

Multilevel Nested Simulation for Efficient Risk Estimation*

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Abstract. We investigate the problem of computing a nested expectation of the form $\mathbb{P}[\mathbb{E}[X|Y] \geq 0] = \mathbb{E}[\mathbb{H}(\mathbb{E}[X|Y])]$ where \mathbb{H} is the Heaviside function. This nested expectation appears, for example, when estimating the probability of a large loss from a financial portfolio. We present a method that combines the idea of using Multilevel Monte Carlo (MLMC) for nested expectations with the idea of adaptively selecting the number of samples in the approximation of the inner expectation, as proposed by [M. Broadie, Y. Du, and C. C. Moallemi, *Manag. Sci.*, 57 (2011), pp. 1172–1194]. We propose and analyze an algorithm that adaptively selects the number of inner samples on each MLMC level and prove that the resulting MLMC method with adaptive sampling has an $\mathcal{O}(\varepsilon^{-2}|\log \varepsilon|^2)$ complexity to achieve a root mean-squared error ε . The theoretical analysis is verified by numerical experiments on a simple model problem. We also present a stochastic root-finding algorithm that, combined with our adaptive methods, can be used to compute other risk measures such as Value-at-Risk (VaR) and Conditional Value-at-Risk (CVaR), the latter being achieved with $\mathcal{O}(\varepsilon^{-2})$ complexity.

Key words. Monte Carlo, nested simulation, risk estimation, multilevel Monte Carlo

AMS subject classifications. 65C05, 62P05

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1. Introduction. Our focus in the current work is on computing the quantity of interest
(1.1)
$$\eta = \mathbb{E}[\mathbb{H}(\mathbb{E}[X | Y])],$$

where \mathbb{H} is the Heaviside step function (i.e., $\mathbb{H}(x) = 1$ for $x \geq 0$ and 0 otherwise), and the inner expectation of the one-dimensional random variable, X , is conditional on the value of the outer multidimensional random variable, Y . This problem appears in many settings. However, our main motivation for looking at this problem is to compute the probability of a large loss from a financial portfolio; see, for example, [11, 2]. In such a context, X would be a one-dimensional random variable equal to the sum of losses at maturity from the options in the portfolio in excess of some threshold value, while Y would be a multidimensional random variable that includes the values of the underlying stocks and other risk factors at some short risk horizon.

Our approach to approximating η in (1.1) draws upon the work of Gordy and Juneja [11]. There, the authors expressed the probability of a large loss as a nested expectation then proposed using nested Monte Carlo samplers to estimate both the outer and inner expectations. They proved that using $\mathcal{O}(\varepsilon^{-1})$ samples in the inner Monte Carlo sampler and $\mathcal{O}(\varepsilon^{-2})$ samples in the outer Monte Carlo sampler is sufficient, under certain conditions, to achieve a root

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mean squared (RME) error of $\mathcal{O}(\varepsilon)$ in the estimation of η . Thus the total cost of their method is $\mathcal{O}(\varepsilon^{-3})$. See [10] for sharper and extended analysis of their results. In [2], Broadie, Du, and Moallemi improved the complexity of the nested Monte Carlo method by adapting the number of samples in the inner Monte Carlo sampler to the specific sample of the outer random variable, Y . The basic idea relies on the fact that the step function in (1.1) does not change value when a large error is committed in the estimation of the inner conditional expectation, $\mathbb{E}[X|Y]$, provided it is sufficiently far from 0. Hence, depending on $|\mathbb{E}[X|Y]|$ and the size of the statistical error that is committed when approximating $\mathbb{E}[X|Y]$ with a Monte Carlo sampler, the required number of samples is determined with a cap, which is again $\mathcal{O}(\varepsilon^{-1})$. Using this idea, it was shown in [2] that, under certain conditions, the expected required number of samples in the inner Monte Carlo estimator is $\mathcal{O}(\varepsilon^{-1/2})$, bringing the total cost of the nested Monte Carlo method down to $\mathcal{O}(\varepsilon^{-5/2})$. We will review in more detail the nested Monte Carlo method and the adaptive method to select the number of inner samples in section 2.1.

In parallel, the Multilevel Monte Carlo (MLMC) method was introduced in [7] to reduce the complexity of Monte Carlo methods when only approximate samples of a random variable can be generated and, hence, Monte Carlo approximations are necessarily biased. Assume we wish to estimate $\mathbb{E}[g]$ for some random variable g . Denoting the ℓ th level approximation of $\mathbb{E}[g]$ by $\mathbb{E}[g_\ell]$ such that $|\mathbb{E}[g_\ell] - \mathbb{E}[g]| = \mathcal{O}(2^{-\alpha\ell}) \xrightarrow{\ell \rightarrow \infty} 0$ for some $\alpha > 0$, the first step to approximate $\mathbb{E}[g]$, up to an RMS error ε , is to select the approximation level, L , such that $|\mathbb{E}[g] - \mathbb{E}[g_L]| = \mathcal{O}(\varepsilon)$. A standard Monte Carlo method then approximates $\mathbb{E}[g_L]$ with a sufficient number of samples such that the standard deviation of the approximation is also $\mathcal{O}(\varepsilon)$. If we assume that the cost of computing a single sample of g_ℓ is $\mathcal{O}(2^{\gamma\ell})$, the complexity of this Monte Carlo method is $\mathcal{O}(\varepsilon^{-2-\gamma/\alpha})$. On the other hand, MLMC is based on the telescopic sum

$$\mathbb{E}[g_L] = \mathbb{E}[g_0] + \sum_{\ell=1}^L \mathbb{E}[g_\ell - g_{\ell-1}].$$

Then, we estimate $\mathbb{E}[g_0]$ and $\mathbb{E}[g_\ell - g_{\ell-1}]$, for $\ell \leq L$, with independent Monte Carlo samplers, with the number of samples decreasing as $\ell \rightarrow 0$. Provided that g_ℓ and $g_{\ell-1}$ are sufficiently correlated such that $\text{Var}[g_\ell - g_{\ell-1}] = \mathcal{O}(2^{-\beta\ell})$ for $\beta > 0$, the complexity of MLMC is $\mathcal{O}(\varepsilon^{-2-\max(0, (\gamma-\beta)/\alpha)})$ for $\gamma \neq \beta$ and $\mathcal{O}(\varepsilon^{-2}|\log \varepsilon|^2)$ for $\gamma = \beta$ [8].

Bujok, Hambly, and Reisinger [3] applied MLMC to nested expectations of the form $\mathbb{E}[\phi(\mathbb{E}[X|Y])]$ for a piecewise linear function, ϕ , with X being a Bernoulli random variable. Giles [8] considers the case in which X is a more general random variable, with ϕ being a twice differentiable function. In any case, approximate samples of the random variable $\mathbb{E}[X|Y]$ are generated with a Monte Carlo sampler with $N_\ell = 2^\ell$ samples, and then a hierarchy of approximations based on the number of inner samples is used in an MLMC setting. The authors of both papers proved that MLMC in this case has an $\mathcal{O}(\varepsilon^{-2}|\log \varepsilon|^2)$ complexity. Moreover, they showed that using an antithetic estimator improves the complexity of MLMC to $\mathcal{O}(\varepsilon^{-2})$. On the other hand, if ϕ is a step function, as is the case when computing the probability of large loss, then we will prove in section 2.2 and show numerically in section 3 that MLMC with deterministic sampling has $\mathcal{O}(\varepsilon^{-5/2})$ complexity. Moreover, in this case, using antithetic sampling does not improve the complexity.

The main contribution of this work is to further reduce the complexity of the MLMC

method for step functions to $\mathcal{O}(\varepsilon^{-2}|\log \varepsilon|^2)$ by using ideas from [2] to adapt the number of inner samples on each level of the MLMC method, based on the particular realization of the random variable, Y , of the outer Monte Carlo sampler. We start in section 2, where we recall in more detail the work and results of [11, 2] on nested Monte Carlo estimators (see also [14] for a more thorough review) and [8] on using MLMC to estimate nested expectations. Then, in section 2.3 we start by motivating an algorithm, inspired by [2], that selects the number of inner samples given a realization of the outer random variable, Y . Section 2.3 also includes an analysis of the adaptive algorithm to show that an MLMC estimator that uses this adaptive strategy has levels whose variance of differences converges with rate $\mathcal{O}(2^{-\ell})$ while the work increases with rate $\mathcal{O}(2^\ell)$ as ℓ increases; hence the complexity of MLMC is $\mathcal{O}(\varepsilon^{-2}|\log \varepsilon|^2)$ in this case.

