\Delta\overline{Z}_i^N + \frac{1}{2}\sum_{i=0}^{N-1}\big(\Delta\overline{Z}_i^N\big)^2\overline{\partial_n^2 v}(t_{i+1}, \overline{X}_{i+1}^N).$$

Remark 4.2.12. In the d-dimensional situation with $d > 1$, we can use the same finite difference approximation as (4.20), i. e.

$$v_{nn}(t,x) = \frac{v_n(t, x + \Delta x n(x)) - h(x)}{\Delta x} + \mathcal{O}(\Delta x),$$

where v_n and v_{nn} are the needed normal derivatives, $x \in \partial D$. Unless $n(x)$ is a constant vector (corresponding to a half-space domain), we do not get a PDE for v_n. However, using the stochastic representation of the original problem, we get

$$v_n(t, x + \Delta x n(x)) = E\Big(\Big\langle \nabla v\big(\tau, X_\tau^{t, x+\Delta x n(x)}\big)\, , J_{t\to\tau}(x + \Delta x n(x)) n(x)\Big\rangle\Big),$$

where $X^{t,x+\Delta xn(x)}$ denotes the solution of the SDE started at time t with $X_t^{t,x+\Delta xn(x)} = x+\Delta xn(x)$ and τ denotes the first hitting time of $X^{t,x+\Delta xn(x)}$ at ∂D (or $\tau = T$ if no such hit occurs before T). $J_{t\to s}(x+\Delta xn(x))$ is the first variation, i. e. the (path-wise) Jacobi matrix of the map $y \mapsto X_s^{t,y}$ evaluated at $y = x + \Delta xn(x)$. By the boundary condition,

$$\Big\langle \nabla v\big(\tau, X_\tau^{t,x+\Delta xn(x)}\big)\,, n\big(X_\tau^{t,x+\Delta xn(x)}\big)\Big\rangle = h\big(X_\tau^{t,x+\Delta xn(x)}\big),$$

but

$$J_{t\to\tau}(x+\Delta xn(x))n(x) \neq n\big(X_\tau^{t,x+\Delta xn(x)}\big)$$

in general. Nevertheless, we might boldly use

$$v_n(t, x+\Delta xn(x)) \approx E\big(h\big(X_\tau^{t,x+\Delta xn(x)}\big)\big),$$

giving us an additional error of

$$E\Big(\Big\langle \nabla v\big(\tau, X_\tau^{t,x+\Delta xn(x)}\big)\,, \\ J_{t\to\tau}(x+\Delta xn(x))\big(n(x) - J_{t\to\tau}(x+\Delta xn(x))^{-1} n\big(X_\tau^{t,x+\Delta xn(x)}\big)\big)\Big\rangle\Big).$$

Assuming that n is defined as a vector field on $\overline{D}$, we can write down the SDE of its pull-back $J_{t\to\tau}(x+\Delta xn(x))^{-1} n\big(X_\tau^{t,x+\Delta xn(x)}\big)$, namely

$$J_{t\to\tau}(x+\Delta xn(x))^{-1} n\big(X_\tau^{t,x+\Delta xn(x)}\big) - n(x) = \\ \int_t^\tau [V_0, n]\big(X_s^{t,x+\Delta xn(x)}\big)ds + \sum_{l=1}^n \int_t^\tau [V_l, n]\big(X_s^{t,x+\Delta xn(x)}\big) \circ dB_s^l.$$

This shows that the above approximation is exact if and only if $[V_l, n] = 0$, $l = 0, \ldots, n$, which is the case if and only of n commutes with L. But in the latter case, we might have worked with the stochastic representation of v_n to begin with. If this is not the case, one can bound the error, using the Itô isometry, by

$$\sqrt{C_1 E(\tau) + C_2 E(\tau^2)}.$$

By the above Remark 4.2.10, this error bound (divided by Δx) does not converge for $\Delta x \to 0$.

4.2.2 The adaptive algorithm

The idea of adaptive algorithms for SDEs is the following: given a certain computational error that one is willing to tolerate, one wants to *minimize* the *work* in order to guarantee that the computational error is smaller than the error tolerance. A few remarks are in order. First, for "work" we substitute the number of time-steps used. In fact, since the number of time-steps will be

random, we try to minimize the average number of time-steps. Notice that all our comments only refer to the algorithm discretizing the SDE in order to produce random samples for the final Monte Carlo simulation. For the general theory of adaptive weak algorithms for SDEs see Szepessy, Tempone and Zouraris [79].

Contrary to Algorithm 4.2.11, the adaptive algorithm works in all dimensions d. As already mentioned before, its advantages are generally expected to show in situations with inherent singularities. We do not have a proof for a certain convergence rate, but notice that for problems with very low regularity most traditional convergence results fail, too. In particular, we have examples in mind where the uniform Euler scheme presented in Algorithm 4.1.11 has a smaller order of convergence than $\frac{1}{2}$.

Our starting point is the error expansion (4.13), which we rewrite as

$$E\left(\sum_{i=0}^{N-1}\left(\Delta\overline{Z}_i^N\right)^2\left|v_{nn}\left(t_{i+1},\overline{X}_{i+1}^N\right)\right|\right) \tag{4.25}$$

where we use the shorthand notation

$$v_{nn}\left(t_{i+1},\overline{X}_{i+1}^N\right)=\int_0^1(1-\theta)\frac{\partial^2}{\partial n\left(\overline{X}_{i+1}^N\right)^2}v\left(t_{i+1},\overline{X}_{i+1}^N-\theta\Delta\overline{Z}_i^N n\left(\overline{X}_{i+1}^N\right)\right)d\theta.$$

Define auxiliary functions $\Delta t^N:[0,T]\to\mathbb{R}$ by $\Delta t^N(t)=\Delta t_i=t_{i+1}-t_i$ and $\overline{Z}^N:[0,T]\to\mathbb{R}$ by $\overline{Z}^N(t)=\overline{Z}_{i+1}^N$ for $t\in]t_i,t_{i+1}]$. Let $\widetilde{N}$ denote the number of hits at the boundary for the given time grid. We approximate

$$E\left(\widetilde{N}\right)\approx E\left(\int_0^T\frac{d\overline{Z}^N(t)}{\sqrt{\Delta t^N(t)}}\right). \tag{4.26}$$

Remark 4.2.13. We do not have a valid theory for (4.26), but the approximation is justified by numerical experiments. Note, however, that (4.26) is certainly only valid for a uniform time grid. For an adaptive, and therefore non-uniform time grid we expect a much higher number of hits at the boundary, since we expect to refine close to the boundary. (Recall that we only consider the reflection error from the boundary.) Indeed, numerical experiments show that e. g. $E\left(\widetilde{N}\right)=\mathcal{O}(N^{0.9})$ for some particular refined meshes, in comparison to $E\left(\widetilde{N}\right)=\mathcal{O}(\sqrt{N})$ for uniform meshes as suggested by (4.26).

We want to minimize (4.26) subject to the constraint that the error term (4.25) is smaller than a given error tolerance TOL. In order to avoid non-adapted stochastic processes entering the picture at this stage, let us

approximate the error term by

$$E\Big(\sum_{i=0}^{N-1}\big(\Delta\overline{Z}_i^N\big)^2\,\Big|v_{nn}\big(t_{i+1},\overline{X}_{i+1}^N\big)\Big|\Big)\approx$$
$$E\Big(\sum_{i=0}^{N-1}\Big|v_{nn}\big(t_{i+1},\overline{X}_{i+1}^N\big)\Big|\,\Delta\overline{Z}_i^N E\big(\Delta\overline{Z}_i^N\big|\overline{X}_i^N,\ \Delta t_i\big)\Big).$$

An easy calculation shows that

$$E\big(\overline{Z}_i^N\big|\overline{X}_i^N=x,\ \Delta t_i=\Delta t\big)=-x\Phi\Big(-\frac{d(x)}{\sqrt{\Delta t}}\Big)+\sqrt{\frac{\Delta t}{2\pi}}\exp\Big(-\frac{d(x)^2}{2\Delta t}\Big),$$

where Φ denotes the cumulative distribution function of the standard Gaussian distribution, provided that D is a half space, and $d(x)$ is the distance of x to the reflecting boundary ∂D. In the general case we use the above equation as an approximation, where we think of the tangent hyperplane on D at x, cf. [28]. Moreover, the derivative of the quantity is given by

$$\frac{\partial}{\partial\Delta t}E\big(\overline{Z}_i^N\big|\overline{X}_i^N=x,\ \Delta t_i=\Delta t\big)=\frac{1}{2\sqrt{2\Delta t\pi}}\exp\Big(-\frac{d(x)^2}{2\Delta t}\Big).$$

Combining these results and rewriting everything in terms of integrals instead of sums, we get the Lagrangian of the minimization problem at hand:

$$\mathcal{L}(\Delta t)=E\Big[\int_0^T\frac{d\overline{Z}(s)}{\sqrt{\Delta t(s)}}+\lambda\Big(\int_0^T\big|v_{nn}\big(s,\overline{X}(s)\big)\big|\,E\big(\Delta\overline{Z}(s)\big|\overline{X}(s),\ \Delta t(s)\big)d\overline{Z}(s)-\mathrm{TOL}\Big)\Big]. \tag{4.27}$$

$\mathcal{L}$ is understood as a function defined on the set of positive, piecewise constant functions on $[0,T]$. Note that we have tacitly omitted the dependence on N in the above equation, because N is now a function of the mesh function Δt, which is no longer fixed. The derivative in direction of the piecewise constant function ϕ is then given by

$$\mathcal{L}'(\Delta t)\cdot\phi=E\Big[\int_0^T\Big(-\frac{\phi}{2\Delta t(s)^{3/2}}+\lambda\phi\frac{\big|v_{nn}\big(s,\overline{X}(s)\big)\big|}{2\sqrt{2\Delta t(s)\pi}}\exp\Big(-\frac{d\big(\overline{X}(s)\big)^2}{2\Delta t(s)}\Big)\Big)d\overline{Z}(s)\Big].$$

$\mathcal{L}'(\Delta t)\cdot\phi=0$ for all functions ϕ implies

$$\mathrm{const}=\frac{1}{\lambda}=\frac{\Delta t(t)}{\sqrt{2\pi}}\exp\Big(-\frac{d\big(\overline{X}(t)\big)^2}{2\Delta t(t)}\Big)\,\big|v_{nn}\big(t,\overline{X}(t)\big)\big| \tag{4.28}$$

for all $t\in[0,T]$. Notice that (4.28) can already be understood as a refinement rule, because it shows the dependence of the grid on the position.

There is, however, no direct dependence on the tolerance level TOL included, yet. To this end, we have the re-insert the expression (4.28) into the error representation (4.27), giving us the const in (4.28). More precisely, we get (4.29)

$$\Delta t(t) = 2\sqrt{2\pi}\frac{\mathrm{TOL} + E\Big(\int_0^T \overline{X}(s)\Phi\Big(-\frac{d\big(\overline{X}(s)\big)}{\sqrt{\Delta t(s)}}\Big)\,\big|v_{nn}\big(s,\overline{X}(s)\big)\big|\,d\overline{Z}(s)\Big)}{E\Big(\int_0^T \frac{d\overline{Z}(s)}{\sqrt{\Delta t(s)}}\Big)\exp\Big(-\frac{d\big(\overline{X}(s)\big)^2}{2\Delta t(t)}\Big)\,\big|v_{nn}\big(t,\overline{X}(t)\big)\big|}.$$

This term is too complicated for the implementation. Two simplifications are immediately possible. First note that the second term in the numerator of (4.29) is always positive. Omitting this term therefore means that the mesh is refined too often. Moreover, the term seems insignificant as compared to the exponential term in the denominator. Secondly, we may again apply (4.26), this time in the other direction, which gives a term $E\big(\widetilde{N}\big)$ in the denominator. In practice, we do not know this expected value, especially since it highly depends on the grid, which is no longer fixed. Therefore, the idea is to run the adaptive algorithm once in order to compute an approximation for $E\big(\widetilde{N}\big)$, and then a second time, using the approximation and a different batch of (pseudo) random numbers, in order to compute the quantity of interest. These two simplifications lead to

$$\Delta t(t) \simeq 2\sqrt{2\pi}\frac{\mathrm{TOL}\exp\Big(\frac{d\big(\overline{X}(t)\big)^2}{2\Delta t(t)}\Big)}{E\big(\widetilde{N}\big)\,\big|v_{nn}\big(t,\overline{X}(t)\big)\big|}. \tag{4.30}$$

There is still the unknown term $\big|v_{nn}\big(t,\overline{X}(t)\big)\big|$ left in equation (4.30). We propose two possible approaches to it, depending on the problem at hand.

- If the problem is simple enough or we have some a-priori information, we can replace $\big|v_{nn}\big(t,\overline{X}(t)\big)\big|$ by the constant 1 or by some approximation based on our knowledge of the problem, respectively. For instance, if v is well behaved but for one singularity at a known point $x_0 \in \mathbb{R}^n$, we could replace $\big|v_{nn}\big(t,\overline{X}(t)\big)\big|$ with 1 far away from x_0 and with $1/\left\|x - x_0\right\|^\alpha$ close to x_0, with α depending on the type of singularity. Notice, however, that in this situation the true computational error can only be proportional to the error estimate given by the local error density (4.30). Therefore, it is not possible to guarantee – within the limitations of a Monte-Carlo setup and our further assumptions – the computational error to be bounded by TOL, but one has to observe the dynamics of the results for smaller and smaller TOL.

- In general, $\big|v_{nn}\big(t,\overline{X}(t)\big)\big|$ can be approximated by the *discrete dual functions*, see [79] for more details. The use of the dual functions introduces some subtleties into the algorithm, because they are computed

by backward recursion. Thus, they are not adapted to the filtration. In this case, the error representation based on the local error density is precise, again under the limitations of the setup, in particular keeping in mind that the discrete dual functions are only approximations of the true second normal derivative.

Let us summarize the adaptive algorithm. In the following, $\mathfrak{t}$ will denote a partition of $[0,T]$, i. e. $\mathfrak{t} = (t_i)_{i=0}^{N(\mathfrak{t})}$ with $0 = t_0 < \cdots < t_{N(\mathfrak{t})} = T$. Given a partition $\mathfrak{t}$, we will denote $\Delta t_i^{\mathfrak{t}} = t_{i+1} - t_i$, $0 \le i \le N(\mathfrak{t}) - 1$. Moreover, $\overline{B}^{\mathfrak{t}}$, $\overline{X}^{\mathfrak{t}}$, $\overline{Z}^{\mathfrak{t}}$ will denote discrete processes defined on the grid $\mathfrak{t}$, i. e. $\overline{B}^{\mathfrak{t}} = (\overline{B}_{t_i})_{i=0}^{N(\mathfrak{t})}$ and we will also use $\Delta\overline{B}_i^{\mathfrak{t}} = \overline{B}_{t_{i+1}} - \overline{B}_{t_i}$, $\Delta\overline{Z}_i^{\mathfrak{t}} = \overline{Z}_{i+1}^{\mathfrak{t}} - \overline{Z}_i^{\mathfrak{t}}$, $0 \le i \le N(\mathfrak{t}) - 1$.

Algorithm 4.2.14 (Refinement)**.** *Given a time grid* $\mathfrak{t}$*, the Brownian motion* $\overline{B}^{\mathfrak{t}}$ *sampled according to* $\mathfrak{t}$*, the process* $\overline{X}^{\mathfrak{t}}$ *sampled on* $\mathfrak{t}$ *and a local error tolerance* TOL*. Set* $i = 0$*.*

(1) Compute a local error density by

$$l_i = \frac{1}{2\sqrt{2\pi}} E\big(\widetilde{N}\big) \Big| v_{nn}\big(t_i, \overline{X}_i^{\mathfrak{t}}\big) \Big| \exp\Big(-\frac{d\big(\overline{X}_i^{\mathfrak{t}}\big)^2}{2\Delta t_i}\Big) \Delta t_i,$$

where $\Big| v_{nn}\big(t_i, \overline{X}_i^{\mathfrak{t}}\big) \Big|$ *is chosen by one of the two approaches mentioned above.*

(2) If $l_i <$ TOL *and* $i < N(\mathfrak{t}) - 1$*, then set* $i = i + 1$ *and go back to (1). If* $l_i <$ TOL *and* $i = N(\mathfrak{t}) - 1$*, then stop. Else go to (3).*

(3) Insert $t = \frac{t_i + t_{i+1}}{2}$ *into* $\mathfrak{t}$*, i. e. set* $\mathfrak{t} = (t_0, \ldots, t_i, t, t_{i+1}, \ldots, t_N)$*, and sample the corresponding Brownian motion* $\overline{B}_t$ *using a Brownian bridge between* $\overline{B}_{t_i}$ *and* $\overline{B}_{t_{i+1}}$*, i. e.*

$$\overline{B}_t = \overline{B}_{t_i} + \frac{1}{2}(\overline{B}_{t_{i+1}} - \overline{B}_{t_i}) + \frac{1}{2}\sqrt{t_{i+1} - t_i}\, Y,$$

where $Y \sim \mathcal{N}(0, \mathrm{id}_d)$ *independent of all previously sampled random variables. Furthermore, insert the new term* $\overline{X}_{i+1}^{\mathfrak{t}} = 0$ *(or any other value). If* $t_{i+1} < T$*, set* $i = i + 2$ *(note that the size of the grid has changed) and go back to (1), else stop.*

Remark 4.2.15. In practice, it is advisable to set a bound on the possible refinements, e. g. one could fix some $\Delta t_{\min}$ and only refine between t_{i+1} and t_i of $l_i \ge$ TOL *and* $t_{i+1} - t_i > \Delta t_{\min}$. Moreover, to ensure convergence of the algorithm one should refine all steps until $\Delta t_i < \Delta t_{\max}$ for some fixed $\Delta t_{\max}$. This guarantees convergence for $\Delta t_{\max} \to 0$, at least with the speed of the uniform Euler scheme – but, in fact, much faster in most situations.

Remark 4.2.16. Of course, it is also possible to sample the Brownian motion in a weak way. In this situation, one has to use the weak analogue of the above Brownian bridge formula.

Algorithm 4.2.17. *Start with an initial mesh* $\mathfrak{t}$ *and the corresponding Brownian motion* $\overline{B}^{\mathfrak{t}}$.

(1) Set $\overline{X}_0^{\mathfrak{t}} = x$, $\overline{Z}_0^{\mathfrak{t}} = 0$, *and* $i = 0$.

(2) Set

$$\hat{X}_{i+1}^{\mathfrak{t}} = \overline{X}_i^{\mathfrak{t}} + V\big(\overline{X}_i^{\mathfrak{t}}\big)\Delta t_i + \sum_{j=1}^{d} V_j\big(\overline{X}_i^{\mathfrak{t}}\big)\Delta \overline{B}_i^j.$$

(3) Set

$$\overline{X}_{i+1}^{\mathfrak{t}} = \begin{cases} \hat{X}_{i+1}^{\mathfrak{t}}, & \hat{X}_{i+1}^{\mathfrak{t}} \in \overline{D}, \\ \Pi(\hat{X}_{i+1}^{\mathfrak{t}}), & \hat{X}_{i+1}^{\mathfrak{t}} \notin \overline{D}, \end{cases}$$

$$\overline{Z}_{i+1}^{\mathfrak{t}} = \begin{cases} \overline{Z}_i^{\mathfrak{t}}, & \hat{X}_{i+1}^{\mathfrak{t}} \in \overline{D}, \\ \overline{Z}_i^{\mathfrak{t}} + \left\| \Pi(\hat{X}_{i+1}^{\mathfrak{t}}) - \hat{X}_{i+1}^{\mathfrak{t}} \right\|, & \hat{X}_{i+1}^{\mathfrak{t}} \notin \overline{D}. \end{cases}$$

(4) Increase i *by one. If* $i < N(\mathfrak{t})$, *go back to (2).*

(5) Refine the grid $\mathfrak{t}$ *using Algorithm 4.2.14. If the grid has changed during refinement, then set* $i = 0$ *and go back to (2), using the refined grid.*

(6) Calculate

$$\overline{F}^{\mathfrak{t}} = f\big(\overline{X}_{N(\mathfrak{t})}^{\mathfrak{t}}\big) - \sum_{i=0}^{N(\mathfrak{t})-1} h\big(\overline{X}_{i+1}^{\mathfrak{t}}\big)\Delta \overline{Z}_i^{\mathfrak{t}}.$$

4.3 Numerical experiments

4.3.1 One-dimensional example

We start with a one-dimensional example, which mainly serves as illustration of the algorithm with correction, cf. Algorithm 4.2.11. Because we are only interested in the error coming from the reflection at the boundary, we use a problem without interior discretization error, i. e. in the interior of the domain $D = [0, \infty[$. The solution process X is the driving Brownian motion B reflected at the boundary $\partial D = \{0\}$. The Neumann boundary condition and the initial condition are fixed as follows:

$$\begin{cases} \dfrac{\partial}{\partial t}u(t,x) = -\dfrac{1}{2}\Delta u(t,x), & (t,x) \in [0,2] \times [0,\infty[, \\ u(2,x) = e^2(\sin(\sqrt{2}x) + \cos(\sqrt{2}x)), & x \in [0,\infty[, \\ \dfrac{\partial}{\partial x}u(t,0) = \sqrt{2}e^t, & t \in [0,2]. \end{cases} \tag{4.31}$$

Obviously, problem (4.31) has the explicit solution

$$u(t,x) = e^t(\sin(\sqrt{2}x) + \cos(\sqrt{2}x)). \tag{4.32}$$

Remark 4.3.1. In [16], the authors prove that the uniform Euler algorithm for the Brownian motion reflected at 0 (but with different boundary and initial conditions) does not converge faster than with rate one half. We have changed the boundary conditions because the third derivative of the solution of their problem vanishes, which would lead to untypically fast convergence rates for the algorithm with second order correction terms, because its leading order error term involves the third derivative. As can be easily checked, the third derivative of (4.32) does not vanish for $x = 0$.

We compute the value $u(0, x_0)$ for $x_0 = 0.5$ using three different methods: the uniform Euler method, cf. Algorithm 4.1.11, the uniform Euler method with second order correction term computed using a stopped diffusion approximated by the adaptive algorithm of [21], cf. Algorithm 4.2.11. Finally, we also compute the outcome with the adaptive Algorithm 4.2.17. Notice that the exact value is $u(0, 0.5) = 1.4099$.

N	M	Error	$\mathcal{S}$
2	80 080	0.3811	0.0416
4	80 320	0.5986	0.0386
8	56 400	0.6252	0.0448
16	62 800	0.5417	0.0420
32	75 600	0.4493	0.0382
64	101 200	0.3581	0.0329
128	152 400	0.2461	0.0269
256	254 800	0.1822	0.0208
512	459 600	0.1330	0.0155
1024	869 200	0.0881	0.0113
2048	1 688 400	0.0638	0.0081
4096	3 326 800	0.0496	0.0058

Table 4.1: Results of the uniform Euler Monte-Carlo algorithm for problem (4.31)

Table 4.1 gives the results for the uniform algorithm. Here, and in all the subsequent examples, M denotes the number of paths used in the Monte Carlo simulation for $u(0, 0.5)$. The "Error" in the table is the computational error in the sense that

$$\text{Error} = \overline{u}(0, 0.5) - u(0, 0.5),$$

where $\overline{u}(0, 0.5)$ denotes the computed approximation to the true value $u(0, 0.5)$. $\mathcal{S}$ gives an estimate for the possible "statistical" error component

caused by the computation of the expected value of the random variable $\overline{F}^N$ constructed in Algorithm 4.1.11 by Monte-Carlo simulation. Indeed, let $\overline{F}_i^N$ denote the ith sample of $\overline{F}^N$, $i = 1, \dots, M$. Ideally, these samples are independent and identically distributed samples of $\overline{F}^N$, which allows us to appeal to the central limit theorem, giving

$$\sqrt{M}\Big(E\big(\overline{F}^N\big) - \frac{1}{M}\sum_{i=1}^{M}\overline{F}_i^N\Big) \xrightarrow[M\to\infty]{} \mathcal{N}(0,\sigma^2),$$

where the convergence is understood as convergence in distribution and σ^2 denotes the variance of $\overline{F}^N$. Heuristically, we may assume that M is already large enough that the convergence in the central limit theorem has already taken place, i. e.

$$\text{Error} \approx \mathcal{N}\Big(0, \frac{\overline{\sigma}^2}{M}\Big),$$

where $\overline{\sigma}^2$ denotes the empirical variance of the sample $\big(\overline{F}_i^N\big)_{i=1}^M$. This gives us a 90%-confidence interval,

$$E\big(\overline{F}^N\big) - u(0,0.5) \in \Big[\text{Error} - 1.65 \times \frac{\overline{\sigma}}{\sqrt{M}}\,,\, \text{Error} + 1.65 \times \frac{\overline{\sigma}}{\sqrt{M}}\Big] \tag{4.33}$$

with probability close to 0.9. We denote

$$\mathcal{S} = 1.65 \times \frac{\overline{\sigma}}{\sqrt{M}} \tag{4.34}$$

and report it in Table 4.1 and all the subsequent tables.

