Adaptive Multilevel Monte Carlo Approximation of Distribution Functions

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Abstract. We analyse a multilevel Monte Carlo method for the approximation of distribution functions of univariate random variables. Since, by assumption, the target distribution is not known explicitly, approximations have to be used. We provide an asymptotic analysis of the error and the cost of the algorithm. Furthermore we construct an adaptive version of the algorithm that does not require any a priori knowledge on weak or strong convergence rates. We apply the adaptive algorithm to smooth path-independent and path-dependent functionals and to stopped exit times of SDEs.

Key words. adaptive multi-level Monte Carlo, approximation of distribution functions, stochastic differential equations, path-(in)dependent functionals, stopped exit times, smoothing

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1. Introduction. Let $Y$ denote a real-valued random variable with distribution function $F$. We study the approximation of $F$ with respect to the supremum norm on a compact interval $[S_0, S_1]$, without assuming that the distribution of $Y$ is explicitly known or that the simulation of $Y$ is feasible. Instead, we suppose that a sequence of random variables $Y^{(\ell)}$ is at hand that converge to $Y$ in a suitable way and that are suited to simulation.

The general approach for this problem, based on the multilevel Monte Carlo (MLMC) approach [9, 6], has been presented in [8] and applied in the context of stochastic differential equations (SDEs). The suggested algorithm has already been used in stochastic oil reservoir simulations, which is based on numerical approximation of large-scale stochastic subsurface simulations [12], while the suggested smoothing technique has been used for analysis in [13].

In outline, one approach is to use the standard MLMC algorithm to approximate $F(s_i) = E(1_{]-\infty,s_i]}(Y))$, for a finite set of $k$ spline points $s_i$, and then use spline interpolation to define the approximation to $F(s)$ for the whole interval. The drawback of this approach is that the discontinuity in the indicator function leads to a high variance for the MLMC estimator. Instead, in [8] we introduce smoothing and approximate $E(g((Y - s_i)/\delta))$, where $g$ is a smooth approximation to the indicator function $1_{]-\infty,0]}$, and $\delta \ll S_1 - S_0$. This leads to an approximation of $F$ which has four error components:

- spline interpolation error, which depends on the number $k$ of spline knots;
- smoothing error, which depends on the smoothing parameter $\delta$;
- discretisation bias, which additionally depends on the accuracy of $Y^{(L)}$ on the finest level $L$;
- Monte Carlo sampling error, which additionally depends on the number $N_\ell$ of samples on each level.

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The standard MLMC algorithm has analysis and heuristics to determine near-optimal values for $L$ and $N^\ell$ [6, 7]. This paper addresses the question of how to adaptively determine the values for $k$ and $\delta$ to minimize the computational cost to achieve a prescribed accuracy. This extends the asymptotic analysis in [8] which, roughly speaking, assumes that the orders of weak and strong convergence of $Y^{(\ell)}$ towards $Y$ are known a priori.

The paper is organized as follows. In Section 2 we recall briefly the algorithm strategy, and present updated bounds on the cost and the assumptions under which they were derived. In Section 2.5 we present the error decomposition. Section 3 analyses the complexity of the MLMC algorithm, i.e., it provides a new asymptotic upper bound of the cost of the MLMC algorithm in terms of its error. In Section 4 we describe the adaptive approach for distribution function approximation. Finally, Section 5 is devoted to the numerical experiments.

For an alternative approach to the use of MLMC to construct approximations of distribution functions with error analysis in different norm, see the recent work of Bierig and Chernov [1, 2] who use the Maximum Entropy method to approximate the distribution, and MLMC to obtain estimates for the required moments.

2. Approximation of Distribution Functions on Compact Intervals via MLMC. In this section we present the multilevel algorithm for the approximation of a distribution function $F$ of a real-valued random variable $Y$ on a compact interval $[S_0, S_1]$. In particular, we discuss the smoothing and interpolation steps of the algorithm, which are not present in the standard setting for MLMC, namely the approximation of the expectation $E(Y)$. Our approach basically follows [8]. However, through an improvement in the implementation of the algorithm we derive a new cost bound, which leads to an improved upper bound for the cost of the algorithm in terms of its error, see Section 3.

2.1. Smoothing. For the approximation of the distribution function $F$ of $Y$ a straightforward application of the MLMC approach based on

$$F(s) = E(1_{(-\infty,s]}(Y))$$

would suffer from the discontinuity of $1_{(-\infty,s]}$. This can be avoided by a smoothing step, provided that a density exists and is sufficiently smooth. Specifically, we assume that

(A1) the random variable $Y$ has a density $\rho$ on $\mathbb{R}$ that is $r$-times continuously differentiable on $[S_0 - \delta_0, S_1 + \delta_0]$ for some $r \in \mathbb{N}_0$ and $\delta_0 > 0$.

The smoothing is based on rescaled translates of a function $g : \mathbb{R} \to \mathbb{R}$ with the following properties:

(S1) The cost of computing $g(s)$ is bounded by a constant, uniformly in $s \in \mathbb{R}$.
(S2) $g$ is Lipschitz continuous.
(S3) $g(s) = 1$ for $s < -1$ and $g(s) = 0$ for $s > 1$.
(S4) $\int_{-1}^{1} s^j \cdot (1_{(-\infty,0]}(s) - g(s)) \, ds = 0$ for $j = 0, \ldots, r-1$.

Obviously, $g$ is bounded due to (S2) and (S3).

Remark 1. Such a function $g$ is easily constructed as follows. There exists a uniquely determined polynomial $p$ of degree at most $r+1$ such that

$$\int_{-1}^{1} s^j \cdot p(s) \, ds = (-1)^j/(j+1), \quad j = 0, \ldots, r-1,$$
as well as \( p(1) = 0 \) and \( p(-1) = 1 \). The extension \( g \) of \( p \) with \( g(s) = 1 \) for \( s < -1 \) and \( g(s) = 0 \) for \( s > 1 \) has the properties as claimed. Since \( \frac{g-1}{2} \) is an odd function, the same function \( g \) arises in this way for \( r \) and \( r+1 \), if \( r \) is even.

For \( r = 3 \), which will be considered in the numerical experiments, we obtain

\[
p(s) = \frac{1}{2} + \frac{5s^3 - 9s}{8}.
\]

Using \( \| \cdot \|_\infty \) to denote the supremum norm on \( C([S_0, S_1]) \), we have the following estimate for the bias that is induced by smoothing with parameter \( \delta \), i.e., by approximation of \( 1_{]-\infty,s]} \) by \( g(\cdot - s)/\delta) \), see \cite[Lemma 2.2]{8}.

**Lemma 1.** There exists a constant \( c > 0 \) such that

\[
\| F - E(g((Y - \cdot)/\delta)) \|_\infty \leq c \cdot \delta^{r+1}
\]

holds for all \( \delta \in [0, \delta_0] \).

**Proof.** Clearly

\[
F(s) - E(g((Y - s)/\delta)) = \int_{-\infty}^\infty \rho(u) \cdot (1_{]-\infty,s]}(u) - g((u - s)/\delta)) \, du
\]

\[
\quad = \delta \cdot \int_{-1}^1 \rho(s + \delta u) \cdot (1_{]-\infty,0]}(u) - g(u)) \, du,
\]

so that the statement follows in the case \( r = 0 \). For \( r \geq 1 \) the Taylor expansion

\[
\rho(s + \delta u) = \sum_{j=0}^{r-1} \rho^{(j)}(s) \cdot (\delta u)^j/j! + R(\delta u, s)
\]

yields

\[
F(s) - E(g((Y - s)/\delta)) = \delta \cdot \int_{-1}^1 R(\delta u, s) \cdot (1_{]-\infty,0]}(u) - g(u)) \, du
\]

\[
= \frac{\delta^{r+1}}{(r-1)!} \int_{-1}^1 \int_0^u (u-t)^{r-1} \cdot \rho^{(r)}(s + \delta t) \, dt \cdot (1_{]-\infty,0]}(u) - g(u)) \, du,
\]

which completes the proof. \( \square \)

**Remark 2.** Consider \( g \) according to Remark 1, and assume that \( r \) is odd. Since

\[
\int_{-1}^1 \int_0^u (u-t)^{r-1} \cdot \rho^{(r)}(s + \delta t) \, dt \cdot (1_{]-\infty,0]}(u) - g(u)) \, du
\]

\[
\quad = - \int_0^1 \int_t^1 (u-t)^{r-1} \cdot g(u) \, du \cdot (\rho^{(r)}(s + \delta t) + \rho^{(r)}(s - \delta t)) \, dt,
\]

we have

\[
|F(s) - E(g((Y - s)/\delta))| \leq \frac{2\delta^{r+1}}{(r-1)!} \int_0^1 \int_t^1 (u-t)^{r-1} \cdot g(u) \, du \, dt \cdot \sup_{s \in [S_0-\delta_0,S_1+\delta]} |\rho^{(r)}(s)|.
\]
In particular, for $r = 3$,

$$\int_0^1 (u - t)^2 \cdot g(u) \, du = \frac{-1}{96} \cdot (t - 1)^4 \cdot (t^2 + 4t + 1),$$

and therefore

$$\|F - E(g((Y - \cdot) / \delta))\|_\infty \leq \frac{\delta^4}{280} \cdot \sup_{s \in [S_0 - d, S_1 + d]} |\rho^{(3)}(s)|.$$

### 2.2. Interpolation and Monotonicity Corrections.

In the sequel $| \cdot |_\infty$ denotes the $\ell_\infty$-norm on $\mathbb{R}^k$.

The approximation of $F$ on the interval $[S_0, S_1]$ is based on its approximation at finitely many points $S_0 \leq s_1 < \cdots < s_k \leq S_1$, followed by a suitable extension to $[S_0, S_1]$. For the extension we take a sequence of mappings $Q_r^k : \mathbb{R}^k \to C([S_0, S_1])$ with the following properties for some constant $c > 0$:

(E1) For all $k \in \mathbb{N}$ and $x \in \mathbb{R}^k$ the cost for computing $Q_r^k(x)$ is bounded by $c \cdot k$.

(E2) For all $k \in \mathbb{N}$ and $x, y \in \mathbb{R}^k$

$$\|Q_r^k(x) - Q_r^k(y)\|_\infty \leq c \cdot |x - y|_\infty.$$

(E3) For all $k \in \mathbb{N}$

$$\|F - Q_r^k(F(s_1), \ldots, F(s_k))\|_\infty \leq c \cdot k^{-(r+1)}.$$

These properties are easily achieved, e.g., by piecewise polynomial interpolation with degree $\max(r, 1)$ at equidistant points.

In terms of the spacing parameter $\tau$ of equidistant points, the interpolation error is of the order $\tau^{r+1}$. Since the smoothing error is of the order $\delta^{r+1}$ then to balance these errors one has to take $\tau$ and $\delta$ of the same order.