In section 3, a simple model problem that mimics the problem of computing the probability of a large loss from a financial portfolio is presented. We apply the MLMC method with adaptive and deterministic sampling and show that our analysis matches well with numerical experiments. In section 4 we discuss how our methods can be combined with a simple root-finding algorithm to compute other risk measures, namely, the Value-at-Risk (VaR) and the Conditional Value-at-Risk (CVaR). Somewhat surprisingly, we prove in the case of CVaR that the complexity of MLMC with deterministic sampling is the optimal $\mathcal{O}(\varepsilon^{-2})$. Finally, conclusions and future work directions are discussed in section 5.

2. Nested estimators for nested expectations.

2.1. Nested Monte Carlo estimators. In this section we review the works of Gordy and Juneja [11] and Broadie, Du, and Moallemi [2] which are based on approximating the inner and outer expectations in (1.1) using Monte Carlo. In [11], the conditional *inner* expectation $\mathbb{E}[X | Y = y]$, for a given y , is estimated using an unbiased Monte Carlo estimator with N samples as follows:

$$(2.1) \quad \widehat{\mathbb{E}}_N(y) = \frac{1}{N} \sum_{n=1}^N x^{(n)}(y),$$

where $x^{(n)}(y)$ is the n th sample of the random variable X given $Y = y$, and $\{x^{(n)}\}_n$ are mutually independent, conditional on $Y = y$. Then, Monte Carlo is used again to approximate the *outer* expectation as follows:

$$(2.2) \quad \eta \approx \frac{1}{M} \sum_{m=1}^M \mathbb{H}(\widehat{\mathbb{E}}_N(y^{(m)})),$$

where $y^{(m)}$ is the m th sample of the random variable Y , and $\{y^{(m)}\}_m$ are mutually independent. Denote the joint density of the two random variables $\mathbb{E}[X | Y]$ and $\widehat{\mathbb{E}}_N(Y)$ by $p_N(y, z)$. Moreover, for $i = 0, 1$, and 2 , assume that $\frac{\partial^i}{\partial y^i} p_N(y, z)$ exists and that there exists a nonnegative function, $p_{i,N}$, such that

$$\left| \frac{\partial^i}{\partial y^i} p_N(y, z) \right| \leq p_{i,N}(z) \text{ for all } N, y, \text{ and } z$$

$$\text{and } \sup_N \int_{-\infty}^{\infty} |z|^q p_{i,N}(z) dz < \infty$$

for all $0 \leq q \leq 4$. Then, by [11, Proposition 1], the RMS error of the estimator (2.2) is $\mathcal{O}(M^{-1/2} + N^{-1})$. Hence, to get an RMS error of $\mathcal{O}(\varepsilon)$, we require $M = \mathcal{O}(\varepsilon^{-2})$ and $N = \mathcal{O}(\varepsilon^{-1})$, and the total complexity is $\mathcal{O}(\varepsilon^{-3})$.

Note that, given a sample of the random variable Y , we want to evaluate a step function that is based on the expectation $\mathbb{E}[X|Y]$, which is approximated using a Monte Carlo estimator with N samples. However, depending on how far the expectation $\mathbb{E}[X|Y]$ is from zero, where the step function changes value, a very rough approximation of $\mathbb{E}[X|Y]$ might still give the correct value for the step function $H(\mathbb{E}[X|Y])$. This motivates adapting the number of samples based on the value of $|\mathbb{E}[X|Y]|$. Such a method was introduced and analyzed in [2] for a nested Monte Carlo approximation.

Heuristically, assuming that given Y we have an estimate $\hat{E}_N(Y) > 0$, the authors in [2] ask: What is the probability that adding an extra sample will produce a negative estimate? Denoting the random variables $\mu := \mathbb{E}[X|Y]$ and $\sigma^2 := \text{Var}[X|Y]$ and using Chebyshev's inequality yields

$$\begin{aligned} \mathbb{P}[\hat{E}_{N+1}(Y) \leq 0 \mid \hat{E}_N(Y)] &= \mathbb{P}\left[N\hat{E}_N(Y) + \mu \leq \mu - x^{(N+1)}(Y) \mid \hat{E}_N(Y)\right] \\ &\leq \mathbb{P}\left[N\hat{E}_N(Y) + \mu \leq \left|\mu - x^{(N+1)}(Y)\right| \mid \hat{E}_N(Y)\right] \\ &\leq \frac{\sigma^2}{(N\hat{E}_N(Y) + \mu)^2} \approx \frac{\sigma^2}{N^2\mu^2}. \end{aligned}$$

Then, for $d := |\mu|$, we need only $N \geq \varepsilon^{-1/2}\sigma/d$ in order to ensure that adding a new inner sample does not change the value of the step function with probability $1 - \varepsilon$, i.e., that our estimate $H(\hat{E}_N(Y)) = H(\hat{E}_{N+1}(Y)) \approx H(\mathbb{E}[X|Y])$ is correct with probability $1 - \varepsilon$. In [2], two algorithms were introduced to adaptively determine the number of samples in the inner Monte Carlo sampler of a nested Monte Carlo method. The first is based on minimizing the total required number of samples for all inner Monte Carlo samplers subject to some error tolerance. The second algorithm is iterative such that in every iteration estimates of d and σ given Y are computed using N inner samples. Then more inner samples are added until Nd/σ exceeds some error margin threshold. In the current work, we instead start by adding a cap on the number of samples and set

$$(2.3) \quad N = \left\lceil \min\left(\mathcal{O}(\varepsilon^{-1}), \varepsilon^{-1/2} \frac{\sigma}{d}\right) \right\rceil.$$

Hence when $\delta := d/\sigma = o(\varepsilon^{1/2})$, we would use the maximum number of samples, otherwise, fewer samples are used and we still get the same estimate for $H(\hat{E}_N(Y))$ with probability $1 - \varepsilon$. Assuming that the random variable δ has a distribution with a bounded density near 0, the average number of samples is then $\mathcal{O}(\varepsilon^{-1/2})$ and the complexity of the nested Monte Carlo method with this choice of number of samples is $\mathcal{O}(\varepsilon^{-5/2})$.

2.2. MLMC for nested expectation. In this section, based on ideas in [3, 8, 13], we will use an MLMC estimator to approximate the *outer* expectation, using the number of samples in the inner Monte Carlo as a discretization parameter, as follows:

$$(2.4) \quad \hat{\eta} := \sum_{\ell=0}^L \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} H\left(\hat{E}_{N_\ell}^{(f,\ell,m)}(y^{(\ell,m)})\right) - H\left(\hat{E}_{N_{\ell-1}}^{(c,\ell,m)}(y^{(\ell,m)})\right),$$

where the estimator of the inner expectation, \widehat{E}_{N_ℓ} , is as defined in (2.1), where, as before,

$$(2.5) \quad \widehat{E}_{N_\ell}^{(f,\ell,m)}(y) := \frac{1}{N_\ell} \sum_{n=1}^{N_\ell} x^{(f,\ell,m,n)}(y)$$

with $\widehat{E}_{N_{\ell-1}}^{(c,\ell,m)}$ defined similarly but with $H(\widehat{E}_{N_{\ell-1}}^{(c,0,\dots)}(\cdot)) := 0$. Here, $\{x^{(\cdot,\ell,m,n)}(y)\}_n$ are i.i.d. samples of X given $Y = y$. Moreover, the samples of the random variable, X , used in $\widehat{E}_{N_\ell}^{(f,\ell,m)}$ and $\widehat{E}_{N_{\ell-1}}^{(c,\ell,m)}$ are mutually independent, but conditional on the same y , and independent from the samples used in $\widehat{E}_{N_\ell}^{(f,\ell',m')}$ and $\widehat{E}_{N_{\ell-1}}^{(c,\ell',m')}$ for any $\ell' \neq \ell$ or $m' \neq m$.

Again, due to [11, Proposition 1] and under the assumptions listed therein, and recalled in section 2.1, we have

$$(2.6) \quad \left| \mathbb{E} \left[H \left(\widehat{E}_{N_\ell}(Y) \right) - H(\mathbb{E}[X | Y]) \right] \right| = \mathcal{O}(N_\ell^{-1}).$$

Moreover, the cost to generate samples of $H(\widehat{E}_{N_\ell}(\cdot))$ is $\mathcal{O}(N_\ell)$. Unlike standard Monte Carlo, MLMC also requires strong convergence of the estimators. More specifically, the variance of the difference $H(\widehat{E}_{N_\ell}(y)) - H(\widehat{E}_{N_{\ell-1}}(y))$ must converge sufficiently fast.