Remark 4.3.2. $\mathcal{S}$ as defined in (4.34) is an indicator for the size of the statistical error, possibly overlapping the error from the time discretization in the observed computational error. Recall that the computational error can be decomposed as

$$u(0,0.5) - \underbrace{\frac{1}{M}\sum_{i=1}^{M}\overline{F}_i^N}_{=\overline{u}(0,0.5)} = \underbrace{u(0,0.5) - E\big(\overline{F}^N\big)}_{=\mathrm{E}_{\mathrm{disc}}} + \underbrace{E\big(\overline{F}^N\big) - \frac{1}{M}\sum_{i=1}^{M}\overline{F}_i^N}_{=\mathrm{E}_{\mathrm{stat}}}.$$

$\mathrm{E}_{\mathrm{disc}}$ can be naturally interpreted as the error caused by the time-discretization of the dynamics of the (reflected) SDE, whereas $\mathrm{E}_{\mathrm{stat}}$ is the "statistical" error caused by Monte-Carlo simulation, i. e. the integration error. In this study, we are *only* interested in the discretization error $\mathrm{E}_{\mathrm{disc}}$, since we want to analyze the behavior of special time-discretization algorithms. Consequently, we need to make sure that our results are not overshadowed by the statistical error. In practice, we choose M large enough such that $\mathcal{S} = \mathcal{S}(M)$ is much smaller than the observed computational error. For a thorough treatment of the types of errors involved in Euler Monte-Carlo schemes, we refer to [79].

Remark 4.3.3. Continuing the discussion in Remark 4.3.2, we would like to stress that the statistical error is, in practice, a very important part of the overall computational error, and the strategy advocated in Remark 4.3.2, namely to choose M large enough such that the statistical error can be neglected, is not suited for true computations, but only for the purpose of analysis of algorithms as mentioned above. Indeed, such a strategy grossly increases the over-all amount of work for the computations, as the statistical error usually is the dominant part of the error decomposition.

Heuristically, we may argue as follows: assume that we compute a quantity of interest $u = E(F)$ by Monte-Carlo simulation with M paths, sampling from an approximation $\overline{F}^N \approx F$, i. e. we approximate

$$u \approx \frac{1}{M} \sum_{i=1}^{M} \overline{F}_i^N = \overline{u}^{N,M}.$$

Assume that $\overline{F}^N$ converges to F with a weak rate γ in the sense of Definition 1.3.5 (for $\mathcal{G}$ containing the identity function). Using the above decomposition of the computational error, we obtain

$$\left|\overline{u}^{N,M} - u\right| \leq \frac{C_1}{N^\gamma} + \frac{C_2}{\sqrt{M}}.$$

Given an error tolerance $\epsilon = \epsilon_1 + \epsilon_2$, let us impose an error tolerance of ϵ_1 for the discretization error and of ϵ_2 for the statistical error. This means we have to choose

$$N = N(\epsilon_1) = \left(\frac{C_1}{\epsilon_1}\right)^{1/\gamma}$$

and

$$M = M(\epsilon_2) = \left(\frac{C_2}{\epsilon_2}\right)^2.$$

Write $\epsilon_1 = \lambda\epsilon$ and $\epsilon_2 = (1-\lambda)\epsilon$, $0 < \lambda < 1$, and minimize the total work

$$N(\epsilon_1) \times M(\epsilon_2) = C\lambda^{-1/\gamma}(1-\lambda)^{-2}\epsilon^{-(2+1/\gamma)}. \tag{4.35}$$

Equation (4.35) is already quite remarkable, because it shows that the work is proportional to $\epsilon^{-(2+1/\gamma)}$, which implies that the total work can no longer be improved dramatically if $\gamma > 1$. Minimizing (4.35) with respect to λ gives $\lambda = \frac{1}{2\gamma+1}$, e. g. for $\gamma = 1$ the error tolerance for the statistical error should already be $2/3$ of the total error tolerance.

The results in Table 4.1 show the typical convergence order $\frac{1}{2}$ of the reflected uniform Euler method, as theoretically described. See also Figure 4.1 for comparisons of the different algorithms used.

Table 4.2 shows the results for the algorithm with second order correction term, cf. Algorithm 4.2.11. The correction term $\overline{G}^{ad}$ is calculated using the

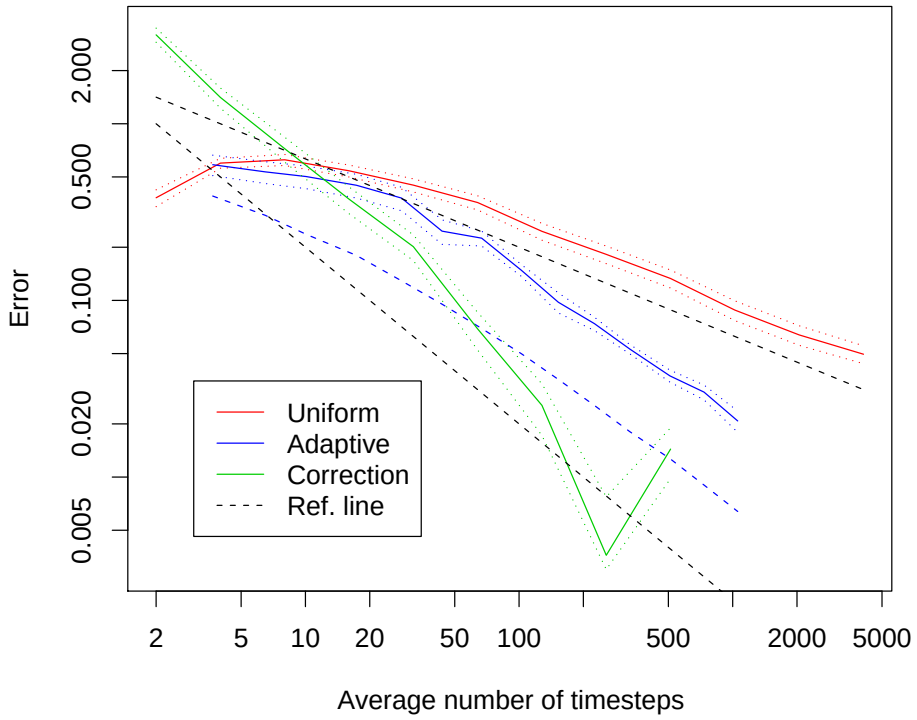


Figure 4.1: Absolute value of the computational error for problem (4.31). The dotted lines show confidence areas for the true error in the sense of equation (4.33) and the dashed lines in black are reference lines of order $1/N$ and $1/\sqrt{N}$, respectively. Notice that the "Average number of timesteps" is understood as the work in the sense of Example 4.3.4 in the case of the algorithm with a second order correction term and as average size of the refined mesh in the case of the adaptive algorithm. The dashed line for the adaptive algorithm corresponds to the error estimate computed for the refinement algorithm and is clearly proportional to the observed computational error.

adaptive Euler algorithm for stopped diffusions presented in [21]. The local error tolerance parameter is chosen to be

$$\mathrm{TOL} = \frac{1}{\log(N)},$$

which is consistent with the observation that the error decreases exponentially fast, implying an approximation error proportional to $\frac{1}{N}$ for the correction term using the above local error tolerance.

As before, N is the size of the uniform base grid of the discretization of the reflected diffusion. Work denotes the average work per realization, i. e. for

N	Work	M	Error	$\mathcal{S}$
2	2.45	5 400	−3.1856	0.2928
4	7.74	6 600	−1.4092	0.1838
8	19.35	11 400	−0.7224	0.1163
16	43.66	30 600	−0.3743	0.0647
32	92.22	107 400	−0.2014	0.0333
64	193.13	414 600	−0.0690	0.0166
128	401.43	1 643 400	−0.0255	0.0083
256	831.52	6 558 600	−0.0036	0.0041
512	3065.85	5 262 880	−0.0144	0.0046

Table 4.2: Results of the uniform Euler Monte-Carlo algorithm with second order correction term calculated using an adaptive algorithm for problem (4.31).

one single realization, the corresponding work is N plus the total work for each stopped diffusion, which is computed in order to get the respective correction terms. The work of one trajectory of the adaptive algorithm of the stopped diffusion is understood as in the following example.

Example 4.3.4. Assume that we start with the initial mesh $\mathfrak{t}_0 = \{0, 1, 2\}$, i. e. the initial step-size is $N(\mathfrak{t}_0) = 2$. In the first step, the mesh is refined everywhere, i. e. $\mathfrak{t}_1 = \{0, 0.5, 1, 1.5, 2\}$, $N(\mathfrak{t}_1) = 4$. Then only the second half of the mesh is refined, i. e. $\mathfrak{t}_2 = \{0, 0.5, 1, 1.25, 1.5, 1.75, 2\}$ with $N(\mathfrak{t}_2) = 6$. Finally, yet another refinement in the middle of the mesh takes place, i. e. $\mathfrak{t}_3 = \{0, 0.5, 1, 1.125, 1.25, 1.5, 1.75, 2\}$ with $N(\mathfrak{t}_3) = 7$. Then the refinement stops. The total work of this trajectory is given as follows. First we compute the process along $\mathfrak{t}_0$, which gives $\mathrm{Work}_0 = 2$. After the refinement, the whole process has to be computed again, along $\mathfrak{t}_1$, giving

$$\mathrm{Work}_1 = \mathrm{Work}_0 + 4 = 6.$$

For the refinement from $\mathfrak{t}_1$ to $\mathfrak{t}_2$, we only need to recompute the process for the second half of the mesh, i. e. for $t > 1$. Therefore,

$$\mathrm{Work}_2 = \mathrm{Work}_1 + 4 = 10.$$

For the final refinement, the process has to be recomputed after the newly inserted point, i. e. again for $t > 1$. Consequently,

$$\mathrm{Work}_3 = \mathrm{Work}_2 + 5 = 15,$$

which is the final work along this trajectory. While this number might not record the actual work of the computer, i. e. the time spent on the computation, it should be proportional to it.

Notice that the hitting time at the boundary is increasing with the fineness of the mesh: i. e. if $\mathfrak{t}_1 \subset \mathfrak{t}_2$, then the observed stopping times satisfy $\overline{\tau}(\mathfrak{t}_1) \geq \overline{\tau}(\mathfrak{t}_2)$. The reason for this behavior is that there is no interior error, i. e. up to the true first hitting time the discrete approximation of the process is exact. Consequently, the first observed hitting time can only take place at or after the first true hitting time.

The results of the algorithm with correction show an empirical order of convergence one, i. e. like $1/N$, even if the total work in the above sense is used as reference. As remarked above Algorithm 4.2.11, this is only possible since the approximation is precise in the interior of the domain. Compare also Figure 4.1, which shows the superiority of the algorithm with correction over the other two proposed algorithms. (Notice that the confidence interval for the last but second result of this algorithm could not be plotted in Figure 4.1, because it contains negative numbers. Therefore, this confidence interval was changed manually.)

Finally, Table 4.3 shows the results of the adaptive Algorithm 4.2.17 applied to problem (4.31).

TOL	N	M	Error	$\mathcal{S}$
125.00×10^{-3}	3.68	20 051	0.5864	0.0776
62.50×10^{-3}	6.49	20 204	0.5342	0.0754
31.25×10^{-3}	10.08	20 819	0.5025	0.0735
15.63×10^{-3}	17.34	23 276	0.4485	0.0689
7.81×10^{-3}	28.20	33 107	0.3794	0.0577
3.91×10^{-3}	43.61	72 428	0.2466	0.0390
1.95×10^{-3}	66.82	229 715	0.2251	0.0219
0.98×10^{-3}	102.56	858 860	0.1481	0.0113
0.49×10^{-3}	152.79	691 088	0.0976	0.0126
0.24×10^{-3}	225.44	2 704 354	0.0739	0.0064
0.12×10^{-3}	330.04	10 757 418	0.0530	0.0032
0.05×10^{-3}	508.65	13 000 000	0.0374	0.0029
0.02×10^{-3}	734.23	13 000 000	0.0303	0.0029
0.01×10^{-3}	1055.59	13 501 772	0.0208	0.0029

Table 4.3: Results of the adaptive Euler Monte-Carlo algorithm for problem (4.31).

TOL is the local error tolerance used for the adaptive algorithm, cf. Algorithm 4.2.14. The second order normal derivative in the local error term (4.30) is approximated by the constant 1. The size of the uniform initial grid is always 2, which is, of course, unrealistically small but probably useful for the theoretical understanding of the refinements. The value N as reported in the second column of Table 4.3 corresponds to the average size of the final mesh (after refinements). Notice that this value is proportional

to the work in the sense of Example 4.3.4.

The observed computational error of the adaptive algorithm lies between the errors for the uniform Euler algorithms with and without correction term, as expected. For high TOL, the dynamics of the computational error is similar to the error dynamics of the uniform Euler algorithm without correction. For smaller values of TOL, however, it seems to be rather proportional to the error of the uniform Euler algorithm with correction, see Figure 4.1. Therefore, it is rather difficult to compute a meaningful empirical convergence rate.

4.3.2 Two-dimensional example

For multi-dimensional examples the choice of the domain D is critical for the applicability of algorithms, which usually require some smoothness assumptions on D. In the following, we present two examples in dimension $d = 2$ based on a rectangular domain D presented in Figure 4.2.

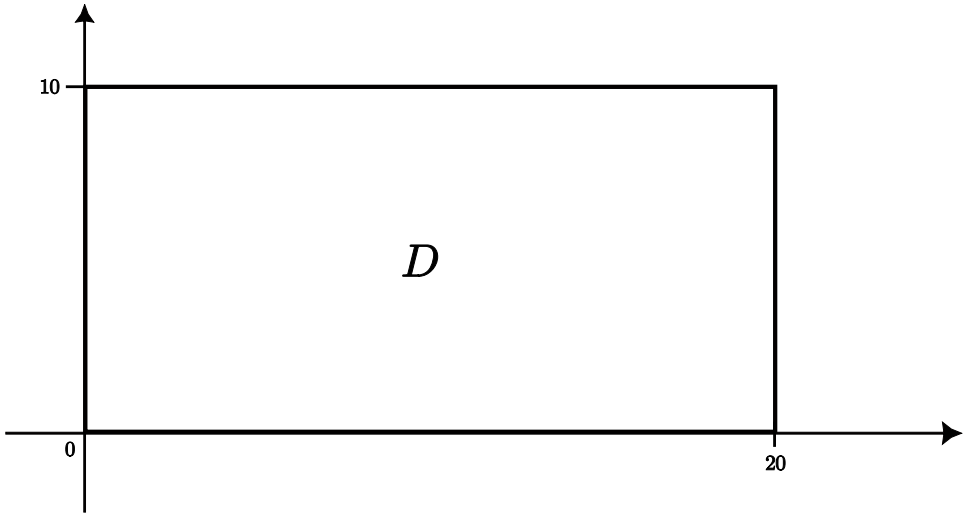


Figure 4.2: Domain of the two-dimensional example.

The first example is an ordinary reflected diffusion in D, where the exact solution is known. It is not an optimal example in so far as that other methods, in particular Gobet's half-space scheme, [28], seem to be better suited for this problem.

$$
\begin{cases}
\dfrac{\partial}{\partial t}u(t,x) = -\dfrac{1}{2}\Delta u(t,x), \quad (t,x) \in [0,1] \times D, \\
\quad u(1,x) = (2\cos(x_1 - x_2) + \cos(x_1 + x_2)), \quad x \in \overline{D}, \\
\dfrac{\partial}{\partial n}u(t,x) = h(t,x), \quad (t,x) \in [0,1] \times \partial D,
\end{cases}
\tag{4.36}
$$

where $h(t,x)$ is the normal derivative of the exact solution

$$u(t,x) = (2\cos(x_1 - x_2) + \cos(x_1 + x_2))e^{-(1-t)} \tag{4.37}$$

at $x \in \partial D$. Once again, the solution of the corresponding reflected SDE is a Brownian motion orthogonally reflected at the boundary of D. This time, we only implemented the uniform Euler method, Algorithm 4.1.11, and the adaptive method, cf. Algorithm 4.2.17, since Algorithm 4.2.11 is not directly applicable. We compute

$$u(0,x_0), \text{ for } x_0 = (10, 0.2) \in D,$$

which evaluates to

$$u(0, 10, 0.2) = -0.9473.$$

Remark 4.3.5. Since is is rather unlikely for a path started at x_0 to ever hit another boundary of D but the bottom boundary $[0,20] \times \{0\}$, even an implementation based on the explicit form of the distribution of a Brownian motion reflected at a half-space and its local time might be a serious alternative in this particular case.

N	M	Error	$\mathcal{S}$
2	28 000	−0.1686	0.0146
4	36 000	−0.1312	0.0126
8	52 000	−0.1128	0.0103
16	84 000	−0.0788	0.0080
32	148 000	−0.0610	0.0060
64	276 000	−0.0448	0.0043
128	532 000	−0.0356	0.0031
256	1 044 000	−0.0229	0.0022
512	2 068 000	−0.0163	0.0016
1024	4 116 000	−0.0118	0.0011

Table 4.4: Results of the uniform algorithm for problem (4.36).

The results of the uniform algorithm, which is also used as benchmark for this example, are presented in Table 4.4. Notice that the theoretical rate of convergence $N^{-1/2}$ is, once again, nicely recovered by our empirical results.

Table 4.5 shows the results of the adaptive Algorithm 4.2.17. For calculation of the error density, see (4.30) and Algorithm 4.2.14, we replace the estimator for the second normal derivative v_{nn} by the constant 1. As before, the initial grid only has size 2 for the adaptive algorithm. Once again, N (in the above table as well as in Figure 4.3) denotes the average size of the final grid produced by refining according to Algorithm 4.2.14. Of course, the average computational work in the sense of Example 4.3.4 is much higher

TOL	N	M	Error	$\mathcal{S}$
1.2500	3.81	28 000	−0.1291	0.0144
0.6250	7.00	36 000	−0.1030	0.0124
0.3125	12.35	52 000	−0.0835	0.0102
0.1563	20.96	84 000	−0.0632	0.0079
0.0781	34.55	148 000	−0.0498	0.0059
0.0391	54.24	276 000	−0.0330	0.0043
0.0195	84.96	532 000	−0.0274	0.0031
0.0098	129.44	1 044 000	−0.0156	0.0022
0.0049	194.50	2 068 000	−0.0121	0.0016
0.0024	290.19	4 116 000	−0.0078	0.0011
0.0012	426.58	8 212 000	−0.0065	0.0008

Table 4.5: Results of the adaptive algorithm for problem (4.36).

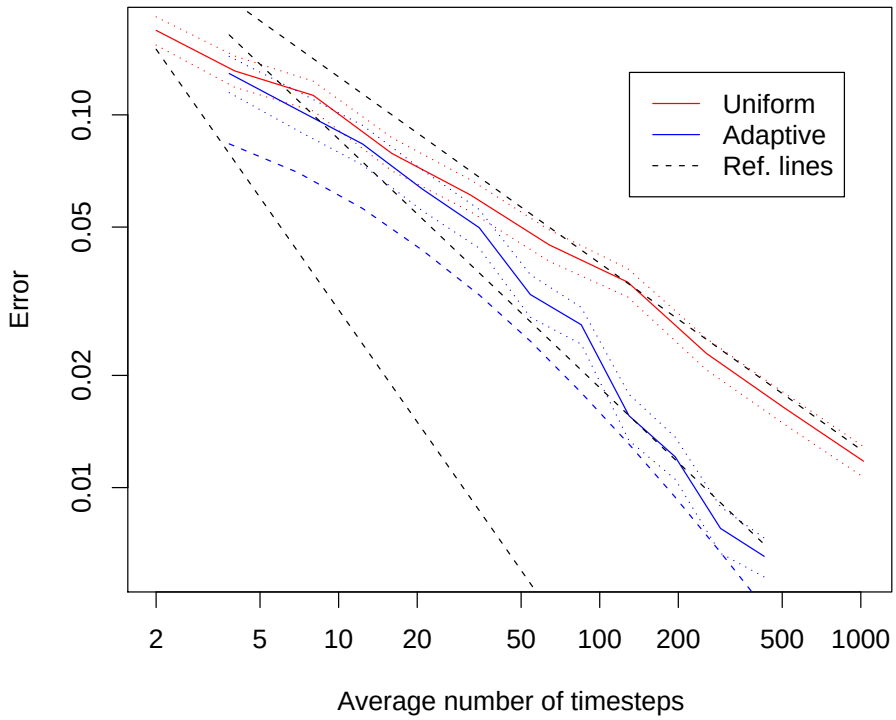


Figure 4.3: Absolute value of the error for problem (4.36). The dotted lines show confidence intervals for the true error in the sense of (4.33). The reference lines are lines with slopes $1/\sqrt{N}$ and $\frac{1}{N^{2/3}}$, respectively. The dashed line in color is proportional to the error estimate computed for the refinement algorithm.

than the value N, but proportional to it. The empirical order of convergence (in terms of N, and consequently also in terms of overall work) is

$$\text{Error} \simeq 0.44 \times N^{-0.67},$$

if, however, the first two lines in Table 4.5 are discarded, then the same computation yields an empirical order of convergence like

$$\text{Error} \simeq 0.67 \times N^{-0.76},$$

i. e. the results seem to indicate an order of convergence of 3/4. Notice, however, that the computational cost for the adaptive results are higher than those for the uniform algorithm for all the results of Table 4.4 – in the sense that obtaining the same level of exactness using the uniform algorithm was computationally cheaper than for the adaptive algorithm. This, however, changes fast if the desired level of precision is increased.

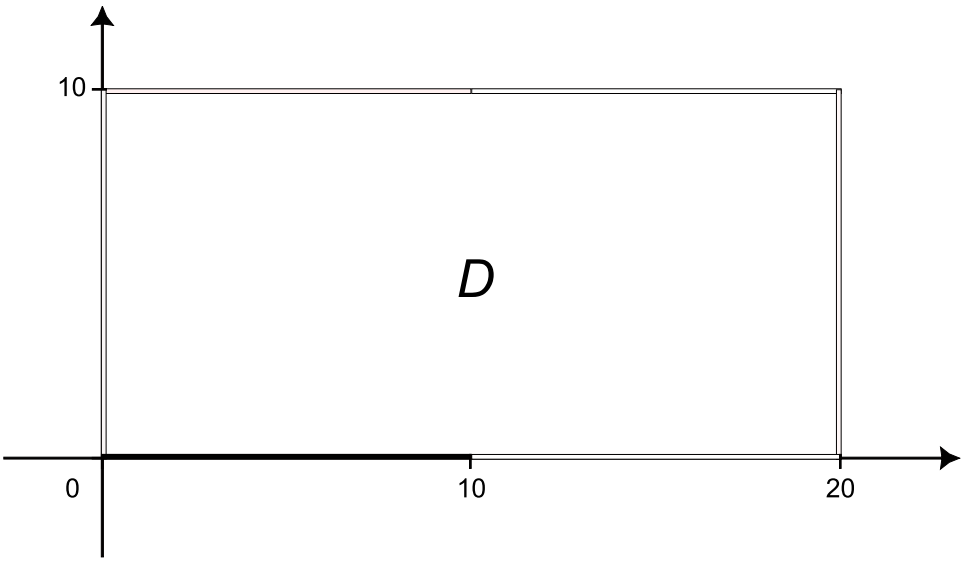


Figure 4.4: Domain for the two-dimensional example with mixed boundary conditions. The solid line denotes the reflecting boundary, the "empty" lines belong to the stopping boundary.