**Remark 3.** In the numerical experiments we will first consider the following simple cubic interpolant which is linear with respect to its inputs. Let $r = 3$, assume that $k = 3n + 1$ with $n \in \mathbb{N}$, and put

$$\tau = (S_1 - S_0)/n$$

as well as

$$s_j = S_0 + (j - 1) \cdot (S_1 - S_0)/(k - 1), \quad j = 1, \ldots, k.$$

Furthermore, let $Q_r^3$ denote the piecewise polynomial interpolation of degree three at four consecutive knots. The classical error estimate for polynomial interpolation yields

$$\|F - Q_r^3(F(s_1), \ldots, F(s_k))\|_\infty \leq \frac{\tau^4}{1944} \cdot \|\rho^{(3)}\|_\infty.$$

Furthermore, the corresponding Lipschitz constant is easily computed explicitly, giving

$$\|Q_r^3(x) - Q_r^3(y)\|_\infty \leq c \cdot |x - y|_\infty, \quad c = \frac{7 \cdot (2\sqrt{7} + 1)}{27} \approx 1.63.$$
The resulting vectors of data $y = (y_1, \ldots, y_k) \in \mathbb{R}^k$ generated by the multilevel construction are not necessarily non-decreasing. Even when they are, there is the possibility that a piecewise polynomial interpolant may not be non-decreasing. Therefore we employ a two stage post-processing for the resulting approximation as described in Remark 4.

**Remark 4.** For $y = (y_1, \ldots, y_k) \in \mathbb{R}^k$ we define $u_0 = 0$ and

$$u_j = \min(\max(y_j, u_{j-1}), 1)$$



to get a non-decreasing sequence $u = (u_1, \ldots, u_k) \in [0, 1]$. For symmetry reasons we also define $v = (v_1, \ldots, v_k) \in [0, 1]$ with

$$v_j = \max(\min(y_j, v_{j+1}), 0),$$

where $v_{k+1} = 1$. Observe that $y \mapsto (u + v)/2$ defines a Lipschitz continuous mapping with Lipschitz constant 1 w.r.t. $|\cdot|_\infty$. In the second stage of the post-processing the piecewise polynomial interpolant $\varphi$ of $(u + v)/2$, as described in Remark 3, is transformed into a non-decreasing function that coincides with $\varphi$ at the knots $s_j$. To this end we put

$$f(s) = \min\left(\max_{t \in [s_{j-1}, s_j]} \varphi(t), \varphi(s_j)\right)$$

and

$$h(s) = \max\left(\min_{t \in [s, s_{j-1}]} \varphi(t), \varphi(s_{j-1})\right)$$

for $s \in [s_{j-1}, s_j]$. Observe that $\varphi \mapsto (f + h)/2$ defines a Lipschitz continuous mapping with Lipschitz constant 1 w.r.t. $\|\cdot\|_\infty$.

Instead of the plain interpolation according to Remark 3, in the numerical experiments we now consider

$$Q_k^3(y) = (f + h)/2.$$ 

Clearly we have (E2) with $c$ given by (2). Furthermore, $u = v = y$ for $y = (F(s_1), \ldots, F(s_k))$ and

$$\max(\|F - f\|_\infty, \|F - h\|_\infty) \leq \|F - \varphi\|_\infty$$

for every distribution function $F$ and every $\varphi \in C([S_0, S_1])$. Consequently, (1) holds true, and in particular we have (E3). To actually compute $(f + h)/2$, which is a piecewise polynomial of degree three, one has to solve at most $2k$ polynomial equations of degree two or three, and therefore we also have (E1).

### 2.3. The MLMC Algorithm

Our multilevel Monte Carlo construction is based on a sequence $Y^{(\ell)}_{\ell \in \mathbb{N}_0}$ of random variables, defined on a common probability space together with $Y$. Assumptions on the cost for the simulation of the joint distribution of $Y^{(\ell)}$ and $Y^{(\ell-1)}$ and on the weak and strong convergence will be specified in Sections 2.4 and 3.1.

For notational convenience we put

$$g^{k, \delta}(t) = (g((t - s_1)/\delta), \ldots, g((t - s_k)/\delta)) \in \mathbb{R}^k, \quad t \in \mathbb{R}.$$
We choose \( L_0, L_1 \in \mathbb{N}_0 \) with \( L_0 \leq L_1 \) as the minimal and the maximal level, respectively, and we choose replication numbers \( N_\ell \in \mathbb{N} \) for all levels \( \ell = L_0, \ldots, L_1 \), as well as \( k \in \mathbb{N} \) and \( \delta \in [0, \delta_0] \). The corresponding MLMC algorithm for the approximation at the points \( s_j \) is defined by

\[
\mathcal{M}^{k,\delta,L_0,L_1}_{N_{L_0},\ldots,N_{L_1}} = \frac{1}{N_{L_0}} \sum_{i=1}^{N_{L_0}} g^{k,\delta}(Y_i^{(L_0)}) + \sum_{\ell=L_0+1}^{L_1} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} \left( g^{k,\delta}(Y_i^{(\ell)}) - g^{k,\delta}(Z_i^{(\ell)}) \right)
\]

with an independent family of \( \mathbb{R}^2 \)-valued random variables \((Y_i^{(\ell)}, Z_i^{(\ell)})\) for \( \ell = L_0, \ldots, L_1 \) and \( i = 1, \ldots, N_\ell \) such that equality in distribution holds for \((Y_i^{(\ell)}, Z_i^{(\ell)})\) and \((Y_i^{(\ell)}, Y_i^{(\ell-1)})\) if \( \ell > L_0 \) as well as for \( Y_i^{(L_0)} \) and \( Y_i^{(L_0)} \).

In the particular case \( L = L_0 = L_1 \), i.e., in the single-level case, we actually have a classical Monte Carlo algorithm, based on independent copies of \( Y^{(L)} \) only. In addition to

\[
\mathcal{S}^{k,\delta,L}_{N} = \mathcal{M}^{k,\delta,L,L}_{N} = \frac{1}{N} \sum_{i=1}^{N} g^{k,\delta}(Y_i^{(L)})
\]

with \( \delta > 0 \), we also consider the single-level algorithm without smoothing. Hence we put

\[
g^{k,0}(t) = (1_{-\infty,s_1]}(t), \ldots, 1_{-\infty,s_k]}(t)) \in \mathbb{R}^k, \quad t \in \mathbb{R},
\]

to obtain

\[
\mathcal{S}^{k,0,L}_{N} = \mathcal{M}^{k,0,L,L}_{N} = \frac{1}{N} \sum_{i=1}^{N} g^{k,0}(Y_i^{(L)})
\]

Observe that \( \mathcal{S}^{k,0,L}_{N} \) yields the values of the empirical distribution function, based on \( N \) independent copies of \( Y^{(L)} \), at the points \( s_j \).

We employ \( Q^r_k(\mathcal{M}) \) with

\[
\mathcal{M} = \mathcal{M}^{k,\delta,L_0,L_1}_{N_{L_0},\ldots,N_{L_1}}
\]

as a randomized algorithm for the approximation of \( F \) on \([S_0, S_1]\).

### 2.4. Cost Bounds.

In our analysis of the computational cost we assume the following for some constant \( c > 0 \):

(A2) There exists a constant \( M > 1 \) such that the simulation of the joint distribution of \( Y^{(\ell)} \) and \( Y^{(\ell-1)} \) is possible at cost at most \( c \cdot M^\ell \) for every \( \ell \in \mathbb{N} \).

Typically, \( M \) is a refinement factor, e.g., for the time-step of a numerical approximation scheme for a stochastic differential equation.

Together with the property (S1) for \( g \), the assumption (A2) yields the following upper bound. There exists a constant \( c > 0 \) such that, for all \( k, \delta, L_0, L_1, N_{L_0}, \ldots, N_{L_1} \),

\[
\text{cost}(Q^r_k(\mathcal{M})) \leq c \cdot \sum_{\ell=L_0}^{L_1} N_\ell \cdot (M^\ell + k)
\]
for the cost of $Q_{M}^{L}(\mathcal{M})$, see [8, Eqn. (2.16)]. In fact, for every replication on level $\ell$ the simulation cost is at most of the order $M^{\ell}$, while the cost to evaluate $g^{k,\delta}$ is of the order $k$.

The number of arithmetic operations that are needed additionally is of the order $\sum_{\ell=L_{0}+1}^{L_{1}} N_{\ell}$, plus an additional order $k$ for the interpolation.

As an extension to the analysis in [8], we derive an improved cost bound in the case of equidistant knots. Observe that every realization of $\mathcal{M}$ is of the form $\sum_{i=1}^{N} a_{i} g^{k,\delta}(t_{i})$, where

$$N = N_{L_{0}} + 2 \sum_{\ell=L_{0}+1}^{L_{1}} N_{\ell},$$

$$a = (a_{1}, \ldots, a_{N}) \in \mathbb{R}^{N}$$

with $|a_{i}| \in \{1/N_{L_{0}}, \ldots, 1/N_{L_{1}}\}$, and

$$t = (t_{1}, \ldots, t_{N}) \in \mathbb{R}^{N}$$

being a realization of $(Y_{1}^{(L_{0})}, \ldots, Z_{N_{L_{1}}}, Y_{N_{L_{1}}}^{(L_{1})})$. Taking into account that $g = 1$ on $]-\infty, -1]$ and $g = 0$ on $[1, \infty[$, the sum $\sum_{i=1}^{N} a_{i} g^{k,\delta}(t_{i})$ may be evaluated in the following, efficient way, if the knots $s_{j}$ are chosen equidistantly. Put

$$j^{*}(t) = \min\{j \in \{1, \ldots, k\} : s_{j} > t + \delta\}$$

for $t \in \mathbb{R}$ with $\min \emptyset = \infty$, and define $g_{1}^{k,\delta}(t) \in \mathbb{R}^{k}$ by

$$g_{1,j}^{k,\delta}(t) = \begin{cases} 1, & \text{if } j = j^{*}(t), \\ 0, & \text{otherwise}, \end{cases}$$

for $j = 1, \ldots, k$. Due to the uniform spacing of the knots, the cost to compute $j^{*}(t)$ is bounded by a constant, uniformly in $t$ and $k$. Hence we have a uniform cost bound of order $N$ to compute

$$g_{2}^{k,\delta}(a, t) = \sum_{i=1}^{N} a_{i} g_{1,i}^{k,\delta}(t_{i}) \in \mathbb{R}^{k}$$

for $N, k \in \mathbb{N}$ and $a, t \in \mathbb{R}^{N}$. Consider $\psi : \mathbb{R}^{k} \rightarrow \mathbb{R}^{k}$ given by $\psi(x) = (x_{1} + x_{2}, \ldots, \sum_{j=1}^{k} x_{j})$, which is sometimes called the scan function or the cumulative summation function. The vector $g_{3}^{k,\delta}(a, t) = \psi(g_{2}^{k,\delta}(a, t)) \in \mathbb{R}^{k}$ of successive partial sums of $g_{2}^{k,\delta}(a, t)$ may therefore be computed at a cost uniformly bounded by a multiple of $\max(N, k)$. Finally, let $g_{4}^{k,\delta}(t) \in \mathbb{R}^{k}$ be given by

$$g_{4,j}^{k,\delta}(t) = 1_{[t-\delta, t+\delta]}(s_{j}) \cdot g((t - s_{j})/\delta)$$

for $j = 1, \ldots, k$ and $t \in \mathbb{R}$. Due to the uniform spacing of the knots, $g_{4}^{k,\delta}(t)$ may be computed at a cost uniformly bounded by $\max(k \cdot \delta, 1)$ for $t \in \mathbb{R}$, $k \in \mathbb{N}$, and $\delta > 0$. Since

$$\sum_{i=1}^{N} a_{i} g_{4,i}^{k,\delta}(t_{i}) = g_{3}^{k,\delta}(a, t) + \sum_{i=1}^{N} a_{i} g_{4,i}^{k,\delta}(t_{i}),$$
the cost to compute this sum is uniformly bounded by \( k + N \cdot \max(k \cdot \delta, 1) \), up to a constant. Altogether this yields the cost bound

