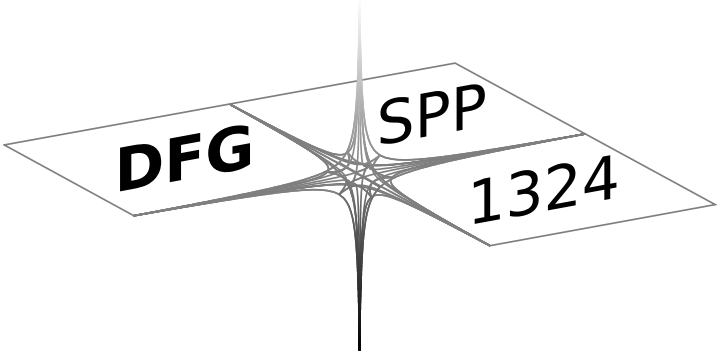
DFG-Schwerpunktprogramm 1324

„Extraktion quantifizierbarer Information aus komplexen Systemen”

On the Complexity of Computing Quadrature Formulas for SDEs

S. Dereich, T. Müller-Gronbach, K. Ritter

Preprint 109



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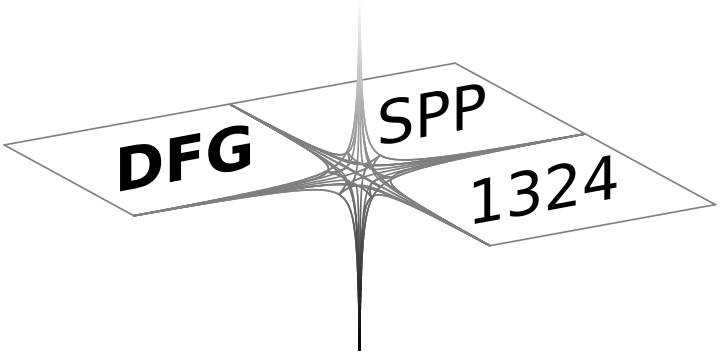

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On the Complexity of Computing Quadrature Formulas for SDEs

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Abstract

We survey recent results on the constructive approximation of the distribution of the solution of an SDE by probability measures with finite support, i.e., by quadrature formulas with positive weights summing up to one. Here we either consider the distribution on the path space or a marginal distribution on the state space. We provide asymptotic results on the N-th minimal error of deterministic and randomized algorithms, which is the smallest error that can be achieved by any such algorithm not exceeding the cost bound N.

1 Introduction

Consider a stochastic differential equation (SDE)

$$dX(t) = a(X(t))\,dt + b(X(t))\,dW(t), \qquad t \in [0,1],$$

driven by a Brownian motion W and, for simplicity, with a deterministic initial value $X(0) = x_0$. Assuming at least existence of a weak solution and uniqueness in distribution, we study the constructive approximation of

- the distribution $\mu = P_X$ of the solution on the path space $\mathfrak{X}$ or
- the marginal distribution $\mu = P_{X(1)}$ of the solution at time $t = 1$ on the state space $\mathfrak{X}$

by probability measures $\hat{\mu}$ with finite support. Hence

$$\hat{\mu} = \sum_{i=1}^{n} c_i \cdot \delta_{x_i}$$

with $n \in \mathbb{N}$, $x_1, \ldots, x_n \in \mathfrak{X}$ and $c_1, \ldots, c_n > 0$ such that $\sum_{i=1}^n c_i = 1$.

In both cases μ is given only implicitly, which constitutes a major challenge. Obviously $\hat{\mu}$ yields a quadrature formula

$$\int_{\mathfrak{X}} f \, d\hat{\mu} = \sum_{i=1}^{n} c_i \cdot f(x_i)$$

for the integral $\int_{\mathfrak{X}} f \, d\mu$ of any μ-integrable function $f \colon \mathfrak{X} \to \mathbb{R}$.

We study deterministic as well as randomized algorithms in a worst case analysis with respect to classes of SDEs, i.e., classes of parameters (x_0, a, b). Typically, these classes are defined in terms of smoothness and degeneracy constraints for the drift coefficient a and the diffusion coefficient b, and x_0 is assumed to belong to a bounded set in $\mathbb{R}^d$. The coefficients a and b are accessible only via an oracle that provides function values or derivative values of these functions at arbitrary points in $\mathbb{R}^d$, and the real number model is used to define the notions of an algorithm.

The worst case error $e(\hat{S})$ of an algorithm $\hat{S}$ is defined in terms of a metric on the space of probability measures on $\mathfrak{X}$, and we are interested in algorithms $\hat{S}$ with an (almost) optimal relation between $e(\hat{S})$ and $\mathrm{cost}(\hat{S})$, the worst case computational cost. To this end we study the N-th minimal errors

$$e_N^{\mathrm{ran}} = \inf\{e(\hat{S}) : \hat{S} \text{ randomized algorithm with } \mathrm{cost}(\hat{S}) \leq N\}$$

and

$$e_N^{\mathrm{det}} = \inf\{e(\hat{S}) : \hat{S} \text{ deterministic algorithm with } \mathrm{cost}(\hat{S}) \leq N\}.$$

Actually we survey asymptotic upper and lower bounds for these quantities as well as algorithms that achieve the upper bounds. The results and the technique are very different in the cases $\dim(\mathfrak{X}) = \infty$ and $\dim(\mathfrak{X}) < \infty$, i.e., whether we aim at the distribution on the path space or at a marginal distribution on the state space.

The problem of approximating a probability measure on $\mathfrak{X}$ by a probability measure with finite support w.r.t. a Wasserstein metric is called the quantization problem, see, e.g., [7, 10, 28]. We use this terminology for a general metric as well, and accordingly construction of quadrature formulas may also be called constructive quantization.

We briefly outline the content of this survey. In Section 2 we introduce the basic notions of algorithms, error, and cost for the construction of quadrature formulas. In Section 3 we study deterministic algorithms for approximation on the path space, see [5, 6, 18, 19, 24, 29], while

Section 4 is devoted to the analogous problem on the state space, see [3, 14, 15, 16, 21, 25]. In Section 5 we analyze randomized algorithms for marginal distributions on the state space by means of a randomized quantization technique, see [9].

In the sequel we use $a_n \approx b_n$ to denote the strong asymptotic equivalence of sequences of positive reals, i.e., $\lim_{n\to\infty} a_n/b_n = 1$. Furthermore, $a_n \preceq b_n$ means $a_n \le \kappa\, n_n$ with a constant $\kappa > 0$. Finally $a_n \asymp b_n$ is used to denote the weak asymptotic equivalence, i.e., $a_n \preceq b_n$ and $b_n \preceq a_n$.