The second example is a mixed Neumann-Dirichlet boundary value problem. More precisely, let $D =]0, 20[\times]0, 10[$ as before, and let $D_N =]0, 10[\times\{0\}$ be the Neumann boundary, see Figure 4.4. Consider the prob-

lem

(4.38)
$$\begin{cases} \dfrac{\partial}{\partial t}u(t,x) = -\dfrac{1}{2}\Delta u(t,x), \quad (t,x) \in [0,2] \times D, \\ \quad u(2,x) = 10\exp\Big(-\sqrt{(10-x_1)^2+x_2^2}\Big), \quad x \in D, \\ \dfrac{\partial}{\partial n}u(t,x) = x_1, \quad (t,x) \in [0,2] \times D_N, \\ \quad u(t,x) = 10\exp\Big(-\sqrt{(10-x_1)^2+x_2^2}\Big), \quad (t,x) \in [0,2] \times (\partial D \setminus D_N). \end{cases}$$

Notice that the solution $u(t,x)$ of (4.38) has singularities at $x = (0,0)$ and at $x = (10,0)$, where the Neumann and the Dirichlet boundaries collide. The stochastic representation is given by a Brownian motion X_t^x reflected at D_N and killed when hitting $\partial D \setminus D_N$. More precisely, fix $t \in [0,T]$, let $X_s^{t,x}$ be a Brownian motion reflected at D_N and started at $X_t^x = x \in D$ and let $\tau^{t,x}$ be its first hitting time at $\partial D \setminus D_N$ (after t). Then

$$u(t,x) = E\bigg(g\big(X^{t,x}_{\min(2,\tau^{t,x})}\big) - \int_t^{\min(2,\tau^{t,x})} h\big(X_s^{t,x}\big)dZ_s^{t,x}\bigg), \tag{4.39}$$

where $h(x) = x_1$, $x \in D_N$,

$$g(x) = 10\exp\Big(-\sqrt{(10-x_1)^2+x_2^2}\Big), \quad x \in \overline{D},$$

and $Z^{t,x}$ denotes the local time corresponding to $X^{t,x}$. Once again, we compute $u(0,x_0)$ with $x_0 = (10,0.2)$, close to the singularity at $(10,0)$. Using the commercial finite-element package FEMLAB, see [15], we have computed

$$u(0,10,0.2) = 4.352,$$

which is used as reference value for the reported computational errors.

Since the stochastic representation (4.39) involves sampling from a mixed reflected-stopped diffusion, we cannot directly use the algorithms presented before. An adaption of the uniform Euler Algorithm 4.1.11 to the present situation is very simple, since we only additionally have to observe the first hitting time of $\overline{X}$ at the killing boundary $\partial D \setminus D_N$. More precisely, we start with $\overline{X}_0 = x_0$ and $\overline{Z}_0 = 0$ and $\overline{\tau} = 2$. Then, for $i = 0, \ldots, N-1$, we compute

$$\hat{X}_{i+1} = \overline{X}_i + \Delta B_i, \quad \overline{X}_{i+1} = \Pi\big(\hat{X}_{i+1}\big).$$

If $\hat{X}_{i+1} \in D$, we set $\overline{Z}_{i+1} = \overline{Z}_i$. If $\hat{X}_{i+1} \notin D$, but $\overline{X}_{i+1} \in D_N$, then we compute

$$\overline{Z}_{i+1} = \overline{Z}_i + \Big\|\overline{X}_{i+1} - \hat{X}_{i+1}\Big\|.$$

If, however, $\overline{X}_{i+1} \in \partial D \setminus D_N$, then we set $\overline{Z}_{i+1} = \overline{Z}_i$ and $\overline{\tau} = t_{i+1}$ and stop the procedure. In any case, the approximate version of the stochastic

representation is given by the discretized version of (4.39), where X^x is replaces by $\overline{X}$, Z is replaced by $\overline{Z}$ and τ is replaced by $\overline{\tau}$.

Remark 4.3.6. Notice that the simulation of the mixed reflected-killed diffusion as given above introduces a third source of error: besides the interior error and the error from the reflection at the reflecting boundary, there is also the error in determining the first hitting time at the killing boundary. Even very small perturbations of the Brownian path or even of the starting vector x_0 can lead to big changes in the first hitting time at the killing boundary. A-fortiori, the convergence of the first observed hitting time of the discretized process to the first hitting time of the true, continuous solution is not unproblematic. This is probably the reason for the big advantage of using adaptive schemes for stopped diffusions as in Dzougoutov et al. [21].

N	M	Error	$\mathcal{S}$	N_{tot}
2	20 020	−3.3371	0.0643	1.79
4	20 040	−3.1662	0.0681	3.18
8	20 080	−2.7336	0.0687	5.63
16	20 160	−2.2720	0.0715	10.04
32	20 320	−1.7794	0.0710	18.12
64	20 640	−1.2920	0.0698	33.39
128	21 280	−1.0527	0.0698	63.16
256	22 560	−0.7367	0.0673	118.4
512	25 120	−0.5640	0.0639	228.9
1 024	30 240	−0.4172	0.0581	445.7
2 048	40 480	−0.2975	0.0505	861.2
4 096	60 960	−0.1921	0.0404	1 704
8 192	101 920	−0.1617	0.0315	3 357
16 384	183 840	−0.1311	0.0236	6 669
32 768	347 680	−0.0878	0.0171	13 247
65 536	675 360	−0.0556	0.0122	26 331
131 072	1 330 720	−0.0342	0.0087	52 427

Table 4.6: Results of the uniform Euler Monte-Carlo algorithm for problem (4.38).

Table 4.6 gives the results of the uniform Euler scheme for equation (4.38). While N denotes the size of the uniform grid, N_{tot} denotes the average grid size until the algorithm stops. Since the iteration only needs to be computed until the first (observed) hitting time of the discretized process at the killing boundary, this value corresponds to the final grid size of an adaptive scheme for a stopped diffusion. Note that Table 4.6 shows that the uniform Euler scheme still seems to converge with order $\frac{1}{2}$ in the singular situation (4.38), even though the starting vector $x_0 = (10, 0.2)$ is close to one singularity of the solution u. Indeed, a numerical estimate gives an estimated

order of convergence of 0.46 with respect to N_{tot} provided that the first four results of Table 4.6 are discarded and similar results hold for convergence with respect to N. Comparison with Table 4.4 shows that a much larger grid size N (or N_{tot}) is necessary to achieve a similar level of precision for the more irregular problem (4.38) than for (4.36), even if the relative error is considered.

For the adaptive algorithm, the necessary changes to Algorithm 4.2.17 correspond precisely to the adaptions to the uniform algorithm prescribed above. We need, however, also to change the local error density as given in Algorithm 4.2.14. Basically, the new local error density is chosen to be the sum of the local error density already given in Algorithm 4.2.14 and the corresponding local error density given in Dzougoutov et al. [21]. More precisely, we choose

$$l_i = l_i^{(\mathrm{ref})} + l_i^{(\mathrm{stop})},$$

where $l_i^{(\mathrm{ref})}$ is given as before, i. e.

$$l_i^{(\mathrm{ref})} = \frac{1}{2\sqrt{2\pi}} E\big(\widetilde{N}\big) \Big| v_{nn}\big(t_i, \overline{X}_i^{\mathrm{t}}\big) \Big| \exp\Big(-\frac{d\big(\overline{X}_i^{\mathrm{t}}\big)^2}{2\Delta t_i}\Big) \Delta t_i,$$

where $d(x)$ now denotes the distance of x to the reflecting boundary only. We choose v_{nn} according to

$$\Big| v_{nn}\big(t_i, \overline{X}_i^{\mathrm{t}}\big) \Big| = \frac{1}{\Big\| \overline{X}_i^{\mathrm{t}} - x_{\mathrm{sing}} \Big\|^{\beta} + \mathrm{TOL}^{\alpha}}, \tag{4.40}$$

where $x_{\mathrm{sing}} = (10, 0)$, the place of one singularity of u, and α and β are two parameters. β gives the order of the singularity of u at x_{sing}, which general theory suggests to be $\frac{1}{2}$. We have also used $\beta = 0$, which corresponds to not using the a-priori information on the singularity at x_{sing}. Adding TOL^{α} smoothes the singularity out, we choose $\alpha = 2$. Moreover, since we are only interested in the asymptotic speed of convergence, we may set $E\big(\widetilde{N}\big) = 1$. Of course, this implies that the actual computational error can only be proportional to TOL and to the error estimate used for the refinements.

For the definition of $l_i^{(\mathrm{stop})}$ we have [21, Theorem 2.1 and formula (2.8)] in mind. Intuitively $l_i^{(\mathrm{stop})}$ is decomposed of two factors: the probability that the process X^x hits the killing boundary in the interval $]t_i, t_{i+1}]$ for the first time but the discrete approximation does not hit the killing boundary, and, secondly, the path-wise error from non-detecting the hit at the killing boundary provided that this happens. Following [21], let $\hat{P}_{X,i}$ be the conditional probability that the process X^x hits the killing boundary for the first time during the interval $]t_i, t_{i+1}]$ given the past history $X_0^x, X_{t_1}^x, \ldots, X_{t_{i+1}}^x$, $i = 0, \ldots, N-1$. Moreover, $P_{X,i}$ denotes the conditional probability that

the process hits the killing boundary during the interval $]t_i, t_{i+1}]$ given $X^x_{t_i}$ and $X^x_{t_{i+1}}$ (and the implicit assumption that the process has not been killed before), $i = 0, \ldots, N-1$. Obviously, we have

$$\hat{P}_{X,i} = P_{X,i} \prod_{j=0}^{i-1} (1 - P_{X,j}), \quad i = 0, \ldots, N-1.$$

For the computations we approximate $P_{X,i}$ by

$$P_{\overline{X},i} = \exp\left(-2 \frac{\operatorname{dist}\big(\overline{X}_i\big) \operatorname{dist}\big(\overline{X}_{i+1}\big)}{\Delta t_i}\right), \quad i = 0, \ldots, N-1, \tag{4.41}$$

where dist denotes the distance to the killing boundary, i. e. in our situation we have

$$\operatorname{dist}(x) = \operatorname{dist}(x, \partial D \setminus D_N), \quad x \in \overline{D}.$$

$\hat{P}_{\overline{X},i}$ is then computed by the same formula as $\hat{P}_{X,i}$, but based on the approximations $P_{\overline{X},i}$, $i = 0, \ldots, N$.

Remark 4.3.7. Notice that (4.41) gives exactly the conditional probability for a Brownian motion W to hit a hyperplane through 0 during the interval $]t_i, t_{i+1}]$ conditioned on $W_{t_i} = \overline{X}_i$ and $W_{t_{i+1}} = \overline{X}_{i+1}$. In the general case, this formula can be used as an approximation based on local replacement of the killing boundary with its tangent hyperplane.

If the true solution process is killed during the interval $]t_i, t_{i+1}]$, but the discrete process is not, then the contribution of the stopped diffusion to the stochastic representation (4.39) is $g\big(\overline{X}_{\min(\overline{\tau},2)}\big)$ for some $\overline{\tau} > t_{i+1}$ instead of $g\big(\overline{X}_{t_{i+1}}\big)$. (In fact, we ignore the dependence of the integral term in (4.39) on the stopping time $\overline{\tau}$ right now.) Therefore, the path-wise error from the wrong detection of the first hitting time is given by

$$g\big(\overline{X}_{t_{i+1}}\big) - g\big(\overline{X}_{\min(\overline{\tau},2)}\big),$$

and we set

$$l_i^{(\mathrm{stop})} = \big(g\big(\overline{X}_{t_{i+1}}\big) - g\big(\overline{X}_{\min(\overline{\tau},2)}\big)\big)\hat{P}_{\overline{X},i}, \quad i = 0, \ldots, N-1.$$

Remark 4.3.8. $l_i^{(\mathrm{stop})}$ is not adapted to the filtration. See [21] and [79] for detailed discussions of the subtle difficulties arising from this fact.

The empirical rate of convergence for the results of the adaptive Euler algorithm in Table 4.7 is $\gamma = -1.05$, and it even changes to

$$\text{Error} \simeq 69 \times N^{-1.3}$$

if the first three entries in the table are discarded. This empirical convergence rate is in apparent contradiction to the one-dimensional example, see

TOL	N	M	Error	$\mathcal{S}$
0.3086	3.37	5 500	−3.5984	0.1284
0.1715	5.26	6 000	−3.3227	0.1293
0.0953	7.89	7 000	−2.6912	0.1247
0.0529	9.55	9 000	−2.5931	0.1058
0.0294	13.57	13 000	−1.9168	0.0888
0.0163	19.02	21 000	−1.4781	0.0703
0.0091	24.74	37 000	−1.2832	0.0532
0.0050	33.20	69 000	−0.8673	0.0390
0.0028	43.73	133 000	−0.5987	0.0279
0.0016	55.35	261 000	−0.4496	0.0198
0.0009	67.82	517 000	−0.2922	0.0140
0.0005	87.57	1 029 000	−0.1894	0.0128
0.0003	113.33	2 053 000	−0.1269	0.0070
0.0001	147.43	4 101 000	−0.0851	0.0049

Table 4.7: Results of the adaptive Euler Monte-Carlo algorithm with $\beta = 0$ and $\alpha = 2$ for problem (4.38).

Table 4.3, and to the two-dimensional problem (4.36), see Table 4.5, where we have clearly observed empirical convergence rates below 1. It seems plausible that the fast convergence of the adaptive algorithm in the case of mixed Neumann and Dirichlet conditions is caused by the extremely fast convergence of the adaptive algorithm for stopped diffusions. Indeed, from the problem formulation (4.38) it is rather apparent that the Dirichlet boundary condition contributes to the solution much stronger than the Neumann boundary. This explains why the slower convergence rate of the adaptive algorithm for reflected diffusions is overshadowed by the faster convergence of the adaptive algorithm for stopped diffusions, at least as far as the results reported in this study reach. In the end, the asymptotic rate of convergence should again be lower than 1, as before.

Notice in particular that the estimated error used for the refinement algorithm as depicted in Figure 4.5 shows the same asymptotic behavior as the computational error. Furthermore, a comparison to Table 4.6 shows that comparable levels of precision can be obtained with a much lower grid size using the adaptive algorithm with $\beta = 0$. In particular, in this situation the adaptive algorithm is also much more efficient in terms of computer time.

Even faster convergence can be obtained by using $\beta = \frac{1}{2}$, see Table 4.8. However, Figure 4.5 shows that the error estimate used for the refinement part deviates rather strongly from the actual computational error in this case. The empirical rate of convergence of the results in Table 4.8 is even slightly larger than for Table 4.7.

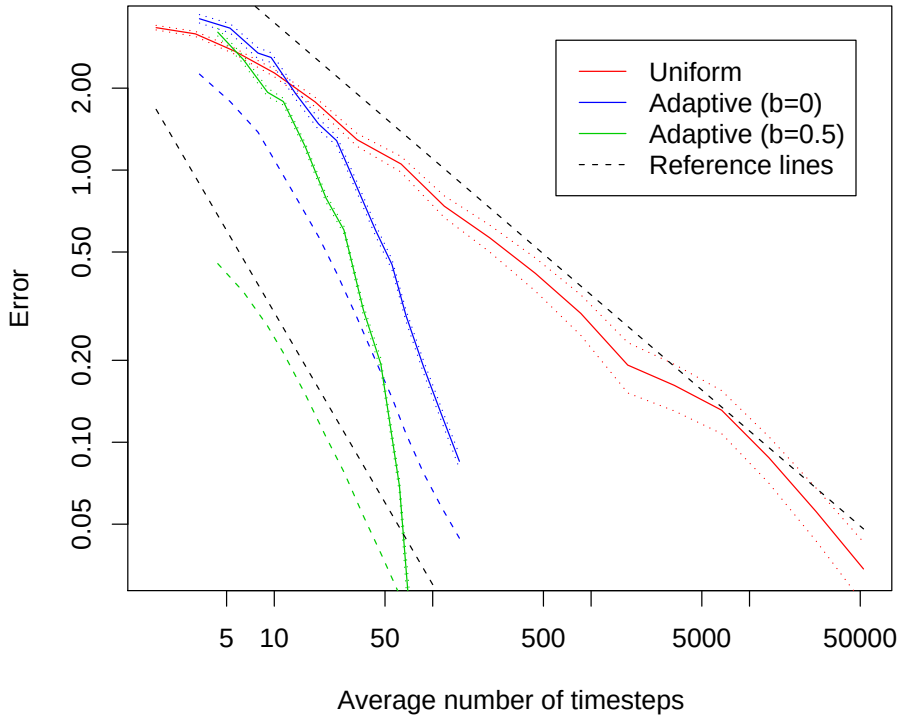


Figure 4.5: Absolute value of the error for problem (4.38). The reference lines have slopes $1/N$ and $1/\sqrt{N}$, respectively. The dashed line in color is proportional to the error estimate computed for the refinement algorithm, whereas the dotted lines correspond to 90% confidence intervals around the error.

TOL	N	M	Error	$\mathcal{S}$
0.3086	4.40	9 000	−3.2112	0.1024
0.1715	6.39	13 000	−2.5444	0.0848
0.0953	9.07	21 000	−1.9312	0.0680
0.0529	11.41	37 000	−1.7854	0.0511
0.0294	15.73	69 000	−1.2149	0.0375
0.0163	21.22	133 000	−0.7889	0.0273
0.0091	27.52	261 000	−0.6025	0.0194
0.0050	36.51	517 000	−0.3061	0.0138
0.0028	47.06	1 029 000	−0.1938	0.0098
0.0016	61.68	5 125 000	−0.0691	0.0044
0.0009	78.06	10 245 000	−0.0124	0.0031

Table 4.8: Results of the adaptive Euler algorithm with $\alpha = 2$ and $\beta = 1/2$ for problem (4.38).

Chapter 5

Implementation of hypo-elliptic simulated annealing

This chapter is based on the Bayer, Teichmann and Warnung [8], which, in turn, is largely based on Baudoin, Hairer and Teichmann [4].

Given a potential U on some state space E. By this we mean that $U : E \to \mathbb{R}$ is a rather general function possessing a global minimum $\min U$ with, possibly non-unique minimizer (set) $\arg\min U$. *Simulated Annealing* is a stochastic algorithm to find the global minimum.

It was first proposed by S. Kirkpatrick, C. D. Gelett and M. P. Vecchi [41] and, independently, by V. Černy [84] for finite state space E. Both articles are motivated by combinatorial optimization problems, in case of Kirkpatrick and his co-authors more precisely by applied problems of physical design of computers. The algorithm itself was motivated by a problem from statistical mechanics, namely the problem of finding low-temperature states of materials by slowly lowering the temperature, known as *annealing*. Already in 1953, Metropolis et al. [55] had proposed a simple but powerful algorithm allowing to simulate groups of atoms in equilibrium at a certain temperature. Consequently, the simulated annealing algorithm – for a finite state space and in discrete time – consists of applying the *Metropolis algorithm* over and over again while lowering the "temperature" until the minimum is reached. Of course, for the purposes of optimization, the "temperature" is just the name of a parameter borrowed from the Metropolis algorithm.

Before going further, let us very briefly recall the Metropolis algorithm: in order to calculate the equilibrium value of a quantity of interest in statistical mechanics, one has to integrate with respect to the *Gibbs measure*

$$\mu_U^T(dx) = C_U^T \exp(-U(x)/T)\lambda(dx), \tag{5.1}$$

where U is a potential on the phase space E of the system, e. g. the potential energy, T is the temperature and $\lambda(dx)$ is a volume element in the phase space. Finally, C_U^T is the normalizing constant such that μ_U^T is a probability

measure. In particular, we assume that $U \geq 0$ and $\int_E \exp(-U(x)/T)dx < \infty$. Since the dimension of the phase space is usually very large, Monte-Carlo simulation is the method of choice for calculating integrals with respect to μ_U^T. Therefore, we need to have an efficient way of sampling points from the distribution μ_U^T, and this is provided by the Metropolis algorithm.

When the temperature T is slowly decreasing to 0, the mass of μ_U^T at areas with large values of the potential are decreasing. Since the total mass stays constant, the effect is that the measure is concentrated more and more around $\arg\min U$. If we assume that there is a unique minimizer

$$x_0 = \arg\min_{x \in E} U(x),$$

then $\lim_{T \to 0} \mu_U^T = \delta_{x_0}$, a Dirac measure at x_0, where convergence is understood in the sense of convergence of distributions, provided that the temperature is decreased slowly enough. If $T \to 0$ too fast, then the paths may get stuck in local minima. A similar result holds if $\arg\min U$ is a finite set. On the other hand, if the volume of $\arg\min U$ is positive, then the limiting distribution is the uniform distribution. Also in the intermediate case, i. e. $\arg\min U$ is infinite but has volume 0, precise descriptions of the limiting distribution are possible provided some regularity conditions are satisfied. For more information see Hwang [37].

The simulated annealing technique consists in constructing a Markov chain (in discrete time), where the transition probabilities are given as in the Metropolis algorithm but with temperature T being decreased from step to step. In comparison to other, local optimization techniques, the randomization with the Metropolis algorithm allows the Markov chain to overcome local minima of the potential.

As already indicated above, the simulated annealing method makes, of course, also sense for continuous optimization problems. Then E is a Euclidean vector space. See the excellent review article of M. Locatelli [50] for more information about this context, in particular about useful techniques for speeding up the rather slow overall convergence of the method – i. e. the decreasing of the temperature T – without sacrificing convergence to $\arg\min U$.

We are more interested in a related technique which could be called simulated annealing in continuous time. The basic idea of this method is to add a random perturbation to a gradient flow, which allows it to overcome local minima. Let the state space be given by $E = \mathbb{R}^n$ and introduce the non-autonomous *Langevin equation*

$$dX_t^x = -\frac{1}{2}\nabla U(X_t^x)dt + \sqrt{\sigma(t)}dB_t, \tag{5.2}$$

with initial value $X_0^x = x \in \mathbb{R}^n$. Here, B_t denotes an n-dimensional Brownian motion and $\sigma : [0, \infty[\to [0, \infty[$ is called temperature. Under certain

regularity conditions on U, the process X_t^x will, for any initial value x, converge to $\arg\min U$ in law provided that the temperature $\sigma(t)$ converges to 0 slowly enough for $t \to \infty$.

Recently, F. Baudoin, M. Hairer and J. Teichmann [4] have proved a *hypo-elliptic* version of the above convergence result. By hypo-elliptic we mean that we may work with a d-dimensional Brownian motion with $d < n$, i. e. the dimension of the Brownian motion might be lower than the space dimension. Of course, we have to pay a price: the drift term of the diffusion needs to be changed and we have to use non-trivial volatility vector fields.

Remark 5.0.9. The classical view to (elliptic) simulated annealing can be described as follows: we are given a potential U and perturb the corresponding gradient flow with an n-dimensional Brownian motion B. It turns out that the Gibbs measure for U is a "locally invariant" measure (in a sense to be made precise below) for the resulting perturbed gradient flow.

Conversely, the point of view underlying hypo-elliptic simulated annealing is: given a process W (in turn driven by a d-dimensional Brownian motion with $d < n$) and the Gibbs measure of the potential U, how do we have to choose the drift in order to obtain a Markov process such that the Gibbs measure is locally invariant for the process? It will turn out that this drift term can be interpreted as a horizontal gradient related to W.

The potential benefits of hypo-elliptic simulated annealing are two-fold: first simulation of normal random variables is numerically quite expensive in many situations, therefore a reduction of the number of Brownian motions might speed up the method in certain cases, especially if we can identify "unproblematic" dimensions by inspection of the potential before starting the optimization. Moreover, it might allow us to extend simulated annealing to infinite dimensional situations, where the elliptic formulation (5.2) is not feasible. Let us mention that infinite dimensional optimization is an interesting subject in certain applications, for instance in calibration of the jump measure of models driven by Lévy processes in finance.

On the other hand, [4] actually allows the extension of simulated annealing to Lie groups with a natural sub-Riemannian geometry such as Heisenberg groups. Until now, the extension of simulated annealing to compact Riemannian manifolds has been successfully carried out, see Holley, Kusuoka and Stroock [35], but the extension to Lie groups without such a structure is new.

In the present study, we have implemented the abstract theory of [4], in order to see whether numerical calculations based on it are feasible.

5.1 Theory and implementation of hypo-elliptic simulated annealing

5.1.1 Simulated annealing in continuous time

In this section, we once again consider elliptic simulated annealing. More precisely, we report the results of L. Miclo [57], which are representative for the field. Let $U : \mathbb{R}^n \to \mathbb{R}$ be a potential satisfying

Assumption 5.1.1. $U \in C^2(\mathbb{R}^n; \mathbb{R})$ such that both U and $\|\nabla U\|$ converge to infinity as $\|x\| \to \infty$. Moreover, we assume boundedness of

$$\|\nabla U\|^2 - \Delta U$$

from below, where Δ, as usual, denotes the Laplace operator, and $\|\cdot\|$ denotes the Euclidean norm on $\mathbb{R}^n$.

We may, without loss of generality, assume that $U \geq 0$.

Remark 5.1.2. Assumption 5.1.1 basically means that U grows like $\|x\|^\alpha$ for some $1 < \alpha \leq 2$ outside some compact set. For different growth conditions, which include potentials increasing like $\|x\|^\alpha$ for $0 < \alpha < 1$, see Zitt [90]. See also Chiang, Hwang and Sheu [14] for a different method of proof and Holley and Stroock [34].

For a deterministic function $\sigma : [0, \infty[\to]0, \infty[$, consider the stochastic differential equation (5.2) driven by an n-dimensional Brownian motion $B = (B_t)_{t \in [0,\infty[}$ defined on the filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \in [0,\infty[}, P)$. As before, it will be helpful to take a look at the autonomous situation at first.