(3) \[
\text{cost} \left( Q^r_k(M) \right) \leq c \cdot \left( k + \sum_{\ell=L_0}^{L_1} N_\ell \cdot (M^\ell + k \cdot \delta) \right)
\]

with a constant \( c > 0 \) for all \( k, \delta, L_0, L_1, N_{L_0}, \ldots, N_{L_1} \). Typically \( N_{L_0} \cdot M^{L_0} \) dominates \( k \) and \( M^{L_0} \) dominates \( k \cdot \delta \), so that the upper bound is of the order \( \sum_{\ell=L_0}^{L_1} N_\ell \cdot M^\ell \) and neither smoothing nor interpolation affects the cost bound.

The adaptive MLMC algorithm that will be introduced in Section 4 involves, in particular, a variance estimation step. It is crucial that the cost for this step also stays within the cost bound (3).

2.5. Error Decomposition. Observe that \( M \) is square-integrable, since \( g \) is bounded, so that (E2) yields \( \|Q^r_k(M)\|_\infty^2 < \infty \). The error of \( Q^r_k(M) \) is defined by

(4) \[
\text{error}\left( Q^r_k(M) \right) = \left( \mathbb{E} \|F - Q^r_k(M)\|_\infty^2 \right)^{1/2}.
\]

The variance of any square-integrable \( \mathbb{R}^k \)-valued random variable \( M \) is defined by

\[
\text{Var}(M) = \mathbb{E} |M - \mathbb{E}(M)|_\infty^2,
\]

and

\[
\mathbb{E} |x - M|_\infty^2 \leq 2 \cdot (|x - \mathbb{E}(M)|_\infty^2 + \text{Var}(M))
\]

for \( x \in \mathbb{R}^k \).

For \( \delta > 0 \) the error of \( Q^r_k(M) \) may be decomposed into the interpolation error

\[
e_1 = \|F - Q^r_k(F(s_1), \ldots, F(s_k))\|_\infty,
\]

the smoothing error

\[
e_2 = \left( |(F(s_1), \ldots, F(s_k)) - \mathbb{E}(g^{k,\delta}(Y))|_\infty \right),
\]

and the bias

\[
e_3 = \left| \mathbb{E}(g^{k,\delta}(Y)) - \mathbb{E}(g^{k,\delta}(Y^{(L_1)})) \right|_\infty
\]

as well as the variance

\[
e_4 = \text{Var}(M)
\]

of \( M \). In fact, we have

\[
\text{error}(Q^r_k(M)) \leq e_1 + \left( \mathbb{E} \|Q^r_k((F(s_1), \ldots, F(s_k)) - M)\|_\infty^2 \right)^{1/2}
\]

\[
\leq e_1 + \|Q^r_k\| \cdot \left( \mathbb{E} |(F(s_1), \ldots, F(s_k)) - M|_\infty^2 \right)^{1/2},
\]

where \( \|Q^r_k\| \) denotes the Lipschitz constant of \( Q^r_k \). Since

\[
\left( \mathbb{E} |(F(s_1), \ldots, F(s_k)) - M|_\infty^2 \right)^{1/2} \leq e_2 + \left( \mathbb{E} |\mathbb{E}(g^{k,\delta}(Y)) - M|_\infty^2 \right)^{1/2}
\]

\[
\leq e_2 + \sqrt{2} \cdot (e_3^2 + e_4^2)^{1/2},
\]
we obtain
\begin{equation}
\text{error}(Q_k^r(\mathcal{M})) \leq e_1 + \|Q_k^r\| \cdot \left( e_2 + \sqrt{2} \cdot (e_3^2 + e_4^{1/2}) \right).
\end{equation}

If we do not apply smoothing, i.e., for $\delta = 0$, we formally have $e_2 = 0$, which leads to
\begin{equation}
\text{error}(Q_k^r(\mathcal{M})) \leq e_1 + \sqrt{2} \cdot \|Q_k^r\| \cdot \left( \|F(s_1), \ldots, F(s_k)\|_\infty^2 + e_4^{1/2} \right).
\end{equation}

The Bienaymé formula for real-valued random variables turns into the inequality
\begin{equation}
\text{Var}(\mathcal{M}) \leq c(k) \cdot \sum_{i=1}^n \text{Var}(\mathcal{M}_i),
\end{equation}
if $\mathcal{M} = \sum_{i=1}^n \mathcal{M}_i$ with independent square-integrable random variables $\mathcal{M}_i$ taking values in $\mathbb{R}^k$. Here $c(k)$ only depends on the dimension $k$, and there exist $c_1, c_2 > 0$ such that
\begin{equation}
c_1 \cdot \log(k + 1) \leq c(k) \leq c_2 \cdot \log(k + 1)
\end{equation}
for every $k \in \mathbb{N}$. In the context of multilevel algorithms this is exploited in [9] for the first time. We refer to (48) and (50) in the Supplementary Materials for an explicit value of $c(k)$.

Consequently,
\begin{equation}
\text{Var}(\mathcal{M}) \leq c(k) \cdot \left( \frac{\text{Var}(g^{k,\delta}(Y^{L_0}))}{N_{L_0}} + \sum_{\ell = L_0 + 1}^{L_1} \frac{\text{Var}(g^{k,\delta}(Y^{(\ell)})) - g^{k,\delta}(Y^{(\ell-1)}))}{N_{\ell}} \right)
\end{equation}
for the variance of the multilevel algorithm $\mathcal{M}$.

3. Asymptotic Analysis of the MLMC Algorithm. Using the improved cost bound (3) we derive an improved version of [8, Thm. 2.6], which gives an asymptotic upper bound of the cost of the multilevel algorithm in terms of its error.

3.1. Assumptions on Weak and Strong Convergence. In our analysis of the bias and the variance of the multilevel algorithm $\mathcal{M}$ we assume that the following properties hold for some constant $c > 0$ with $M$ according to (A2):

(A3) There exist constants $\alpha_1 \geq 0$, $\alpha_2 > 0$, and $\alpha_2 \geq \alpha_3 \geq 0$ such that the weak error estimate
\begin{equation}
\sup_{s \in [S_0, S_1]} \left| \mathbb{E}\left( g((Y - s)/\delta) - g((Y^{(\ell)} - s)/\delta) \right) \right| \leq c \cdot \min\left( \delta^{-\alpha_1} \cdot M^{-\ell \cdot \alpha_2}, M^{-\ell \cdot \alpha_3} \right)
\end{equation}
holds for all $\delta \in [0, \delta_0]$ and $\ell \in \mathbb{N}_0$.

(A4) There exist constants $\beta_4 \geq 0$ and $\beta_5 > 0$ such that the strong error estimate
\begin{equation}
\mathbb{E} \min((Y - Y^{(\ell)})^2/\delta^2, 1) \leq c \cdot \delta^{-\beta_4} \cdot M^{-\ell \cdot \beta_5}
\end{equation}
holds for all $\delta \in [0, \delta_0]$ and $\ell \in \mathbb{N}_0$.

Assumption (A4) and the Lipschitz continuity and boundedness of $g$ immediately yield the following fact, see [8, Lemma 2.4].
Lemma 2. There exists a constant $c > 0$ such that
\[ E \sup_{s \in [S_0, S_1]} \left( g((Y - s)/\delta) - g((Y^{(\ell)} - s)/\delta) \right)^2 \leq c \cdot \min(\delta^{-\beta_4} \cdot M^{-\ell \beta_5}, 1) \]
holds for all $\delta \in [0, \delta_0]$ and $\ell \in \mathbb{N}_0$.

Remark 5. For the analysis of the single-level algorithm $S^k_{N, L}$, i.e., for $L = L_0 = L_1$, it suffices to assume that the simulation of the distribution of $Y^{(\ell)}$ is possible at cost at most $c \cdot M^\ell$ for every $\ell \in \mathbb{N}_0$, cf. (A2). Furthermore, there is no need for a strong error estimate like (A4), and if we do not employ smoothing, then (A3) may be replaced by the following assumption. There exist a constant $\alpha > 0$ such that the weak error estimate
\[ \sup_{s \in [S_0, S_1]} \left| E \left( 1_{]-\infty,s]}(Y) - 1_{]-\infty,s]}(Y^{(\ell)}) \right) \right| \leq c \cdot M^{-\ell \alpha} \]
holds for all $\ell \in \mathbb{N}_0$. It turns out that the analysis of single-level algorithms $S^k_{N, 0, L}$ without smoothing is formally reduced to the case $\delta > 0$ if we take
\[ \alpha_1 = 0, \quad \alpha_2 = \alpha, \quad \alpha_3 = \alpha. \]

3.2. Main Result. We say that a sequence of randomized algorithms $A_n$ converges with order $(\gamma, \eta) \in \mathbb{R} \times \mathbb{R}$ if $\lim_{n \to \infty} \text{error}(A_n) = 0$ and if there exists a constant $c > 0$ such that
\[ \text{cost}(A_n) \leq c \cdot (\text{error}(A_n))^{\gamma} \cdot (-\log \text{error}(A_n))^\eta. \]
Moreover, we put
\[ q = \min \left( \frac{r + 1 + \alpha_1}{\alpha_2}, \frac{r + 1}{\alpha_3} \right). \]

Theorem 3. Assume that the cost bound (3) is satisfied. The following order, with $\eta = 1$, is achieved by algorithms $Q^k_r(M^{k, \delta}_{N_{L_0}, \ldots, N_{L_1}})$ with suitably chosen parameters:
\begin{align*}
q \leq \beta_4 / \beta_5 & \quad \Rightarrow \quad \gamma = 2 + \frac{q}{r + 1}, \\
q > \beta_4 / \beta_5 \land \beta_5 > 1 & \quad \Rightarrow \quad \gamma = 2 + \frac{\beta_4 / \beta_5}{r + 1}, \\
q > \beta_4 / \beta_5 \land \beta_5 < 1 & \quad \Rightarrow \quad \gamma = 2 + \frac{\beta_4 + (1 - \beta_5) \cdot q}{r + 1}.
\end{align*}
Moreover, with $\eta = 3$,
\[ q > \beta_4 \land \beta_5 = 1 \quad \Rightarrow \quad \gamma = 2 + \frac{\beta_4}{r + 1}. \]

The proof of this result, which also includes the choice of the parameters of the multilevel algorithm, follows the one presented in [8] and can be seen in Section 6 in the Supplementary Materials.