At this point, we will prove another general result regarding nested Monte Carlo samplers. To begin, we list the first of two main assumptions in the current work. In what follows, we define the one-dimensional random variables $d := |\mathbb{E}[X | Y]|$, $\sigma^2 := \text{Var}[X | Y]$, and $\delta := d/\sigma$.

Assumption 2.1. We assume that the probability density function of the nonnegative, one-dimensional random variable, δ , denoted by ρ , exists. Moreover, we assume that there exist constants $\rho_0 > 0$ and $\delta_0 > 0$ such that $\rho(\delta) \leq \rho_0$ for all $\delta \in [0, \delta_0]$.

Based on this assumption and for a positive, nonincreasing function a , we have

$$(2.7) \quad \int_0^\infty a(\delta) \rho(\delta) d\delta \leq \rho_0 \int_0^\infty a(\delta) d\delta + a(\delta_0),$$

which can be shown by splitting the integral at δ_0 and then bounding ρ using Assumption 2.1. We will also make repeated use of the following identity for a $q > 1$ and a constant $b > 0$:

$$(2.8) \quad \int_0^\infty \min(1, bx^{-q}) dx = \frac{q b^{1/q}}{q-1},$$

which can be shown by splitting the integral at $b^{1/q}$.

Proposition 2.2 (variance of the inner Monte Carlo). Let X, Y be two random variables satisfying Assumption 2.1. Then

$$(2.9) \quad \begin{aligned} \text{Var} \left[H \left(\widehat{E}_N(Y) \right) - H(\mathbb{E}[X | Y]) \right] &\leq \mathbb{E} \left[\left(H \left(\widehat{E}_N(Y) \right) - H(\mathbb{E}[X | Y]) \right)^2 \right] \\ &= \mathcal{O}(N^{-1/2}). \end{aligned}$$

Proof. We start from

$$\begin{aligned} & \mathbb{E} \left[\left(H(\widehat{E}_N(Y)) - H(\mathbb{E}[X | Y]) \right)^2 \middle| Y \right] \\ &= \mathbb{P} \left[\left| H(\widehat{E}_N(Y)) - H(\mathbb{E}[X | Y]) \right| = 1 \middle| Y \right] \\ &\leq \mathbb{P} \left[\left| \widehat{E}_N(Y) - \mathbb{E}[X | Y] \right| \geq d \middle| Y \right], \end{aligned}$$

where, by Chebyshev's inequality and bounding the probability by 1, we have

$$(2.10) \quad \mathbb{P} \left[\left| \widehat{E}_N(Y) - \mathbb{E}[X | Y] \right| \geq d \middle| Y \right] \leq \min \left(1, d^{-2} \text{Var} \left[\widehat{E}_N(Y) \middle| Y \right] \right) = \min \left(1, \delta^{-2} N^{-1} \right).$$

Taking expectation over Y yields

$$\begin{aligned} \mathbb{E} \left[\left(H(\widehat{E}_N(Y)) - H(\mathbb{E}[X | Y]) \right)^2 \right] &\leq \int_0^\infty \min(1, \delta^{-2} N^{-1}) \rho(\delta) d\delta \\ &\leq \rho_0 \int_0^\infty \min(1, \delta^{-2} N^{-1}) d\delta + \min(1, \delta_0^{-2} N^{-1}) \\ &\leq 2\rho_0 N^{-1/2} + \delta_0^{-2} N^{-1}. \end{aligned}$$

Here we first used (2.7) and then (2.8). Hence, the variance is $\mathcal{O}(N^{-1/2})$. ■

Based on this proposition and under [Assumption 2.1](#), for a *deterministic* choice of N_ℓ , increasing with each level, we have

$$(2.11) \quad \text{Var} \left[H(\widehat{E}_{N_\ell}(Y)) - H(\widehat{E}_{N_{\ell-1}}(Y)) \right] = \mathcal{O}(N_{\ell-1}^{-1/2}),$$

since for any two random variables V and W , we have $\text{Var}[V+W] \leq 2\text{Var}[V] + 2\text{Var}[W]$. Hence, if we make a simple choice of $N_\ell = N_0 2^\ell$, and provided the assumptions of [11, Proposition 1] are satisfied so that we have (2.6), we can conclude, according to standard MLMC complexity analysis (with $\alpha = 2\beta = \gamma = 1$), that the cost to approximate η to an error tolerance of ε is $\mathcal{O}(\varepsilon^{-5/2})$.

Remark 2.3 (using antithetic sampling). In some nested simulation applications, it is possible to use an antithetic estimator, where all samples in the fine estimator, $\widehat{E}^{(f, \dots)}$, are used in the coarse estimator, $\widehat{E}^{(c, \dots)}$, in each level to increase the correlation between the fine and coarse estimators of the inner conditional expectation; see, for example, [8] or [section 3](#) for more details. In fact, such an estimator was used to compute the moments of the total loss from a portfolio at a risk horizon in [12]. However, using antithetic sampling does not change the variance convergence rate in our setting because the discontinuity in the step function violates the differentiability requirements of the antithetic estimator. In fact, the main correlation between the fine and coarse samples is due to the strong convergence of the inner Monte Carlo estimator (2.9), and using independent samples is sufficient to get the rate in (2.11). Nevertheless, using an antithetic estimator might reduce the variance by a constant, as we will discuss in [section 3](#). We do not emphasise this in the presented theorems to simplify presentation.

2.3. Adaptive sampling for MLMC. In this section, we apply the adaptive sampling method mentioned in section 2.1 to the MLMC estimator of the outer expectation and analyze the resulting algorithm. Our aim is to increase the variance convergence to $\mathcal{O}(2^{-\ell})$ while still using $\mathcal{O}(2^\ell)$ inner samples per level on average, so that the MLMC complexity is $\mathcal{O}(\varepsilon^{-2}|\log \varepsilon|^2)$. In this section, in addition to Assumption 2.1, we also work under the following assumption.

Assumption 2.4. We assume that for some $2 < q < \infty$, the q th normalized, central moment of X given Y is uniformly bounded for all values of Y , i.e.,

$$\kappa_q := \sup_y \mathbb{E} \left[\sigma^{-q} |X - \mathbb{E}[X | Y]|^q \mid Y = y \right] < \infty.$$

Moreover, we will make repeated use of the following lemma.

Lemma 2.5. Let \bar{Z}_N be an average of N i.i.d. samples of a random variable, Z , with zero mean and finite q th moment for $q \geq 1$. Then for any $z > 0$ there exists a constant, C_q , depending only on q , such that

$$\begin{aligned} \mathbb{E}[|\bar{Z}_N|^q] &\leq C_q N^{-q/2} \mathbb{E}[|Z|^q] \\ \text{and} \quad \mathbb{P}[|\bar{Z}_N| > z] &\leq \min\left(1, C_q z^{-q} N^{-q/2} \mathbb{E}[|Z|^q]\right). \end{aligned}$$

Proof. Denoting by $\{Z_n\}_{n=1}^N$ the N samples of Z , the discrete Burkholder–Davis–Gundy inequality gives

$$\begin{aligned} \mathbb{E}[|\bar{Z}_N|^q] &\leq C_q \mathbb{E} \left[\left(N^{-2} \sum_{n=1}^N Z_n^2 \right)^{q/2} \right] \\ &\leq C_q \mathbb{E} \left[N^{-q/2-1} \sum_{n=1}^N |Z_n|^q \right] \\ &= C_q N^{-q/2} \mathbb{E}[|Z|^q], \end{aligned}$$

where C_q is a constant depending only on q [4]. The second result follows immediately using Markov's inequality and bounding the probability by 1. ■

In particular, given Y , letting $Z = X(Y) - \mathbb{E}[X | Y]$ and $\bar{Z}_N = \hat{\mathbb{E}}_N(Y) - \mathbb{E}[X | Y]$ and using the definition of κ_q , we have

$$(2.12) \quad \mathbb{P} \left[\left| \hat{\mathbb{E}}_N(Y) - \mathbb{E}[X | Y] \right| > d \mid Y \right] \leq \min \left(1, C_q \kappa_q \left(\delta N^{1/2} \right)^{-q} \right).$$

This is a generalization of (2.10) when we have bounded q -moments.