Fix $\sigma > 0$ and consider the homogeneous Markov-process

$$dY_t^y = -\frac{1}{2}\nabla U(Y_t^y)dt + \sqrt{\sigma}dB_t \tag{5.3}$$

with $Y_0^y = y \in \mathbb{R}^n$. It is well-known that Y_t^y converges, for $t \to \infty$, to its invariant measure, which coincides with the Gibbs measure μ_U^σ introduced before.

Note that μ_U^σ is a *reversible measure* for the process $Y^y = (Y_t^y)_{t \in [0,\infty[}$, i. e. the infinitesimal generator, see (1.4),

$$L^\sigma f = -\frac{1}{2}\langle \nabla U, \nabla f \rangle + \frac{\sigma}{2}\Delta f \tag{5.4}$$

(defined for $f : \mathbb{R}^n \to \mathbb{R}$ smooth enough) is a symmetric operator on the Hilbert space $L^2(\mathbb{R}^n, \mu_U^\sigma)$. The self-adjoint negative extension of L^σ (Friedrich's extension) will also be denoted by L^σ – and in the sequel we will always refer to the extension. It is well known, e. g. see Reed and Simon [66],

that L^σ has a discrete, non-positive spectrum. The largest eigenvalue is 0 and the second-largest is given by the formula

$$\lambda^\sigma = -\frac{\sigma}{2} \inf\left\{ \|\nabla f\|_{L^2(\mu_U^\sigma)} \;\middle|\; \|f\|_{L^2(\mu_U^\sigma)} = 1 \text{ and } \int_{\mathbb{R}^n} f d\mu_U^\sigma = 0 \right\}. \tag{5.5}$$

The *spectral gap* λ^σ controls the convergence of the distribution of Y_t^y towards the equilibrium, i. e. towards the measure μ_U^σ. Roughly speaking, given $f : \mathbb{R}^n \to \mathbb{R}$ measurable and integrable such that

$$\int_{\mathbb{R}^n} f(x)\mu_U^\sigma(dx) = 0,$$

then $E(f(Y_t^y))$ converges to 0 for $t \to \infty$ like $e^{\lambda^\sigma t}$, as can be seen by Fourier expansion in terms of the eigenvectors of L^σ in $L^2(\mathbb{R}^n, \mu_U^\sigma)$.

Note that simulated annealing in the sense of equation (5.2) also works on compact Riemannian manifolds for elliptic diffusions, see Holley, Kusuoka and Stroock [35].

Moreover, we would also like to mention recent results of I. Pavlyukevich, who considers the Langevin equation (5.2) driven by α-stable Lévy processes. Under suitable regularity conditions – and, of course, not too fast cooling – he finds that the solution converges, in law, to a Markov chain jumping between the local minima of the potential. In particular, if there are only finitely many local minima, the Lévy driven simulated annealing process can identify them and we can then find the global minimum by comparison of all the local minima.

5.1.2 The setting of hypo-elliptic simulated annealing

Before being able to explain what we understand by hypo-elliptic simulated annealing, we want to introduce the setting, in which it will be available.

The state space of hypo-elliptic simulated annealing will be *compact homogenous spaces*, in particular compact nilmanifolds, i. e. compact homogenous spaces with respect to the action of a nilpotent Lie group. More precisely, let G be a connected, finite dimensional Lie group with Lie algebra $\mathfrak{g}$, which we understand as the space of *left-invariant* vector fields on G. Moreover, we denote the *right-invariant* Haar measure on G by λ. We mainly have the following examples in mind, which provide a natural link to optimization problems in Euclidean vector spaces. The following examples are used as a reminder on the definitions of Section 2.1.

Example 5.1.3. Fix p generators denoted by $\{e_1, \ldots, e_p\}$ and let $\mathbb{A}_p^m$ denote the space of all non-commutative polynomials of degree less than or equal to m. By usual – non-commutative – multiplication of polynomials (and cutting off all terms of order higher than two), $\mathbb{A}_p^m$ is an associative algebra with unit, namely the *free associative, step m nilpotent algebra with unit*

generated by p generators, see Definition 2.1.9. Note, however, that we do not use the special degree deg as in Section 2.1, but rather the ordinary degree of polynomials. Again, we introduce the commutator bracket

$$[x, y] = xy - yx, \quad x, y \in \mathbb{A}_p^m,$$

and note that $\mathbb{A}_p^m$ endowed with $[\cdot, \cdot]$ is a *Lie algebra*. We consider the sub-Lie-algebra generated by $\{e_1, \ldots, e_p\}$ and denote it by $\mathfrak{g}_p^m$, the *free, step m nilpotent Lie algebra with p generators*, cf. Definition 2.1.13.

The step m nilpotent Lie group is the Lie group corresponding to the Lie algebra $\mathfrak{g}_p^m$, and it can be constructed as follows. Consider the exponential map $\exp : \mathfrak{g}_p^m \to \mathbb{A}_p^m$ defined by

$$\exp(x) = 1 + x + \frac{1}{2}x^2 + \cdots + \frac{1}{m!}x^m, \quad x \in \mathfrak{g}_p^m, \tag{5.6}$$

where the multiplication is understood in the sense of A_p^m, i. e. all terms of degree larger than m are cut off. As in Definition 2.1.13,

$$G_p^m = \exp(\mathfrak{g}_p^m)$$

is the *free, step m nilpotent Lie group with p generators*, which is known as *Heisenberg group* for $m = 2$ – notice that this group is more commonly denoted by $H_{\dim(\mathfrak{g}_p^2)}$ and $\mathfrak{g}_p^2$ is mostly denoted by $\mathfrak{h}_{\dim(\mathfrak{g}_p^2)}$, where $\dim \mathfrak{g}_p^2 = \frac{1}{2}(p^2 + p)$.

Remark 5.1.4. The exponential map $\exp : \mathfrak{g}_p^m \to G_p^m$ is a global chart of the Lie group G_p^m. Thus, a global optimization method for G_p^m will immediately give us a global optimization method for the vector space $\mathfrak{g}_p^m$ and hence for any Euclidean vector space with the same dimension.

Of course, the orthogonal groups are not nilpotent groups, however, similar results as in [4] also apply in this situation.

Example 5.1.5. The *special orthogonal group* $SO(n)$ of orthogonal $n \times n$-matrices with determinant one is a connected Lie group. Its Lie algebra is the space $\mathfrak{so}(n)$ of skew-symmetric matrices. For $n = 3$, a simple formula for the Haar measure is available. Indeed, use the parameterization of $SO(3)$ by Euler angles, i. e.

$$SO(3) = \{g_\varphi h_\psi g_\theta \mid \varphi, \theta \in [0, 2\pi],\ \psi \in [0, \pi]\}$$

with

$$g_\varphi = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad h_\psi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & -\sin\psi \\ 0 & \sin\psi & \cos\psi \end{pmatrix}.$$

Then the normalized Haar measure on $SO(3)$ is given by

$$\int_{SO(3)} f(x)\lambda(dx) = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} f(g_\varphi h_\psi g_\theta)\sin(\psi)d\varphi d\psi d\theta$$

for bounded measurable functions $f : SO(3) \to \mathbb{R}$.

We will next introduce the notion of a homogenous space, see Michor [56]. Let M be a smooth, finite dimensional manifold and consider a *right action* $r : M \times G \to M$ of the Lie group G on M, i. e. a smooth map such that

$$r(r(x,h),g) = r(x,hg) \in M, \quad \forall g,h \in G,\ x \in M.$$

An action is called *transitive* if M is one single *orbit*, i. e. if for all $x, y \in M$ we can find a $g \in G$ such that $y = r(x,g)$. If we fix some point $o \in M$, we can define a surjective map $\pi : G \to M$ by

$$\pi(g) = r(o,g), \quad g \in G. \tag{5.7}$$

A manifold M with a transitive G-action as above is called *homogenous space*. If the Lie group is nilpotent, then M is also known as *nilmanifold*. We will additionally require the manifold M to be compact. Below, we give a few examples of homogenous spaces.

Remark 5.1.6. We have the following construction in mind. Let G denote a Lie group as before and $\Gamma \subset G$ a discrete, co-compact subgroup of G and consider the factor group $\Gamma\backslash G$, i. e. the space of all left cosets of G with respect to Γ, $\Gamma\backslash G = \{\Gamma g \mid g \in G\}$. Then G transitively acts on $\Gamma\backslash G$ by $r(\Gamma g, h) = \Gamma(gh)$. Consequently, $\Gamma\backslash G$ is a homogenous space, which is compact by assumption on Γ.

Example 5.1.7. Take the Heisenberg group G_p^2 (cf. Example 5.1.3) and let it act on itself, i. e. let $r(g,h) = gh$, $g,h \in G_p^2$. Obviously, this defines a transitive group action. Using the exponential map $\exp : \mathfrak{g}_p^2 \to G_p^2$ once again, it is not difficult to construct a discrete subgroup. For simplicity, we only consider the case $p = 2$. Define $e_3 = \frac{1}{2}[e_1, e_2] \in \mathfrak{g}_2^2$ and let

$$\mathfrak{l}_2^2 = \langle\{e_1, e_2, e_3\}\rangle_{\mathbb{Z}},$$

the $\mathbb{Z}$-module generated by e_1, e_2, e_3. Of course, we understand $\mathfrak{l}_2^2 \subset \mathfrak{g}_2^2$. The exponential image $L_2^2 = \exp(\mathfrak{l}_2^2) \subset G_2^2$ is a discrete subgroup of the Heisenberg group. Indeed, fix

$$x = x_1e_1 + x_2e_2 + x_3e_3 \in \mathfrak{l}_2^2,$$
$$y = y_1e_1 + y_2e_2 + y_3e_3 \in \mathfrak{l}_2^2.$$

By the *Baker-Campbell-Hausdorff formula*

$$\exp(x)\exp(y) = \exp\Big(x + y + \frac{1}{2}[x,y] + \frac{1}{12}([x,[x,y]] - [y,[y,x]]) + \cdots\Big),$$

see Serre [75], we get

$$\begin{aligned}\exp(x)\exp(y) &= \exp\Big(x+y+\frac{1}{2}[x,y]\Big)\\ &= \exp\Big((x_1+y_1)e_1+(x_2+y_2)e_2+(x_1y_2-x_2y_1+x_3+y_3)e_3\Big) \in L_2^2\end{aligned}$$

because the coefficients with respect to e_1, e_2, e_3 are again in $\mathbb{Z}$ – we needed to choose $e_3 = \frac{1}{2}[e_1, e_2]$ because of the "$\frac{1}{2}$" term in the Baker-Campbell-Hausdorff formula. Noting that $\exp(x)^{-1} = \exp(-x)$, this shows that L_2^2 is a discrete subgroup of G_2^2. We get a compact nilmanifold $M = L_2^2 \backslash G_2^2$, the so-called *Heisenberg torus*.

Remark 5.1.8. L_2^2 is not a normal subgroup of G_2^2, consequently the Heisenberg torus is not a group anymore.

Example 5.1.9. The same construction as in Example 5.1.7 also works in the case of step m-nilpotent free Lie groups. In particular, for $p = 2$ and $m = 3$, we may define a basis of $\mathfrak{g}_2^3$ by $e_3 = \frac{1}{2}[e_1, e_2]$, $e_4 = \frac{1}{12}[e_1, [e_1, e_2]]$ and $e_5 = \frac{1}{12}[e_2, [e_1, e_2]]$. Once again, a discrete subgroup is given as exponential image $L_2^3 = \exp(\mathfrak{l}_2^3)$ of the $\mathbb{Z}$ module

$$\mathfrak{l}_2^3 = \langle \{e_1, e_2, e_3, e_4, e_5\} \rangle_{\mathbb{Z}} \subset \mathfrak{g}_2^3.$$

Example 5.1.10. The special orthogonal group $SO(3)$ is itself a compact Lie group, therefore the right action of $SO(3)$ on itself trivially makes it a compact homogenous space.

Finally, we have to relate the remaining available structures to the homogenous space. We assume that there is a measure λ^M on M which is invariant under the action, i. e. for any $g \in G$ and any bounded measurable function $f : M \to \mathbb{R}$ we have

$$\int_M f(r(x,g))\lambda^M(dx) = \int_M f(x)\lambda^M(dx).$$

Given a left invariant vector field V on G, i. e. $V \in \mathfrak{g}$, we define a vector field V^M on M by

$$(V^M f) \circ \pi = V(f \circ \pi) \tag{5.8}$$

for all smooth functions $f : M \to \mathbb{R}$, where we recall the definition of π given in (5.7).

Remark 5.1.11. In the setting of Remark 5.1.6, but under some minor additional assumption, there is always a measure on $\Gamma \backslash G$ which is invariant under the right action of G. Moreover, a celebrated formula of A. Weil, see Elstrodt [22], relates it in terms of the Haar measures on Γ and G. Moreover, Weil's formula implies uniqueness of the invariant measure.

Example 5.1.12. A Haar measure for the Heisenberg group G_p^2 is given by the Lebesgue measure on $\mathfrak{g}_p^2$. More precisely, the Haar measure λ on G_p^2 is the image measure of the Lebesgue measure on $\mathfrak{g}_p^2$ under the exponential map, i. e.

$$\int_{G_p^2} f(x)\lambda(dx) = \int_{\mathfrak{g}_p^2} f(\exp(y))dy$$

for bounded measurable functions $f : G_p^2 \to \mathbb{R}$.

Example 5.1.13. We give an explicit construction of the invariant measure as guaranteed in Remark 5.1.11 in the case of the Heisenberg torus $L_2^2 \diagdown G_2^2$ defined in Example 5.1.7. To this end, we introduce special coordinates on $L_2^2 \diagdown G_2^2$, which allow us to identify the Heisenberg torus with the three dimensional torus $\mathbb{T}^3$, where we think of the torus $\mathbb{T}$ as $[0, 1[$ and denote the rest class operation by $[\cdot]$, i. e. $[x] = x \mod 1$ for $x \in \mathbb{R}$.

Let $z = z_1e_1 + z_2e_2 + z_3e_3 \in \mathfrak{g}_2^2$. We define a map $\phi : \mathfrak{g}_2^2 \to \mathbb{T}^3$ by

$$\phi(z) = ([z_1], [z_2], [z_3 - [z_2]z_1 + [z_1]z_2]).$$

Then $L_2^2 \diagdown G_2^2 \simeq \mathbb{T}^3$ via the diffeomorphism $\phi \circ \exp^{-1} : L_2^2 \diagdown G_2^2 \to \mathbb{T}^3$. The invariant measure is then given by the Lebesgue measure on $\mathbb{T}^3$, more precisely it is the image measure of the Lebesgue measure under the map $\exp \circ \phi^{-1} : \mathbb{T}^3 \to L_2^2 \diagdown G_2^2$.

For future reference, let us summarize the setting developed in this section.

Assumption 5.1.14. Let G be a connected, finite dimensional Lie group with Lie algebra $\mathfrak{g}$ and right-invariant Haar measure λ. The state space M is a compact homogenous space with respect to G and λ^M denotes a positive, finite measure invariant with respect to the right action of G on M.

Remark 5.1.15. Assumption 5.1.14 is often too restrictive, since it only allows us to work in a manifold which is diffeomorphic to the torus, but not in the Euclidean space. In many situations, we may, however, ignore this fact and still work in the full space. Indeed, provided that we may find, for each $\epsilon > 0$ a compact subset of $\mathbb{R}^n$ such that the process under consideration remains in the set until some large time T with probability larger than $1 - \epsilon$, we may rescale the problem in such a way that the process always stays in the torus, with probability larger than $1 - \epsilon$, where the torus is understood as subset of $\mathbb{R}^n$. Then we can apply our theory, with the specification that observed trajectories leaving the torus at some point are rejected.

On the other hand, a much more elegant approach to the non-compact situation works by suitable modification of the potential outside a compact set. Note that the potential needs to be modified in a time-dependent way. We will come back to this possibility shortly

5.1.3 Hypo-elliptic simulated annealing

This section is devoted to a presentation of the results of Baudoin, Hairer and Teichmann [4]. In our point of view, their result has two different consequences for global optimization:

(1) It allows simulated annealing style global optimization on Lie groups.

(2) It can be seen as hypo-elliptic simulated annealing algorithm in Euclidean vector spaces of certain dimensions.

The connection of these two points is very simple, because the Euclidean spaces of (2) will be the Lie algebras of the Lie groups of (1).

Before getting more concrete, let us delve a little bit into the ubiquitous notion of *hypo-ellipticity*, see also Definition 1.1.8 and the related Definition 1.1.9. Just as the stronger notion of *ellipticity*, it has its origins in the theory of (semi-linear) partial differential equations. In the context of stochastic differential equations, the notions are important in their own right, and, at least in the case of hypo-ellipticity, maybe even easier to understand than in the broader PDE context. Consider a general, n-dimensional (Stratonovich) stochastic differential equation driven by a d-dimensional Brownian motion, i. e.

$$dX_t^x = V_0(X_t^x)dt + \sum_{i=1}^{d} V_i(X_t^x) \circ dB_t^i, \tag{5.9}$$

where $X_0^x = x \in \mathbb{R}^n$, $V_0, V_1, \ldots, V_d : \mathbb{R}^n \to \mathbb{R}^n$ are smooth vector fields satisfying usual growth and Lipschitz conditions and $B_t = (B_t^1, \ldots, B_t^d)$, $t \in [0, \infty[$, is a d-dimensional Brownian motion, see also (1.3). Unlike before, we do not require that $n = d$!

The SDE (5.9) is called *elliptic* if the vector fields $V_1, \ldots, V_d$ span the whole space $\mathbb{R}^n$ for each $x \in \mathbb{R}^n$, i. e. if

$$\forall x \in \mathbb{R}^n : \ \langle \{V_1(x), \ldots, V_d(x)\} \rangle_{\mathbb{R}} = \mathbb{R}^n,$$

where $\langle \cdot \rangle_{\mathbb{R}}$ again denotes the linear hull of a set. In particular, an SDE can only be elliptic for $d \geq n$, that is we need at least as many Brownian motions as space dimensions. The prime example of an elliptic diffusion is the n-dimensional Brownian motion itself, corresponding to the Laplace operator in the PDE formulation. Therefore, we may say that elliptic diffusions have the same local behavior as the Brownian motion. In particular, they fill up the space in the sense that

$$P(X_t^x \in O) > 0$$

for any $x \in \mathbb{R}^n$, any open, non-empty set $O \subset \mathbb{R}^n$ and any $t > 0$. This now provides us with a probabilistic intuition for the classical continuous-time

simulated annealing: the process (5.3) traverses, in law, the whole search space thus allowing it to identify the global minimum of the potential U. Provided that the variance of the stochastic perturbation is decreased slowly enough, the process then converges to the global minimum. For obvious reasons, (5.3) may be called elliptic simulated annealing.

Recall that the diffusion process X^x of (5.9) is called *hypo-elliptic*, if it has a smooth transition density $p_t(x,y)$ in the sense that $y \mapsto p_t(x,y)$ is the density of X_t^x. *Hörmander's theorem* states that the diffusion (5.9) is hypo-elliptic if the Lie algebra generated by the vector fields at each point $x \in \mathbb{R}^n$ spans the whole space. More precisely, the *Hörmander condition*, see Definition 1.1.9, states that

$$\{V_1(x), \dots, V_d(x)\} \cup \{[V_i, V_j](x) \mid i,j \in \{0,\dots,d\}\} \cup \\ \cup \{[[V_i, V_j], V_k](x) \mid i,j,k \in \{0,\dots,d\}\} \cup \cdots$$

is a generating set for $\mathbb{R}^n$ for each $x \in \mathbb{R}^n$, where we implicitly assume that the vector fields are C^∞-bounded, see Hörmander [36]. The proof that Hörmander's condition implies hypo-ellipticity in the above stochastic sense goes back to P. Malliavin [54]. In fact, Hörmander's condition only needs to be satisfied in the initial value $x \in \mathbb{R}^n$ of X^x.

Going further, there are conditions available, which do not only ensure existence and regularity but even positivity of the density, i. e. that the process again enters every open set with positive probability, see Ben Arous and Léandre [9], without being elliptic. Hence, the intuitive explanation of the success of simulated annealing should also apply to the hypo-elliptic situation.

In what follows, we mainly have the Heisenberg groups, Example 5.1.3, in mind. Given any group G satisfying Assumption 5.1.14, we have to fix some way to introduce stochasticity into our system.

Assumption 5.1.16. Fix $d \geq 1$ and left invariant vector fields $V_1, \dots, V_d$ on G. We assume that *Hörmander's condition* holds true, i. e. the sub-Lie-algebra of $\mathfrak{g}$ generated by $V_1, \dots, V_d$ equals $\mathfrak{g}$, where we used the well-known identification of $\mathfrak{g}$ with the space of left invariant vector fields on G.

Fix a d-dimensional Brownian motion $B_t = (B_t^1, \dots, B_t^d)$ and consider a stochastic process on G solving the Stratonovich SDE

$$dX_t^x = \sum_{i=1}^d V_i(X_t^x) \circ dB_t^i \tag{5.10}$$

with initial value $x \in G$. For readers unfamiliar with stochastic integration on manifolds, we refer to Ikeda and Watanabe [38]. Notice, however, that in all the above examples, the Lie group is naturally embedded into some vector space, therefore we may use ordinary stochastic calculus as defined

thereon. (In Example 5.1.3, this vector space is given by the respective nilpotent algebra $\mathbb{A}_p^m$.)

In any case, by the existence and uniqueness theorem for SDEs, there is a unique strong solution of (5.10) in G. Moreover, the process X_t^x is hypo-elliptic on G. Conceptually, X_t^x will play the rôle of Brownian motion in the elliptic situation, cf. (5.2). By hypo-ellipticity, X^x is well-suited for this task, since it will allow us to search globally on G, because it traverses everywhere in distribution. There are, however, some subtle differences to the elliptic situation, i. e. to the situation of dynamics driven by an n-dimensional Brownian motion, which affect the appropriate choice of drift.

Geometrically, the choice of the drift as gradient of the potential U as in (5.2) corresponds to a Riemannian geometry, where the gradient is the direction of steepest decent with respect to the Riemannian metric. In the setting of Assumptions 5.1.14 and 5.1.16, however, there is no Riemannian geometry available, or, if the group happens to be endowed with a Riemannian structure, it is not appropriate for the problem at hand. Indeed, while the n-dimensional Brownian motion can locally go in each direction of the n-dimensional space without discrimination, the "hypo-elliptic Brownian motion" X_t^x can only follow *horizontal* directions, i. e. directions given as linear combinations of $V_1(X_t^x), \dots, V_d(X_t^x)$. Therefore, the appropriate geometry on G is the sub-Riemannian geometry generated by the driving vector fields $V_1, \dots, V_d$, see Montgomery [59]. Roughly speaking, the sub-Riemannian distance between two points $x, y \in G$ is the infimum of the length of all paths joining x and y, which are always tangential to the space generated by $V_1, \dots, V_d$ along the way. To identify the natural notion of "gradient" in the present setting, having simulated annealing in mind, is one of the accomplishments of [4].

To this end, let us denote the infinitesimal generator of (5.10) by L, i. e.

$$Lf(x) = \frac{1}{2} \sum_{i=1}^{d} V_i^2 f(x), \quad x \in G, \tag{5.11}$$

for smooth functions $f : G \to \mathbb{R}$. Following, for instance, Revuz and Yor [68], we define the *carré-du-champs operator* Γ by

$$\Gamma(f, g)(x) = L(fg)(x) - f(x)Lg(x) - g(x)Lf(x), \quad x \in G, \tag{5.12}$$

again for smooth functions $f, g : G \to \mathbb{R}$. We can calculate

$$\Gamma(f, g)(x) = \sum_{i=1}^{d} V_i f(x) V_i g(x). \tag{5.13}$$

This shows that the map $\Gamma(f, \cdot) = (g \mapsto \Gamma(f, g))$ is a vector field, i. e. a first order differential operator, for any fixed f, which, moreover, is horizontal in the sense that

$$\Gamma(f, \cdot)(x) \in \langle \{V_1(x), \dots, V_d(x)\} \rangle_{\mathbb{R}}$$

for any $x \in G$. It turns out that $\Gamma(f, \cdot)(x)$ is precisely the natural horizontal gradient of f in the current setting. Consequently, under appropriate conditions on the potential $U : G \to \mathbb{R}$, the stochastic differential equation for simulated annealing on G – corresponding to the Langevin equation (5.2) in the elliptic setting – will be given by

$$dX_t^x = -\frac{1}{2}\Gamma(U, \cdot)(X_t^x)dt + \sqrt{\sigma(t)}\sum_{i=1}^{d} V_i(X_t^x) \circ dB_t^i, \tag{5.14}$$

with initial value $x \in G$. Notice that the usual global existence and uniqueness theorems for SDEs do not work for equation (5.14), because $\Gamma(U, \cdot)$ might not satisfy common growth and global Lipschitz conditions, even if U is "well-behaved", i. e. regular enough for elliptic simulated annealing. It is, however, possible to show existence and uniqueness using a special technique devised in Li [49] based on the theory of Dirichlet forms, provided that $U : G \to \mathbb{R}$ is a smooth function with

$$\int_G \exp(-U(x))\lambda(dx) < \infty,$$

see [4, Proposition 2.1].