Theorem 3 improves [8, Thm. 2.6], if (3) is satisfied. This improved cost bound also leads to improved versions of [8, Thm. 3.3, Thm. 4.3], which deal with the approximation of densities on compact intervals and distribution functions at a single point, respectively.
Example 1. Suppose that \( Y = \varphi(X) \), where \( X \) is a sufficiently smooth Gaussian process (or random field) on a compact domain and \( \varphi \) is a Lipschitz continuous real-valued functional with respect to the supremum norm, say, the supremum norm itself. Using appropriate approximations \( X^{(\ell)} \) of \( X \) and putting \( Y^{(\ell)} = \varphi(X^{(\ell)}) \) the estimate (5.1) in [8] is satisfied with a large value of \( \beta \) due to the smoothness of \( X \). It what follows, \( \varepsilon > 0 \) may be chosen arbitrarily small.

We obtain \( \beta_4 = 2 \) and \( \beta_5 = \beta \) as well as \( \alpha_1 = \varepsilon \), \( \alpha_2 = \beta/2 \), and \( \alpha_3 = \beta/2 - \varepsilon \), see [8, Sec. 5]. This leads to \( q = 2(r+1)/\beta + \varepsilon \), while \( \beta_4/\beta_5 = 2/\beta \). Hence (11) yields

\[
\gamma = 2 + \frac{2}{\beta \cdot (r+1)}.
\]

Since \( \max(1, \beta_4/\beta_5) = 1 \), the case (2.10) in [8, Thm. 2.6] only yields

\[
\gamma = 2 + \frac{1}{r + 1}.
\]

Remark 6. In the limit \( r \to \infty \) we obtain \( \gamma = 2 + \max(1 - \beta_5,0)/\alpha_2 \) in Theorem 3, i.e., we recover the order of convergence for the standard MLMC application, namely, the approximation of expectations.

4. Sketch of the Adaptive MLMC Algorithm. We present an MLMC algorithm, which assumes that the parameters for the weak and the strong convergence are unknown and have to be substituted by suitable estimates during the algorithm run. Based on these estimates we determine the replication numbers, the range of levels, the smoothing parameter, and the number of interpolation points adaptively. For simplicity, the minimal level is chosen as \( L_0 = 0 \), and we use \( L = L_1 \) to denote the maximal level.

We do not address the issue how to detect the smoothness \( r \) of the density \( \rho \) from simulation data, and how to choose an interpolation scheme that exploits the smoothness in an optimal way. Instead, we assume a known \( r \geq 1 \), and we take a function \( g \) with the properties (S1)–(S4). Furthermore, we use piecewise polynomial interpolation of degree \( r \) at equidistant points. The number \( k_n \) of interpolation points is given by

\[
k_n = \left\lceil \frac{2^n}{r} \right\rceil \cdot r + 1,
\]

where \( n \in \mathbb{N} \) with \( 2^{n+1} > r \), and the points themselves are given by

\[
s_j = s_{j,n} = S_0 + (j-1) \cdot (S_1 - S_0)/(k_n - 1)
\]

for \( j = 1, \ldots, k_n \). We use

\[
Q_n = Q_{k_n}^r
\]

to denote the piecewise polynomial interpolation of degree \( r \) at these points, together with the monotonicity corrections as described in Remark 4, and we put

\[
F_n = (F(s_1), \ldots, F(s_{k_n})).
\]

Obviously, (E1) and (E2) are satisfied, and the Lipschitz constant \( \|Q_n\| \) of \( Q_n \) does not depend on \( n \). In the numerical experiments we take \( r = 3 \) and \( g \) according to Remark 1.
The smoothing parameter $\delta$ is chosen from the discrete set of values
$$\delta_m = (S_1 - S_0)/2^m,$$
where $m \in \mathbb{N}$. With a slight abuse of notation we put
$$g^{n,m} = g^{k,m}.$$ For a given $\epsilon > 0$ we wish to select the parameters of the MLMC algorithm such that its error is at most $\epsilon$ and its cost is as small as possible. Our approach to the selection of the replication numbers and of the maximal level follows [7], who studies MLMC algorithms with values in $\mathbb{R}$. The latter is adapted to the present case of vector-valued algorithms and extended to also handle the selection of the smoothing parameter and the number of interpolation points.

In order to achieve
$$\text{error}(Q_n(\mathcal{M})) \leq \epsilon$$
we have to assign certain proportions of $\epsilon$ to the four sources of the error, which have been introduced in Section 2.5. The analysis presented in Theorem 3 yields an asymptotically optimal choice of the parameters of the multilevel algorithm, in which case the cost is asymptotically bounded by $\sum_{\ell=0}^{L} N_\ell \cdot M^\ell$, see (43), and $k \cdot \delta$ is of the order one, see (40) and (41). This suggests assigning only a small part of $\epsilon$ to the interpolation error $e_1$ and to the smoothing error $e_2$. While $k$ only has an impact on the error and cost of $\mathcal{M}$ via a factor of order log($k$), a small value of $\delta$ might harm the decay of the bias and the variances, see (39). Accordingly, we aim at $e_1$ being smaller than $e_2$. Specifically we wish to choose the parameters of our algorithm such that

$$e_1 \leq \|Q_n\| \cdot \epsilon_\ast, \quad e_2 \leq 4 \cdot \epsilon_\ast, \quad e_3 \leq 16 \cdot \epsilon_\ast, \quad e_4 \leq 256 \cdot \epsilon_\ast^2,$$

where
$$\epsilon_\ast = \frac{\epsilon}{37 \cdot \|Q_n\|}.$$ By (5) we get (14), if (15) holds true. Recall that Remark 3 provides the explicit value $\|Q_n\| \approx 1.63$ in the case $r = 3$.

It is possible that a different assignment of $\epsilon$ to the four sources of the error may lead to better results, numerically. Concerning the upper bounds (3) and (39) of the cost and the error, however, an improvement is possible at most by a multiplicative constant, which does not depend on $\epsilon$. In the standard setting of MLMC to compute expectations, this assignment problem is further analyzed and a new algorithm is constructed in [4].

The present stage of the MLMC algorithm is defined, in particular, by the parameter values $n$ and $m$ for interpolation and smoothing, and the values of the maximal level $L$ and of the replication numbers $N_\ell$. We always have $L \geq 2$ and $N_\ell \geq 100$ for $\ell = 0, \ldots, L$. By the latter we ensure a reasonable accuracy in certain estimates to be introduced below. We use $y_{i,0}$ to denote samples of the random variable $Y^{(0)}$ and $(y_{i,\ell}, y_{i,\ell-1})$ to denote samples of the random vector $(Y^{(\ell)}, Y^{(\ell-1)})$ for $\ell = 1, \ldots, L$. During the computation the values of $n$, $m$, $L$, and $N_\ell$ are updated and all samples are stored.
4.1. Assumptions. For sequences of real numbers \( u_\ell \) and positive real numbers \( w_\ell \) we write \( u_\ell \approx w_\ell \), if
\[
\lim_{\ell \to \infty} \frac{u_\ell}{w_\ell} = 1,
\]
and \( u_\ell \lesssim w_\ell \), if
\[
\limsup_{\ell \to \infty} \frac{u_\ell}{w_\ell} \leq 1.
\]
Assumption (A2) on the computational cost of simulating the joint distribution of \( Y(\ell) \) and \( Y(\ell-1) \) is assumed to hold. Assumption (A3) on the weak convergence, which is used in our asymptotic analysis, is replaced as follows. For every \( n \) and \( m \), we suppose that there exists \( c, \alpha > 0 \) such that
\[
|E(g_{n,m}(Y)) - E(g_{n,m}(Y))|_\infty \approx c \cdot M^{-\ell-\alpha}.
\]
Furthermore, we assume that
\[
\lim_{\ell \to \infty} E(g_{n,m}(Y)) = E(g_{n,m}(Y)).
\]
This yields the asymptotic upper bound
\[
|E(g_{n,m}(Y)) - E(g_{n,m}(Y))|_\infty \lesssim (M^\alpha - 1) \cdot |E(g_{n,m}(Y)) - E(g_{n,m}(Y))|_\infty
\]
for the bias at level \( \ell \). In contrast to our asymptotic analysis, which makes use of (A4), the construction of the adaptive MLMC algorithm is not based on any assumption on the strong convergence.

Put
\[
C_r = 2^{r+1}.
\]
For every \( n \), we suppose that there exists \( c > 0 \) such that
\[
|E(g_{n,m}(Y)) - E(g_{n,m-1}(Y))|_\infty \approx c \cdot \delta_m^{r+1}.
\]
This yields the asymptotic upper bound
\[
|F_n - E(g_{n,m}(Y))|_\infty \lesssim (C_r - 1)^{-1} \cdot |E(g_{n,m}(Y)) - E(g_{n,m-1}(Y))|_\infty
\]
for the smoothing error with parameter \( \delta_m \).

We suppose that there exists \( c > 0 \) such that
\[
\|Q_n(F_n) - Q_n(F_{n-1})\|_\infty \approx c \cdot C_r^{-n}.
\]
This yields the asymptotic upper bound
\[
\|F - Q_n(F_n)\|_\infty \lesssim (C_r - 1)^{-1} \cdot \|Q_n(F_n) - Q_n(F_{n-1})\|_\infty
\]
for the interpolation error with \( k_n \) equidistant points.

Formally, (A1) is not assumed to hold for the chosen value of \( r \), but of course the convergence order \( r + 1 \) in the assumptions (19) and (21) corresponds to \( \rho \) being at least \( r \) times continuously differentiable.
Remark 7. Let $[z]_i$ denote the $i$-th component of $z \in \mathbb{R}^k$. In the context of SDEs weak error results of the form

$$[E(g^{n,m}(Y)) - E(g^{n,m}(Y^{(l)}))]_i \approx c_i \cdot M^{-\ell \cdot \alpha}$$

with $c_i \neq 0$ and $\alpha > 0$ are known to hold for fixed $n$ and $m$ and all $i = 1, \ldots, k_n$ under suitable assumptions. Note that (23) implies (17) as well as (16) with

$$c = (M^n - 1) \cdot ||(c_1, \ldots, c_{k_n})||_{\infty}.$$

Suppose that (A1) is satisfied for the chosen value of $r$ and that $\rho^{(r)}(s_j) \neq 0$ for $j = 1, \ldots, k_n$ as well as

$$\int_{-1}^{1} u^r \cdot (1_{-\infty,0}(u) - g(u)) \, du \neq 0.$$

From the proof of Lemma 1 we get

$$[F_n - E(g^{n,m}(Y))]_i \approx c_i \cdot \delta_m^{r+1}$$

with $c_i \neq 0$ for fixed $n$ and all $i = 1, \ldots, k_n$. Note that (24) implies (19) with

$$c = (C_r - 1) \cdot ||(c_1, \ldots, c_{k_n})||_{\infty}.$$

Roughly speaking, our MLMC algorithm is based on the following heuristics: the asymptotic bounds (18), (20), and (22) are replaced by the corresponding inequalities, and estimators for means and variances are assumed to be nearly exact.