2.3.1. Algorithm. Recall the choice (2.3) for the adaptive number of samples that was made in [2]. Another choice can be motivated by the central limit theorem. We know that a Monte Carlo estimate of $\mathbb{E}[X | Y]$ with N samples, denoted by $\hat{\mathbb{E}}_N$, has an error that is roughly bounded by $C \sqrt{\text{Var}[X | Y]/N}$, where C is a confidence constant. Then, we need

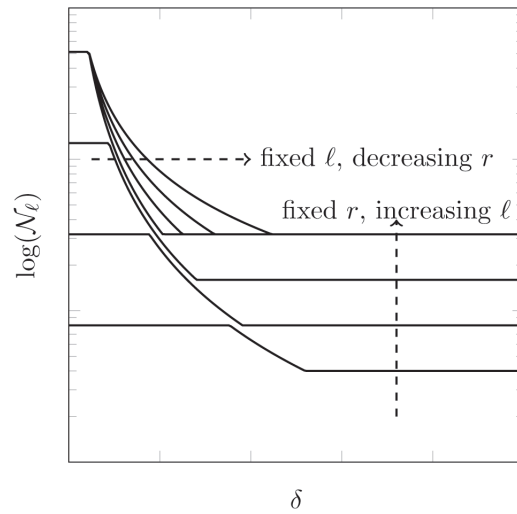


Figure 1. The function N_ℓ in (2.14) as a function of $\delta = d/\sigma$ for different values of ℓ and r .

only $N \geq C^2 \sigma^2 / d^2$ in order to ensure that our estimate $H(\hat{E}_N(Y)) \approx H(\mathbb{E}[X|Y])$ is correct. Imposing, again, a maximum number of samples of $\mathcal{O}(\varepsilon^{-1})$, we get

$$(2.13) \quad N = \left\lceil \max\left(\mathcal{O}(\varepsilon^{-1}), C^2 \frac{\sigma^2}{d^2}\right) \right\rceil.$$

Compare this to (2.3) and note the different power of (d/σ) and the introduction of the confidence constant C .

More generally, in the context of MLMC, the algorithm we would like to use should ensure, conditioned on Y , that the number of samples, N_ℓ , on level ℓ satisfies $N_\ell = \lceil \mathcal{N}_\ell \rceil$, where

$$(2.14) \quad \mathcal{N}_\ell = N_0 4^\ell \max\left(2^{-\ell}, \min\left(1, \left(C^{-1} N_0^{1/2} 2^\ell \frac{d}{\sigma}\right)^{-r}\right)\right)$$

for some given confidence constant C and $1 < r < 2$ as we shall see later. The choice (2.14) is motivated from (2.3) and (2.13), with the following changes: (i) the number of samples on level ℓ is now bounded below by $N_0 2^\ell$ and bounded above by $N_0 4^\ell$, (ii) we introduce a generic power r , where, for a given value of Y , the number of samples increases as r decreases; see Figure 1, and (iii) we introduce a confidence constant $C \geq 1$.

The difficulty with (2.14) is that we do not know a priori the values of d and σ , given Y , so instead we use an iterative algorithm, inspired by [2, Algorithm 3], that doubles the number of samples N_ℓ at every iteration and then estimates d and σ . The algorithm then terminates when N_ℓ satisfies $N_\ell \geq \hat{N}_\ell$, where \hat{N}_ℓ is the same as \mathcal{N}_ℓ , but computed with the current estimates of d and σ , denoted by \hat{d} and $\hat{\sigma}$, respectively. Hence, the output of the algorithm, N_ℓ satisfies

$$(2.15) \quad \hat{N}_\ell \leq N_\ell < 2\hat{N}_\ell.$$

The full algorithm is listed in Algorithm 1. Note that the number of inner samples that this algorithm uses to determine N_ℓ is, at most, $(2 - 2^{-\ell})N_\ell < 2N_\ell$.

Algorithm 1 Adaptive algorithm to determine N_ℓ .

Data: ℓ, y, N_0, r **Result:** N_ℓ set $N_\ell := N_0 2^\ell$ set done := false**repeat**
 /* If we continue the adaptive algorithm, at least $2N_\ell$ inner samples
 will be used (N_ℓ samples in this step and then another N_ℓ samples
 when computing the Monte Carlo estimate). Hence, terminate if $2N_\ell$
 is greater than the maximum number of inner samples. */
if $2N_\ell \geq N_0 4^\ell$ **then**| set $N_\ell := N_0 4^\ell$ set done := true**else**| generate N_ℓ new, and independent, inner samples compute new estimates \hat{d} and $\hat{\sigma}^2$ | given $Y = y$ **if** $N_\ell \geq N_0 4^\ell \left(C^{-1} N_0^{1/2} 2^\ell \frac{\hat{d}}{\hat{\sigma}} \right)^{-r}$ **then**

| | set done := true

| **else**| | set $N_\ell := 2N_\ell$ | **end****end****until** done;**return** N_ℓ

2.3.2. Numerical analysis. In this section we will show that, under [Assumptions 2.1](#) and [2.4](#), the adaptive algorithm has a random output, N_ℓ , that satisfies $\mathbb{E}[N_\ell] = \mathcal{O}(2^\ell)$. Moreover, we will show that, with this random choice of number of inner samples, we have $\text{Var}[\text{H}(\hat{\text{E}}_{N_\ell}(Y)) - \text{H}(\mathbb{E}[X | Y])] = \mathcal{O}(2^{-\ell})$. From here, using standard MLMC complexity analysis, the complexity of our method is $\mathcal{O}(\varepsilon^{-2} |\log \varepsilon|^2)$. We start in [Lemma 2.6](#) by proving the results when we have perfect knowledge of d and σ^2 . Then in [Theorem 2.7](#) we consider the case when \hat{d} and $\hat{\sigma}^2$ are Monte Carlo estimates of d and σ^2 , given Y . In what follows, we will denote a “normalized δ ” by

$$(2.16) \quad \nu := C^{-1} N_0^{1/2} 2^\ell \delta.$$

Lemma 2.6 (perfect adaptive sampling). Under [Assumptions 2.1](#) and [2.4](#), for the estimator [\(2.5\)](#) and the number of samples N_ℓ obtained using [Algorithm 1](#) for $1 < r < 2 - 2/q$, $\hat{d} = d = |\mathbb{E}[X | Y]|$, and $\hat{\sigma}^2 = \sigma^2 = \text{Var}[X | Y]$ we have

$$\mathbb{E}[N_\ell] = \mathcal{O}(2^\ell) \quad \text{and} \quad \text{Var}[\text{H}(\hat{\text{E}}_{N_\ell}(Y)) - \text{H}(\mathbb{E}[X | Y])] = \mathcal{O}(2^{-\ell}).$$

Comment. Even though the setting of this lemma is idealistic in that it assumes perfect knowledge of d and σ^2 , its proof still illustrates important points. The first point is the usage

of (2.12) to bound the tail probability of a Monte Carlo average. The second point is that the bounds on the value of $r \in (1, 2 - 2/q)$ are needed even with such perfect knowledge.

As stated previously, as r increases, the required number of inner samples, for the same value of y , decreases. This means that, subject to the condition $r < 2 - 2/q$ or when $q \rightarrow \infty$, we want to take r as close as possible to 2 to reduce the total number of inner samples needed while still maintaining the same variance convergence rate. On the other hand, if, for example, we only have bounded fourth moments, i.e., $q = 4$, then we must have $r < 3/2$ to maintain the same convergence rate of the variance.

Proof. In this lemma, we are supposing that we have perfect knowledge of d and σ , and hence $\hat{\mathcal{N}} = \mathcal{N}$. Recall that the output of the adaptive algorithm satisfies (2.15). Then, given $N_\ell < 2\mathcal{N}_\ell$, we have

$$\begin{aligned}
 (2.17) \quad \mathbb{E}[N_\ell] &\leq 2N_0 4^\ell \int_0^\infty \max\left(2^{-\ell}, \min\left(1, \left(C^{-1}N_0^{1/2}2^\ell \delta\right)^{-r}\right)\right) \rho(\delta) d\delta \\
 &\leq 2N_0 2^\ell + 2N_0 4^\ell \int_0^\infty \min\left(1, \left(C^{-1}N_0^{1/2}2^\ell \delta\right)^{-r}\right) \rho(\delta) d\delta \\
 &\leq 2N_0 2^\ell + 2N_0 4^\ell \rho_0 \int_0^\infty \min\left(1, \left(C^{-1}N_0^{1/2}2^\ell \delta\right)^{-r}\right) d\delta \\
 &\quad + 2N_0 4^\ell \min\left(1, \left(C^{-1}N_0^{1/2}2^\ell \delta_0\right)^{-r}\right) \\
 &\leq 2N_0 2^\ell + 2CN_0^{1/2} \rho_0 \frac{r}{r-1} 2^\ell + 2C^r N_0^{(2-r)/2} \delta_0^{-r} 2^{(2-r)\ell},
 \end{aligned}$$

where we first used (2.7) and then (2.8). Since $2 - r < 1$, we have $\mathbb{E}[N_\ell] = \mathcal{O}(2^\ell)$.