Let $p_t(x, y)$, $x, y \in G$, denote the density of the law of X_t^x with respect to λ, i. e.

$$E(f(X_t^x)) = \int_G f(y)p_t(x, y)\lambda(dy)$$

for any bounded measurable function $f : G \to \mathbb{R}$. By hypo-ellipticity, we know that $p_t : G \times G \to \mathbb{R}$ is a smooth function for any $t > 0$. Furthermore, let $d : G \times G \to [0, \infty[$ be the sub-Riemannian or *Carnot-Carathéodory metric* on G generated by $V_1, \ldots, V_d$, i. e.

$$d(g, h) = \inf_{\gamma} \int_0^1 \sqrt{\langle \dot{\gamma}(s)\,, \dot{\gamma}(s) \rangle_G}\, ds,$$

where the infimum is taken along smooth curves $\gamma : [0, 1] \to G$ with $\gamma(0) = g$ and $\gamma(1) = h$, which are horizontal in the sense that

$$\dot{\gamma}(s) \in \langle \{V_1(\gamma(s)), \ldots, V_d(\gamma(s))\} \rangle_{\mathbb{R}}, \quad s \in [0, 1],$$

and where $\langle \cdot\,, \cdot \rangle_G$ denotes a suitable smooth section of inner products on TG. See Montgomery [59] for details.

We will now use the state space M as given in Assumption 5.1.14. In particular, all the vector fields $V_1, \ldots, V_d$ and $\Gamma(U, \cdot)$ will be interpreted as vector fields on M using the extension by the action given in (5.8). Consequently, we consider the simulated annealing equation on M, which is given by (5.14) interpreted in M, i. e.

$$dX_t^x = -\frac{1}{2}\Gamma^M(U, \cdot)(X_t^x)dt + \sqrt{\sigma(t)}\sum_{i=1}^{d} V_i^M(X_t^x) \circ dB_t^i, \tag{5.15}$$

where the initial value is given by $x \in M$ and the potential $U : M \to \mathbb{R}$ is a smooth function and Γ^M is the carré-du-champs operator with respect to the vector fields $V_1^M, \ldots, V_d^M$.

Remark 5.1.17. By compactness of M, existence of the SDE (5.15) is unproblematic, therefore we do not need the above mentioned existence result for the Langevin equation on the Lie group G. However, if U comes from a related potential on G, for which (5.14) has a global strong solution, then we may actually work in G. We will come back to this point later.

As in (5.1), define the *Gibbs measure* on M by

$$\mu_U^T(dx) = C_U^T \exp(-U(x)/T)\lambda^M(dx), \quad x \in M, \tag{5.16}$$

where C_U^T is once again a normalizing constant such that μ_U^T is a probability measure.

Theorem 5.1.18. *Given Assumptions 5.1.14 and 5.1.16, let* $U_0 = \min_{x\in M} U(x)$ *for the potential* U *on* M *with Gibbs measure* μ_U^T. *There are constants* $R, c > 0$ *such that the solution* X_t^x *of the annealing equation* (5.15) *for any* $x \in M$ *with*

$$\sigma(t) = \frac{c}{\log(R+t)} \tag{5.17}$$

satisfies: for any $\delta > 0$ *let* $A_\delta = \{x \in M \mid U(x) \geq U_0 + \delta\}$, *then*

$$P(X_t^x \in A_\delta) \leq C\sqrt{\mu_{\sigma(t)}^U(A_\delta)} \xrightarrow[t\to\infty]{} 0,$$

where C *denotes a constant independent of* t. *Consequently, the law of* X_t^x *converges weakly to a measure supported on* $\arg\min U$.

Proof. We give a short sketch of the proof given in [4], the above Theorem 5.1.18 corresponds to Theorem 4.8 therein.

The analysis first considers a very special, time-dependent potential, namely $W^\tau(x) = -\log p_\tau(x_0, x)$ for some fixed $x_0 \in M$. The corresponding infinitesimal generator

$$L^\tau = L - \frac{1}{2}\Gamma(W^\tau, \cdot) = \frac{1}{2}\sum_{i=1}^d V_i^2 - \frac{1}{2}\Gamma(W^\tau, \cdot),$$

is the infinitesimal generator of the Langevin equation

$$dY_t^y = -\frac{1}{2}\Gamma(U, \cdot)(Y_t^y)dt + \sqrt{\sigma}\sum_{i=1}^d V_i^M(Y_t^y) \circ dB_t^i \tag{5.18}$$

with constant $\sigma = 1$ and $U = W^\tau$ for fixed $\tau > 0$. Regarded as self-adjoint operator on $L^2(M, \mu_{W^\tau}^1)$, L^τ has a spectral gap of size

$$a^\tau = \frac{1}{2K\tau}$$

for some constant $K > 0$. By compactness, we have

$$\big|d(x_0,x)^2 - tW^t(x)\big| \le D \text{ and } \big|U(x) - d(x_0,x)^2\big| \le D \tag{5.19}$$

for some constant D. This allows us to recover the spectral gap if we use the potential U in equation (5.18) and a general constant σ. More precisely, the infinitesimal generator L^σ of (5.18) satisfies

$$L^\sigma = \frac{\sigma}{2}\sum_{i=1}^{d} V_i^2 - \frac{1}{2}\Gamma(U,\cdot)$$

and has a spectral gap a^σ of size

$$a^\sigma \ge \frac{1}{K}\exp\Big(-\frac{4D}{\sigma}\Big).$$

Now let $u(t)$ denote the norm of the Radon-Nikodym derivative of the law of X_t^x solving (5.15) with respect to the Gibbs measure $\mu_U^{\sigma(t)}$ computed in $L^2(\mu_U^{\sigma(t)})$, where $\sigma(t)$ is given as in the statement of the theorem with $c = 4D$ and R sufficiently big. Then we may conclude that $u(t)$ is (uniformly) bounded from above, which proves the result by the Cauchy-Schwarz inequality. □

Remark 5.1.19. In fact, the proof relies on the following properties of the state space M and the potential U.

(1) The operator L^τ defined on the Lie group G has a spectral gap as an operator on $L^2(\mu_1^{W^\tau})$. The spectral gap is of size $a^\tau > 0$ for a sufficiently regular function a.

(2) M is a homogenous space with respect to G. We are given vector fields $V_1,\dots,V_d$ satisfying Assumption 5.1.16 such that the induced Carnot-Carathéodory metric and the induced heat-kernel on M satisfy that there is a constant $D > 0$ and some $x_0 \in M$ with

$$\forall x \in M,\ \forall t \in]0,1[\colon\ \big|d(x_0,x)^2 + t\log p_t(x_0,x)\big| \le D.$$

(3) The potential is close to the Carnot-Carathéodory metric in the sense that there is a constant $D > 0$ and $x_0 \in M$ such that

$$\forall x \in M\colon\ \big|U(x) - d(x_0,x)^2\big| \le D.$$

The current setting introduced in Assumption 5.1.14 turns out to be convenient, because there all these conditions are automatically satisfied. Indeed, by the Driver-Melcher inequality, cf. Driver and Melcher [19], (1) is satisfied for any connected, finite dimensional, nilpotent Lie group. On the other

hand, it is known since the recent paper by Li [48] that the inequality in (2) is not satisfied for the Heisenberg group (acting on itself). However, by a result of Léandre [46, 47], we have

$$\lim_{t\to 0} t \log(p_t(x_0, x)) = -d(x_0, x)^2$$

uniformly on any compact nilmanifold M. Therefore, the above inequality is satisfied on compact nilmanifolds. The last point (3) is a condition on the potential, which is trivially satisfied in a compact setting. Otherwise, it somehow means that we can a-priori give a compact set, in which $\arg\min U$ lies.

Remark 5.1.20. The condition (2) in Remark 5.1.19 can always be satisfied, even in a non-compact situation, if we are allowed to modify the potential outside of a compact set, e. g. because we know from the beginning that $\arg\min U \subset K$ for some known compact set K. Then we can consider a bump function $0 \leq \varphi \leq 1$ with compact support, such that $\varphi|_K \equiv 1$, and define

$$U_t(x) = \varphi(x)U(x) - (1 - \varphi(x))t \log p_t(x_0, x).$$

This potential certainly satisfies (2), since it is equal to $t \log p_t(x_0, \cdot)$ outside of a compact set, and we can still rely on Léandre's result inside the compact support of φ.

Of course, the modification is harmless for global optimization, if we make sure that $\arg\min U \subset K$.

5.1.4 Implementation

Let us briefly describe the setting for the implementation. Theorem 5.1.18 provides the basis for the hypo-elliptic simulated annealing as a global optimization problem for the potential U on the homogenous space M (over the Lie group G with Lie algebra $\mathfrak{g}$), having Assumption 5.1.14 and 5.1.16 in mind.

If we want to solve an optimization problem given on M, i. e. with a potential $U : M \to \mathbb{R}$, then we can directly solve the corresponding hypo-elliptic equation on M. This case seems to be realistic if G is itself a compact Lie group and $M = G$, e. g. for $G = SO(n)$. Usually, embedding M into a Euclidean space $\mathbb{R}^N$, N large enough, and applying a straight-forward Euler scheme thereon will not give satisfying results, since the approximate solution might rapidly leave M. However, specialized algorithms for SDEs on manifolds are available, see, for instance, Malham and Wiese [53]. In our situation, we can use the exponential coordinates of the Lie group.

For optimization on $\mathbb{R}^n$, we use the following approach. We choose a free Lie group, i. e. we are in the situations introduced in Example 5.1.3 and the compact nilmanifold M is constructed as in Example 5.1.7, respectively. Therefore, keeping Example 5.1.13 in mind, we have a diffeomorphism ϕ :

$M \to \mathbb{T}^n$, where $\mathbb{T}$, once again, denotes the torus and $n = \dim \mathfrak{g}$ is the dimension of the Lie group. In the following, we will always identify the torus $\mathbb{T}^n$ with the nilmanifold M using ϕ.

We start with a family of smooth vector fields $V_1, \dots, V_d : \mathbb{R}^n \to \mathbb{R}^n$, which we will also interpret as vector fields on the torus. Understood as vector fields on the Lie algebra $\mathfrak{g}$, they have to be *left invariant* in the sense that their push forward under $\exp : \mathfrak{g} \to G$ is a left invariant vector field on the Lie group G.

Remark 5.1.21. Left-invariance of the vector fields guarantees that the infinitesimal generator of the simulated annealing process on the group G defined in (5.14) is a symmetric operator on the Hilbert space $L^2(G, \mu_U^T)$. Therefore, left-invariance is a critical requirement on the vector fields, and one cannot expect convergence otherwise, cf. the proof of Theorem 5.1.18.

As before, let Y^y denote the Langevin equation

$$dY_t^y = -\frac{1}{2}\Gamma(U, \cdot)(Y_t^y)dt + \sqrt{\sigma(t)} \sum_{i=1}^{d} V_i(Y_t^y) \circ dB_t^i \tag{5.20}$$

on $\mathbb{T}^n$.

In order to solve the global minimization problem in $\mathbb{R}^n$ for the potential $U : \mathbb{R}^n \to \mathbb{R}$, we assume that

- there is a compact set $K \subset \mathbb{R}^n$ with $\arg\min U \subset K$ which is a-priori given,
- the vector fields $V_1, \dots, V_d : \mathbb{R}^n \to \mathbb{R}^n$ are such that the Langevin equation (5.20) understood as SDE in $\mathbb{R}^n$ has a global solution.

Basically, we have three options in this moment. First, we may solve the hypo-elliptic simulated annealing equation (5.20) on the torus $\mathbb{T}^n$. To this end, we need to choose the torus $\mathbb{T}^n$ in such a way that $K \subset \mathbb{T}^n \subset \mathbb{R}^n$ and restrict it to a potential on $\mathbb{T}^n$. More precisely, we can (easily) diffeomorphically transform the space $\mathbb{R}^n$ such that the potential takes its minimum in $[0,1[^n$, i. e. such that $K \subset [0,1[^n \simeq \mathbb{T}^n$. (More precisely, we need to make sure that $K \subset]\delta, 1-\delta[^n$ for some $\delta > 0$.) Notice that this transformation can be performed explicitly since we have assumed that K is a-priori given. Then we need to restrict U to a potential on $\mathbb{T}^n$, which we will denote by $U|_{\mathbb{T}^n}$. In fact, a closer look reveals that we only need to restrict $\Gamma(U, \cdot)$ to $\mathbb{T}^n$, which can be simply done by extending it as a periodical function outside of $[0,1[^n$. By Theorem 5.1.18, Y_t^y converges in distribution to a measure concentrated on

$$\arg\min_{x \in \mathbb{T}^n} U|_{\mathbb{T}^n}(x).$$

By construction, the arg min of the restricted potential corresponds to the arg min of the original potential on $\mathbb{R}^n$ by reverting the above transformation.

On the other hand, we may treat the hypo-elliptic annealing equation as an equation on $\mathbb{R}^n$. Since equation (5.20) understood as an SDE on $\mathbb{R}^n$ has a strong solution, for any fixed time $T > 0$ and any $\epsilon > 0$ we may find a compact set $C \subset \mathbb{R}^n$ such that

$$P(\exists t \in [0,T] : \ Y_t^y \notin C) \leq \epsilon.$$

Consequently, by rescaling the problem in such a way that $C \subset [0,1[^n$, the solution Y^y of equation (5.20) understood as equation in $\mathbb{R}^n$ does not leave the torus $\mathbb{T}^n$ understood as a subset of $\mathbb{R}^n$ with probability $1-\epsilon$ until time T. Consequently, we may change the vector fields $V_1, \ldots, V_d : \mathbb{R}^n \to \mathbb{R}^n$ and the potential $U : \mathbb{R}^n \to \mathbb{R}$ to give us vector fields $V_1, \ldots, V_d : \mathbb{T}^n \to \mathbb{R}^n$ and a potential $U : \mathbb{T}^n \to \mathbb{R}$ and then consider the equation (5.20) as equation on $\mathbb{T}^n$, such that the solutions coincide with probability $1-2\epsilon$. Summarizing, the *hypo-elliptic simulated annealing algorithm* on $\mathbb{R}^n$ is given as follows.

(1) Fix a time $T > 0$, until which the solution of the non-autonomous Langevin equation should be computed, and an initial value $y \in \mathbb{R}^n$. Furthermore, fix the *cooling schedule* $\sigma(t)$.

(2) Fix a numerical scheme for the Langevin equation, in particular, fix a time discretization of size N and a number M of trajectories to be approximated.

(3) Solve the equation given the parameters fixed in 1 with the numerical scheme defined in 2.

(4) Find the realized minimum of the potential for the simulated paths.

Remark 5.1.22. In (1), the choice of the cooling schedule is problematic, since the constants c and R in Theorem 5.1.18 are usually very difficult to compute, if at all. Therefore, the usual approach is to guess them, run the simulated annealing algorithm and check whether the process can traverse local maxima of the potential. Moreover, notice that the constants c and R actually are constants for the problem on $\mathbb{T}^n$. Therefore, they depend on ϵ: decreasing ϵ means that c and R need to be increased.

Remark 5.1.23. The convergence in Theorem 5.1.18 is a convergence in distribution, therefore we may use a weak discretization scheme for the equation (5.20) (understood as equation in $\mathbb{R}^n$). Discrete pseudo random numbers for weak schemes can be much faster generated than their continuous counterparts necessary in strong schemes. Moreover, higher order weak Taylor schemes are feasible, in contrast to their strong counterparts (in dimensions $d > 1$).

Remark 5.1.24. Since the convergence of the simulated annealing algorithm to the minimum is a convergence in distribution, one should always solve the Langevin equation along several paths, not only along one path.

The third and most elegant option has already been described in Remark 5.1.20.

5.2 Numerical examples

5.2.1 Two test problems

Let us first present the test potentials used in the sequel. In order to test hypo-elliptic simulated annealing as well as to compare it to the elliptic algorithm we considered the following two potentials $U : \mathbb{R}^n \to \mathbb{R}$.

The Rastrigin potential (see e. g. Törn and Zilinskas [82]), is defined by

$$U(x) = 10n + \sum_{i=1}^{n}(x_i^2 - 10 \cdot \cos(2\pi x_i)). \tag{5.21}$$

Obviously this potential has its unique global minimum at the origin. The plot of the potential in $\mathbb{R}^2$ in Figure 5.1 shows that the potential has infinitely many local minima due to the cosine term. Obviously it grows like $\|x\|^2$ for big x.

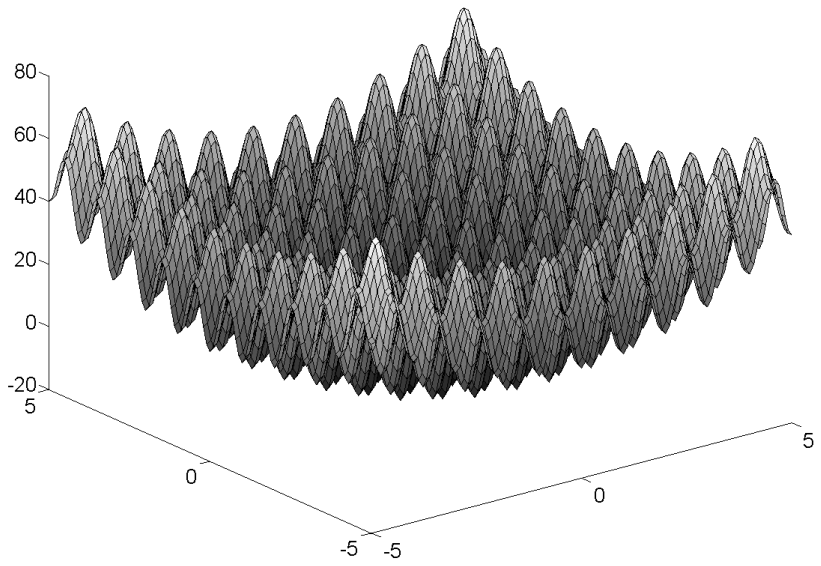


Figure 5.1: Rastrigin potential in $\mathbb{R}^2$

The second potential that we consider is an adoption of the Drop Wave

potential (see e. g. Molga and Smutnicki [58]), defined by

$$U(x) = 1 + \frac{\|x\|^2}{100} - \frac{2 + 2\cos(12\|x\|)}{\|x\|^2 + 2}. \tag{5.22}$$

Again we find the unique, global minimum at the origin. Note that the potential usually called Drop Wave potential is defined without the term $1 + \|x\|^2/100$. We added this term in order to have non-negativity and again growth of the order of $\|x\|^2$. In the following we will refer to (5.22) simply as the Drop Wave potential. The plot in $\mathbb{R}^2$ in Figure 5.2 shows that this potential offers different features than the Rastrigin potential. As it only depends on the norm of x it is radially symmetric. But it features potential walls that would be impossible for deterministic gradient flows to traverse. Moreover, hypo-elliptic simulated annealing does not use the Euclidean geometry, anyway.

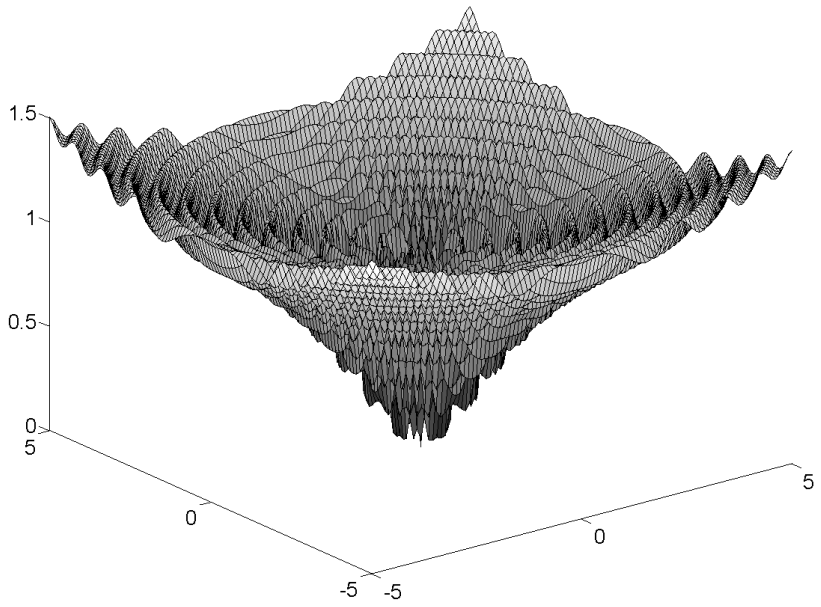


Figure 5.2: Drop Wave potential in $\mathbb{R}^2$

We considered the simulated annealing algorithm applied to the above potentials in dimension three, five and six. As mentioned before we are not free to apply the hypo-elliptic algorithm to any dimension. In particular, using the Heisenberg groups only dimensions $(p^2 + p)/2$ are possible, which is the reason why, e. g., dimension four can not be treated by our approach. We were able to derive useful and efficient set-ups for dimensions three and

six, while dimension five does not seem feasible to us as explained in Remark 5.2.1. Details on the corresponding vector fields follow below.

The SDE for the elliptic approach is given by (5.2) with as many Brownian motions as space dimensions. For the hypo-elliptic approach we fixed the following set-up.

For dimension three we considered two independent Brownian motions $(B_t^1)_{t\geq 0}$ and $(B_t^2)_{t\geq 0}$, the volatility vector fields

$$V_1(x) = \begin{pmatrix} 1 \\ 0 \\ -x_2 \end{pmatrix}, V_2(x) = \begin{pmatrix} 0 \\ 1 \\ x_1 \end{pmatrix} \tag{5.23}$$

and the horizontal gradient given by formula (5.13), i. e.

$$\Gamma(U,\cdot)(x) = \begin{pmatrix} U_{x_1}(x) - x_2 U_{x_3}(x) \\ U_{x_2}(x) + x_1 U_{x_3}(x) \\ x_1 U_{x_2}(x) - x_2 U_{x_1}(x) + (x_1^2 + x_2^2) U_{x_3}(x) \end{pmatrix}, \tag{5.24}$$

where we used the notation U_{x_i} for $\frac{\partial U}{\partial x_i}$ for $i = 1, 2, 3$. This choice of the vector fields leads to the following SDE

$$dY_t^y = -\frac{1}{2}\Gamma(U,\cdot)(Y_t^y)dt + \sqrt{\sigma(t)}V_1(Y_t^y)dB_t^1 + \sqrt{\sigma(t)}V_2(Y_t^y)dB_t^2. \tag{5.25}$$

Note that the SDE (5.20) is written in Stratonovich form. Due to the choice of the vector fields in the case of (5.25) the Stratonovich correction term is zero and the Itô form coincides with the Stratonovich form.

In dimension six we used three independent Brownian motions $(B_t^1)_{t\geq 0}, (B_t^2)_{t\geq 0}$ and $(B_t^3)_{t\geq 0}$ and applied the following vector fields:

$$V_1(x) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -x_2 \\ -x_3 \\ 0 \end{pmatrix}, V_2(x) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ x_1 \\ 0 \\ -x_3 \end{pmatrix}, V_3(x) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ x_1 \\ x_2 \end{pmatrix}. \tag{5.26}$$

In this setting the horizontal gradient given by formula (5.13) equals

$$\Gamma(U,\cdot)(x) = \begin{pmatrix} U_{x_1}(x) - x_2 U_{x_4}(x) - x_3 U_{x_5}(x) \\ U_{x_2}(x) + x_1 U_{x_4}(x) - x_3 U_{x_6}(x) \\ U_{x_3}(x) + x_1 U_{x_5}(x) + x_2 U_{x_6}(x) \\ x_1 U_{x_2}(x) - x_2 U_{x_1}(x) + (x_1^2 + x_2^2) U_{x_4}(x) + x_2 x_3 U_{x_5}(x) - x_1 x_3 U_{x_6}(x) \\ x_1 U_{x_3}(x) - x_3 U_{x_1}(x) + (x_1^2 + x_3^2) U_{x_5}(x) + x_2 x_3 U_{x_4}(x) + x_1 x_2 U_{x_6}(x) \\ x_2 U_{x_3}(x) - x_3 U_{x_2}(x) + (x_2^2 + x_3^2) U_{x_6}(x) - x_1 x_3 U_{x_4}(x) + x_1 x_2 U_{x_5}(x) \end{pmatrix}. \tag{5.27}$$

Thus in dimension six the SDE for the hypo-elliptic setting is given by

$$\begin{aligned} dY_t^y = &-\frac{1}{2}\Gamma(U,\cdot)(Y_t^y)dt \\ &+ \sqrt{\sigma(t)}V_1(Y_t^y)dB_t^1 + \sqrt{\sigma(t)}V_2(Y_t^y)dB_t^2 + \sqrt{\sigma(t)}V_3(Y_t^y)dB_t^3. \end{aligned} \tag{5.28}$$

Again the Stratonovich form equals the Itô form.