2 Algorithms, Error, and Cost

We informally introduce the notions of deterministic and randomized algorithms, and we define their cost and their error for approximation of P_X or $P_{X(1)}$ by measures with finite support. Actually, we are interested in the approximation problem for a whole class of SDEs, which is defined by constraints on the parameters x_0, a and b. We assume that

$$(x_0, a, b) \in H = H_0 \times H_1 \times H_2,$$

where $H_0 \subset \mathbb{R}^d$ and where H_1 and H_2 are classes of functions $\mathbb{R}^d \to \mathbb{R}^d$ and $\mathbb{R}^d \to \mathbb{R}^{d\times d}$, resp., that are at least Lipschitz continuous. Hence $\mathrm{E}\,\|X\|_\infty^s < \infty$ for every SDE with $(x_0, a, b) \in H$ and every $s \ge 1$.

We take $\mathfrak{X} = C([0,1], \mathbb{R}^d)$ or $\mathfrak{X} = L_p([0,1], \mathbb{R}^d)$ for $1 \le p < \infty$ with the corresponding norms, if we study approximation of the distribution on the path space, and we take $\mathfrak{X} = \mathbb{R}^d$, if we study approximation of the marginal distribution at $t = 1$. Finally, we use $M(\mathfrak{X})$ to denote the space of Borel probability measures μ on $\mathfrak{X}$ such that

$$\int_{\mathfrak{X}} \|x\|_{\mathfrak{X}}^s \, d\mu(x) < \infty$$

for every $s \ge 1$, and we consider a metric ρ on this space. We study the mapping

$$S\colon H \to M(\mathfrak{X}),$$

where

$$S(x_0, a, b) = P_X \qquad \text{or} \qquad S(x_0, a, b) = P_{X(1)}.$$

In the framework of information-based complexity S is the so-called solution operator, see [33]. Our computational task is to approximate S by means of algorithms that yield measures in

$$M_0(\mathfrak{X}) = \{\mu \in M(\mathfrak{X}) : |\operatorname{supp}(\mu)| < \infty\}.$$

In particular, $(x_0, a, b) \in H$ is the input to any algorithm, but a and b are accessible only via an oracle that provides function values or derivative values of these coefficients at arbitrary points in $\mathbb{R}^d$. The output of an algorithm, assuming termination, is a list $c_1, x_1, \ldots, c_n, x_n$, where $c_1, \ldots, c_n$ are probability weights and $x_1, \ldots, x_n$ are points in $\mathfrak{X}$, suitably coded if $\dim \mathfrak{X} = \infty$. Computations with real numbers and with elementary functions like exp and floor are carried out exactly, and an algorithm has access to a perfect random number generator for the uniform distribution on $[0, 1]$. For a formal definition of this model of computation we refer to [26].

Accordingly, to any algorithm we associate a mapping

$$\hat{S} \colon H \times \Omega \to M_0(\mathfrak{X})$$

given by

$$\hat{S}((x_0, a, b), \omega) = \sum_{i=1}^{n} c_i \cdot \delta_{x_i}.$$

Here $(\Omega, \mathfrak{A}, Q)$ is an underlying computational probability space that carries an independent sequence of random variables, each uniformly distributed on $[0, 1]$, which is used to model the random number generator. Moreover, n as well as the c_i and x_i are random quantities, which depend on (x_0, a, b), too. We put

$$\hat{S}(x_0, a, b) = \hat{S}((x_0, a, b), \cdot) \colon \Omega \to M_0(\mathfrak{X}),$$

and, in an abuse of notation, we also use $\hat{S}$ to denote the randomized algorithm itself.

The cost of applying $\hat{S}$ to (x_0, a, b) is a random quantity, which is denoted by $\mathrm{cost}(\hat{S}, (x_0, a, b))$. It is given by the sum of the number of evaluations of a, b, a', b' etc., the number of arithmetical operations etc., and the number of calls of the random number generator that are carried out by $\hat{S}$ for this input. In particular, we have

$$\mathrm{cost}(\hat{S}, (x_0, a, b)) \geq 2 \cdot |\operatorname{supp}(\hat{S}(x_0, a, b))| \tag{1}$$

for all $(x_0, a, b) \in H$. The worst case cost of $\hat{S}$ on H is defined by

$$\mathrm{cost}(\hat{S}) = \sup_{(x_0,a,b)\in H} \mathrm{E}(\mathrm{cost}(\hat{S}, (x_0, a, b))),$$

assuming measurability. Likewise the error of applying $\hat{S}$ to (x_0, a, b) is a random quantity, and the worst case error of $\hat{S}$ on H w.r.t. the metric

ρ is defined by

$$e(\hat{S}) = \sup_{(x_0,a,b)\in H} \big(\mathrm{E}(\rho^2(S(x_0,a,b), \hat{S}(x_0,a,b)))\big)^{1/2},$$

assuming measurability.

Deterministic algorithms are a particular case of randomized algorithms, namely, $\hat{S}$ is not calling the random number generator for any $(x_0,a,b) \in H$, which implies that $\hat{S}(x_0,a,b)$ is a constant mapping for every (x_0,a,b). In the definition of $\mathrm{cost}(\hat{S})$ and $e(\hat{S})$ the expectation may therefore be dropped.

The key quantities are the N-th minimal errors

$$\begin{aligned} e_N^{\mathrm{ran}} &= e_N^{\mathrm{ran}}(H, \mathfrak{X}, \rho) \\ &= \inf\{e(\hat{S}) : \hat{S} \text{ randomized algorithm with } \mathrm{cost}(\hat{S}) \le N\} \end{aligned}$$

of randomized algorithms and the N-th minimal errors

$$\begin{aligned} e_N^{\mathrm{det}} &= e_N^{\mathrm{det}}(H, \mathfrak{X}, \rho) \\ &= \inf\{e(\hat{S}) : \hat{S} \text{ deterministic algorithm with } \mathrm{cost}(\hat{S}) \le N\} \end{aligned}$$

of deterministic algorithms. Clearly $e_N^{\mathrm{ran}} \le e_N^{\mathrm{det}}$.