4.2. Variance Estimation and Selection of the Replication Numbers. The innermost loop of the algorithm performs, in particular, a variance estimation with fixed parameters $n$, $m$, and $L$. It is important for the overall performance of the adaptive algorithm that the cost for the variance estimation is of the order $O(k_n + c(N_0, \ldots, N_L))$, where

$$c(n_0, \ldots, n_L) = \sum_{\ell=0}^{L} n_\ell \cdot (M^\ell + k_n \cdot \delta_m),$$

cf. (3). We stress that there is no such constraint needed in the standard MLMC application, which only involves expectations and variances of real-valued random variables.

At first we estimate the expectation and the variance of the random vectors $g^{n,m}(Y^{(0)})$ and $g^{n,m}(Y^{(\ell)}) - g^{n,m}(Y^{(\ell-1)})$ for $\ell = 1, \ldots, L$. To estimate the expectations we employ

$$\hat{b}_0 = \frac{1}{N_0} \cdot \sum_{i=1}^{N_0} g^{n,m}(y_{i,0})$$

and

$$\hat{b}_\ell = \frac{1}{N_\ell} \cdot \sum_{i=1}^{N_\ell} (g^{n,m}(y_{i,\ell}) - g^{n,m}(y_{i,\ell-1})).$$
As we have shown in Section 2.4, the total cost for this step does not exceed the cost bound \( O(k_n + c(N_0, \ldots, N_L)) \). To estimate the variances we cannot afford to use the whole data set. Instead, we only use
\[
N'_\ell = \min(N_\ell, \max(\zeta, N_\ell \cdot M^\ell)/k_n)
\]
samples on level \( \ell \), where
\[
\zeta = \frac{1}{L} \cdot (k_n + c(N_0, \ldots, N_L)).
\]
Accordingly, the variances are estimated by
\[
(26) \hat{v}_0 = \frac{1}{N'_0} \cdot \sum_{i=1}^{N'_0} |g^{n,m}(y_{i,0}) - \hat{b}_0|_\infty^2
\]
and
\[
(27) \hat{v}_\ell = \frac{1}{N'_\ell} \cdot \sum_{i=1}^{N'_\ell} |g^{n,m}(y_{i,\ell}) - g^{n,m}(y_{i,\ell-1}) - \hat{b}_\ell|_\infty^2.
\]
Since \( \hat{v}_\ell \) can be computed at cost \( O(\max(\zeta, N_\ell \cdot M^\ell)) \) for \( \ell = 0, \ldots, L \), the total cost for this step also stays within the cost bound \( O(k_n + c(N_0, \ldots, N_L)) \). Obviously \( \zeta \geq N_0/L \), and \( N_0/L \) is of the order \( \epsilon^{-1} \), while \( k_n \) is of the order \( \epsilon^{-1/(r+1)} \), cf. (41), (42), and (44). Hence \( \zeta/k_n \) tends to infinity as \( \epsilon \to 0 \). On the other hand, \( M^L \) is of the order \( \epsilon^{-q/(r+1)} \), and therefore \( M^L/k_n \) tends to infinity as \( \epsilon \to 0 \) if \( q > 1 \).

With \( c(k) \) given by (50) from the Supplementary Materials,
\[
\hat{v}(n_0, \ldots, n_L) = c(k_n) \cdot \sum_{\ell=0}^{L} \frac{1}{n_\ell} \cdot \hat{v}_\ell
\]
serves as an empirical upper bound for the variance of the MLMC algorithm with any choice of replication numbers \( n_\ell \). If, for the present choice of replication numbers, this bound is too large compared to the upper bound for \( \text{Var}(\mathcal{M}) \) in (15), i.e., if the variance constraint
\[
(28) \hat{v}(N_0, \ldots, N_L) \leq 256 \cdot \epsilon^2
\]
is violated, we determine new values of \( N_0, \ldots, N_L \) by minimizing \( c(n_0, \ldots, n_L) \) subject to the constraint \( \hat{v}(n_0, \ldots, n_L) \leq 256 \cdot \epsilon^2 \). This leads to
\[
(29) n_\ell = \frac{\hat{v}^{1/2}_{\ell}}{(M^\ell + k_n \cdot \delta_m)^{1/2}} \cdot \sum_{\ell=0}^{L} \left( \hat{v}_{\ell} \cdot (M^\ell + k_n \cdot \delta_m) \right)^{1/2} \cdot c(k_n) \cdot 256 \cdot \epsilon^{-2},
\]
and extra samples of \( Y^{(0)} \) and \( (Y^{(\ell)}, Y^{(\ell-1)}) \) have to be generated accordingly. Note that the updated estimates for the expectations and variances can be computed within the updated cost bound.
4.3. Bias Estimation and Selection of the Maximal Level. For fixed \( n \) and \( m \), we wish to determine the smallest value of \( L \) such that
\[
\left| E(g^{n,m}(Y^{(L)})) - E(g^{n,m}(Y^{(L-1)})) \right|_\infty \leq 16 \cdot (M^a - 1) \cdot \epsilon_*
\]
is satisfied, which corresponds to the upper bound for \( e_3 \) in (15) together with (18). Initially we try \( L = 2 \).

For \( \left| E(g^{n,m}(Y^{(\ell)})) - E(g^{n,m}(Y^{(\ell-1)})) \right|_\infty \) the estimate \( |\hat{b}_\ell|_\infty \) is available on the levels \( \ell = 1, \ldots, L \), see (25). To ensure a reasonable accuracy in these estimates we only consider those levels, where the replication number \( N_\ell \) exceeds a certain threshold, and we let \( L \) denote the corresponding subset of \( \{1, \ldots, L\} \); in the numerical experiments we choose \( 10^4 \) as the threshold value. We estimate \( \alpha \) and \( c \) in (16) by a least-squares fit, i.e., we take \( \hat{\alpha} \) and \( \hat{c} \) to minimize
\[
(\alpha, c) \mapsto \sum_{\ell \in L} \left( \log |\hat{b}_\ell|_\infty + \ell \cdot \alpha \log M + \log c \right)^2.
\]

While the value of \( \hat{c} \) is irrelevant, an upper bound for the norm of \( E(g^{n,m}(Y^{(L)})) - E(g^{n,m}(Y^{(L-1)})) \) is given by \( |\hat{b}_L|_\infty \), or, more generally, by \( M^{(\ell-L)\hat{\alpha}} \cdot |\hat{b}_\ell|_\infty \) with \( \ell \leq L \). Hence we put
\[
\hat{B}_2 = \max(|\hat{b}_2|_\infty, |\hat{b}_1|_\infty/M^{\hat{\alpha}})
\]
for \( L = 2 \) and
\[
\hat{B}_L = \max(|\hat{b}_L|_\infty, |\hat{b}_{L-1}|_\infty/M^{\hat{\alpha}}, |\hat{b}_{L-2}|_\infty/M^{2\hat{\alpha}})
\]
for \( L \geq 3 \).

The present value of \( L \) is accepted as the maximal level, if the bias constraint
\[
\hat{B}_L \leq 16 \cdot (M^{\hat{\alpha}} - 1) \cdot \epsilon_*
\]
is satisfied. Otherwise, \( L \) is increased by one, and new samples will be generated. As already mentioned, we take \( N_L = 100 \) as a default value.

In our simulations we will ignore the cost for the performing the regression (30), as its cost is absolutely negligible, compared to number of other operations, performed by the algorithm.

4.4. Selection of the Smoothing Parameter. Our approach to choose the smoothing parameter closely follows the approach for the selection of the maximal level, as we consider two values, \( \delta_m \) and \( \delta_{m-1} \), of the smoothing parameter at the same time.

The parameter \( n \), which determines the number \( k_n \) of interpolation points, is fixed. We wish to determine the smallest value of \( m \), i.e., the largest value of \( \delta_m \), such that
\[
\left| E(g^{n,m}(Y)) - E(g^{n,m-1}(Y)) \right|_\infty \leq 4 \cdot (C_r - 1) \cdot \epsilon_*
\]
is satisfied, which corresponds to the upper bound for \( e_2 \) in (15) together with (20). Initially we try \( m = 2 \). Actually, \( Y \) is approximated by \( Y^{(L)} \), and an upper bound for \( \left| E(g^{n,m}(Y^{(L)})) - E(g^{n,m-1}(Y^{(L)})) \right|_\infty \) is given by
\[
\hat{s} = \left| \frac{1}{N_L} \sum_{i=1}^{N_L} (g^{n,m}(y_i,L) - g^{n,m-1}(y_i,L)) \right|_\infty.
\]
The present value of $\delta_m$ is accepted as the smoothing parameter, if the smoothing constraint
\begin{equation}
\hat{s} \leq 4 \cdot (C_r - 1) \cdot \epsilon_*
\end{equation}
is satisfied. Otherwise, $m$ is increased by one. Due to the update for the smoothing parameter $\delta$, we need to update all the estimates for the bias and the variance, which increases the overall cost of the algorithm by $O(k_n + \max(k_n \cdot \delta_m, 1) \cdot \sum_{\ell=0}^{L} N_\ell)$.

Alternatively, the explicit error bound from Remark 2 may be used to select the smoothing parameter, if an upper bound or reliable estimate for $|\rho^{(3)}|$ is available.

4.5. Selection of the Number of Interpolation Points. The procedure to choose the number $k_n$ of interpolation points mimics our approach to choose the smoothing parameter, i.e., we consider two interpolation schemes, $Q_n$ and $Q_{n-1}$, at the same time.

We wish to determine the smallest value of $n$, i.e., the smallest number $k_n$ of interpolation points, such that
\begin{equation}
\|Q_n(F_n) - Q_{n-1}(F_{n-1})\|_\infty \leq \|Q_n\| \cdot (C_r - 1) \cdot \epsilon_*
\end{equation}
which corresponds to the upper bound for $c_1$ in (15) together with (22). Initially we try $n = 2$. Actually, $F_n$ and $F_{n-1}$ are approximated by $\mathbb{E}(g^{n,m}(Y^{(L)}))$ and $\mathbb{E}(g^{n-1,m}(Y^{(L)}))$, respectively, and an upper bound for the norm of $Q_n(\mathbb{E}(g^{n,m}(Y^{(L)})) - Q_{n-1}(\mathbb{E}(g^{n-1,m}(Y^{(L)}))))$ is given by
\begin{equation}
\hat{i} = \|Q_n \left( \frac{1}{N_L} \sum_{i=1}^{N_L} g^{n,m}(y_i,L) \right) - Q_{n-1} \left( \frac{1}{N_L} \sum_{i=1}^{N_L} g^{n-1,m}(y_i,L) \right) \|_\infty.
\end{equation}
The present value $k_n$ is accepted as the number of interpolation points, if the interpolation constraint
\begin{equation}
\hat{i} \leq \|Q_n\| \cdot (C_r - 1) \cdot \epsilon_*
\end{equation}
is satisfied. Otherwise, $n$ is increased by one. Again, as in Section 4.4, we need to include the cost for evaluating the estimator at new points, and the added cost is of order $O(k_n + \max(k_n \cdot \delta_m, 1) \cdot \sum_{\ell=0}^{L} N_\ell)$.