Finally we have to consider the order of the drift term. Both potentials (5.21) and (5.22) are of growth of the order two and the partial derivatives grow linearly. Thus we have order two in the first two components of the drift (5.24) resp. in the first three components of (5.27). The crucial point making the numerical treatment of the SDE (5.25) resp. (5.28) subtle is that the third component of (5.24) and the last three components of (5.27) have growth like a polynomial of degree three. Thus, we can reduce the number of Brownian motions by using slightly more complex volatility vector fields but we have to use a much more complex drift term. The higher order of the drift forces us to reduce the step size of the time discretization in order to avoid numerical instability. Additionally the evaluation of the drift part is usually more costly than in the elliptic case.

Remark 5.2.1 (The five dimensional case). We wanted to find a hypo-elliptic simulated annealing algorithm in dimension five using only two Brownian motions. Possible volatility vector fields are

$$V_1(x) = \begin{pmatrix} 1 \\ 0 \\ -\frac{1}{2}x_2 \\ -\left(\frac{1}{12}x_1x_2 + \frac{1}{2}x_3\right) \\ -\frac{1}{12}x_2^2 \end{pmatrix}, V_2(x) = \begin{pmatrix} 0 \\ 1 \\ \frac{1}{2}x_1 \\ \frac{1}{12}x_1^2 \\ \frac{1}{12}x_1x_2 - \frac{1}{2}x_3 \end{pmatrix}. \tag{5.29}$$

Consider that the highest order among the components of the vector fields in (5.29) is two, while the vector fields used in (5.23) and (5.26) are affine functions in x. One can show that this is true for any choice of *left-invariant* vector fields using two Brownian motions for five space dimensions. This higher order of the volatility vector fields is reflected in a higher order in the components of the drift calculated according to (5.13). To deal with such a drift we had to choose the step size of our discretization scheme extremely small ($\Delta t \approx 10^{-6}$) in order to avoid numerical explosion phenomena. But then for a numerical solution of the corresponding SDE up to the horizon $T = 2500$ approximately $2,500,000,000$ evaluations of the drift and generations of Brownian increments would be necessary. Furthermore note that we simulated between 100 and 500 paths together in order to get a feeling for the distribution. Due to the exceptional run time needed we dismissed such an algorithm.

Remark 5.2.2. Recently, we have also implemented a test problem in $SO(3)$. There, the elliptic simulated annealing algorithm is clearly inferior to the

hypo-elliptic one, because the reduction of the number of Brownian motions is not compensated by a more complex drift and volatility vector fields, since there is no such thing as a "flat", constant tangential vector field on $SO(3)$.

For the discretization of the SDEs (5.2) and (5.20) we chose a standard strong Euler scheme in the sense of Definition 1.3.3.

Furthermore we had to choose the constants c and R in the cooling schedule $\sigma(t)$ in (5.17). The numerical analysis in Section 5.2.2 shows that the choice of c in the case of our problems depends on the dimension. For both potentials we chose the same c for the hypo-elliptic algorithm as for the elliptic one and a higher c for the problem in dimension six. Namely, we took the ad-hoc choice of $R = 2$ for both problems and empirically chose for the Rastrigin potential c to be $c = 15$ for the elliptic and for the hypo-elliptic algorithm in dimension three and even $c = 100$ for dimension six. For the Drop Wave potential we used $c = 1$ for both algorithms in dimension three. Since annealing for the Drop Wave potential in dimension six does not exhibit remarkable differences to dimension three, we omit a detailed description.

Note that the choice of c is crucial for the performance of the algorithm. If c is chosen too small then the algorithm gets stuck in local minima. On the other hand it can, in practice, not be chosen arbitrary high as the temperature decays logarithmically in time. If we stop the algorithm at high temperature then the variance of the end points of the sample paths is simply too high to allow any analysis of the global minimum.

Remark 5.2.3. Recall that the convergence Theorem 5.1.18 only holds for the problem on the compact homogenous space $\mathbb{T}^n$, not on $\mathbb{R}^n$. Therefore, we may anyway not expect convergence of the algorithm in $\mathbb{R}^n$. The above comments are to be understood as referring to the underlying process on the torus, which, by construction, coincides with the process on $\mathbb{R}^n$ with probability $1 - \epsilon$. See also, however, Remark 5.1.20.

Remark 5.2.4. While solving an SDE numerically, the horizon T is usually fixed. We need to increase the horizon when going further in the annealing process. Therefore using a uniform grid with step size Δt the discretization error depends on the step size Δt as well as on the horizon T. The following estimate [42, Theorem 14.5.1] of the weak error holds for a fixed horizon T

$$|E[g(Y_T^y)] - E[g(Y_T^y(\Delta t))]| \leq C(T)\Delta t,$$

where $Y_T^y(\Delta t)$ denotes the end point at T of a discretization of the SDE (5.25) using a step size of Δt and g is a suitable test function. The constant C in fact depends on the horizon T in a linear way. Thus if we want to keep the error bound constant while increasing the horizon from to kT for some $k > 0$ then we have to reduce the step size from Δt to $\frac{\Delta t}{k}$. For simplicity, we chose the step size Δt sufficiently small for the highest horizon T under consideration and used this value also for smaller horizons.

We could use the rather big step size of $\Delta t = 0.01$ for the Drop Wave potential as the drift vector field in (5.25) resp. in (5.28) did not cause any numerical problems for this choice. The Rastrigin potential is more difficult to handle and we used a step size of $\Delta t = 0.001$. But as the order of the drift components does not depend in the dimension of the problem we could use the same Δt in dimension six as in dimension three.

Remark 5.2.5. As an alternative to the strong Euler scheme a weak Euler scheme with e. g. $\{+1, -1\}$-valued random variates with the correct expectation and covariance matrix could have been used as well (see Kloeden and Platen [42, Chapter 14] for details). Weak schemes often reduce run-time as the generation of normal variates is more complex than the generation of discrete ones.

5.2.2 Results and interpretation

In Tables 5.1– 5.5 we show certain statistics of the samples resulting from the algorithms applied to the Rastrigin as well as to the Drop Wave potential in dimension three respectively six. The tables provide four statistics calculated from 500 paths. Recall that both potentials have their global minimum at the origin. Therefore the norm of the end points tells us how close to the global minimum the points are in the mean. Furthermore, the empirical 80% quantile of the norm is displayed. This means that considering just one path we can expect that the norm of the end point is smaller than $q_{0.8}(\text{norm})$ with a probability 0.8. The other two statistics tell us how close the observed function values are to the minimum of the potential. Therefore we display the average value of the function values as well as the smallest value in the sample. Notice that the Rastrigin potential has rather high function values even very close to the origin, e. g. $U(0.1, 0.1, 0.1) = 5.7595$ and $U(0.2, 0.2, 0.2) = 20.8495$. Therefore the numbers in Table 5.1 and Table 5.2 are more satisfying than they look at first sight. The same reasoning applies to dimension six in Table 5.5.

Remark 5.2.6. We have also tested shifted potentials where the global minimum is attained at points $x_0 \neq 0$. Since we did not find remarkable differences we concentrated on the non-shifted case, note however the Rastrigin example in dimension six below.

Consider that the convergence of both algorithms – the elliptic as well as the hypo-elliptic simulated annealing algorithm – is slow. Moreover, note that the convergence of the computed statistics is not monotonous. The fact that the temperature decays at a rate of $\sqrt{1/\log(t)}$ for $t \to \infty$ of course causes the slow convergence. Furthermore, the path-wise non-monotonicity of the algorithms is indeed their strength. The paths also climb up areas of high values of the potential in order to finally reach the global minimum. This nature of simulated annealing can be seen in the tables.

Figure 5.3 shows the histograms of 500 paths at $t = 1$ and $t = 4000$ of the hypo-elliptic simulated annealing algorithm applied to the Rastrigin potential in dimension three. The starting position for all paths was $(5, 5, -5)$ and the constant c was chosen to be $c = 15$. We see that the paths quickly explore the space in the beginning. The statistics in Table 5.2 show that the distance of the paths from the origin decreases slowly but steadily. As mentioned before this slow convergence is unavoidable in our setting.

In Figure 5.4 we illustrate the failure of the annealing if the constant c is chosen too small. The histograms of the position of the end points at $t = 4000$ show that the first and the second components of most of the paths are stuck around the values 2 and 3 which is far away from the optimal 0. The scatter plot in Figure 5.4 also shows that the end points of the paths are stuck in local minima. One sees the failure of the algorithm in Table 5.3 as the statistics improve much less after $t = 512$ than in Table 5.2.

Figure 5.5 shows hypo-elliptic simulated annealing of 500 paths for the Drop Wave potential in $\mathbb{R}^3$. The starting point of all paths is $(5, 5, -5)$. The histogram of the position of the end points at $t = 4000$ shows that local minima are less attractive than for the Rastrigin potential (compare Figure 5.3). The influence of the randomness is less damped and thus the end points fall in a larger range. Nevertheless the concentration at the global minimum makes convergence plausible. Table 5.4 gives the corresponding statistics.

Finally to illustrate the performance of hypo-elliptic simulated annealing for problems in dimension six, we present the statistics in Table 5.5. After trying several values for the constant c we chose the rather high value $c = 100$ in order to avoid paths getting stuck in local minima.

Table 5.1: Statistics of elliptic simulated annealing for the Rastrigin potential in $\mathbb{R}^3$, $c = 15$ starting at $(5, 5, -5)$

time	mean(norm)	$q_{0.8}$(norm)	mean(f)	min(f)
0	8.66	8.66	50.25	50.25
1	5.43	7.04	55.25	4.45
256	1.81	2.41	8.84	1.14
512	1.78	2.39	7.89	0.29
1024	1.69	2.30	7.30	0.43
2048	1.62	2.25	6.77	0.12

Table 5.2: Statistics of hypo-elliptic simulated annealing for the Rastrigin potential in $\mathbb{R}^3$, $c = 15$ starting at $(5, 5, -5)$

time	mean(norm)	$q_{0.8}$(norm)	mean(f)	min(f)
0	8.66	8.66	50.25	50.25
1	5.92	8.46	68.85	6.89
256	1.88	2.43	10.19	0.02
512	1.78	2.35	8.42	0.17
1024	1.67	2.28	7.41	0.51
2048	1.58	2.18	6.50	0.32

Table 5.3: Statistics of hypo-elliptic simulated annealing for the Rastrigin potential in $\mathbb{R}^3$, with $c = 3$ starting at $(5, 5, -5)$

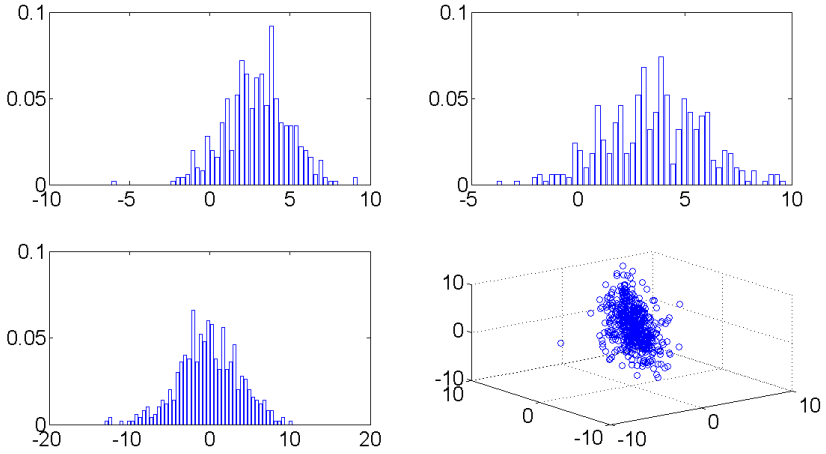
time	mean(norm)	$q_{0.8}$(norm)	mean(f)	min(f)
0	8.66	8.66	50.25	50.25
1	5.38	6.20	50.19	8.89
256	3.42	3.99	16.81	4.48
512	3.37	3.78	16.26	4.56
1024	3.33	3.74	16.00	4.38
2048	3.31	3.67	15.14	3.85

Table 5.4: Statistics of hypo-elliptic simulated annealing for the Drop Wave potential in $\mathbb{R}^3$, $c = 1$ starting at $(5, 5, -5)$

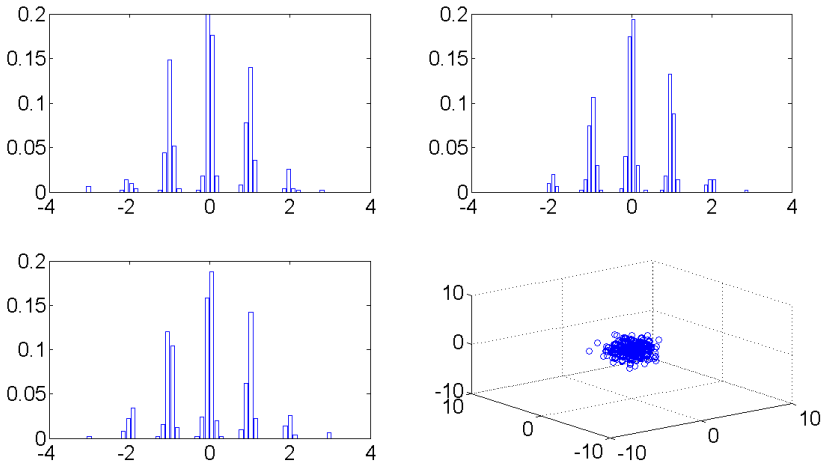
time	mean(norm)	$q_{0.8}$(norm)	mean(f)	min(f)
0	8.66	8.66	1.75	1.75
1	9.25	11.17	1.77	0.78
256	3.67	5.51	0.79	0.12
512	2.82	4.28	0.63	0.12
1024	2.43	3.62	0.57	0.12
2048	1.97	2.97	0.47	0.12

Table 5.5: Statistics of hypo-elliptic simulated annealing for the Rastrigin potential in $\mathbb{R}^6$, $c = 100$ starting at $(5, 5, -5, 5, -5, 5)$ with the potential shifted such that the minimum 0 is attained at $x_0 = (10, 10, 10, 10, 10, 10)$, where *dist* means the distance from x_0.

time	mean(dist)	$q_{0.8}$(dist)	mean(f)	min(f)
0	12.25	12.25	150.00	150.00
1	20.87	23.95	477.10	168.03
256	11.00	13.12	182.01	50.60
512	9.37	11.53	148.89	42.73
1024	8.15	10.54	127.52	30.37
2048	7.39	9.69	114.21	26.29



(a) $t = 1$



(b) $t = 4000$

Figure 5.3: Hypo-elliptic simulated annealing of the Rastrigin Potential in 3D with histograms for components 1 (top left), 2 (top right) and 3 (lower left), and a scatter plot of the simulated points (lower right) with $c = 15$ starting at $(5, 5, -5)$.

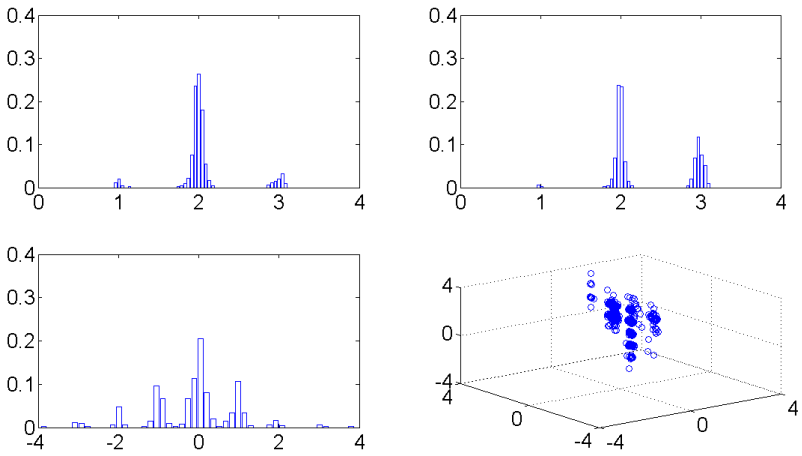


Figure 5.4: Hypo-elliptic simulated annealing of the Rastrigin Potential in 3D with histograms for components 1 (top left), 2 (top right) and 3 (lower left), and a scatter plot of the simulated points (lower right) at $t = 4000$ with $c = 3$ starting at $(5, 5, -5)$.

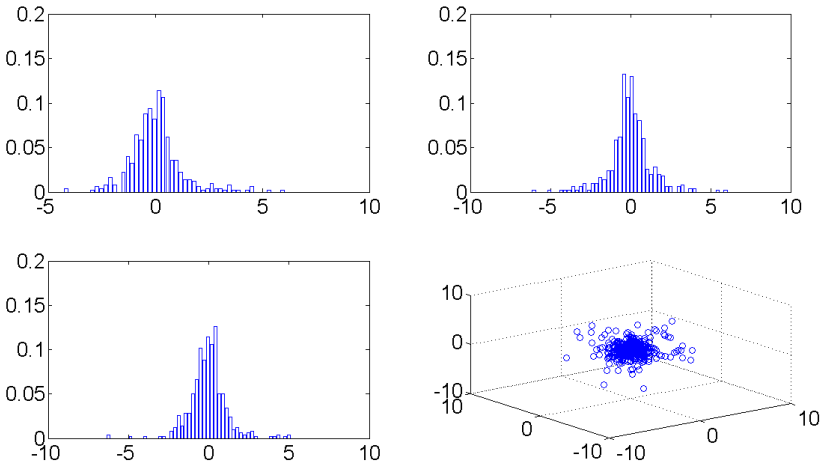
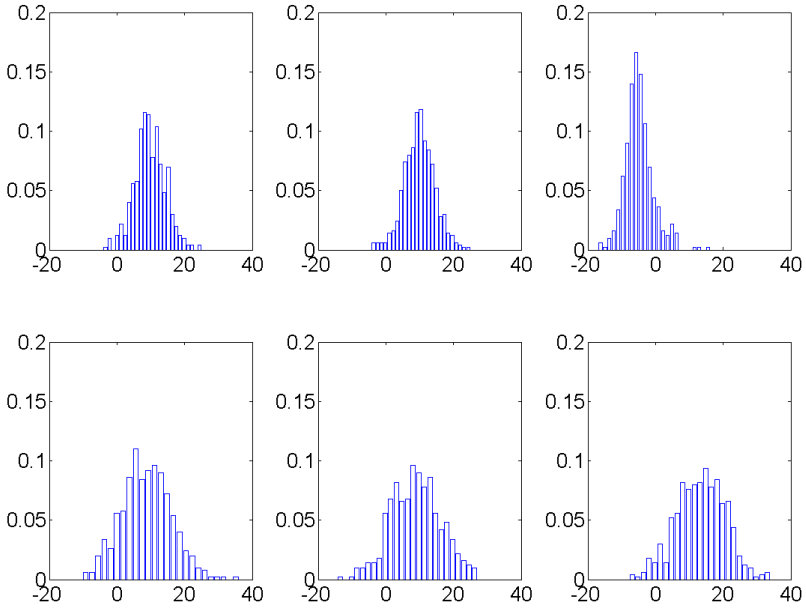
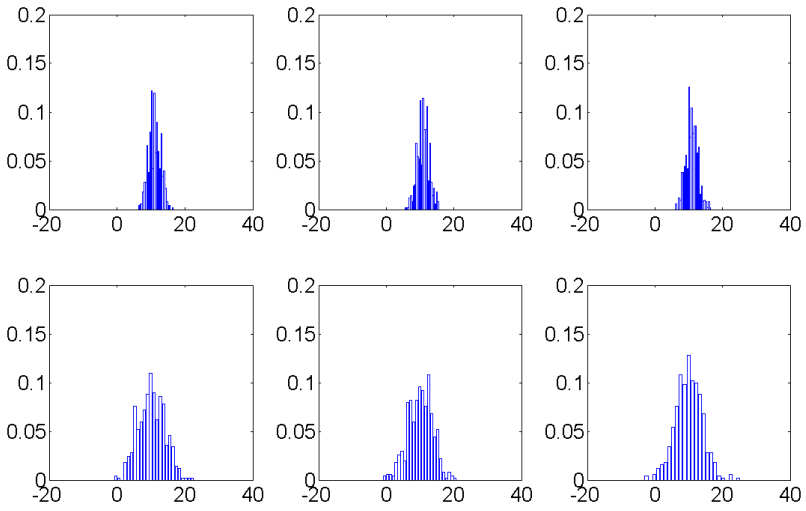


Figure 5.5: Hypo-elliptic simulated annealing of the Drop Wave potential in 3D with histograms for components 1 (top left), 2 (top right) and 3 (lower left), and a scatter plot of the simulated points (lower right) at $t = 4000$ with $c = 1$ starting at $(5, 5, -5)$.



(a) $t = 1$



(b) $t = 4000$

Figure 5.6: Hypo-elliptic simulated annealing of the Rastrigin Potential in 6D with histograms for components $1, 2, 3, 4, 5$ and 6 (from top left to lower right) at $t = 1$ in 5.6(a) and $t = 4000$ in 5.6(b) with $c = 100$ starting at $(5, 5, -5)$ with the potential shifted such that the minimum 0 is attained at $(10, 10, 10, 10, 10, 10)$.

Appendix

A.1 Proofs and constructions

A.1.1 Proof of Proposition 1.1.6

We re-formulate Proposition 1.1.6 in a slightly more general way and give the straight-forward proof.

Proposition A.1.1. *Let N be a finite-dimensional smooth manifold, $V_0, V_1, \dots, V_d$ C^∞-bounded smooth vector fields thereon and B a d-dimensional Brownian motion as usual. Consider $x \in N$ and the solution $X^x = (X_t^x)_{t\in[0,\infty[}$ of the Stratonovich SDE*

$$dX_t^x = V_0(X_t^x)dt + \sum_{i=1}^{d} V_d(X_t^x) \circ dB_t^i,$$

for details see Ikeda and Watanabe [38]. Given a submanifold $M \subset N$ such that the vector fields $V_0, \dots, V_d$ are tangential to M, then M is locally invariant under X in the sense of Definition 1.1.5. Conversely, if M is locally invariant, then $V_0, \dots, V_d$ are tangential to it.

Proof. Let $m = \dim N$, $n = \dim M$, fix $x_0 \in M$ and consider a submanifold chart ϕ of M around x_0, i. e. $\phi : U \to W$ is a diffeomorphism, where $x_0 \in U \subset N$, $0 \in W \subset \mathbb{R}^m$ are open sets, $\phi(x_0) = 0$ and

$$\phi(M \cap U) = (\mathbb{R}^n \times \{0\}) \cap W,$$

in the sense that

$$\mathbb{R}^n \times \{0\} = \left\{ y \in \mathbb{R}^m \;\middle|\; y^{n+1} = 0, \dots, y^m = 0 \right\}.$$

Let $Y_t = \phi(X_t^{x_0})$, $0 \le t < \tau^{x_0}$, where τ^{x_0} denotes the first exit time of U by the process X^{x_0}. Obviously, $Y_0 = 0$ and Itô's formula implies

$$dY_t = \phi_* V_0(Y_t)dt + \sum_{i=1}^{d} \phi_* V_i(Y_t) \circ dB_t^i,$$

where $\phi_* V(y) = T_{\phi^{-1}(y)}\phi V(\phi^{-1}(y)) \in \mathbb{R}^m$ is the push-forward of the vector field V. Notice that

$$\phi_* V : \mathbb{R}^n \times \{0\} \cap W \to \mathbb{R}^n \times \{0\}$$

for vector fields V tangential to M.