Concerning the metric ρ on $M(\mathfrak{X})$ the following two cases will be considered in the sequel. Let $\mu_1, \mu_2 \in M(\mathfrak{X})$. The Wasserstein metric $\rho^{(s)}$ of order $1 \le s < \infty$ is defined by

$$\rho^{(s)}(\mu_1,\mu_2) = \inf_{\xi} \left(\int_{\mathfrak{X}\times\mathfrak{X}} \|x_1 - x_2\|_{\mathfrak{X}}^s \, d\xi(x_1,x_2) \right)^{1/s},$$

where the infimum is taken over all Borel probability measures ξ on $\mathfrak{X} \times \mathfrak{X}$ with marginals μ_1 and μ_2, respectively. Furthermore, we study metrics

$$\rho_F(\mu_1,\mu_2) = \sup_{f\in F} \left| \int_{\mathfrak{X}} f \, d\mu_1 - \int_{\mathfrak{X}} f \, d\mu_2 \right|$$

given in a dual representation in terms of a class F of functions $f\colon \mathfrak{X} \to \mathbb{R}$ that satisfies

$$\sup_{f\in F} \sup_{x\in\mathfrak{X}} \frac{|f(x) - f(0)|}{1 + \|x\|_{\mathfrak{X}}^s} < \infty$$

for some $1 \le s < \infty$. In particular, ρ_F is called a metric with ζ-structure, if all functions $f \in F$ are bounded, see [31, p. 72].

Consider $F = \mathrm{Lip}(1)$, i.e., F consists of all functions $f\colon \mathfrak{X} \to \mathbb{R}$ with

$$|f(x_1) - f(x_2)| \le \|x_1 - x_2\|_{\mathfrak{X}}, \qquad x_1, x_2 \in \mathfrak{X}.$$

Then, by the Kantorovich-Rubinstein Theorem,

$$\rho_{\mathrm{Lip}(1)} = \rho^{(1)}.$$

Remark 1 We relate our computational problem to an approximation theoretical question. For $\mu \in M(\mathfrak{X})$ and $n \in \mathbb{N}$ let

$$q_n(\mu) = q_n(\mu, \rho) = \inf\{\rho(\mu, \hat{\mu}) : \hat{\mu} \in M_0(\mathfrak{X}),\ |\operatorname{supp}(\hat{\mu})| \leq n\}.$$

If $\rho = \rho^{(s)}$ then $q_n(\mu)$ is called the n-th quantization number of μ, see [7, 10, 28]. We use this terminology for a general metric ρ, and accordingly construction of quadrature formulas may also be called constructive quantization.

Consider a randomized algorithm $\hat{S}$ with $\mathrm{cost}(\hat{S}) \leq N$, let $(x_0, a, b) \in H$, and put $A = \{\mathrm{cost}(\hat{S}, (x_0, a, b)) \leq 2N\}$. Clearly, $Q(A) \geq 1/2$ and $|\operatorname{supp}(\hat{S}(x_0, a, b))| \leq N$ on A due to (1). Therefore

$$e_N^{\mathrm{ran}} \geq \tfrac{1}{2} \cdot \sup_{(x_0,a,b)\in H} q_N(S(x_0, a, b)). \tag{2}$$

Since the asymptotic behavior of the quantization numbers is known in many cases, we may obtain lower bounds for the minimal errors in this way. Note that this argument does not at all exploit the fact that algorithms only have partial information about a and b in the following sense. For every algorithm $\hat{S}$ the number of evaluations of a or b is bounded from above by $\mathrm{cost}(\hat{S}, (x_0, a, b))$, and for a non-trivial class H a finite number of such evaluations does not suffice to determine $S(x_0, a, b)$ exactly. We refer to [30] for lower bounds based on partial information about the drift coefficient a.

Remark 2 Consider the marginal case $\mathfrak{X} = \mathbb{R}^d$ and let $\rho = \rho_F$. We compare the construction of quadrature formulas and the actual quadrature problem on F. For the latter task an oracle for $f \in F$ is needed, too, and algorithms yield real numbers as output. The worst case error of a randomized algorithm $\tilde{S}\colon H \times F \times \Omega \to \mathbb{R}$ is defined by

$$\Delta(\tilde{S}) = \sup_{(x_0,a,b)\in H, f\in F} \left(\mathrm{E}\Big(\int_{\mathfrak{X}} f\, dS(x_0, a, b) - \tilde{S}(x_0, a, b, f)\Big)^2\right)^{1/2},$$

and the number of evaluations of f has to be added as another term in the definition of the computational cost. The minimal errors Δ_N^{ran} and Δ_N^{det} for the quadrature problem are defined in the canonical way.

Clearly, every algorithm $\hat{S}$ for construction of quadrature formulas

yields an algorithm $\tilde{S}$ for quadrature by

$$\tilde{S}((x_0, a, b), f, \omega) = \int_{\mathfrak{X}} f \, d\hat{S}((x_0, a, b), \omega),$$

and we have $\Delta(\tilde{S}) \leq e(\hat{S})$ as well as $\mathrm{cost}(\hat{S}) \leq \mathrm{cost}(\tilde{S}) \leq 3\,\mathrm{cost}(\hat{S})$. Hence

$$\Delta_{3N}^{\mathrm{ran}} \leq e_N^{\mathrm{ran}} \qquad \text{and} \qquad \Delta_{3N}^{\mathrm{det}} \leq e_N^{\mathrm{det}}.$$

We stress that the minimal errors $\Delta_{3N}^{\mathrm{ran}}$ and e_N^{ran} may differ substantially, because of the order of taking suprema over F and expectations. For instance, let $H_0 \subset \mathbb{R}^d$ be a bounded set, let

$$H_1 = \{h \in C^1(\mathbb{R}^d, \mathbb{R}^d) \colon |h(0)|, \|\nabla h\|_\infty \leq K\}$$

with $K > 0$, and let H_2 be defined analogously for functions with values in $\mathbb{R}^{d \times d}$. Moreover, let $F = \mathrm{Lip}(1)$. By a well known result, the Monte Carlo Euler scheme yields

$$\Delta_N^{\mathrm{ran}} \preceq N^{-1/3},$$

while

$$e_N^{\mathrm{ran}} \succeq N^{-1/d} \tag{3}$$

follows from $q_n(\mu) \asymp n^{-1/d}$ for every normal distribution $\mu \in S(H)$ with full support in $\mathbb{R}^d$, see [10, p. 78] and (2). We therefore conclude that, at least for $d \geq 4$, the construction of quadrature formulas is substantially harder than quadrature, if randomized algorithms may be used in both cases.

We do not discuss quadrature problems on the path space here, since this requires to introduce an appropriate cost model for evaluating functions on infinite dimensional spaces $\mathfrak{X}$, see [2, 13].

Remark 3 Precomputing is permitted in our model of computation, and it is actually used in a number of rather different algorithms for the construction of quadrature formulas; we refer to the subsequent sections. Precomputing allows to solve auxiliary problems that do not involve the parameters x_0, a and b of the SDE beforehand. The computational effort for precomputing is not taken into account by $\mathrm{cost}(\hat{S})$.