Alternatively, the explicit error bound from Remark 3 may be used to select the number of interpolation points, if an upper bound or reliable estimate for $|\rho^{(3)}|$ is available.

4.6. The Algorithm. The desired accuracy $\epsilon$ is the input to our MLMC algorithm.

\begin{verbatim}
n = 1;
m = 2;
L = 2;
N_0 = N_1 = N_2 = 10^2;
Generate these numbers of samples of $Y^{(0)}$ and $(Y^{(\ell)}, Y^{(\ell-1)})$ for $\ell = 1, 2$;
Compute $\hat{v}_0, \hat{v}_1, \hat{v}_2$, see (26) and (27);
repeat  /* interpolation */
n = n + 1;
m = m - 1;
\end{verbatim}
repeat /* smoothing */
  \( m = m + 1; \)
  \( \text{newlevel} = \text{false}; \)
repeat /* bias */
  if newlevel then
    \( L = L + 1; \)
    \( N_L = 100; \)
    Generate this number of samples of \((Y^{(L)}, Y^{(L-1)})\);
    Compute \( \hat{v}_L \), see (27);
  endif;
repeat
  Compute \( n_0, \ldots, n_L \), see (29);
  \( N_\ell = \max(N_\ell, n_\ell) \) for \( \ell = 0, \ldots, L \);
  Generate extra samples of \( Y^{(0)} \) and \((Y^{(\ell)}, Y^{(\ell-1)})\) for \( \ell = 1, \ldots, L \)
  as needed;
  Compute \( \hat{v}_0, \ldots, \hat{v}_L \), see (26) and (27);
until the variance constraint (28) is satisfied;
Compute \( \hat{\alpha} \), see (30), and \( \hat{B}_L \), see (31) and (32);
\( \text{newlevel} = \text{true}; \)
until the bias constraint (33) is satisfied;
Compute \( \hat{s} \), see (34);
until the smoothing constraint (35) is satisfied;
Compute \( \hat{i} \), see (36);
Compute \( Q_n(M^{k_n, \delta_m, 0, L}) \);

We comment on the cost for the individual steps of the algorithm and their contributions to
the overall cost. By assumption (A2), samples of \( Y^{(0)} \) or \((Y^{(\ell)}, Y^{(\ell-1)})\) can be generated at cost \( O(1) \) or \( O(M^\ell) \), respectively. For the present values of \( L, n, m, \) and \( N_0, \ldots, N_L \) the variance
estimates \( \hat{v}_0, \ldots, \hat{v}_L \) can be compute at cost \( O(k_n + c(N_0, \ldots, N_L)) \), see Section 4.2. Moreover,
these two steps are the dominating ones, i.e., the cost for all other steps of the algorithm is
negligible. Actually, the whole bias loop with terminal values \( L \) and \( N_0, \ldots, N_L \) can be
executed at cost \( O(k_n + c(N_0, \ldots, N_L)) \), see Section 4.2. Summing up these quantities over
all iterations of the interpolation and the smoothing loops yields a bound for the overall cost
of the algorithm including an additional cost for the updating the smoothing coefficient, see
Section 4.4, and number of interpolation points, see Section 4.5. In the numerical experiments,
which are presented in the following section, the constant in the \( O \)-notation is taken to be
one.

5. Numerical Experiments. In this section we will apply our adaptive general approach
for approximating the distribution function, based on the multilevel Monte Carlo approach,
in the context of stochastic differential equations. We would like to point at the fact, that all
the previous presentation does not assume in any way that we work in the SDE context.

We consider three benchmark problems for a simple, scalar SDE, where the solutions are
known analytically. Our numerical experiments show the computational gain in terms of upper bounds, achieved by the adaptive multilevel Monte Carlo approach with smoothing in comparison to a non-adaptive single-level Monte Carlo approach without smoothing. Furthermore, we compare the error of the multilevel algorithm with the accuracy demand $\epsilon$, which serves as an input to the algorithm.

Consider a geometric Brownian motion $X$, given by

$$dX_t = \mu \cdot X_t \, dt + \sigma \cdot X_t \, dW_t, \quad t \in [0, T],$$

$$X_0 = 1,$$

where $W$ denotes a scalar Brownian motion. For the approximation of $X$ we use the Milstein scheme with equidistant time-steps $h_\ell = M^{-\ell} T$ with $M = 2$ and with piecewise linear interpolation between the interpolation points.

Given $\epsilon$, we use the algorithm from Section 4.6, which estimates all the necessary parameters on the fly, so no prior knowledge of the convergence properties of the discretization scheme is needed. The cost of an individual run of the algorithm is calculated as described in Section 4.6 and includes path generation and variance and bias estimation (Sections 4.2 and 4.3), functional evaluations due to the updates of the smoothing coefficients (Section 4.4) and interpolation points (Section 4.5). The only costs we do not include, since they are negligible, are the costs for the regression (30) and the monotonicity corrections (Remark 4).

The cost as well as the error, i.e., the supremum norm distance between the output and the true distribution function $F$, for an individual run of the adaptive multilevel algorithm are random quantities, which depend on $\epsilon$. By taking expectations we get two deterministic quantities that characterize the performance of the multilevel algorithm. More precisely, we consider the root mean squared error, cf. (4), which will be denoted by $\text{error}_{\text{ML}}(\epsilon)$, and the expected cost, which will be denoted by $\text{cost}_{\text{ML}}(\epsilon)$.

Since $\text{error}_{\text{ML}}(\epsilon)$ and $\text{cost}_{\text{ML}}(\epsilon)$ are not known exactly, we employ a simple Monte Carlo algorithm with 100 independent replications for each of the values $\epsilon = 2^{-i}$, $i = 3, \ldots, 9$. The corresponding empirical means are denoted by $\hat{\text{error}}_{\text{ML}}(\epsilon)$ and $\hat{\text{cost}}_{\text{ML}}(\epsilon)$, respectively.

To assess the accuracy of the multilevel algorithm, $\text{error}_{\text{ML}}(\epsilon)$ should be compared with the desired accuracy $\epsilon$. Our present approach provides control of the error of the multilevel algorithm for a given $\epsilon$, therefore we aim at $\hat{\text{error}}_{\text{ML}}(\epsilon)$ being less than $\epsilon$.

To specify the computational gain we need to choose the parameters $k_n$, $L$, and $N$ of a single-level Monte Carlo method $S$ without smoothing in a fair way. As we have discussed in Section 2.5, if we do not apply smoothing, i.e., for $\delta = 0$, we formally have $e_2 = 0$, which leads to

$$\text{error}(Q_n(S)) \leq e_1 + \sqrt{2} \cdot \|Q_n\| \cdot (\|F(s_1), \ldots, F(s_{k})\| - \text{E}(S)^2_{\infty} + \text{Var}(S))^{1/2},$$

cf. (6). Hence we aim at

$$e_1 \leq \|Q_n\| \cdot \epsilon_*, \quad \|F(s_1), \ldots, F(s_{k})\| - \text{E}(S)^{\infty} \leq 16 \cdot \epsilon_*, \quad \text{Var}(S) \leq 256 \cdot \epsilon_*^2,$$

where $\epsilon_* = \epsilon/(33 \cdot \|Q_n\|)$ in this case, again with $\|Q_n\| \approx 1.63$. We choose

$$k_n = (\|Q_n\| \cdot \epsilon_*)^{-1/4},$$
up to the appropriate rounding, which corresponds to the assumption that (E3) holds with a constant $c$ close to one. Moreover, based on (8) with $L = L_0 = L_1$ with $\log_2 k_n$ instead of $c(k)$, and with the assumption that $\text{Var}(g^{k_0,0}(Y^{(L)}))$ is approximately one, we take $(\log_2 k_n)/(256 \cdot \epsilon^2)$ replications, up to integer rounding, in the single-level algorithm. Finally, we assume that the weak error, as considered in Remark 5, is bounded from above by $h^{\hat{\alpha}}$, where $h$ denotes the step-size of the Milstein scheme. The exponent $\hat{\alpha}$ is estimated empirically and provided to the single-level algorithm, but the cost for this is not taken into account, since we consider

$$\text{cost}_{\text{SL}}(\epsilon) = \log_2 k_n \cdot \frac{1}{256 \cdot \epsilon^2} \cdot \left( k_n + (16 \cdot \epsilon^2)^{-1/\hat{\alpha}} \right)$$

as the cost for the single-level Monte Carlo algorithm.

The ratio $\text{cost}_{\text{SL}}(\epsilon)/\text{cost}_{\text{ML}}(\epsilon)$ determines how effective is our approach, and consequently we will use $\text{cost}_{\text{SL}}(\epsilon)/\hat{c}_{\text{ML}}(\epsilon)$ to specify the computational gain.

5.1. Smooth Path-independent Functionals for SDEs. In this section we set $\mu = 0.05$, $\sigma = 0.2$, and $T = 1$ in (38), and we approximate the distribution function of $Y = X_T$ on the interval $[S_0, S_1] = [0.5, 1.5]$. Note that $Y$ is lognormally distributed with parameters $\mu - \sigma^2/2$ and $\sigma^2$

The variance and the mean decay with respect to the level $\ell$ for different values of $\delta$ and 7 equidistantly placed points on $[S_0, S_1]$, along with the corresponding quantities of the MLMC algorithm for the indicator function ($\delta = 0$), are estimated based on $10^6$ samples and presented in the top two plots in Figure 1. The empirical values for the order of convergence are close to 2 for the variance if $\delta > 0$, close to 1 for the variance if $\delta = 0$ (see dashed reference lines for first and for second order decay), and close to 1 for the mean for any given $\delta$ (see dashed reference line for first order decay). We stress that this part of the numerical experiments is not a part of our adaptive MLMC algorithm, and, of course, the findings are not provided to the adaptive algorithm.

In the middle left plot in Figure 1 we compare the estimate $\hat{e}_{\text{ML}}(\epsilon)$ (solid line) for the root mean squared error of the multilevel algorithm and the accuracy demand $\epsilon$ (dotted line). The computational gain over the single-level algorithm can be seen in the middle right plot in Figure 1.