If $V_0, \dots, V_d$ are tangential to M, then $Y_t \in \mathbb{R}^n \times \{0\} \cap W$ for $0 \leq t < \tau^{x_0}$, implying that $X_t^{x_0} \in M$ for $0 \leq t < \tau^{x_0}$. Conversely, if M is locally invariant under X, i. e. $X_t^{x_0} \in M$ for $0 \leq t < \tau$ for some positive stopping time $\tau \leq \tau^{x_0}$, then $Y_t \in \mathbb{R}^n \times \{0\}$ up to the same stopping time, implying that $\phi_* V_i(y) \in \mathbb{R}^n \times \{0\}$ for $i = 0, \dots, d$ and y in a neighborhood around $0 \in \mathbb{R}^m$. This implies that $V_0, \dots, V_d$ are tangential to M in a neighborhood of x_0. Consequently, since $x_0 \in M$ was chosen arbitrarily, we may conclude that $V_0, \dots, V_d$ are tangential to M. □

A.1.2 Proof of the Chen-Strichartz formula

Let $X = (X_t^1, \dots, X_t^d)_{t \in [0,\infty[}$ denote a d-dimensional continuous semi-martingale. In slight modification of Definition 2.1.2, let

$$\mathcal{A} = \bigcup_{k=0}^{\infty} \{1, \dots d\}^k$$

be the set of all multi-indices in $\{1, \dots, d\}$ and let $|I|$ be the length of the multi-index $I \in \mathcal{A}$. Similar to Chapter 2, let

$$X_t^I = X_t^{(i_1,\dots,i_k)} = \int_{0<t_1<\cdots<t_k<t} \circ dX_{t_1}^{i_1} \circ \cdots \circ dX_{t_k}^{i_k} \tag{A.1}$$

for a multi-index $I = (i_1, \dots, i_k) \in \mathcal{A}$, denote the iterated Itô-Stratonovich integral of the semi-martingale X. Recall that the Stratonovich integral of a continuous semi-martingale X with respect to a continuous semi-martingale Y is defined by

$$\int_0^t X_s \circ dY_s = \int_0^t X_s dY_s + \frac{1}{2} \langle X, Y \rangle_t ,$$

where $\langle X, Y \rangle$ denotes the quadratic covariation of X and Y, see Protter [64]. Moreover, let $f \in C^2(\mathbb{R}^d)$ and recall that the Itô formula for the continuous semi-martingale X reads

$$f(X_t) = f(X_0) + \sum_{i=1}^{d} \int_0^t \frac{\partial}{\partial x^i} f(X_s) \circ dX_s^i \tag{A.2}$$

when using the Stratonovich integral.

Consider the stochastic process

$$Y_t = \sum_{I \in \mathcal{A}} X_t^I e_I \tag{A.3}$$

where, for $I = (i_1, \dots, i_k) \in \mathcal{A}$,

$$e_I = e_{i_1} \cdots e_{i_k}$$

and (A.3) is considered as a formal series. More precisely, let $\mathbb{A}_d$ denote the free algebra[1] generated by $A = \{e_1, \dots, e_d\}$ and let us denote by $\overline{\mathbb{A}}_d$ the corresponding *space of formal series* in A. As in (2.6), let

$$W_k = \langle \{ e_I \mid I \in \mathcal{A},\ |I| = k \} \rangle_{\mathbb{R}}$$

denote the subspace of polynomials of homogeneous degree k, $k \in \mathbb{N}$. Naturally, any $x \in \overline{\mathbb{A}}_d$ can be written as

$$x = \sum_{k=0}^{\infty} x_k$$

with $x_k \in W_k$, where the infinite sum is again understood as a formal series. Let $\mathfrak{g}_d \subset \mathbb{A}_d$ denote the free Lie algebra generated by A. $x \in \overline{\mathbb{A}}_d$ is called a *Lie series* if

$$\forall k \in \mathbb{N} : \ x_k \in \mathfrak{g}_d.$$

The space of all Lie series is denoted by $\overline{\mathfrak{g}}_d \subset \overline{\mathbb{A}}_d$. Note that $\mathfrak{g}_d \subset \overline{\mathfrak{g}}_d$.

The exponential function and the logarithm are defined as usual, i. e. for $x \in \overline{\mathbb{A}}_d$ let

$$\exp(x) = \sum_{k=0}^{\infty} \frac{1}{k!} x^k \in \overline{\mathbb{A}}_d$$

and for $y \in \overline{\mathbb{A}}_d$ with $y_0 = 1$ let

$$\log(y) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} y^k \in \overline{\mathbb{A}}_d.$$

We prove the following version of the Chen-Strichartz formula.

Proposition A.1.2. *For $I \in \mathcal{A}$ and $t \geq 0$ let*

$$\Lambda_t^I = \sum_{\sigma \in \mathfrak{S}_{|I|}} \frac{(-1)^{e(\sigma)}}{|I|^2 \binom{|I|-1}{e(\sigma)}} X_t^{\sigma^{-1}(I)},$$

[1] Recall Remark 2.1.5.

where $\mathfrak{S}_k$ *denotes the symmetric group in* k *elements,* $e(\sigma) = \#\{\, j \mid \sigma(j) > \sigma(j+1) \,\}$ *and* $\sigma(I) = (i_{\sigma(1)}, \ldots, i_{\sigma(k)})$ *for* $I \in \mathcal{A}$, $|I| = k$, $\sigma \in \mathfrak{S}_k$ *and* $k \in \mathbb{N}$. *Then*

$$Y_t = \exp(Z_t) = \exp\Bigg(\sum_{I \in \mathcal{A} \setminus \{\emptyset\}} \Lambda_t^I e_{[I]} \Bigg),$$

where

$$e_{[I]} = e_{[(i_1,\ldots,i_k)]} = [e_{i_1}, [\cdots, [e_{i_{k-1}}, e_{i_k}] \cdots]$$

for the generic element $I = (i_1, \ldots, i_k) \in \mathcal{A}$, $k \in \mathbb{N}$.

Remark A.1.3. The fact that $\log(Y_t)$ is a Lie series goes back to Chen [13], whereas the explicit formula above is due to Strichartz [77]. See also Baudoin [3] for the generalization to the case of a d-dimensional Brownian motion.

For the proof of Proposition A.1.2, we will need a few results from the theory of free Lie algebras. In order to formulate them, we need three more notions, taken from Reutenauer [67]. Define the linear maps

$$r : \mathbb{A}_d \to \mathfrak{g}_d,$$
$$D : \mathbb{A}_d \to \mathbb{A}_d$$

by specifying that

$$r(e_I) = e_{[I]},$$
$$D(e_I) = |I|\, e_I$$

for $I \in \mathcal{A} \setminus \{\emptyset\}$ and by $r(1) = D(1) = 0$. Moreover, a homomorphism of algebras

$$\delta : \mathbb{A}_d \to \mathbb{A}_d \otimes \mathbb{A}_d,$$

the tensor product of $\mathbb{A}_d$ with itself, is defined by extension of

$$\delta(e_i) = e_i \otimes 1 + 1 \otimes e_i, \quad i = 1, \ldots, d.$$

Notice that both r, D and δ preserve the degree $|\cdot|$ of monomials, where

$$|e_I| = |I|\,.$$

Therefore, the mappings can be easily extended to

$$r : \overline{\mathbb{A}}_d \to \overline{\mathfrak{g}}_d,$$
$$D : \overline{\mathbb{A}}_d \to \overline{\mathbb{A}}_d,$$
$$\delta : \overline{\mathbb{A}}_d \to \overline{\mathbb{A}}_d \otimes \overline{\mathbb{A}}_d.$$

We cite (a part of) Reutenauer [67, Theorem 3.1].

Lemma A.1.4. *Let $y \in \overline{\mathbb{A}}_d$. The following statements are equivalent.*

(1) $y \in \overline{\mathfrak{g}}_d$.

(2) $\delta(y) = y \otimes 1 + 1 \otimes y$ *(Friedrich's criterion).*

(3) $\delta(\exp(y)) = \exp(y) \otimes \exp(y)$.

(4) $y_0 = 0$ *and* $r(y) = D(y)$.

Remark A.1.5. Recall that the Baker-Campbell-Hausdorff formula (2.12) states that

$$\log(\exp(y)\exp(z)) \in \overline{\mathfrak{g}}_d$$

for $y, z \in \mathfrak{g}_d$. Dynkin [20] has given an explicit expression for the above term, which can be easily obtained from part (4) of Lemma A.1.4, provided that we already assume as granted that $\log(\exp(y)\exp(z)) \in \overline{\mathfrak{g}}_d$. Indeed, by the definition of the logarithmic series,

$$\begin{aligned}\log(\exp(y)\exp(z)) &= \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} (\exp(y)\exp(z) - 1)^k \\ &= \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \Big(\sum_{l+m>0} \frac{y^l z^m}{y!z!} \Big)^k \\ &= \sum_{k=1}^{\infty} \sum_{l_1+m_1>0,\ldots,l_k+m_k>0} \frac{(-1)^{k-1}}{k} \frac{y^{l_1} z^{m_1} \cdots y^{l_k} z^{l_k}}{l_1!m_1! \cdots l_k!m_k!}.\end{aligned}$$

For a homogenous Lie polynomial y_n of degree $|y_n| = n$, (3) in Lemma A.1.4 implies that $\frac{1}{n} r(y_n) = y_n$. Assuming $y, z \in A$, we, hence, obtain Dynkin's formula

$$\log(\exp(y)\exp(z)) = \sum_{k=1}^{\infty} \sum_{l_1+m_1>0,\ldots,l_k+m_k>0} \frac{(-1)^{k-1}}{k} \frac{1}{l_1 + \cdots l_k + m_1 + \cdots m_k} \frac{r(y^{l_1} z^{m_1} \cdots y^{l_k} z^{l_k})}{l_1!m_1! \cdots l_k!m_k!}.$$

For general $y, z \in \mathfrak{g}_d$, Dynkin's formula is obtained by passing to the free algebra generated by y and z.

Proof of Proposition A.1.2. We follow the second proof given in Strichartz [77]. The strategy of the proof can be summarized as follows.

(1) Prove that $Z_t \in \overline{\mathfrak{g}}_d$ by applying Friedrich's criterion, in the form of Lemma A.1.4 (3).

(2) Use the same reasoning as in Remark A.1.5 above to pass from polynomials to Lie polynomials.

(3) The formula given in Proposition A.1.2 is finally obtained by some combinatorial simplifications.

In order to prove that $Z_t \in \overline{\mathfrak{g}}_d$, we need to show that

$$\delta(Y_t) = Y_t \otimes Y_t,$$

and we do so by showing that both processes satisfy the same stochastic differential equation.[2] Since Y_t solves the SDE

$$dY_t = \sum_{i=1}^{d} Y_t e_i \circ dX_t^i,$$

with initial value $Y_0 = 1$, compare equation (2.15), $Y_t \otimes Y_t$ solves the initial value problem

$$\begin{cases} d(Y_t \otimes Y_t) = Y_t \otimes Y_t \Big(\sum_{i=1}^{d} e_i \circ dX_t^i \otimes 1 + 1 \otimes \sum_{i=1}^{d} e_i \circ dX_t^i \Big), \\ \quad Y_0 \otimes Y_0 = 1 \otimes 1. \end{cases}$$

We compute the SDE satisfied by $\delta(Y_t)$ by applying Itô's formula, see (A.2). Using linearity and multiplicativity of δ, we obtain

$$\begin{aligned} d\delta(Y_t) &= \delta(dY_t) \\ &= \delta\Big(Y_t \textstyle\sum_{i=1}^{d} e_i \circ dX_t^i\Big) \\ &= \delta(Y_t)\delta\Big(\textstyle\sum_{i=1}^{d} e_i \circ dX_t^i\Big) \\ &= \delta(Y_t)\Big(\sum_{i=1}^{d} e_i \circ dX_t^i \otimes 1 + 1 \otimes \sum_{i=1}^{d} e_i \circ dX_t^i \Big). \end{aligned}$$

Moreover, $\delta(Y_0) = 1 \otimes 1$, which implies that

$$\delta(Y_t) = Y_t \otimes Y_t,$$

and consequently $Z_t \in \overline{\mathfrak{g}}_d$.

Next, we collect all terms of a given degree in the formal series defining Z_t, which will allow us to apply Lemma A.1.4 (4). Let

$$\mathcal{A}_{=k} = \{\, I \in \mathcal{A} \mid |I| = k \,\}$$

[2] At this point, we need to endow $\overline{\mathbb{A}}_d$ with a topological structure. We choose the initial topology of the projections $\overline{\mathbb{A}}_d \to W_k$, $k \in \mathbb{N}$. That is, convergence in $\overline{\mathbb{A}}_d$ means convergence of all the projections to the finite dimensional subspaces W_k.

and let $\mathcal{A}_0 = \mathcal{A} \setminus \{\emptyset\}$. Given a multi-index $I \in \mathcal{A}_0$ and $k \in \mathbb{N}$ such that $1 \leq k \leq |I|$, let

$$\mathcal{A}_0^k(I) = \left\{ (I_1, \ldots, I_k) \in \mathcal{A}_0^k \;\middle|\; I = I_1 * \cdots * I_k \right\},$$

i. e. $\mathcal{A}_0^k(I)$ collects all the possible ways of writing I by concatenation of k non-trivial multi-indices. Then

$$\begin{aligned}
Z_t = \log(Y_t) &= \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} (Y_t - 1)^k \\
&= \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \Big(\sum_{I \in \mathcal{A}_0} X_t^I e_I \Big)^k \\
&= \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} \sum_{(I_1, \ldots I_k) \in \mathcal{A}_0^k} X_t^{I_1} \cdots X_t^{I_k} e_{I_1} \cdots e_{I_k} \\
&= \sum_{m=1}^{\infty} \sum_{I \in \mathcal{A}_{=m}} \sum_{k=1}^{m} \frac{(-1)^{k-1}}{k} \sum_{(I_1, \ldots, I_k) \in \mathcal{A}_0^k(I)} X_t^{I_1} \cdots X_t^{I_k} e_{I_1} \cdots e_{I_k} \\
&= \sum_{m=1}^{\infty} Z_t^m.
\end{aligned}$$

Notice that the last line gives precisely the decomposition of Z_t into homogenous polynomials Z_t^m of degree m, $m \in \mathbb{N}$. Since we have already established that $Z_t \in \overline{\mathfrak{g}}_d$, we may conclude that $Z_t^m \in \mathfrak{g}_d$ is a homogenous Lie polynomial of degree $|Z_t^m| = m$ and part (4) of Lemma A.1.4 implies that

$$Z_t^m = \frac{1}{m} r(Z_t^m),$$

$m \in \mathbb{N}$. Therefore, we get

$$Z_t = \sum_{m=1}^{\infty} \sum_{I \in \mathcal{A}_{=m}} \sum_{k=1}^{m} \frac{(-1)^{k-1}}{km} \sum_{(I_1, \ldots, I_k) \in \mathcal{A}_0^k(I)} X_t^{I_1} \cdots X_t^{I_k} e_{[I]}. \tag{A.4}$$

In order to complete the proof, we are left to show that

$$\Lambda_t^I = \sum_{k=1}^{m} \frac{(-1)^{k-1}}{km} \sum_{(I_1, \ldots, I_k) \in \mathcal{A}_0^k(I)} X_t^{I_1} \cdots X_t^{I_k} =: Z_t^I$$

for multi-indices I of length m and $m \in \mathbb{N}$. As a first step in this direction, let us replace *products* of iterated integrals (as in (A.4)) by *sums* of iterated integrals (as in the definition of Λ_t^I).

For fixed $I \in \mathcal{A}_{=m}$, $1 \leq k \leq m$ and $(I_1, \ldots, I_k) \in \mathcal{A}_0^k(I)$, let $q_0 = 0$ and

$$q_{j+1} = q_j + |I_{j+1}|, \quad j = 0, \ldots, k-1.$$

Notice that $q_k = m$. Moreover, let

$$\mathfrak{S}_m(q_1, \dots, q_k) = \{\, \sigma \in \mathfrak{S}_m \mid \forall j \in \{0, \dots, k-1\} : \ \sigma(q_j + 1) < \cdots < \sigma(q_{j+1}) \,\}.$$

We claim that

$$X_t^{I_1} \cdots X_t^{I_k} = \sum_{\sigma \in \mathfrak{S}_m(q_1, \dots, q_k)} X_t^{\sigma^{-1}(I)}. \tag{A.5}$$

We give a heuristic proof of (A.5), which can be made precise using Itô's formula. Let, for any $l \in \mathbb{N}$, Δ_t^l denote the open l-dimensional simplex with base length t, in the sense that

$$\Delta_t^l = \left\{ x \in \mathbb{R}^l \;\middle|\; 0 < x^1 < x^2 < \cdots < x^l < t \right\}.$$

Furthermore, let

$$A_t(q_1, \dots, q_k) = \Delta_t^{q_1} \times \Delta_t^{q_2 - q_1} \times \cdots \times \Delta_t^{q_k - q_{k-1}} \subset \mathbb{R}^m.$$

Letting $\mathfrak{S}_m$ act on $\mathbb{R}^m$ in the usual way, i. e. by

$$\sigma(x) = (x^{\sigma(1)}, \dots, x^{\sigma(m)}), \quad x \in \mathbb{R}^m, \ \sigma \in \mathfrak{S}_m,$$

it is simple to see that

$$A_t(q_1, \dots, q_k) = \bigcup_{\sigma \in \mathfrak{S}_m(q_1, \dots, q_k)} \sigma(\Delta_t^m) \tag{A.6}$$

(up to a set of m-dimensional Lebesgue measure 0). The union on the right hand side of (A.6) is a disjoint union. Notice that

$$X_t^{I_1} \cdots X_t^{I_k} = \int_{A_t(q_1, \dots, q_k)} \circ dX_{t_1}^{i_1} \circ \cdots \circ dX_{t_m}^{i_m}.$$

Inserting the equality (A.6) and appealing to finite additivity yields

$$\begin{aligned} X_t^{I_1} \cdots X_t^{I_k} &= \sum_{\sigma \in \mathfrak{S}_m(q_1, \dots, q_k)} \int_{\sigma(\Delta_t^m)} \circ dX_{t_1}^{i_1} \circ \cdots \circ dX_{t_m}^{i_m} \\ &= \sum_{\sigma \in \mathfrak{S}_m(q_1, \dots, q_k)} \int_{\Delta_t^m} \circ dX_{t_1}^{i_{\sigma^{-1}(1)}} \circ \cdots \circ dX_{t_m}^{i_{\sigma^{-1}(m)}} \\ &= \sum_{\sigma \in \mathfrak{S}_m(q_1, \dots, q_k)} X_t^{\sigma^{-1}(I)}, \end{aligned}$$

which proves (A.5).[3]

Now we can rewrite, still fixing $m \geq 1$ and $I \in \mathcal{A}_{=m}$,

$$\begin{aligned} Z_t^I &= \sum_{k=1}^{m} \frac{(-1)^{k-1}}{km} \sum_{(I_1,\dots,I_k)\in\mathcal{A}_0^k(I)} \sum_{\sigma\in\mathfrak{S}_m(q_1,\dots,q_k)} X_t^{\sigma^{-1}(I)} \\ &= \sum_{\sigma\in\mathfrak{S}_m} \sum_{k=1}^{m} \frac{(-1)^{k-1}}{km} d(m,k,\sigma) X_t^{\sigma^{-1}(I)}, \end{aligned}$$

where

$$\begin{aligned} &d(m,k,\sigma) = \\ &\#\left\{\, 0 < q_1, < \cdots < q_k = m \mid \forall j \in \{0,\dots,k-1\} :\ \sigma(q_j+1) < \cdots < \sigma(q_{j+1}) \,\right\}. \end{aligned}$$

A short combinatorial argument in [77] shows that

$$d(m,k,\sigma) = \begin{cases} \binom{m-e(\sigma)-1}{k-e(\sigma)-1}, & k \geq e(\sigma)+1, \\ 0, & \text{else.} \end{cases}$$

[3] This argument can be made precise in the case of semi-martingales in the following way. Let $m = 2$ and choose $I = (1,2)$ and $k = 2$. Then the claim is that

$$X_t^1 X_t^2 = X_t^{(1,2)} + X_t^{(2,1)},$$

note that $\mathfrak{S}_2(1,2) = \mathfrak{S}_2$ in this case. Using the above argument, we have

$$A_t(1,2) =]0,t[^2 = \Delta_t^2 \cup \sigma(\Delta_t^2),$$

where $\sigma = (12) \in \mathfrak{S}_2$ and we have neglected the diagonal in $A_t(1,2)$. But, of course, equation (A.5) simply follows from Itô's formula in this situation. More precisely, the above argument involving unions of permutations of the simplex is a short-hand description of the necessary applications of Itô's formula in order to expand the left hand side of (A.5) into iterated integrals of order m.

For fixed $\sigma \in \mathfrak{S}_m$, we compute, using $n = m - e(\sigma) - 1$ and $j = k - e(\sigma) - 1$,

$$\begin{aligned}
\sum_{k=1}^{m} \frac{(-1)^{k-1}}{km} d(m,k,\sigma) &= \sum_{k=e(\sigma)+1}^{m} \frac{(-1)^{k-1}}{km} \binom{m-e(\sigma)-1}{k-e(\sigma)-1} \\
&= \frac{(-1)^{e(\sigma)}}{m} \sum_{j=0}^{n} \frac{(-1)^j}{j+1+e(\sigma)} \binom{n}{j} \\
&= \frac{(-1)^{e(\sigma)}}{m} \sum_{j=0}^{n} (-1)^j \int_0^1 x^{j+e(\sigma)} dx \binom{n}{j} \\
&= \frac{(-1)^{e(\sigma)}}{m} \int_0^1 (1-x)^n x^{e(\sigma)} dx \\
&= \frac{(-1)^{e(\sigma)}}{m} B(n+1, e(\sigma)+1) \\
&= \frac{(-1)^{e(\sigma)}}{m} \frac{(m-e(\sigma)-1)!e(\sigma)!}{m!} = \frac{(-1)^{e(\sigma)}}{m^2 \binom{m-1}{e(\sigma)}},
\end{aligned}$$

where we have used the elementary identity for the Beta function:

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}.$$

Collecting everything, we obtain

$$Z_t^I = \sum_{\sigma \in \mathfrak{S}_m} \frac{(-1)^{e(\sigma)}}{m^2 \binom{m-1}{e(\sigma)}} X_t^{\sigma^{-1}(I)},$$

which concludes the proof. □

A.1.3 Construction for calculating moments

Continuing Subsection 2.4.2, we would like to calculate the moments of Z_t^m, $m \in \mathbb{N}$, $t > 0$, using the formula for the expected value of $\left[Y_t^{1,\tilde{m}}\right]_{m,\tilde{m}}$ given in Theorem 2.4.10. Now we fix $m \in \mathbb{N}$ and drop the dependence of Z^m on m again from the notation, i. e. we want to calculate

$$E\Big((Z_t^1)^{k_1} \cdots (Z_t^N)^{k_N}\Big),$$

where we recall that Z_t^k denotes the kth coefficient of Z_t with respect to the Hall basis $P_H = \{f_1, \ldots, f_N\}$ of $\mathfrak{g}_{d,1}^m$ and $k_1, \ldots, k_N$ are natural numbers. Note that the $(k_1, \ldots, k_N)$-moment of Z_t is contained in $E\big(\left[Y_t^{1,\tilde{m}}\right]_{m,\tilde{m}}\big)$ provided that $k_1 \deg(f_1) + \cdots + k_N \deg(f_N) \leq \tilde{m}$. We can, however, not directly extract the value, because we can only read out the coefficients of

Symbol	Definition	Generic element	degree
$\mathcal{A}$	$\bigcup_{n=0}^{\infty}\{0,\dots,d\}^n$	$I=(i_1,\dots,i_k)$	$\deg$
$\tilde{\mathcal{A}}$	$\bigcup_{n=0}^{\infty}\{1,\dots,N\}^n$	$J=(j_1,\dots,j_r)$	$\widetilde{\deg}$
$\mathbb{N}^N$		$K=(k_1,\dots,k_N)$	$\widetilde{\deg}$

Table A.1: Multi-index sets

$E\big(\big[Y_t^{1,\tilde{m}}\big]_{m,\tilde{m}}\big)$ with respect to the Poincaré-Birkhoff-Witt basis. In this subsection we shall show that efficient calculation of the moments of Z_t given $E\big(\big[Y_t^{1,\tilde{m}}\big]_{m,\tilde{m}}\big)$ is possible.

Fix $\tilde{m}\geq m$ and let $(\cdot,\cdot)$ denote the unique inner product on $\mathbb{A}_{d,1}^{m,\tilde{m}}$ such that the Poincaré-Birkhoff-Witt basis is an orthonormal basis with respect to $(\cdot,\cdot)$. For $J=(j_1,\dots,j_r)\in\tilde{\mathcal{A}}$ with $j_1\geq\cdots\geq j_r$ and $\widetilde{\deg}(J)\leq\tilde{m}$, let

$$V_t^J=\Big(\big[Y_t^{1,\tilde{m}}\big]_{m,\tilde{m}},f_{j_1}\cdots f_{j_r}\Big). \tag{A.7}$$

Equation (A.7) is an equation in $\mathbb{A}_{d,1}^{m,\tilde{m}}$ and we are allowed to omit the $[\cdot]_{m,\tilde{m}}$ in $[f_{j_1}]_{m,\tilde{m}}\cdots[f_{j_r}]_{m,\tilde{m}}$ by appealing to the isomorphism between $\mathbb{A}_{d,1}^{m,\tilde{m}}$ and $\mathcal{U}(\mathfrak{g}_{d,1}^m)/\langle\deg>\tilde{m}\rangle$. The quantities $E(V_t^J)$ will be considered as known and we will use them to calculate the moments of Z_t. But first we will still have to add some shorthand notations.