Remark 4 In this paper we discuss constructive approximation by probability measures with finite support. More generally, one might admit signed measures with finite support, which is motivated by, e.g., the stochastic multi-level construction, or one might omit any constraint,

which means that $\hat{S}\colon H \times \Omega \to M(\mathfrak{X})$. It seems that these variants of the constructive approximation problem for the distribution of SDEs have not been studied so far.

3 Quadrature Formulas on the Path Space

We focus on scalar SDEs, i.e., $d = 1$, and we assume that $H_0 \subset \mathbb{R}$ is a bounded set and

$$H_1 = H_2 = \{h \in C^2(\mathbb{R}) : |h(0)|, |h'|, |h''| \leq K\}$$

with $K > 0$. Moreover, $\mathfrak{X} = \mathfrak{X}_p$ where $\mathfrak{X}_\infty = C([0,1])$ and $\mathfrak{X}_p = L_p([0,1])$ for $1 \leq p < \infty$, and $\rho = \rho^{(s)}$ is the Wasserstein metric of order s on $M(\mathfrak{X}_p)$ for any $1 \leq s < \infty$.

At first we discuss the quantization problem, see Remark .1. We assume $b(x_0) \neq 0$ in order to exclude deterministic equations.

Theorem 5 *For every $(x_0, a, b) \in H$ with $b(x_0) \neq 0$ there exists a constant $\kappa(x_0, a, b, p, s) > 0$ such that*

$$q_n(S(x_0, a, b)) \approx \kappa(x_0, a, b, p, s) \cdot (\ln n)^{-1/2}.$$

In the particular case of a Brownian motion, i.e., for the parameters $(x_0, a, b) = (0, 0, 1)$, this result is due to [4, 17] for $p = 2$ and to [8] for general p. For SDEs the result is established in [5, 6]. The structure of the asymptotic constant $\kappa(x_0, a, b, p, s)$ and its dependence on the parameters of the SDE is as follows. There exist constants $c(p) > 0$ such that

$$\kappa(x_0, a, b, p, s) = c(p) \cdot \left(\mathrm{E}\left(\int_0^1 |b(X(t))|^{2/(1+2/p)}\, dt \right)^{s(1+2/p)/2} \right)^{1/s},$$

where $1/\infty = 0$. In particular, $c(2) = \sqrt{2}/\pi$, while only upper and lower bounds for $c(p)$ are known in the case $p \neq 2$.

From Theorem .5 we immediately get a lower bound for e_N^{ran}, see (2), which turns out to be sharp and attainable already by deterministic algorithms.

Theorem 6 *We have*

$$e_N^{\mathrm{ran}} \asymp e_N^{\mathrm{det}} \asymp (\ln N)^{-1/2}.$$

The upper bound $e_N^{\mathrm{det}} \preceq (\ln N)^{-1/2}$ in Theorem .6 is due to [24], and

we describe the deterministic algorithm that yields this bound in the case $p = s = 2$.

Fix $(x_0, a, b) \in H$. The construction is motivated by the following two-level approximation of the solution process X of the corresponding SDE. For $m \in \mathbb{N}$ we consider the Milstein scheme Y with step-size $1/m$ and with piecewise linear interpolation, and we put $t_k = k/m$. Furthermore, we consider the Brownian bridges

$$B_k(t) = W(t) - W(t_k) - (t - t_k) \cdot m \cdot (W(t_{k+1}) - W(t_k)),$$

where $t \in [t_k, t_{k+1}]$. Note that $Y, B_0, \ldots, B_m$ are independent. As an approximation to X we consider $Y + Z$ with the coarse level approximation Y and with a local refinement

$$Z(t) = \sum_{k=0}^{m-1} b(Y(t_k)) \cdot B_k(t) \cdot 1_{[t_k, t_{k+1}]}(t).$$

Instead of the Gaussian measures that are involved in Y and Z the algorithm employs probability measures with finite support.

For the standard normal distribution γ and the Wasserstein metric ρ of order two on $M(\mathbb{R})$ we have $q_n(\gamma, \rho) \asymp n^{-1}$, and we take a sequence of uniform distributions $\hat{\gamma}_r \in M_0(\mathbb{R})$ with $|\operatorname{supp}(\hat{\gamma}_r)| = r$ and

$$\rho(\gamma, \hat{\gamma}_r) \asymp r^{-1}.$$

We refer to [10, Sec. 7.3] for a general account and to [24] for details and additional requirements concerning $\hat{\gamma}_r$ in the present context.

For the distribution ξ of a Brownian bridge on $[0, 1]$ and the Wasserstein metric $\rho^{(2)}$ of order two on $M(L_2([0, 1]))$ we have $q_n(\xi, \rho^{(2)}) \approx \sqrt{2}/\pi \cdot (\ln n)^{-1/2}$, cf. Theorem .5, and we take a sequence of measures $\hat{\xi}_n \in M_0(L_2([0, 1]))$ with $|\operatorname{supp}(\hat{\xi}_n)| = n$ and

$$\rho^{(2)}(\xi, \hat{\xi}_n) \asymp (\ln n)^{-1/2}. \tag{4}$$

The construction of $\hat{\xi}_n$ is based on the Karhunen-Loève expansion of the Brownian bridge, where the eigenfunctions and eigenvalues are given by $e_\ell(t) = \sqrt{2}\sin(\ell\pi t)$ and $\lambda_\ell = (\ell\pi)^{-2}$, respectively, and on quantization of normal distributions. In particular, $\operatorname{supp}(\hat{\xi}_n) \subset \operatorname{span}\{e_\ell \colon \ell \in \mathbb{N}\}$. In order to achieve

$$\rho^{(2)}(\xi, \hat{\xi}_n) \approx q_n(\xi, \rho^{(2)}) \tag{5}$$

suitable quantizations of multi-dimensional centered normal distributions with covariance matrices of diagonal form are used for quantization of blocks of coefficients of the Karhunen-Loève expansion, and

this approach involves large scale numerical optimization. Alternatively, (4) with reasonable good constants can already be achieved by product quantizers, which merely rely on quantizations of the one-dimensional standard normal distribution. We refer to [7, 19, 20] for surveys and recent results and to the web site [27] for downloads. In any case the construction of suitable measures $\hat{\xi}_n$ is a matter of precomputing.