For the adaptive algorithm the number $k_n$ of interpolation points and the smoothing parameter $\delta_m$ are random quantities, which are updated during the algorithm run and which depend on $\epsilon$. Empirical means of the final values of $k_n$ and of the reciprocal of $\delta_m$, based on 100 samples, are presented in the bottom left plot in Figure 1.

Finally, we show the true distribution function on the interval $[S_0, S_1]$ (dashed line) along with two approximations at different accuracies: $\epsilon = 2^{-3}$ (red line) and $\epsilon = 2^{-9}$ (green line).

5.2. Smooth Path-dependent Functionals for SDEs. Consider the SDE (38) with parameters $\mu = 0.5$, $\sigma = 0.2$, and $T = 1$. In this section we approximate the distribution function of $Y = \max_{t \in [0,T]} X_t$ on the interval $[S_0, S_1] = [1.05, 2.05]$. We have an explicit solution, see [3], also in this case, since

$$F(s) = 1 - \frac{1}{2} \text{erfc}(d_1) - \frac{1}{2} \text{erfc}(d_2) s^{2\mu/\sigma^2-1}$$
with
\[ d_1 = \frac{\ln(s) - (\mu - \frac{\sigma^2}{2}) \cdot T}{\sigma \cdot \sqrt{2 \cdot T}}, \quad d_2 = \frac{\ln(s) + (\mu - \frac{\sigma^2}{2}) \cdot T}{\sigma \cdot \sqrt{2 \cdot T}}. \]

The plots in Figure 2 are obtained and organised in the same way as the plots in Figure 1. The empirical values for the order of convergence are close to 0.85 for the variance if \( \delta > 0 \), close to 0.5 for the variance if \( \delta = 0 \) (see dashed reference line for first order decay), and close to 0.57 for the mean for any given \( \delta \) (see dashed reference line for half order decay). The true distribution function is shown on the interval \([S_0, S_1]\) along with two different approximations at different accuracies: \( \epsilon = 2^{-3} \) (red line) and \( \epsilon = 2^{-9} \) (green line).

5.3. Exit times. Now we choose the parameters \( \mu = 0.01, \sigma = 0.2, \) and \( T = 2 \) in the SDE (38), and we approximate the distribution function of
\[ Y = \inf\{t \geq 0 : X_t \leq b\} \wedge T \]
for \( b = 0.95 \) on the interval \([S_0, S_1] = [0.25, 1.25]\). The distribution of \( \inf\{t \geq 0 : X_t = b\} \) is an inverse Gaussian distribution with parameters \( \ln b / (\mu - \sigma^2 / 2) \) and \( (\ln b)^2 / \sigma^2 \), see [3], and this yields an explicit formula for the distribution function of \( Y \), since \( T > S_1 \).

The numerical studies are performed and presented in the same way as in Sections 5.1 or 5.2, except in order to ensure better mean and variance decay, we use the distribution function

**Figure 1.** Path-independent functional: variance decay (top left), mean decay (top right), computational gain (bottom right), RMSE (bottom left), average smoothing coefficient and number of interpolation points (bottom left), true CDF and estimated for \( \epsilon^{-3} \) and \( \epsilon^{-9} \) CDFs.
The empirical values for the order of convergence of the variance and the mean are both close to 1 (see dashed reference lines for the first order decay) regardless of $\delta$, though the constants are inversely proportional to the value of $\delta$, thus showing the benefits of smoothing. As before, we show the true distribution function $F$ on the interval $[S_0, S_1]$ along with two different approximations at different accuracies: $\epsilon = 2^{-3}$ (red line) and $\epsilon = 2^{-9}$ (green line).

5.4. Conclusions. The two most important findings are as follows. The estimate $\hat{\epsilon}_{\text{ML}}(\epsilon)$ for the root mean squared error of the adaptive MLMC algorithm is in the range of the desired accuracy $\epsilon$ for all three functionals; actually, it is less than $\epsilon$ in our experiments. For all three functionals the adaptive MLMC algorithm achieves a substantial computational gain over the single-level algorithm. For instance, if we ask for accuracy $\epsilon = 2^{-9}$, then this gain is around 840, 70 and 25 times for smooth path-independent, smooth path-dependent and exit time functionals.

We clearly see that a proper choice of $\delta$ decreases the variances and consequently leads to a computational gain. For the smooth path-independent functional this effect is very strong, and it is still substantial for the smooth path-dependent functional. In both cases smoothing

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**Figure 2.** Path-dependent functional: variance decay (top left), mean decay (top right), computational gain (middle right), RMSE (middle left), average smoothing coefficient and number of interpolation points (bottom left), true CDF and estimated for $\epsilon^{-3}$ and $\epsilon^{-9}$ CDFs.
(δ > 0) improves the empirical order of convergence of the variances, compared to the indicator function (δ = 0). For the exit time the effect is much weaker, and we have more or less the same empirical order of convergence of the variances. For all three functionals the mean decay shows basically no dependence on δ.

For all three functionals the empirical means of the number of interpolation points and of the reciprocal of the smoothing parameter, as chosen by our adaptive algorithm, increase similar to each other with respect to ε, which is consistent with the assumptions in Sections 2.2 and 4.1 and with the asymptotic analysis, see (40) and (41) in the Supplementary Materials. The true distribution functions and their approximations with the smaller value of ε are virtually indistinguishable.

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REFERENCES
6. Proof of the Theorem 3. We write $a \preceq b$ if there exists a constant $c > 0$ that does not depend on the parameters $k, \delta, L_0, L_1, N_{L_0}, \ldots, N_{L_1}$ such that $a \leq c \cdot b$. Moreover, $a \asymp b$ stands for $a \preceq b$ and $b \preceq a$.

Recall the error decomposition (5). Use Lemma 2 together with (7), (8), and the boundedness of $g$ to obtain

$$e_4 \preceq \log k \cdot \left( \frac{1}{N_{L_0}} + \sum_{\ell=L_0+1}^{L_1} \min(\delta^{-\beta_4} \cdot M^{-\ell \cdot \beta_5}, 1) \right)$$

for the variance $e_4$ of $M$. Furthermore, (A3) states that

$$e_3 \preceq \min \left( \delta^{-2\alpha_1} \cdot M^{-L_1 \cdot 2\alpha_2}, M^{-L_1 \cdot 2\alpha_3} \right)$$

for the bias $e_3$ of $M$. Use Lemma 1 and assumptions (E2) and (E3) to obtain the error bound

$$\text{error}^2(Q_k(M)) \preceq k^{-2(r+1)} + \delta^{2(r+1)} + \min \left( \delta^{-2\alpha_1} \cdot M^{-L_1 \cdot 2\alpha_2}, M^{-L_1 \cdot 2\alpha_3} \right)$$

$$+ \log k \cdot \left( \frac{1}{N_{L_0}} + \sum_{\ell=L_0+1}^{L_1} \min(\delta^{-\beta_4} \cdot M^{-\ell \cdot \beta_5}, 1) \right)$$

(39)

see [8, Eqn. (2.15)].
We determine parameters of the algorithm \( Q_k^r(\mathcal{M}) \) such that an error of about \( \epsilon \in ]0, \min(1, \delta_0^{-1})[ \) is achieved at a small cost. More precisely, we minimize the upper bound (3) for the cost, subject to the constraint that the upper bound (39) for the squared error is at most \( \epsilon^2 \), up to multiplicative constants for both quantities.

First of all we consider the case \( \delta > 0 \), and we choose

\[(40) \quad \delta = \epsilon^{1/(r+1)} \]

and, up to integer rounding,

\[(41) \quad k = \epsilon^{-1/(r+1)} \]

and

\[(42) \quad N_{L_0} = \epsilon^{-2} \cdot \log_M \epsilon^{-1}. \]

This yields

\[
\text{error}^2(Q_k^r(\mathcal{M})) \leq \epsilon^2 + a^2(L_1) + \log \epsilon^{-1} \cdot \sum_{\ell=L_0+1}^{L_1} \min(\delta^{-\beta_1} \cdot M^{-\ell^{-\beta_5}}, 1) N_{\ell}
\]

with

\[
a(L_1) = \min(\delta^{-\alpha_1} \cdot M^{-L_1^{-\alpha_2}}, M^{-L_1^{-\alpha_3}}).
\]

Since \( k \leq N_{L_0} \) and \( k \cdot \delta \leq 1 \), we obtain

\[(43) \quad \text{cost}(Q_k^r(\mathcal{M})) \leq c(L_0, L_1, N_{L_0}, \ldots, N_{L_1})
\]

with

\[
c(L_0, L_1, N_{L_0}, \ldots, N_{L_1}) = \sum_{\ell=L_0}^{L_1} N_{\ell} \cdot M^\ell
\]

from (3). In contrast to [8, Eqn. (2.16)] this cost bound does not depend on \( k \).

We need \( a(L_1) \leq \epsilon \), which requires \( L_1 \geq q \cdot L^* \) with

\[
L^* = \frac{1}{r+1} \cdot \log_M \epsilon^{-1}.
\]

Consequently, we choose

\[(44) \quad L_1 = q \cdot L^*, \]

up to integer rounding.

For a single-level algorithm with smoothing, i.e., for \( L_0 = L_1 \) and \( \delta > 0 \), all parameters have thus been determined, and we obtain \( \text{error}(Q_k^r(\mathcal{M})) \leq \epsilon \) as well as

\[(45) \quad c(L_1, L_1, N_{L_1}) \propto \epsilon^{-2} \cdot \log \epsilon^{-1} \cdot M^q L^* = \epsilon^{-2-q/(r+1)} \cdot \log \epsilon^{-1}.
\]
For a single-level algorithm without smoothing we obtain the same result, if we formally choose the parameters \( \alpha_i \) by (9), which leads to \( q = (r + 1)/\alpha \).