On the other hand, by (2.12),

$$\begin{aligned}
 \text{Var}\left[\mathbb{H}\left(\hat{\mathbb{E}}_{N_\ell}(Y)\right) - \mathbb{H}(\mathbb{E}[X | Y])\right] &\leq \mathbb{E}\left[\mathbb{P}\left[\left|\hat{\mathbb{E}}_{N_\ell}(Y) - \mathbb{E}[X | Y]\right| > d \mid Y\right]\right] \\
 &\leq \mathbb{E}\left[\min\left(1, C_q \kappa_q \left(\frac{d}{\sigma} N_\ell^{1/2}\right)^{-q}\right)\right].
 \end{aligned}$$

Using the definition of ν in (2.16) and since $N_\ell \geq \mathcal{N}_\ell$, we have

$$\begin{aligned}
 \text{Var}\left[\mathbb{H}\left(\hat{\mathbb{E}}_{N_\ell}(Y)\right) - \mathbb{H}(\mathbb{E}[X | Y])\right] &\leq \mathbb{E}\left[\min\left(1, C_q \kappa_q C^{-q} \nu^{-q} \left(\frac{N_\ell}{N_0 4^\ell}\right)^{-q/2}\right)\right] \\
 &\leq \mathbb{E}\left[\min\left(1, C_q \kappa_q C^{-q} \nu^{-q} \min\left(2^{\ell q/2}, \max(1, \nu^{rq/2})\right)\right)\right] \\
 &\leq \rho_0 \int_0^\infty \min\left(1, C_q \kappa_q C^{-q} \nu^{-q} \max\left(1, \nu^{rq/2}\right)\right) d\nu \\
 &\quad + \min\left(1, C_q \kappa_q 2^{-\ell q/2} N_0^{-q/2} \delta_0^{-q}\right) \\
 &\leq \rho_0 C N_0^{-1/2} 2^{-\ell} \int_0^\infty \min\left(1, C_q \kappa_q C^{-q} \nu^{-q} \left(1 + \nu^{rq/2}\right)\right) d\nu \\
 &\quad + C_q \kappa_q 2^{-\ell q/2} N_0^{-q/2} \delta_0^{-q},
 \end{aligned}$$

where we first used (2.7) and then changed the variable of integration from δ to ν . The integral in the first term is a constant independent of ℓ and can be computed using (2.8) since $q - rq/2 > 1$. Hence, since $q > 2$ the variance is $\mathcal{O}(2^{-\ell})$. ■

Theorem 2.7 (adaptive sampling with \hat{d} and $\hat{\sigma}$ -estimators). *Let Assumptions 2.1 and 2.4 hold, and consider the estimator (2.5) and the number of samples N_ℓ obtained using Algorithm 1 for*

$$(2.18) \quad 1 < r < 2 - \frac{\sqrt{4q+1}-1}{q}.$$

Assume further that in every iteration of the algorithm given Y , the current number of samples, N_ℓ , and $\{x^{(n)}(Y)\}_{n=1}^{N_\ell}$ being i.i.d. samples of X given Y , we estimate d and σ^2 by

$$(2.19) \quad \hat{d} = |\hat{\mathbf{E}}_{N_\ell}(Y)| = \left| \frac{1}{N_\ell} \sum_{n=1}^{N_\ell} x^{(n)}(Y) \right|$$

$$(2.20) \quad \text{and} \quad \hat{\sigma}^2 = \frac{1}{N_\ell} \sum_{n=1}^{N_\ell} \left(x^{(n)}(Y) - \hat{\mathbf{E}}_{N_\ell}(Y) \right)^2,$$

respectively. Then we have

$$\mathbb{E}[N_\ell] = \mathcal{O}(2^\ell) \quad \text{and} \quad \text{Var} \left[\mathbf{H} \left(\hat{\mathbf{E}}_{N_\ell}(Y) \right) - \mathbf{H}(\mathbb{E}[X | Y]) \right] = \mathcal{O}(2^{-\ell}).$$

Before proving this theorem, we will bound the probability of incurring a given error when estimating the variance, σ^2 , with (2.20).

Corollary 2.8. *Let Assumption 2.4 hold. For a fixed $\ell' = \ell, \dots, 2\ell$ and a given Y , denote by $\hat{\sigma}_{\ell'}$ the estimate of σ computed using $N_0 2^{\ell'}$ samples of X given Y by*

$$(2.21) \quad \hat{\sigma}_{\ell'}^2 = \frac{1}{N_0 2^{\ell'}} \sum_{n=1}^{N_0 2^{\ell'}} \left(x^{(n)}(Y) - \hat{\mathbf{E}}_{N_0 2^{\ell'}}(Y) \right)^2.$$

Then, for any constant $c_1 > 0$, there exists a constant c_2 , depending only on N_0 , κ_q , q , and c_1 , such that

$$\mathbb{P} \left[|\hat{\sigma}_{\ell'}^2 - \sigma^2| > c_1 \sigma^2 \mid Y \right] \leq c_2 2^{-q\ell'/4}.$$

Proof. We can write

$$\hat{\sigma}_{\ell'}^2 = \frac{1}{N_0 2^{\ell'}} \sum_{n=1}^{N_0 2^{\ell'}} \left(x^{(n)}(Y) - \mathbb{E}[X | Y] \right)^2 - \left(\hat{\mathbf{E}}_{N_0 2^{\ell'}}(Y) - \mathbb{E}[X | Y] \right)^2.$$

Next, using Lemma 2.5 and the fact that $\mathbb{E}[(X - \mathbb{E}[X|Y])^2 | Y] = \sigma^2$ yields

$$\begin{aligned}
& \mathbb{P}\left[|\hat{\sigma}_{\ell'}^2 - \sigma^2| > c_1 \sigma^2 \mid Y\right] \\
& \leq \mathbb{P}\left[\left|\frac{1}{N_0 2^{\ell'}} \sum_{n=1}^{N_0 2^{\ell'}} \left(x^{(n)}(Y) - \mathbb{E}[X|Y]\right)^2 - \sigma^2\right| > \frac{1}{2} c_1 \sigma^2 \mid Y\right] \\
& \quad + \mathbb{P}\left[\left|\hat{\mathbb{E}}_{N_0 2^{\ell'}}(Y) - \mathbb{E}[X|Y]\right| > \left(\frac{c_1}{2}\right)^{1/2} \sigma \mid Y\right] \\
& \leq 2^{q/2} C_{q/2} c_1^{-q/2} \kappa_q \left(N_0 2^{\ell'}\right)^{-q/4} \\
& \quad + 2^{q/2} C_q c_1^{-q/2} \kappa_q \left(N_0 2^{\ell'}\right)^{-q/2} \\
& \leq c_2 2^{-q\ell'/4}.
\end{aligned}$$

Corollary 2.9. Let Assumption 2.4 hold and assume that at every iteration in the loop inside Algorithm 1, σ is estimated by $\hat{\sigma}$ as in (2.20). Then, there exists a constant c_3 such that

$$\mathbb{P}\left[|\hat{\sigma}^2 - \sigma^2| > c_1 \sigma^2 \mid Y\right] \leq c_3 2^{-q\ell/4}.$$

In particular, this is true for the final estimate of σ computed in Algorithm 1 before returning N_ℓ .

Proof. Using Corollary 2.8,

$$\begin{aligned}
\mathbb{P}\left[|\hat{\sigma} - \sigma^2| > c_1 \sigma^2 \mid Y\right] & \leq \sum_{\ell'=\ell}^{2\ell} \mathbb{P}\left[|\hat{\sigma}_{\ell'} - \sigma^2| > c_1 \sigma^2 \mid Y\right] \\
& \leq c_2 \sum_{\ell'=\ell}^{2\ell} 2^{-q\ell'/4} \leq \frac{c_2}{1 - 2^{-q/4}} 2^{-q\ell/4}.
\end{aligned}$$

We are now ready to prove Theorem 2.7.