We first explain how to approximate the distribution P_Y. The standard normal distribution on $\mathbb{R}^m$, which is the basis for the Milstein scheme, is replaced by the uniform distribution

$$\hat{\gamma} = \bigotimes_{k=0}^{m-1} \hat{\gamma}_r.$$

Note that $\mathrm{supp}(\hat{\gamma})$ is a non-uniform grid in $\mathbb{R}^m$. For every $w \in \mathrm{supp}(\hat{\gamma})$ we define a function $y(\cdot; w) \in C([0,1])$ by $y(0; w) = x_0$ and

$$\begin{aligned} y(t_{k+1}; w) = y(t_k; w) &+ 1/m \cdot a(y(t_k; w)) + 1/\sqrt{m} \cdot b(y(t_k; w)) \cdot w_k \\ &+ 1/(2m) \cdot (b \cdot b')(y(t_k; w)) \cdot (w_k^2 - 1) \end{aligned}$$

and by piecewise linear interpolation. This corresponds to the Milstein scheme with the normalized Brownian increments replaced by the components of w, and as an approximation to the distribution P_Y of the Milstein scheme we use the uniform distribution

$$\hat{\nu} = \frac{1}{r^m} \sum_{w \in \mathrm{supp}(\hat{\gamma})} \delta_{y(\cdot; w)}$$

on a finite set of piecewise linear functions.

Next we turn to the approximation of the distribution P_Z. For every polygon $y \in \mathrm{supp}(\hat{\nu})$ the distribution of the weighted Brownian bridge $b(y(t_k)) \cdot B_k$ on $[t_k, t_{k+1}]$ is approximated by one of the measures $\hat{\xi}_n$, properly rescaled and shifted. Hereby, the size n of the support is chosen in such a way that the local regularity of the solution process X is taken into account. Essentially, we take

$$n = n_k(y) = \max\bigl(\lfloor M^{\eta_k(y)} \rfloor, 1\bigr)$$

with

$$\eta_k(y) = |b(y(t_k))| / \sum_{k=0}^{m-1} |b(y(t_k))|$$

for a given $M \in \mathbb{N}$, see [24] for technical details. This strategy, which is crucial for the overall performance of the algorithm, is similar to asymptotically optimal step-size control for pathwise approximation of SDEs,

see [11, 12, 22, 23]. To approximate the joint distribution of the weighted Brownian bridges $b(y(t_k)) \cdot B_k$ we take the product measure

$$\hat{\xi}(\cdot, y) = \bigotimes_{k=0}^{m-1} \hat{\xi}_{n_k(y)}$$

in $C([0,1])^m$ and use the linear mapping $\psi(\cdot; y)\colon \operatorname{supp}(\hat{\xi}(\cdot, y)) \to C([0,1])$ given by

$$\psi(z; y)(t) = \sum_{k=0}^{m-1} b(y(t_k)) \cdot z_k((t - t_k) \cdot m)/\sqrt{m} \cdot 1_{[t_k, t_{k+1}]}(t).$$

Choose $m = r \asymp (\ln M)^\alpha$ for $\alpha \in]1/2, 1[$, and put $N = m^m \cdot M$. As an approximation to P_{Y+Z}, and thus to P_X, we take

$$\hat{S}_N(x_0, a, b) = \sum_{y \in \operatorname{supp}(\hat{\nu})} \sum_{z \in \operatorname{supp}(\hat{\xi}(\cdot, y))} \frac{\hat{\xi}(\{z\}, y)}{r^m} \cdot \delta_{y + \psi(z; y)}.$$

Clearly

$$|\operatorname{supp}(\hat{S}_N(x_0, a, b))| \le N,$$

and $\hat{\xi}(\{z\}, y)$ is the product of certain probability weights of the measures $\hat{\xi}_n$. The piecewise linear functions y and the functions $\psi(z; y)$, which consist of trigonometric polynomials on the subintervals $[t_k, t_{k+1}]$ can be coded in a natural way. It turns out that $\operatorname{cost}(\hat{S}_N) \preceq m \cdot N$ and $e(\hat{S}_N) \asymp (\ln N)^{-1/2} \asymp (\ln(\operatorname{cost}(\hat{S}_N))^{-1/2}$. Moreover, if (5) is satisfied then we even have

$$\rho^{(2)}(S(x_0, a, b), \hat{S}_N(x_0, a, b)) \approx \kappa(x_0, a, b, 2, 2) \cdot (\ln N)^{-1/2} \tag{6}$$

for every $(x_0, a, b) \in H$ with $b(x_0) \neq 0$, i.e., the algorithm $\hat{S}_N$ achieves strong asymptotic optimality for the quantization problem for every such SDE, see Remark .1 and Theorem .5. We refer to [32] for an efficient implementation of $\hat{S}_N$ and to [24] for the construction of $\hat{S}_N$ in the case $p \neq 2$ or $s \neq 2$.

Remark 7 The algorithm $\hat{S}_N$ can be generalized to handle systems of SDEs, i.e., to the case $d > 1$, in a straightforward manner. For coarse level approximation, however, it no longer suffices to approximate Brownian increments, since multiple Itô integrals are needed, too, in the Milstein scheme. For this task there are several methods available, e.g., the quantization of an approximation to these integrals based on a suitably truncated Karhunen-Loève expansion, see [36], and an empirical

measure approach, see Section 5, but the analysis of error and cost for construction of quadrature formulas on the path space seems to be open for $d > 1$.

Remark 8 The constructive quantization of diffusion processes was initiated by [18], where suitable quantizers for the driving Brownian motion are used as a building block, which is similar to our approach. The approaches differ, however, with respect to the numerical treatment of the SDE. A key assumption in [18] is strict positivity of the diffusion coefficient, which permits to use the Lamperti transform. Along this way one has to solve n deterministic ODEs, in general, to get an approximation $\hat{\mu}_n$ with $\mathrm{supp}(\hat{\mu}_n) = n$ and $\rho^{(2)}(P_X, \hat{\mu}_n) \asymp (\ln n)^{-1/2}$. This work is extended to systems of of SDEs in [29], where rough path theory is used to establish convergence rates in p-variation and in the Hölder metric for ODE-based quantizations. A different approach is developed in [19], where the mean regularity of stochastic processes is exploited. The construction is based on the expansion of X in terms of the Haar basis, and on the availability of optimal quantizations of the corresponding coefficients. It seems that none of these alternative approaches achieves (6) and that the computational cost has not been analyzed so far. As far as we understand, these alternative methods do not achieve a cost bound close to the size of the quantization.