The set $\mathbb{N}^N$ will also be an important class of multi-indices for us and we will denote the generic element of $\mathbb{N}^N$ by

$$K=(k_1,\dots,k_N)\in\mathbb{N}^N.$$

By abuse of notation, we define the degree $\widetilde{\deg}$ also on $\mathbb{N}^N$ by setting

$$\widetilde{\deg}(K)=\widetilde{\deg}((k_1,\dots,k_N))=k_1\deg(f_1)+\cdots+k_N\deg(f_N).$$

Table A.1 shows the sets of multi-indices, which we have defined so far. In the same fashion as the definition of $\mathcal{A}_m$, we introduce $\tilde{\mathcal{A}}_\mu$ and $\mathbb{N}_\mu^N$,

$$\begin{aligned}\mathcal{A}_m&=\{\,I\in\mathcal{A}\mid\deg(I)\leq m\,\},\\ \tilde{\mathcal{A}}_\mu&=\Big\{\,J\in\tilde{\mathcal{A}}\;\Big|\;\widetilde{\deg}(J)=\mu\,\Big\},\\ \mathbb{N}_\mu^N&=\Big\{\,K\in\mathbb{N}^N\;\Big|\;\widetilde{\deg}(K)=\mu\,\Big\}.\end{aligned}$$

Note, however, that we replaced the "$\leq$" by an "$=$" in the definitions of $\tilde{\mathcal{A}}_\mu$ and $\mathbb{N}_\mu^N$. A multi-index $J\in\tilde{\mathcal{A}}$ is called *ordered* if $j_1\geq j_2\geq\cdots\geq j_r$. This name is justified by the Poincaré-Birkhoff-Witt theorem, Proposition 2.4.5, according to which the basis of the universal enveloping algebra can be indexed by the ordered multi-indices $J\in\tilde{\mathcal{A}}$ – in terms of the Hall basis. Let us write $\tilde{\mathcal{A}}_\mu^o$ for all ordered multi-indices in $\tilde{\mathcal{A}}_\mu$.

For $J, J' \in \tilde{\mathcal{A}}_{\tilde{m}}$ such that J, but not necessarily J' is ordered, let

$$\beta^J_{J'} = \left(f_{j'_1} \cdots f_{j'_s}, f_{j_1} \cdots f_{j_r} \right), \tag{A.8}$$

where $J' = (j'_1, \ldots, j'_s)$. By Lemma 2.4.9, the coefficients of $Y^{m,\tilde{m}}$ defined in equation (A.7) satisfy, for $J \in \tilde{\mathcal{A}}_{\tilde{m}}$ ordered,

$$\begin{aligned} V_t^J &= \sum_{J'=(j'_1,\ldots,j'_s)\in\tilde{\mathcal{A}}_{\tilde{m}}} \frac{1}{s!}\beta^J_{J'} Z_t^{j'_1} \cdots Z_t^{j'_s} \\ &= \sum_{K\in\mathbb{N}^N_{\tilde{m}}} \alpha^J_K (Z_t^1)^{k_1} \cdots (Z_t^N)^{k_N}, \end{aligned} \tag{A.9}$$

where

$$\alpha^J_K = \sum_{\substack{J'=(j'_1,\ldots,j'_s)\in\tilde{\mathcal{A}} \\ \chi_1(J')=k_1,\ldots,\chi_N(J')=k_N}} \frac{1}{s!}\beta^J_{J'}, \quad J \in \tilde{\mathcal{A}}^o_{\tilde{m}},\ K \in \mathbb{N}^N_{\tilde{m}}, \tag{A.10}$$

with $\chi_l(J) = \#\{\, 1 \le k \le r \mid j_k = l \,\}$ for $l = 1, \ldots, N$ and any $J \in \tilde{\mathcal{A}}_{\tilde{m}}$.

Remark A.1.6. Note that the functions χ_l, $l = 1, \ldots, N$, provide a one-to-one correspondence between $\tilde{\mathcal{A}}^o_\mu$ and $\mathbb{N}^N_\mu$. More precisely, the map

$$\chi = (\chi_1, \ldots, \chi_N) : \tilde{\mathcal{A}}^o_\mu \to \mathbb{N}^N_\mu$$

is bijective.

To get a better idea of where we are heading to, let us rewrite the system (A.9) of linear equations in a more compact matrix form

$$V_t = AZ_t^*, \tag{A.11}$$

where V_t denotes the vector of all coefficients V_t^J, A denotes the (square) matrix of all α^J_Ks, and Z_t^* denotes the vector of polynomials in Z_t "of degree less than $\tilde{m}$", i. e.

$$\begin{aligned} V_t &= (V_t^J)_{J\in\bigcup_{1\le\mu\le\tilde{m}}\tilde{\mathcal{A}}^o_\mu}, \\ A &= (\alpha^J_K)_{J\in\bigcup_{1\le\mu\le\tilde{m}}\tilde{\mathcal{A}}^o_\mu,\, K\in\bigcup_{1\le\mu\le\tilde{m}}\mathbb{N}^N_\mu}, \\ Z_t^* &= \left((Z_t^1)^{k_1}\cdots(Z_T^N)^{k_N}\right)_{K\in\bigcup_{1\le\mu\le\tilde{m}}\mathbb{N}^N_\mu}. \end{aligned}$$

Our quantity of interest is given by

$$E(Z_t^*) = A^{-1}E(V_t),$$

and $E(V_t)$ is assumed to be given. Therefore, we want to show that A can be inverted in an efficient way.

Lemma A.1.7. *Given* $J = (j_1, \dots, j_r) \in \bigcup_{1 \le \mu \le \tilde{m}} \tilde{\mathcal{A}}^o_\mu$ *and* $K = (k_1, \dots, k_N) \in \bigcup_{1 \le \mu \le \tilde{m}} \mathbb{N}^N_\mu$ *as before. If* $\widetilde{\deg}(J) \neq \widetilde{\deg}(K)$, *then* $\alpha^J_K = 0$.

Proof. We claim that $\beta^{j_1,\dots,j_r}_{j'_1,\dots,j'_s} = 0$ if $J' = (j'_1, \dots, j'_s) \in \tilde{\mathcal{A}}$ with $\widetilde{\deg}(J') \neq \widetilde{\deg}(J)$. Indeed, expanding a polynomial $f_{j'_1} \cdots f_{j'_s}$ in the Poincaré-Birkhoff-Witt basis is done using an algorithm, which, at each step, expresses some polynomial

$$f_{l_1} \cdots f_{l_q} f_{l_{q+1}} \cdots f_{l_p} = f_{l_1} \cdots f_{l_{q+1}} f_{l_q} \cdots f_{l_p} + f_{l_1} \cdots [f_{l_q}, f_{l_{q+1}}] \cdots f_{l_p},$$

where $f_{l_q} < f_{l_{q+1}}$. $[f_{l_q}, f_{l_{q+1}}]$ is a linear combination of Hall-polynomials (or 0 by nil-potency). By this operation, neither the degree nor the length nor the partial length with respect to any letter is changed. Therefore, the coefficient $\left(f_{j'_1} \cdots f_{j'_s}, f_{j_1} \cdots f_{j_r}\right) = 0$ for any such J' with $\widetilde{\deg}(J') = \widetilde{\deg}(K) \neq \widetilde{\deg}(J)$, which shows that $\alpha^J_K = 0$ by (A.10). See Reutenauer [67, Section 4.2] to learn more about the algorithm. □

If we arrange the rows and columns of the matrix A according to the degree, i. e. such that higher rows and further left columns correspond to smaller degrees, then, according to Lemma A.1.7, A has the form of a block diagonal matrix. More precisely, with $A_\mu = \left(\alpha^J_K\right)_{J \in \tilde{\mathcal{A}}^o_\mu,\ K \in \mathbb{N}^N_\mu}$, $\mu = 1, \dots, \tilde{m}$, we have

$$A = \operatorname{diag}(A_1, \dots, A_{\tilde{m}}) = \begin{pmatrix} A_1 & & \\ & \ddots & \\ & & A_{\tilde{m}} \end{pmatrix}. \tag{A.12}$$

Of course, a block diagonal matrix is invertible if and only if all of the blocks on the diagonal are invertible. So we are left with studying invertibility of many smaller matrices. Note, that in some sense we got rid of $\tilde{m}$: if we want to express a monomial in $(Z^1_t, \dots, Z^N_t)$ of $\widetilde{\deg}$-degree μ in terms of a linear combination of V^J_ts, then we need to invert the matrix A_μ. Actually, in the proof of Lemma A.1.7, we have also shown the following

Lemma A.1.8. *Given* $J = (j_1, \dots, j_r) \in \tilde{\mathcal{A}}^o_\mu$, $K = (k_1, \dots, k_N) \in \mathbb{N}^N_\mu$, $1 \le \mu$, *such that*

$$\exists a \in A : \ |f_{j_1} \cdots f_{j_r}|_a \neq \left|f^{k_N}_N \cdots f^{k_1}_1\right|_a.$$

Then $\alpha^J_K = 0$.

Under the assumptions of Lemma A.1.8 it is easy to see that

$$\mu = 2\,|f_{j_1} \cdots f_{j_r}|_{e_0} + \sum_{i=1}^{d} |f_{j_1} \cdots f_{j_r}|_{e_i}.$$

For fixed $(l_0,\dots,l_d)\in\mathbb{N}^{d+1}$ with $2l_0+l_1+\cdots+l_d=\mu$, let

$$A_\mu^{l_0,l_1,\dots,l_d}=\big(\alpha_K^J\big), \tag{A.13}$$

where J runs over all multi-indices in $\tilde{\mathcal{A}}_\mu^o$ with $|f_{j_1}\cdots f_{j_r}|_{e_0}=l_0,\dots,|f_{j_1}\cdots f_{j_r}|_{e_d}=l_d$ and K runs over all multi-indices in $\mathbb{N}_\mu^N$ with $|f_1^{k_1}\cdots f_N^{k_N}|_{e_0}=l_0,\ \dots,\ |f_1^{k_1}\cdots f_N^{k_N}|_{e_d}=l_d$. Then, again after rearranging the columns and rows, we have

$$A_\mu=\operatorname{diag}\Big(A_\mu^{l_0,\dots,l_d}\ \Big|\ (l_0,\dots,l_d)\in\mathbb{N}^{d+1},\,2l_0+l_1+\cdots+l_d=\mu\Big) \tag{A.14}$$

and invertibility of A_μ is equivalent to invertibility of all the $A_\mu^{l_0,\dots,l_d}$.

Fix $1\le\mu$ and $(l_0,\dots,l_d)\in\mathbb{N}^{d+1}$ with $2l_0+l_1+\cdots+l_d=\mu$. In order to study the structure of $A_\mu^{l_0,\dots,l_d}$, we introduce another grading on the Poincaré-Birkhoff-Witt polynomials and thus on the whole algebra $\mathcal{U}(\mathfrak{g}_{d,1}^m)$: The *bracket degree* $\deg_{[\,]}$ counts the number of Lie brackets appearing in the definition of a Poincaré-Birkhoff-Witt polynomial. More precisely, $\deg_{[\,]}$ is recursively defined: for a letter $a\in A$ set $\deg_{[\,]}(a)=0$, for a Hall word $h\in H$ with standard factorization $h=h'h''$ set $\deg_{[\,]}(P_h)=1+\deg_{[\,]}(P_{h'})+\deg_{[\,]}(P_{h''})$, and for a Poincaré-Birkhoff-Witt polynomial $f_{j_1}\cdots f_{j_r}$, $j_1\ge\cdots\ge j_r$ set $\deg_{[\,]}(f_{j_1}\cdots f_{j_r})=\deg_{[\,]}(f_{j_1})+\cdots+\deg_{[\,]}(f_{j_r})$. For convenience, we also define $\deg_{[\,]}(0)=+\infty$. The following lemma shows that $\deg_{[\,]}$ is consistent with our interpretation of counting Lie brackets in the sense that the bracket degree of the bracket of two polynomials is always greater than the sum of their bracket degrees.

Lemma A.1.9. *Given $f_j,f_l\in P_H$ and write $[f_j,f_l]=\sum_{r=1}^k\gamma_r f_{i_r}$ with $\gamma_r\neq0$, for all $r\in\{1,\dots,k\}$. Then*

$$\forall r\in\{1,\dots,k\}:\ \deg_{[\,]}(f_{i_r})>\deg_{[\,]}(f_j)+\deg_{[\,]}(f_l).$$

Proof. Let $f_j=P_h$ and $f_l=P_k$ for Hall words $h,k\in H$. We prove the claim by induction on the pair (h,k) which is equipped with lexicographic order, i. e. $(h_1,k_1)<(h_2,k_2)$ if and only if either $|h_1|+|k_1|<|h_2|+|k_2|$ or $|h_1|+|k_1|=|h_2|+|k_2|$ and additionally $\sup(h_1,k_1)<\sup(h_2,k_2)$ for Hall words h_1,h_2,k_1,k_2. The smallest pairs (h,k) with respect to this order are pairs of letters, and for them the claim is obvious. Now assume the claim to be proven for all pairs smaller than (h,k). We may assume that $h<k$. We distinguish between three cases.
(i) If h is a letter, then hk is a Hall word with standard factorization hk. Thus, $[f_j,f_l]=P_{hk}$ and $\deg_{[\,]}([f_j,f_l])=\deg_{[\,]}(P_{hk})=\deg_{[\,]}(f_j)+\deg_{[\,]}(f_l)+1$ by definition, which shows the claim.
(ii) If h is a Hall word with standard factorization $h'h''$, such that $h''\ge k$, then hk again is a Hall word with standard factorization hk and we proceed as in (i).

(iii) Otherwise, we may assume that $h = h'h''$ is a Hall word but not a letter and $h'' < k$. By Lemma 2.4.1, $h < h'' < k$ and by the Jacobi identity we have

$$[P_h, P_k] = [[P_{h'}, P_{h''}], P_k] = [[P_{h'}, P_k], P_{h''}] + [P_{h'}, [P_{h''}, P_k]].$$

Since $|h'|, |h''| < |h|$ we can apply the induction hypotheses to get

$$[P_{h'}, P_k] = \sum_i \lambda_i P_{u_i}, \quad [P_{h''}, P_k] = \sum_j \mu_j P_{v_j},$$

for some non-zero numbers λ_i and μ_j and Hall words u_i and v_j such that

$$\begin{aligned} \deg_{[\,]}(P_{u_i}) &> \deg_{[\,]}(P_{h'}) + \deg_{[\,]}(P_k) \\ \deg_{[\,]}(P_{v_j}) &> \deg_{[\,]}(P_{h''}) + \deg_{[\,]}(P_k). \end{aligned}$$

Furthermore, the proof of Reutenauer [67, Theorem 4.9] shows that

$$\begin{aligned} |u_i| &= \left|h'\right| + |k| & |v_j| &= \left|h''\right| + |k| \\ u_i'' &\leq \sup(h', k) & v_j'' &\leq \sup(h'', k), \end{aligned}$$

implying that $(u_i, h'') < (h, k)$ and $(v_j, h') < (h, k)$, as well. By the induction hypothesis,

$$\begin{aligned} [P_{u_i}, P_{h''}] &= \sum_\nu \lambda_{i\nu} P_{u_{i\nu}}, \\ [P_{h'}, P_{v_j}] &= \sum_\kappa \mu_{j\kappa} P_{v_{j\kappa}}, \end{aligned}$$

$\lambda_{i,\nu}, \mu_{j\kappa} \neq 0$, where for any i, j, ν, κ,

$$\begin{aligned} &\deg_{[\,]}(P_{u_{i\nu}}) > \deg_{[\,]}(P_{u_i}) + \deg_{[\,]}(P_{h''}) > \deg_{[\,]}(P_{h'}) + \deg_{[\,]}(P_k) + \deg_{[\,]}(P_{h''}), \\ &\deg_{[\,]}(P_{v_{j\kappa}}) > \deg_{[\,]}(P_{v_j}) + \deg_{[\,]}(P_{h'}) > \deg_{[\,]}(P_{h''}) + \deg_{[\,]}(P_k) + \deg_{[\,]}(P_{h'}) \end{aligned}$$

Since $\deg_{[\,]}(P_h) = \deg_{[\,]}(P_{h'}) + \deg_{[\,]}(P_{h''}) + 1$, we can conclude that

$$\begin{aligned} \deg_{[\,]}(P_{u_{i\nu}}) &> \deg_{[\,]}(P_h) + \deg_{[\,]}(P_k), \\ \deg_{[\,]}(P_{v_{j\kappa}}) &> \deg_{[\,]}(P_h) + \deg_{[\,]}(P_k). \end{aligned}$$

By

$$[P_h, P_k] = \sum_i \lambda_i [P_{u_i}, P_{h''}] + \sum_j \mu_j [P_{h'}, P_{v_j}] = \sum_{i,\nu} \lambda_i \lambda_{i\nu} P_{u_{i\nu}} + \sum_{j,\kappa} \mu_j \mu_{j\kappa} P_{v_{j\kappa}},$$

we have proved the induction hypothesis for h, k. □

Now define $\deg_{[\,]}$ for multi-indices $J = (j_1, \dots, j_r) \in \tilde{\mathcal{A}}_\mu^o$ and $K = (k_1, \dots, k_N) \in \mathbb{N}_\mu^N$ by $\deg_{[\,]}(J) = \deg_{[\,]}(f_{j_1} \cdots f_{j_r})$ and $\deg_{[\,]}(K) = \deg_{[\,]}(f_N^{k_N} \cdots f_1^{k_1})$ and rearrange the rows and columns in the matrix $A_\mu^{l_0,\dots,l_d}$ accordingly.

Lemma A.1.10. *Given $J = (j_1, \dots, j_r) \in \tilde{\mathcal{A}}_\mu^o$, $K = (k_1, \dots, k_N) \in \mathbb{N}_\mu^N$, $\mu \geq 1$ and $2l_0 + l_1 + \cdots + l_d = \mu$, and assume that $|f_{j_1} \cdots f_{j_r}|_{e_j} = |f_N^{k_N} \cdots f_1^{k_1}|_{e_j} = l_j$ for $j = 0, \dots, d$.*
(i) If $\deg_{[\,]}(K) > \deg_{[\,]}(J)$ then $\alpha_K^J = 0$.
(ii) If $\deg_{[\,]}(K) = \deg_{[\,]}(J)$ then

$$\alpha_K^J \neq 0 \iff \alpha_K^J = 1 \iff J = (\underbrace{N, \dots, N}_{k_N}, \dots, \underbrace{1, \dots, 1}_{k_1}).$$

Proof. Part (i) is clear by the algorithm performing the expansion of a polynomial in terms of the Poincaré-Birkhoff-Witt basis together with Lemma A.1.9 (interchanging Hall words produces a higher bracket degree).

Given $\deg_{[\,]}(J) = \deg_{[\,]}(K)$ and assume that $J \neq (\underbrace{N, \dots, N}_{k_N}, \dots, \underbrace{1, \dots, 1}_{k_1})$. By the same argument as for part (i) we get $\alpha_K^J = 0$.

Now assume $J = (\underbrace{N, \dots, N}_{k_N}, \dots, \underbrace{1, \dots, 1}_{k_1})$. By definition,

$$\alpha_K^J = \sum_{\substack{J' = (j_1', \dots, j_s') \in \tilde{\mathcal{A}},\ \widetilde{\deg}(J') = \widetilde{\deg}(K) \\ \chi_1(J') = k_1, \dots, \chi_N(J') = k_N}} \frac{1}{s!} \beta_{j_1', \dots, j_s'}^{j_1, \dots, j_r} = \frac{1}{k!} \sum_{\sigma \in \mathfrak{S}_k} \underbrace{\beta_{j_{\sigma(1)}, \dots, j_{\sigma(k)}}^{j_1, \dots, j_r}}_{=1} = 1,$$

where $\mathfrak{S}_k$ is the group of permutations of $\{1, \dots, k\}$. □

Lemma A.1.10 shows that $A_\mu^{l_0,\dots,l_d}$ is a triangular square matrix whose diagonal entries are equal to 1. Lemmas A.1.7, A.1.8 and A.1.10 together give the following theorem.

Theorem A.1.11. *Fix a natural number $\tilde{m} \geq m$. Then the matrix A given in* (A.11) *is a block diagonal matrix*

$$A = \operatorname{diag}\Big(\Big\{ A_\mu^{l_0,\dots,l_d} \;\Big|\; 1 \leq \mu \leq \tilde{m},\ 2l_0 + l_1 + \cdots + l_d = \mu \Big\} \Big).$$

Each block $A_\mu^{l_0,\dots,l_d}$ is, in turn, a triangular square matrix with non-zero diagonal entries. Thus, A is invertible (and the inversion is feasible even for high dimensions).

A.2 Notations

$(A, \mathcal{D}(A))$	The unbounded operator A with domain $\mathcal{D}(A)$
$\langle A \rangle_{\mathbb{R}}$	The linear span of A over the field $\mathbb{R}$, sometimes also the free $\mathbb{R}$ vector space generated by A
$\langle A \rangle_R$	If A is a set and R a ring, then $\langle A \rangle_R$ denotes the R-module generated by A
$\overline{A}$	Topological closure of a set A
A^c	Complement of the set A
∂A	Boundary of the set A, i. e. $\partial A = \overline{A} \setminus \operatorname{int} A$
$\mathbb{A}_{d,1}$	Free algebra, see Subsection 2.1.2
$\mathbb{A}_{d,1}^m$	Free nilpotent algebra, see Definition 2.1.9
B_t^I	Ith iterated Itô-Stratonovich integral of B, see Definition 2.1.3
$B(x, \epsilon)$	Ball of radius ϵ around x
$C(F; G)$	Set of all continuous functions $F \to G$
$C(F)$	$C(F; \mathbb{R})$
$C_b^m(F; G)$	Set of all m-times differentiable bounded functions
$C^\infty(F; G)$	Set of all smooth functions $F \to G$
$C_0([0,T]; \mathbb{R}^d)$	Wiener space, i. e. $\{ f \in C([0,T]; \mathbb{R}^d) \mid f(0) = 0 \}$.
$C_b^\infty(\mathbb{R}^n)$	Set of infinitely differentiable bounded functions
$\operatorname{conv} A$	Convex hull of the set A
$\operatorname{cone} A$	Convex cone generated by the set A
$\overline{\operatorname{cone}}\, A$	Closed cone hull generated by A
$\mathcal{D}(A^k)$	kth Sobolev space, see Definition 1.2.14
Δ_t	Canonical dilatation, see (2.7)
deg	Degree function counting 0s twice, see Definition 2.1.2
e_I	See Remark 2.1.7
$e_{[I]}$	See (2.10)
esupp	Extended support in the sense of (3.3)
$\|f\|_\infty$	Supremum norm of a function f
$\mathfrak{g}_{d,1}^m$	Free nilpotent Lie algebra, see Definition 2.1.13
$G_{d,1}^m$	Free nilpotent Lie group, see Definition 2.1.13
I_d	d-dimensional identity matrix
id_H	Identity map $H \to H$
$\operatorname{int} A$	Interior of the set A
$L(H)$	Space of bounded linear operators on the Banach space H
$\operatorname{ri} A$	Relative interior of the set A
$\rho(A)$	Resolvent set of the operator A
$R(\lambda, A)$	Resolvent map of A at $\lambda \in \rho(A)$
$\operatorname{supp} \mu$	Support of the measure μ

V_I	See (2.27)
$V_{[I]}$	See (2.28)
X_*P	Image measure of the probability measure P under the random variable X, i. e. $\int f(x)(X_*P)(dx) = \int f(X(\omega))P(d\omega)$
$X \sim Y$	The random variables X and Y have the same law
$X \sim \mathcal{N}(m, C)$	The random variable X has a normal distribution with mean vector m and covariance matrix C

A.3 Curriculum Vitae Christian Bayer

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Publications and Preprints

- Christian Bayer, Josef Teichmann: *The proof of Tchakaloff's Theorem*, Proc. Amer. Math. Soc. 134 (2006) 3035–3040.
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Education

- Since March 2004 University of Technology, Vienna.
  - PhD student under supervision of Dr. Josef Teichmann in stochastic analysis with focus on numerical methods.
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  - Teaching of a course "Introduction to financial and actuarial mathematics" (for "Lehramt Mathematik") in Summer term 2007.
- October 1999 – January 2004 University of Technology, Vienna.
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