Proof. First, for a given value of Y and a corresponding $\delta = d/\sigma$, assume that, with perfect knowledge of δ , the adaptive algorithm would return $N_0 2^{\ell^*}$ as the number of inner samples for $\ell \leq \ell^* \leq 2\ell$. Given the stopping condition, we have

$$(2.22) \quad \frac{2^{(\ell^*-1)}}{4^\ell} < \left(C^{-1} N_0^{1/2} 2^\ell \delta\right)^{-r} \leq \frac{2^{\ell^*}}{4^\ell},$$

whenever $\ell < \ell^* \leq 2\ell$ for the left inequality and whenever $\ell \leq \ell^* < 2\ell$ for the right inequality. Moreover, suppose that, for a given Y , Algorithm 1 returns $N_\ell = N_0 2^{\hat{\ell}}$ for $\ell \leq \hat{\ell} \leq 2\ell$, and let \hat{d} and $\hat{\sigma}^2$ be the final estimates of d and σ , respectively, that were computed in Algorithm 1. The proof proceeds by analyzing the probability that $\hat{\ell}$ differs significantly from ℓ^* to bound the variance and work. In what follows, the constants in the $\mathcal{O}(\cdot)$ notation depend on κ_q , q , N_0 , C , and r only.

Bounding the work. To bound the work, we consider the case in which the adaptive algorithm terminates on a level ℓ' such that $\ell' \geq \ell^* + 3$ for $\ell \leq \ell^* \leq 2\ell - 3$,—the case of returning too many inner samples, where “too many” means that the adaptive algorithm returned a factor of at least 2^3 more samples than it would have returned had we used d and σ instead of their approximations, \hat{d} and $\hat{\sigma}$, respectively. The choice $\ell^* + 3$ is somewhat arbitrary; $\ell^* + 2$ is the minimum to ensure the positivity of certain terms in the proof, but this particular choice simplifies the subsequent algebra. In any case, $\ell' \geq \ell^* + 3$ implies that the termination condition of the adaptive algorithm was *not* satisfied in each $(\ell'' - \ell)$ th iteration of the algorithm where $\ell^* + 2 \leq \ell'' < \ell'$. This, with the right inequality in (2.22), yields

$$\left(C^{-1}N_0^{1/2}2^{\ell}\hat{\delta}_{\ell''}\right)^{-r} \geq \frac{2^{\ell''}}{4^{\ell}} \geq 4\frac{2^{\ell^*}}{4^{\ell}} \geq 4\left(C^{-1}N_0^{1/2}2^{\ell}\delta\right)^{-r} \implies \hat{\delta}_{\ell''} < 4^{-1/r}\delta,$$

where $\hat{\delta}_{\ell''} = \hat{d}_{\ell''}/\hat{\sigma}_{\ell''}$ and $\hat{d}_{\ell''}$ and $\hat{\sigma}_{\ell''}^2$ denote the Monte Carlo estimates of d and σ^2 , respectively, using $N_0 2^{\ell''}$ inner samples. Then, since the inner samples used in the iterations of Algorithm 1 are mutually independent, we have

$$\begin{aligned} \mathbb{P}[\hat{\ell} = \ell' \mid Y] &\leq \prod_{\ell''=\ell^*+2}^{\ell'-1} \mathbb{P}\left[\frac{d}{\hat{d}_{\ell''}} \cdot \frac{\hat{\sigma}_{\ell''}}{\sigma} > 4^{1/r} \mid Y\right] \\ &\leq \prod_{\ell''=\ell^*+2}^{\ell'-1} \left(\mathbb{P}\left[d > 2^{1/r}\hat{d}_{\ell''} \mid Y\right] + \mathbb{P}\left[\hat{\sigma}_{\ell''}^2 > 4^{1/r}\sigma^2 \mid Y\right]\right) \end{aligned}$$

for any ℓ' such that $\ell' \geq \ell^* + 3$. Using the right inequality in (2.22) and (2.12) yields

$$\begin{aligned} \mathbb{P}\left[d > 2^{1/r}\hat{d}_{\ell''} \mid Y\right] &= \mathbb{P}\left[d - \hat{d}_{\ell''} > \left(1 - 2^{-1/r}\right)d \mid Y\right] \\ &\leq \mathbb{P}\left[\left|\hat{\mathbb{E}}_{N_0 2^{\ell''}}(Y) - \mathbb{E}[X \mid Y]\right| > \left(1 - 2^{-1/r}\right)C\sigma N_0^{-1/2}2^{-\ell}2^{(2\ell-\ell^*)/r} \mid Y\right] \\ &\leq \left(1 - 2^{-1/r}\right)^{-q} C_q \kappa_q C^{-q} 2^{-q((2\ell-\ell^*)/r-(2\ell-\ell'')/2)} \\ &\leq \mathcal{O}(2^{-q(\ell''-\ell^*)/2}). \end{aligned}$$

Moreover, using Corollary 2.9, we have, for any Y ,

$$\begin{aligned} \mathbb{P}\left[\hat{\sigma}_{\ell''}^2 > 4^{1/r}\sigma^2 \mid Y\right] &\leq \mathbb{P}\left[|\hat{\sigma}_{\ell''}^2 - \sigma^2| > (4^{1/r} - 1)\sigma^2 \mid Y\right] \\ &\leq \mathcal{O}(2^{-q(\ell''-\ell^*)/4}). \end{aligned}$$

Hence for any ℓ' such that $\ell^* + 3 \leq \ell' \leq 2\ell$ and $\ell \leq \ell^* \leq 2\ell - 3$, we have

$$(2.23) \quad \mathbb{P}[\hat{\ell} = \ell' \mid Y] \leq \prod_{\ell''=\ell^*+2}^{\ell'-1} \mathcal{O}(2^{-q(\ell''-\ell^*)/4}) \leq \mathcal{O}(2^{-q(\ell'-\ell^*)^2/8}).$$

In general, this bounds $\mathbb{P}[\hat{\ell} = \ell' \mid Y]$ for all $\ell \leq \ell^* \leq 2\ell$ since $\mathbb{P}[\hat{\ell} = \ell' \mid Y] = 0$ for $\ell^* + 3 \leq \ell' \leq 2\ell$ whenever $2\ell - 3 < \ell^* \leq 2\ell$. Next, conditional on Y we compute the expected number of samples,

N_ℓ , as follows:

$$\begin{aligned} \mathbb{E}\left[\frac{N_\ell}{N_0 4^\ell} \mid Y\right] &= \sum_{\ell'=\ell}^{2\ell} \mathbb{P}[N_\ell = N_0 2^{\ell'} \mid Y] 2^{\ell'-2\ell} \\ &\leq 2^{\ell^*+3-2\ell} + \sum_{\ell'=\ell^*+3}^{2\ell} \mathbb{P}[\widehat{\ell} = \ell' \mid Y] 2^{\ell'-2\ell} \\ &\leq 2^{\ell^*+3-2\ell} + \mathcal{O}\left(2^{\ell^*-2\ell}\right) \sum_{\ell'=\ell^*+3}^{2\ell} 2^{-q(\ell'-\ell^*)^2/8+\ell'-\ell^*}, \end{aligned}$$

where we substituted (2.23) in the last step. Since the sum in the previous equation is bounded for any q , we have, using the bound on ℓ^* in (2.22), the fact that $\ell \leq \ell^* \leq 2\ell$, and the definition of ν in (2.16), that

$$\begin{aligned} \mathbb{E}\left[\frac{N_\ell}{N_0 4^\ell} \mid Y\right] &= \mathcal{O}\left(2^{\ell^*-2\ell}\right) \\ &= \mathcal{O}\left(\min\left(1, \max\left(2^{-\ell}, \nu^{-r}\right)\right)\right) \end{aligned}$$

for all values of ν , and a similar calculation to (2.17) gives the desired bound on the overall expected number of inner samples.