4 Quadrature Formulas on the State Space – Deterministic Algorithms

We study scalar SDEs, i.e., $d = 1$, and we assume that $H_0 \subset \mathbb{R}$ is a bounded set and

$$H_1 = \{h \in C^4(\mathbb{R})\colon |h(0)|, |h^{(j)}| \leq K \text{ for } j = 1, \ldots, 4\},$$
$$H_2 = \{h \in H_1\colon |h| \geq \varepsilon\}$$

with $K > 0$ and $\varepsilon \geq 0$. Thus $H_1 = H_2$ if $\varepsilon = 0$, while $\varepsilon > 0$ corresponds to an additional non-degeneracy constraint on the diffusion coefficient b. Furthermore, $\mathfrak{X} = \mathbb{R}$, and we consider the metric $\rho = \rho_F$, where

$$F = \{f \in C^4(\mathbb{R})\colon |f^{(j)}(x)| \leq K \cdot (1 + |x|^\beta) \text{ for } j = 1, \ldots, 4\}$$

with $\beta \geq 0$.

In this setting we have the following upper bounds for the minimal errors of deterministic algorithms, see [25].

Theorem 9 *For every $\delta > 0$*

$$e_N^{\det} \preceq \begin{cases} N^{-2/3+\delta} & \text{if } \varepsilon > 0, \\ N^{-1/2+\delta} & \text{if } \varepsilon = 0. \end{cases}$$

The central idea to obtain these upper bounds is as follows. We approximate an Euler scheme with step-size $1/m$ by a Markov chain that stays on a grid of small size and has a sparse transition matrix in order to prevent an exponential explosion of the cost. The transition probabilities are chosen in such a way that the central moments of a single Euler step are close to the corresponding moments of a step of the chain. The approximation to the distribution $P_{X(1)}$ is then obtained as the distribution of the Markov chain after m steps.

Here we present this construction in the case $\varepsilon > 1$. Fix $(x_0, a, b) \in H$, let $\delta > 0$ and $m \in \mathbb{N}$, and define the state space of the Markov chain by $\mathcal{Z} = G \cup \{x_0\}$, where

$$G = \left\{ i \cdot m^{-1/2} : i = -\lceil m^{1/2+\delta} \rceil, \dots, \lceil m^{1/2+\delta} \rceil \right\}.$$

In order to define the transition probabilities $q_{y,z} = q_{y,z}(x_0, a, b)$ for $y, z \in \mathcal{Z}$, we consider an Euler step of length $1/m$ starting in $y \in \mathcal{Z}$, i.e.,

$$Y^y = y + a(y) \cdot m^{-1} + b(y) \cdot m^{-1/2} \cdot V$$

with a standard normally distributed random variable V. Let

$$z_y = y + a(y) \cdot m^{-1}, \qquad \sigma_y = |b(y)| \cdot m^{-1/2}$$

denote the expected value and the standard deviation of Y^y and put

$$\bar{z}_y = \lceil z_y \cdot m^{1/2} \rceil \cdot m^{-1/2}, \qquad \bar{\sigma}_y = \lceil \sigma_y \cdot m^{1/2} \rceil \cdot m^{-1/2},$$

which will serve as projections of z_y and σ_y onto G, respectively. Essentially, we replace the Euler step by a step from y to at most six possible positions on G, namely

$$\bar{z}_y, \qquad \bar{z}_y \pm \bar{\sigma}_y, \qquad \bar{z}_y - m^{-1/2}, \qquad \bar{z}_y - m^{-1/2} \pm \bar{\sigma}_y. \tag{7}$$

To be more precise, we distinguish the two cases given by

$$\mathcal{Z}_1 = \left\{ y \in \mathcal{Z} \colon \bar{z}_y - m^{-1/2} - \bar{\sigma}_y, \bar{z}_y + \bar{\sigma}_y \in G \right\}, \quad \mathcal{Z}_2 = \mathcal{Z} \setminus \mathcal{Z}_1.$$

The points $y \in \mathcal{Z}_2$, where z_y is close to the extremal points of G, are absorbing states, i.e.,

$$q_{y,z} = \begin{cases} 1 & \text{if } z = y, \\ 0 & \text{otherwise.} \end{cases}$$

For $y \in \mathcal{Z}_1$ the points given by (7) are members of G, and due to $|b(y)| > 1$ all of them are different. Put

$$u_y = m^{1/2} \cdot (\bar{z}_y - z_y)$$

as well as

$$\vartheta_y^{(1)} = \frac{\sigma_y^2}{2\bar{\sigma}_y^2} + \frac{u_y^2 - 2u_y}{6\bar{\sigma}_y^2 \cdot m}, \qquad \vartheta_y^{(2)} = \frac{\sigma_y^2}{2\bar{\sigma}_y^2} + \frac{u_y^2 - 1}{6\bar{\sigma}_y^2 \cdot m}.$$

Clearly, $0 \le u_y < 1$ and $\vartheta_y^{(j)} \le 1/2$. Moreover, $|b(y)| > 1$ yields $\vartheta_y^{(j)} > 0$. We define

$$q_{y,z} = \begin{cases} (1-u_y) \cdot (1 - 2\vartheta_y^{(1)}) & \text{if } z = \bar{z}_y, \\ (1-u_y) \cdot \vartheta_y^{(1)} & \text{if } z = \bar{z}_y \pm \bar{\sigma}_y, \\ u_y \cdot (1 - 2\vartheta_y^{(2)}) & \text{if } z = \bar{z}_y - m^{-1/2}, \\ u_y \cdot \vartheta_y^{(2)} & \text{if } z = \bar{z}_y - m^{-1/2} \pm \bar{\sigma}_y, \\ 0 & \text{otherwise.} \end{cases}$$

Let $Q = (q_{y,z})_{y,z \in \mathcal{Z}}$ denote the resulting transition matrix. We approximate $S(x_0, a, b)$ by the discrete distribution

$$\hat{S}_m(x_0, a, b) = \sum_{z \in \mathcal{Z}} (e \cdot Q^m)_z \cdot \delta_z, \tag{8}$$

where $e = (e_z)_{z \in \mathcal{Z}}$ is given by $e_{x_0} = 1$ and $e_z = 0$ for $z \neq x_0$.

Consider a random variable $\tilde{Y}^y$ that models a single step of the Markov chain with transition matrix Q and starting at $y \in \mathcal{Z}$, i.e., $P(\tilde{Y}^y = z) = q_{y,z}$ for every $z \in \mathcal{Z}$. We then have

$$|E(Y^y - z_y)^p - E(\tilde{Y}^y - z_y)^p| \le c \cdot (1 + |y|^{p+1/\delta}) \cdot m^{-2}$$

for every $p \in \mathbb{N}$, where the constant $c > 0$ only depends on K, δ, p, and this estimate is a key property to obtain $e(\hat{S}_m) \preceq m^{-1}$. Moreover, we have $\mathrm{cost}(\hat{S}_m) \asymp m^{3/2+\delta}$, which results from the number of arithmetical operations that are used to compute to the matrix-vector product $e \cdot Q^m$.