For a multi-level algorithm with \( L_0 < L_1 \) we obtain

\[
\text{error}^2(Q^*_k(M)) \preceq \epsilon^2 + \log \epsilon^{-1} \cdot \sum_{\ell=L_0+1}^{L_1} \frac{v_\ell}{N_\ell}
\]

with

\[
v_\ell = \min(M^{L^* \cdot \beta_4 \cdot M^{-\ell \cdot \beta_5}}, 1)
\]

as well as

\[
c(L_0, L_1, N_{L_0}, \ldots, N_{L_1}) \approx \epsilon^{-2} \cdot \log \epsilon^{-1} \cdot M^{L_0} + \sum_{\ell=L_0+1}^{L_1} N_\ell \cdot M^\ell.
\]

We fix \( L_0 \) for the moment, and we minimize

\[
h(L_0, N_{L_0+1}, \ldots, N_{L_1}) = \epsilon^{-2} \cdot \log \epsilon^{-1} \cdot M^{L_0} + \sum_{\ell=L_0+1}^{L_1} N_\ell \cdot M^\ell
\]

subject to

\[
\sum_{\ell=L_0+1}^{L_1} \frac{v_\ell}{N_\ell} \leq \epsilon^2 / \log \epsilon^{-1}.
\]

A Lagrange multiplier leads to

\[
N_\ell = \epsilon^{-2} \cdot \log \epsilon^{-1} \cdot G(L_0) \cdot \left( v_\ell \cdot M^{-\ell} \right)^{1/2},
\]

up to integer rounding, which satisfies the constraint with

\[
G(L_0) = \sum_{\ell=L_0+1}^{L_1} \left( v_\ell \cdot M^\ell \right)^{1/2} = \sum_{\ell=L_0+1}^{L_1} \left( \min(M^{L^* \cdot \beta_4 \cdot M^{-\ell \cdot \beta_5}}, 1) \cdot M^\ell \right)^{1/2}.
\]

Moreover, this choice of \( N_{L_0+1}, \ldots, N_{L_1} \) yields

\[
(46) \quad h(L_0, N_{L_0+1}, \ldots, N_{L_1}) = \epsilon^{-2} \cdot \log \epsilon^{-1} \cdot (M^{L_0} + G^2(L_0)).
\]

Put \( L^* = \beta_4 / \beta_5 \cdot L^* \). Consider the case \( q \leq \beta_4 / \beta_5 \). Then we have \( L_1 \leq L^* \), and therefore

\[
M^{L_0} + G^2(L_0) = M^{L_0} + \left( \sum_{\ell=L_0+1}^{L_1} M^{\ell/2} \right)^2 \preceq M^{L_0} + M^{L_1} \approx M^{L^* - q}.
\]

Observing (45) we get (10) in the present case already by single-level algorithms.
From now on we consider the case $q > \beta_4 / \beta_5$. Suppose that $L_0 < L^\dagger$. Then we get
\[
M^{L_0} + G^2(L_0) \asymp M^{L_0} + \left( \sum_{L_0 + 1}^{L_1} M^{L/2} \right)^2 + M^{L^* \cdot \beta_4} \cdot \left( \sum_{L_0 + 1}^{L_1} M^{L \cdot (1 - \beta_5)/2} \right)^2 
\asymp M^{L^\dagger} + G^2(L^\dagger).
\]
It therefore suffices to study the case $L_0 \geq L^\dagger$, where we have
\[
M^{L_0} + G^2(L_0) = M^{L_0} + M^{L^* \cdot \beta_4} \cdot \left( \sum_{L_0 + 1}^{L_1} M^{L \cdot (1 - \beta_5)/2} \right)^2.
\]

Note that
\[
\beta_5 = 1 \quad \Rightarrow \quad M^{L_0} + G^2(L_0) \asymp M^{L_0} + M^{L^* \cdot \beta_4} \cdot (L_1 - L_0)^2,
\]
\[
\beta_5 > 1 \quad \Rightarrow \quad M^{L_0} + G^2(L_0) \asymp M^{L_0} + M^{L^* \cdot \beta_4} \cdot M^{L_0 \cdot (1 - \beta_5)} \asymp M^{L_0},
\]
\[
\beta_5 < 1 \quad \Rightarrow \quad M^{L_0} + G^2(L_0) \asymp M^{L_0} + M^{L^* \cdot \beta_4} \cdot M^{L_1 \cdot (1 - \beta_5)}.
\]

Hence we choose
\[
L_0 = \beta_4 / \beta_5 \cdot L^*
\]
in all these cases. Hereby we obtain
\[
M^{L_0} + G^2(L_0) \asymp M^{L^* \cdot \beta_4 / \beta_5} \cdot \begin{cases} (L^*)^2, & \text{if } \beta_5 = 1, \\ 1, & \text{if } \beta_5 > 1, \end{cases}
\]
as well as
\[
M^{L_0} + G^2(L_0) \asymp M^{\max(\beta_4 / \beta_5, \beta_4 (1 - \beta_5) \cdot q) \cdot L^*} \quad \text{if } \beta_5 < 1.
\]

In any case, under the condition $q > \beta_4 / \beta_5$, these estimates are superior to $M^{L^* \cdot q}$, cf. (45). Use (46) and $M^{L^*} = \epsilon^{1/(r+1)}$ to derive (11)–(13).

7. On the Type-2 Constant of $(\mathbb{R}^k, | \cdot |_\infty)$. From [9, p. 159] we know how to exploit the type of a Banach space $E$ in the analysis of multilevel algorithms taking values in $E$. The key ingredient is the existence of a constant $c > 0$ (as small as possible) such that

\[
(47) \quad \text{Var}(\sum_{i=1}^{n} \mathcal{M}_i) \leq c^2 \cdot \sum_{i=1}^{n} \text{Var}(\mathcal{M}_i)
\]
holds for every $n \in \mathbb{N}$ and every independent sequence $\mathcal{M}_1, \ldots, \mathcal{M}_n$ of $E$-valued square-integrable random elements. The smallest such constant is called the type-2 constant of the space $E$.

In the sequel we focus on the space $E = \mathbb{R}^k$, equipped with the $\ell_\infty$-norm $| \cdot |_\infty$, and we provide an explicit value for
\[
c = c(k),
\]
i.e., an explicit upper bound for the type-2 constant of this space.

The following result is due to [11, Lemma 6], and stated there in a slightly different setting. For convenience of the reader we present the proof from [11] in the setting of the present paper. Let $Z_1, \ldots$ be an independent sequence of standard normally distributed random variables. Moreover, let

\begin{equation}
\gamma^2(k) = \ln(k + 1) + \frac{(8/\pi)^{1/2}}{k+1} \sum_{j=2}^{k+1} \frac{1}{(\ln(j))^{1/2} \cdot j^2}.
\end{equation}

**Lemma 4.** For $n \in \mathbb{N}$ and $x_1, \ldots, x_n \in \mathbb{R}^k$ let

$$X = \sum_{i=1}^{n} Z_i \cdot x_i.$$  

Then

$$E(|X|_\infty^2) \leq \gamma^2(k) \cdot \sum_{i=1}^{n} |x_i|_\infty^2.$$  

**Proof.** It suffices to show $E(|X|_\infty^2) \leq \gamma^2(k)$ in the case $\sum_{i=1}^{n} |x_i|_\infty^2 = 1$. Put

$$F(s) = P(|X|_\infty^2 \leq s)$$

and

$$G(s) = P(|Z_1|_\infty^2 \leq s)$$

for $s \geq 0$.

Use integration by parts to obtain

$$1 - G(s) = (2\pi)^{-1/2} \int_{s}^{\infty} y^{-1/2} \cdot \exp(-y/2) \, dy$$

$$= (2/\pi)^{1/2} \cdot s^{-1/2} \cdot \exp(-s/2) - (2\pi)^{-1/2} \int_{s}^{\infty} y^{-3/2} \cdot \exp(-y/2) \, dy$$

$$\leq (2/\pi)^{1/2} \cdot s^{-1/2} \cdot \exp(-s/2) = 2G'(s),$$

see [11, Lemma 4], where $1 - G(s) \geq G'(s)$ for $s \geq 2$ is shown as well.

The $j$-th component $X_j$ of $X$ is normally distributed with zero mean and variance

$$\sigma_j^2 = \sum_{i=1}^{n} x_{i,j}^2 \leq 1.$$  

Let $G(\infty) = 1$, $G'(\infty) = 0$, and $s/0 = \infty$ if $s > 0$ for notational convenience. For $s > 0$,

$$P(|X_j^2 > s|) = 1 - G(s/\sigma_j^2) \leq 2G'(s/\sigma_j^2),$$

and therefore

$$1 - F(s) \leq \sum_{j=1}^{k} P(|X_j^2 > s|) \leq 2 \sum_{j=1}^{k} G'(s/\sigma_j^2).$$
Hence, for every $\nu > 0$,

$$E(|X|_\infty^2) \leq \nu + \int_{\nu}^\infty (1 - F(s)) \, ds \leq \nu + 2 \sum_{j=1}^{k} \int_{\nu}^\infty G'(s/\sigma_j^2) \, ds$$

$$= \nu + 2 \sum_{j=1}^{k} \sigma_j^2 \left(1 - G(\nu/\sigma_j^2)\right) \leq \nu + 4 \sum_{j=1}^{k} \sigma_j^2 G'(\nu/\sigma_j^2)$$

$$= \nu + (8/\pi)^{1/2} \sum_{j=1}^{k} \left(\sigma_j/\nu^{1/2} \cdot \exp\left(-\nu/(2\sigma_j^2)\right)\right).$$

Choose

$$\nu = \sup_{1 \leq j \leq k} \left(\sigma_j^2 \cdot \ln(j + 1)\right) \leq \ln(k + 1)$$

to obtain $\nu/\sigma_j^2 \geq \ln(j + 1)$ and therefore

$$E(|X|_\infty^2) \leq \ln(k + 1) + (8/\pi)^{1/2} \sum_{j=2}^{k+1} \frac{1}{(\ln(j))^{1/2} \cdot j^2},$$

as claimed.

In addition to the normally distributed random variables $Z_i$ and the corresponding random vectors $X$ we also consider an independent sequence $\varepsilon_1, \ldots$ of Bernoulli (or Rademacher) random variables, i.e., $\varepsilon_i$ takes the values $\pm 1$ with probability $1/2$. For $n \in \mathbb{N}$ and $x_1, \ldots, x_n \in \mathbb{R}^k$ we define

$$\tilde{X} = \sum_{i=1}^{n} \varepsilon_i \cdot x_i.$$}

We have

$$E(|\tilde{X}|_\infty^2) \leq \pi/2 \cdot E(|X|_\infty^2)$$

as a particular case of Pisier (1973, Prop. 1), which deals with arbitrary normed spaces and symmetric random variables $Z_i$.

The Rademacher type 2 constant of the space $\mathbb{R}^k$, which we denote by $T_2(k)$, is the smallest constant $\tilde{c} > 0$ such that

$$E(|\tilde{X}|_\infty^2) \leq \tilde{c}^2 \cdot \sum_{i=1}^{n} |x_i|_\infty^2$$

for every $n \in \mathbb{N}$ and all $x_1, \ldots, x_n \in \mathbb{R}^k$. Observe that the latter is an estimate for the variance of $\tilde{X}$ in terms of the variances $|x_i|_\infty^2$ of the random vectors $\varepsilon_i \cdot x_i$. This estimate actually extends to every independent sequence of random vectors, at the expense of a slightly larger constant. More precisely, for every $n \in \mathbb{N}$ and every independent sequence $M_1, \ldots, M_n$ of square-integrable random vectors with values in $\mathbb{R}^k$, we have (47) with

$$c(k) = 2T_2(k).$$
This result actually holds true with the corresponding type 2 constant for every Banach space \( E \) of this type, see [10, Prop. 9.11].

Lemma 4 together with (49) provides an explicit constant for (47) to hold in the case \( E = \mathbb{R}^k \), namely

\[
(50) \quad c(k) = (2\pi)^{1/2} \cdot \gamma(k).
\]

This constant is of the order \((\ln(k))^{1/2}\), which is known to be optimal for the spaces \( \mathbb{R}^k \).