Bounding the variance. When bounding the variance, we want to control the probability of $\widehat{\ell}$ being significantly smaller than ℓ^* , i.e., the probability of returning a significantly smaller number of inner samples than we would have returned had we used d and σ instead of their approximations, \widehat{d} and $\widehat{\sigma}$, respectively. In particular, $\widehat{\ell} < \ell^*$ implies that \widehat{d} overestimates d and/or $\widehat{\sigma}$ underestimates σ . We first deal with the latter case by denoting $G_\ell := \mathbb{H}(\widehat{E}_{N_\ell}(Y)) - \mathbb{H}(\mathbb{E}[X \mid Y])$ and writing the variance as

$$\begin{aligned} \text{Var}[G_\ell] &\leq \mathbb{E}[\mathbb{E}[G_\ell^2 \mid Y]] = \mathbb{E}[\mathbb{E}[G_\ell^2 \mid Y, b^2\sigma^2 > \widehat{\sigma}^2] \mathbb{P}[b^2\sigma^2 > \widehat{\sigma}^2 \mid Y]] \\ &\quad + \mathbb{E}[\mathbb{E}[G_\ell^2 \mathbf{1}_{b^2\sigma^2 \leq \widehat{\sigma}^2} \mid Y]] \end{aligned} \quad (2.24)$$

for some constant $0 < b < 1$, independent of ℓ , ℓ^* , and $\widehat{\ell}$. The first term in (2.24) deals with the case when $\widehat{\sigma}$ underestimates σ , while the second term deals with the opposite case. Using Corollary 2.9, we have, for any Y ,

$$\mathbb{P}[b^2\sigma^2 > \widehat{\sigma}^2 \mid Y] \leq \mathbb{P}[|\sigma^2 - \widehat{\sigma}^2| > (1 - b^2)\sigma^2 \mid Y] \leq \mathcal{O}(2^{-q\ell/4}).$$

On the other hand, since the inner samples used to compute G_ℓ are independent from those used to compute N_ℓ , we can bound, for any Y ,

$$\begin{aligned} \mathbb{E}[G_\ell^2 \mid Y, b\sigma^2 > \widehat{\sigma}^2] &= \mathbb{E}[\mathbb{E}[G_\ell^2 \mid N_\ell] \mid Y, b\sigma^2 > \widehat{\sigma}^2] \\ &= \mathbb{E}[\mathbb{P}[|\widehat{E}_{N_\ell}(Y) - \mathbb{E}[X \mid Y]| \geq d \mid N_\ell] \mid Y, b\sigma^2 > \widehat{\sigma}^2] \\ &\leq \mathbb{E}[\min(1, \delta^{-2} N_\ell^{-1}) \mid Y, b\sigma^2 > \widehat{\sigma}^2] \\ &\leq \min(1, \delta^{-2} N_0^{-1} 2^{-\ell}). \end{aligned}$$

Here, we used (2.10), then the fact that $N_\ell \geq N_0 2^\ell$. Taking expectation with respect to Y and using (2.7) and (2.8) we have that

$$\mathbb{E}[\mathbb{E}[G_\ell^2 \mid Y, b\sigma^2 > \hat{\sigma}^2]] \leq 2\rho_0 N_0^{-1/2} 2^{-\ell/2} + \delta_0^{-2} N_0^{-1} 2^{-\ell}.$$

Hence, we have that the first term in (2.24) is $\mathcal{O}(2^{-\ell/2-q\ell/4}) = \mathcal{O}(2^{-\ell})$, since $q \geq 2$.

Now, we turn our attention to the second term in (2.24), where the estimator $\hat{\sigma}$ does not significantly underestimate σ , i.e., given $b^2\sigma^2 \leq \hat{\sigma}^2$. First, for some $p \in (2/(2-r), q)$, we bound by (2.12),

$$\begin{aligned} \mathbb{E}[G_\ell^2 \mathbf{1}_{b^2\sigma^2 \leq \hat{\sigma}^2} \mid Y] &= \mathbb{E}\left[\mathbb{E}[G_\ell^2 \mid Y, \hat{d}, \hat{\sigma}^2] \mathbf{1}_{b^2\sigma^2 \leq \hat{\sigma}^2} \mid Y\right] \\ &\leq \mathbb{E}\left[\mathbb{P}\left[\left|\hat{E}_{N_\ell}(Y) - \mathbb{E}[X \mid Y]\right| > d \mid Y, \hat{d}, \hat{\sigma}^2\right] \mathbf{1}_{b^2\sigma^2 \leq \hat{\sigma}^2} \mid Y\right] \\ &\leq \mathbb{E}\left[\min\left(1, C_p \kappa_p \left(\delta N_\ell^{1/2}\right)^{-p}\right) \mathbf{1}_{b^2\sigma^2 \leq \hat{\sigma}^2} \mid Y\right] \\ &\leq \mathbb{E}\left[\min\left(1, C_p \kappa_p \left(\delta N_\ell^{1/2}\right)^{-p} \mathbf{1}_{b^2\sigma^2 \leq \hat{\sigma}^2}\right) \mid Y\right] \\ &\leq \min\left(1, C_p \kappa_p C^{-p} \nu^{-p} \mathbb{E}\left[\left(\frac{N_\ell}{N_0 4^\ell}\right)^{-p/2} \mathbf{1}_{b^2\sigma^2 \leq \hat{\sigma}^2} \mid Y\right]\right). \end{aligned}$$

Here we used that fact that the inner samples used to compute G_ℓ are independent from those used to compute \hat{d} and $\hat{\sigma}$. We will proceed by bounding the probability of N_ℓ being too small, then using this probability to bound the conditional expectations $\mathbb{E}[(N_\ell/(N_0 4^\ell))^{-p/2} \mathbf{1}_{b^2\sigma^2 \leq \hat{\sigma}^2} \mid Y]$. Finally, we conclude by following the same steps as in the proof of Lemma 2.6. To start, the question we will address is: What is the probability that the adaptive algorithm terminates on a level ℓ' given that $\ell' \leq \ell^* - 3$ and $b^2\sigma^2 \leq \hat{\sigma}^2$? That is, what is the probability of returning too few inner samples, “too few” here meaning that the adaptive algorithm returned a fraction of at most $1/2^3$ samples of what it would have returned had we used d and σ instead of their approximations, \hat{d} and $\hat{\sigma}$, respectively. The choice $\ell^* - 3$ is somewhat arbitrary; $\ell^* - 2$ is the maximum to ensure the positivity of certain terms in the proof, but this particular choice simplifies the subsequent algebra. In any case, $\ell' \leq \ell^* - 3$, the termination condition in Algorithm 1, and the left inequality in (2.22) imply that

$$\left(C^{-1} N_0^{1/2} 2^\ell \hat{\delta}\right)^{-r} \leq \frac{2^{\ell'}}{4^\ell} \leq \frac{1}{4} \cdot \frac{2^{(\ell^*-1)}}{4^\ell} < \frac{1}{4} \left(C^{-1} N_0^{1/2} 2^\ell \delta\right)^{-r} \implies \hat{\delta} > 4^{1/r} \delta$$

for $\ell \leq \ell' \leq \ell^* - 3$ and $\ell + 3 \leq \ell^* \leq 2\ell$. Hence, choosing b such that $4^{-1/r} < b < 1$, we have

$$\begin{aligned} \mathbb{P}[\widehat{\ell} = \ell', b^2 \sigma^2 \leq \widehat{\sigma}^2 \mid Y] &\leq \mathbb{P}\left[\frac{\widehat{d}}{d} \cdot \frac{\sigma}{\widehat{\sigma}} > 4^{1/r}, b^2 \sigma^2 \leq \widehat{\sigma}^2 \mid Y\right] \\ &\leq \mathbb{P}\left[\widehat{d} > 4^{1/r} b d, b^2 \sigma^2 \leq \widehat{\sigma}^2 \mid Y\right] \\ &\leq \mathbb{P}\left[\widehat{d} - d > (1 - 4^{-1/r} b^{-1}) \widehat{d}, b^2 \sigma^2 \leq \widehat{\sigma}^2 \mid Y\right] \\ &\leq \mathbb{P}\left[|\widehat{d} - d| > (b - 4^{-1/r}) C \sigma N_0^{-1/2} 2^{-\ell} 2^{(2\ell - \ell')/r}, b^2 \sigma^2 \leq \widehat{\sigma}^2 \mid Y\right] \\ &\leq \mathbb{P}\left[|\widehat{\mathbb{E}}_{N_0 2^{\ell'}}(Y) - \mathbb{E}[X \mid Y]| > (b - 4^{-1/r}) C \sigma N_0^{-1/2} 2^{-\ell} 2^{(2\ell - \ell')/r} \mid Y\right] \\ &\leq (b - 4^{-1/r})^{-q} C_q \kappa_q C^{-q} 2^{-q(2\ell - \ell')(1/r - 1/2)}. \end{aligned}$$