Remark 10 We consider, more generally, the case of d-dimensional systems of SDEs with coefficients that satisfy a smoothness constraint of degree $r \in \mathbb{N}$. Fix $K > 0$. For $\beta \ge 0$ we use F^β to denote the class of functions $f\colon \mathbb{R}^d \to \mathbb{R}$ that have continuous partial derivatives $f^{(\alpha)}$ with

$$|f^{(\alpha)}(x)| \le K \cdot (1 + |x|^\beta)$$

for every $x \in \mathbb{R}^d$ and every $\alpha \in \mathbb{N}_0^d$ with $1 \le \sum_{i=1}^d \alpha_i \le r$. We take $\mathfrak{X} = \mathbb{R}^d$, and we consider the metric ρ_F with $F = F^\beta$.

Assume that $H_0 \subset \mathbb{R}^d$ is bounded,

$$H_1 = \{h \in C^r(\mathbb{R}^d, \mathbb{R}^d) \colon |h(0)| \le K,\, h_1, \dots, h_d \in F^0\} \tag{9}$$

and H_2 is defined analogously to H_1 for functions $h \colon \mathbb{R}^d \to \mathbb{R}^{d\times d}$ with the additional uniform ellipticity constraint that $|y'h(x)| \ge \varepsilon \cdot |y|$ for all $x, y \in \mathbb{R}^d$.

Assume $r \ge 4$. We conjecture that a construction, similar to the Markov chain for $d = 1$, leads to upper bounds

$$e_N^{\mathrm{det}} \preceq \begin{cases} N^{-(r-2)/(d+2)+\delta} & \text{if } \varepsilon > 0, \\ N^{-(r-2)/(2d+2)+\delta} & \text{if } \varepsilon = 0 \end{cases} \tag{10}$$

for the minimal errors of deterministic algorithms for every $\delta > 0$. Note that (10) holds true for $d = 1$ and $r = 4$ due to Theorem .9.

Alternatively, the connection between SDEs and initial value problems for the associated parabolic PDEs could be employed, and numerical methods for PDEs could be used to construct deterministic quadrature formulas on the state space. It would be interesting to investigate the potential of finite difference methods for the latter problem.

We turn to lower bounds for the minimal errors via quantization numbers, which hold for randomized algorithms, too. Consider a probability measure $\mu \in M(\mathbb{R}^d)$ with a continuous Lebesgue density that satisfies suitable decay properties. Then

$$q_n(\mu, \rho_F) \asymp n^{-r/d} \tag{11}$$

follows from results on weighted approximation and integration in [34, 35]. In particular, (11) holds for any non-degenerate d-dimensional normal distribution $\mu \in S(H)$, which implies

$$e_N^{\mathrm{ran}} \succeq N^{-r/d} \tag{12}$$

due to (2).

Specifically, for $r = 4$ and $d = 1$ we get a lower bound of order four in (12), which differs substantially from the upper bounds of order $2/3$ or $1/2$ in Theorem .9. It would be interesting to know whether the fact that any algorithm only has partial information about a and b can be used to improve the lower bound, cf. Remark .1.

Remark 11 Quadrature formulas on the Wiener space, which are based on paths of bounded variation and are exact for iterated integrals up to a fixed degree m, are introduced in [14, 15] and further developed in [3, 21]. The construction of such formulas is a matter of precomputing.

For d-dimensional systems of SDEs with smooth coefficients a and b an approximation to the marginal distribution $P_{X(1)}$ of the solution X is obtained by iteratively solving a collection of ODEs on k non-equidistant time intervals. The error is defined in terms of metrics ρ_F with different spaces F. For $F = \mathrm{Lip}(1)$ an error bound of order $k^{-(m-1)/2}$ is achieved. However, the number of ODEs to be solved grows polynomially in k. To cope with this difficulty a recombination technique has been introduced in [16].

Remark 12 Let us compare the results from Section 3 (for $s = 1$) and 4. In both cases we assume a finite degree of smoothness for the coefficients of the SDE and for the elements in F, together with some boundedness or growth constraints. For the problem on the path space we merely achieve a logarithmic convergence of the minimal errors, and the computational cost of the almost optimal algorithm $\hat{S}_N$ presented in Section 3 is only slightly larger than $|\operatorname{supp}(\hat{S}_N(x_0, a, b))|$. Furthermore, $\operatorname{supp}(\hat{S}_N(x_0, a, b))$ strongly depends on the SDE, i.e., on x_0, a, and b. For the marginal distribution problem we have a polynomial rate of convergence, and the computational cost of the corresponding algorithm $\hat{S}_m$ is substantially larger than $|\operatorname{supp}(\hat{S}_m(x_0, a, b))|$. Furthermore, $\operatorname{supp}(\hat{S}_m(x_0, a, b))$ is essentially a grid that does not depend on the SDE.

5 Quadrature Formulas on the State Space – Randomized Algorithms

In this section we consider systems of SDEs, and we employ random quantization techniques for the marginal distributions $P_{X(1)}$ to obtain randomized algorithms for the construction of quadrature formulas on the state space.

We first present a general result on quantization by empirical measures. For a probability measure μ on $\mathfrak{X} = \mathbb{R}^d$ and $n \in \mathbb{N}$ we use $\hat{\mu}_n$ to denote the empirical measure that is induced by a sequence of n independent random variables $Y_1, \ldots, Y_n$ with $P_{Y_1} = \mu$, i.e.,

$$\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{Y_i}.$$

The following upper bound for the average Wasserstein distance of μ and $\hat{\mu}_n$ is due to [9].

Theorem 13 *Let $1 \le s < d/2$ and $q > ds/(d-s)$. There exists a constant $\kappa(d,s,q) > 0$ such that*

$$\Big(\mathrm{E}\big(\big(\rho^{(s)}(\mu,\hat{\mu}_n)\big)^s\big)\Big)^{1/s} \le \kappa(d,s,q) \cdot \left(\int_{\mathbb{R}^d} |x|^q \, d\mu(x)\right)^{1/q} \cdot n^{-1/d}$$

for any probability measure μ on $\mathbb{R}^d$ and all $n \in \mathbb{N}$.

Note that the bound stated in Theorem .13 allows to control the approximation error in terms of moments of the probability measure μ. Results of this type are commonly referred to as Pierce type estimates in quantization.

We add that the n-th quantization numbers satisfy

$$q_n(\mu, \rho^{(s)}) \asymp n^{-1/d} \tag{13}$$

if μ has a finite moment of order $s+\delta$ for some $\delta > 0$ and a nonvanishing absolute continuous part w.r.t. the Lebesgue measure on $\mathbb{R}^d$. See [10, Thm. 6.2] for further details and for results on the strong asymptotic behavior of $q_n(\mu, \rho^{(s)})$, too.

In the sequel we consider systems of SDEs with the same constraints as in Remark .2. Thus $H_0 \subset \mathbb{R}^d$ is a bounded set,

$$H_1 = \{h \in C^1(\mathbb{R}^d, \mathbb{R}^d) \colon |h(0)|, \|\nabla h\|_\infty \le K\}$$

with $K > 0$, and H_2 is defined analogously for functions with values in $\mathbb{R}^{d\times d}$. Moreover, $\mathfrak{X} = \mathbb{R}^d$, and we consider the Wasserstein metric $\rho^{(s)}$ of order $1 \le s < d/2$ on $M(\mathfrak{X})$.

Theorem 14 *For $d \ge 5$ we have*

$$N^{-1/d} \preceq e_N^{\mathrm{ran}} \preceq N^{-1/(d+2)}.$$

The lower bound in this result is a consequence of (2) and (13), and in fact it holds for every $d \in \mathbb{N}$ and $s \ge 1$.

Note that Theorem .13 is not directly applicable to derive an upper bound for the minimal error e_N^{ran}, since one cannot sample from the marginal distribution $P_{X(1)}$ in general. More precisely, there is no randomized algorithm $A : H \times \Omega \to \mathbb{R}^d$, which uses partial information about a and b, such that the distribution of $A((x_0,a,b),\cdot)$ coincides with $P_{X(1)}$ for every $(x_0,a,b) \in H$.

We show that the upper bound in Theorem .14 is obtained by the empirical measure based on the Euler scheme. Let $m, n \in \mathbb{N}$, and let

$V_1, \dots, V_m$ denote an independent sequence of standard normally distributed d-dimensional random vectors. Fix $(x_0, a, b) \in H$. Put $Y^{(0)} = x_0$ and

$$Y^{(k+1)} = Y^{(k)} + a(Y^{(k)}) \cdot m^{-1} + b(Y^{(k)}) \cdot m^{-1/2} \cdot Z^{(k)}$$

for $k = 0, \dots, m-1$, and take n independent copies $Y_1^{(m)}, \dots, Y_n^{(m)}$ of $Y^{(m)}$. We define

$$\hat{S}_{m,n}((x_0, a, b), \omega) = \frac{1}{n} \sum_{i=1}^{n} \delta_{Y_i^{(m)}(\omega)}.$$

We briefly analyze the error and the cost of $\hat{S}_{m,n}$. Fix $(x_0, a, b) \in H$, and put $\mu^{(m)} = P_{Y^{(m)}}$ and $\hat{\mu}_n^{(m)} = \hat{S}_{m,n}(x_0, a, b)$. Then

$$\Big(\mathrm{E}\Big(\big(\rho^{(s)}(S(x_0, a, b), \hat{S}_{m,n}(x_0, a, b))\big)^2\Big)\Big)^{1/2}$$
$$\leq \rho^{(s)}(P_{X(1)}, P_{Y^{(m)}}) + \Big(\mathrm{E}\Big(\big(\rho^{(s)}(\mu^{(m)}, \hat{\mu}_n^{(m)})\big)^2\Big)\Big)^{1/2}.$$

Put $s^* = \max(s, 2)$ and apply Theorem .13 with any $q > ds^*/(d - s^*)$ to obtain

$$\Big(\mathrm{E}\Big(\big(\rho^{(s)}(P_{Y^{(m)}}, \hat{\mu}_{m,n})\big)^2\Big)\Big)^{1/2} \leq \kappa_1 \cdot n^{-1/d}$$

for every $m \in \mathbb{N}$, with a constant $\kappa_1 > 0$ that only depends on d, s, x_0, K. Similarly, we have

$$\rho^{(s)}(P_{X(1)}, P_{Y^{(m)}}) \leq E(|X(1) - Y^{(m)}|^s)^{1/s} \leq \kappa_2 \ \cdot m^{-1/2}, \tag{14}$$

for every $m \in \mathbb{N}$, with a constant $\kappa_2 > 0$ that only depends on d, s, x_0, K. Hence

$$e(\hat{S}_{n,m}) \preceq m^{-1/2} + n^{-1/d}.$$

Clearly,

$$\mathrm{cost}(\hat{S}_{m,n}) \leq \kappa \cdot d^2 \cdot n \cdot m$$

with a constant $\kappa > 0$. Choose $m \asymp n^{2/d}$ to obtain the estimate in Theorem .14.

We add that the upper bound in Theorem .14 is valid for $d \geq 3$, if the worst case error $e(\hat{S})$ of an algorithm $\hat{S}$ is defined in terms of moments of order one rather than two.

Remark 15 Under stronger assumptions on the parameters of the SDE, i.e., for smaller classes H, improved upper bounds should hold for e_N^{ran}.

In [1] the Euler scheme is studied for SDEs with C^∞-coefficients that have bounded partial derivatives of any order and satisfy a nondegeneracy condition. For every bounded measurable function $f : \mathbb{R}^d \to \mathbb{R}$ an upper bound of order $1/m$ is obtained for the so-called weak error $\left|\int_{\mathbb{R}^d} f\, dP_{X(1)} - \int_{\mathbb{R}^d} f\, dP_{Y^{(m)}}\right|$. A careful adaptation of [1] should therefore lead to an upper bound of order m^{-1} in (14) and, consequently, to an upper bound of order $1/N^{1/(d+1)}$ in Theorem .14 in the case $s = 1$ for an appropriate class H.

An alternative approach is to employ Itô-Taylor schemes of higher order instead of the Euler scheme, which leads to faster convergence in (14) under appropriate assumptions on H_1 and H_2. Actually, for each $\delta > 0$ one can determine classes of coefficients such that an upper bound of order $1/N^{1/d-\delta}$ is valid in Theorem .14. However, this approach makes use of iterated integrals, and the effort for precomputation may therefore be prohibitively large if δ is small.

Acknowledgement

This work was supported by the Deutsche Forschungsgemeinschaft (DFG) within the Priority Programme 1324. We are grateful to Stefan Heinrich, Henryk Woźniakowki and Larisa Yaroslavtseva for stimulating discussions.

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