Moreover, $\mathbb{P}[\widehat{\ell} = \ell' \mid Y] = 0$ for $\ell \leq \ell' \leq \ell^* - 3$ whenever $\ell \leq \ell^* < \ell + 3$. Hence

$$(2.25) \quad \mathbb{P}[\widehat{\ell} = \ell', b^2 \sigma^2 \leq \widehat{\sigma}^2 \mid Y] = \mathcal{O}(2^{-q(2\ell - \ell')(1/r - 1/2)})$$

for $\ell \leq \ell' \leq \ell^* - 3$ and $\ell \leq \ell^* \leq 2\ell$. Now, we have that

$$\begin{aligned} &\mathbb{E}\left[\left(\frac{N_\ell}{N_0 4^\ell}\right)^{-p/2} \mathbf{1}_{b^2 \sigma^2 \leq \widehat{\sigma}^2} \mid Y\right] \\ &= \sum_{\ell'=\ell}^{2\ell} \mathbb{P}[N_\ell = N_0 2^{\ell'}, b^2 \sigma^2 \leq \widehat{\sigma}^2 \mid Y] 2^{p(2\ell - \ell')/2} \\ &\leq 2^{p(2\ell - \ell^* + 2)/2} + \sum_{\ell'=\ell}^{\ell^* - 3} \mathbb{P}[\widehat{\ell} = \ell', b^2 \sigma^2 \leq \widehat{\sigma}^2 \mid Y] 2^{p(2\ell - \ell')/2}. \end{aligned}$$

Substituting (2.25) and denoting $u := q(r - 2)/r + p$ yields

$$\begin{aligned} \mathbb{E}\left[\left(\frac{N_\ell}{N_0 4^\ell}\right)^{-p/2} \mathbf{1}_{b^2 \sigma^2 \leq \widehat{\sigma}^2} \mid Y\right] &\leq 2^{p(2\ell - \ell^* + 2)/2} + \sum_{\ell'=\ell}^{\ell^* - 3} \mathcal{O}(2^{u(2\ell - \ell')/2}) \\ &\leq 2^{p(2\ell - \ell^* + 2)/2} + \mathcal{O}\left(\frac{2^{u(2\ell - \ell^* + 2)/2} - 2^{u\ell/2}}{2^{-u/2} - 1}\right). \end{aligned}$$

Note that $(2 - r)^2 q = 2r$ has roots $r = 2 - (\pm\sqrt{4q + 1} - 1)/q$, and hence from (2.18) we have that $q > 2r/(2 - r)^2$. Therefore, we can choose p to satisfy $2/(2 - r) < p < q(2 - r)/r$, in which case we have $u < 0 < p$ and the previous conditional expectation is $\mathcal{O}(2^{p(2\ell - \ell^*)/2})$ whenever $\ell \leq \ell^* \leq 2\ell$. Using the bound on ℓ^* in (2.22), the fact that $\ell \leq \ell^* \leq 2\ell$, and the definition of ν in (2.16) yields

$$\begin{aligned} \mathbb{E}\left[\left(\frac{N_\ell}{N_0 4^\ell}\right)^{-p/2} \mathbf{1}_{b^2 \sigma^2 \leq \widehat{\sigma}^2} \mid Y\right] &= \mathcal{O}(2^{p(2\ell - \ell^*)/2}) \\ &= \mathcal{O}\left(\max\left(1, \min\left(2^{\ell p/2}, \nu^{rp/2}\right)\right)\right) \end{aligned}$$

for all values of ν . The condition $p > 2/(2-r)$ implies that $r < 2-2/p$, and hence a similar calculation to (2.18) yields that the second term in (2.24) is again $\mathcal{O}(2^{-\ell})$. Hence $\text{Var}[G_\ell] = \mathcal{O}(2^{-\ell})$. ■

3. A model problem. In this section, we will look at a simple example that mimics many of the challenges of computing the probability of a large loss from a financial portfolio. In fact, the underlying model problem can be seen as the loss from a single option with a stock following a Brownian motion and a final payoff function, $f(x) = -x^2$ evaluated at maturity, $T = 1$. This is a model for a delta-hedged portfolio with negative Gamma such that a large loss is incurred with very low probability under extreme circumstances.

Problem setup. Defining, for $\tau \ll 1$,

$$\begin{aligned} P(y, z) &:= -\left(\tau^{1/2} y + (1-\tau)^{1/2} z\right)^2 \\ &= -\tau y^2 - 2\tau^{1/2}(1-\tau)^{1/2} yz - (1-\tau)z^2, \end{aligned}$$

we will compute the following:

$$(3.1) \quad \eta = \mathbb{E}\left[\mathbb{H}\left(\mathbb{E}[P(\tilde{Y}, Z)] - \mathbb{E}[P(Y, Z) | Y] - L_\eta\right)\right],$$

where \tilde{Y} , Y , and Z are independent standard normal random variables, and L_η is a constant. In financial applications, η corresponds to the probability the portfolio loss will exceed a given loss level, L_η , over a short risk horizon, τ , with the portfolio loss defined as the difference between current and future risk-neutral portfolio expectations.

Alternatively, we will later specify $\eta \ll 1$ and determine the corresponding loss level, L_η using the relation (3.1). Note that only the second inner expectation in (3.1) is conditioned on samples of the outer random variable, Y . When approximating the inner expectations for a given Y , we could use the exact value of $\mathbb{E}[P(\tilde{Y}, Z)] = -1$ and set $X := -1 - P(Y, Z) - L_\eta$. However, the variance is $\text{Var}[X | Y] = 4\tau(1-\tau)Y^2 + 2(1-\tau)^2 = \mathcal{O}(1)$. We could also use independent samples of Z to compute both $\mathbb{E}[P(\tilde{Y}, Z)]$ and $\mathbb{E}[P(Y, Z) | Y]$, setting $X := P(\tilde{Y}, \tilde{Z}) - P(Y, Z) - L_\eta$ for independent standard normal variables Z , \tilde{Z} , and \tilde{Y} . The variance would then be $\text{Var}[X | Y] = 2(1-\tau)^2 + 4\tau(1-\tau)Y^2 + 2 = \mathcal{O}(1)$.

Instead, we use the same samples of Z when estimating both inner expectations. Moreover, for increased variance reduction, we also use an antithetic control variate based on the fact that \tilde{Y} is identically distributed to $-\tilde{Y}$. In summary, we set, for a given Y ,

$$\begin{aligned} (3.2) \quad X &:= \frac{1}{2} \left(P(\tilde{Y}, Z) + P(-\tilde{Y}, Z) \right) - P(Y, Z) - L_\eta \\ &= \tau(Y^2 - \tilde{Y}^2) + 2\tau^{1/2}(1-\tau)^{1/2} YZ - L_\eta. \end{aligned}$$

Here again, \tilde{Y} and Z are independent standard normal random variables. The variance in this case is reduced to

$$\sigma^2 = \text{Var}[X | Y] = 2\tau^2 + 4\tau(1-\tau)Y^2 = \mathcal{O}(\tau),$$

and we can also compute analytically

$$d = |\mathbb{E}[X | Y]| = |\tau(Y^2 - 1) - L_\eta|.$$

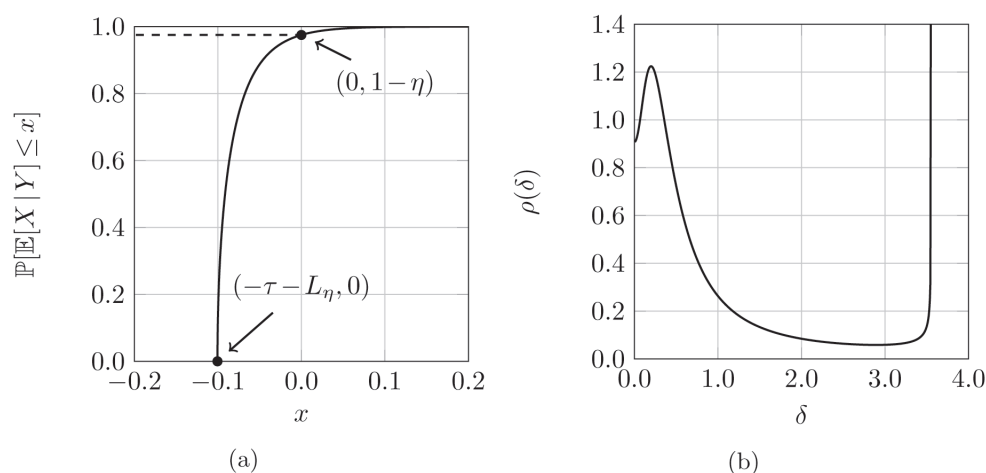


Figure 2. (a) The cumulative distribution function of $\mathbb{E}[X|Y]$ with X as defined in (3.2) and Y a standard normal variable. This figure illustrates the square-root behavior in the neighborhood of $x = -\tau - L_\eta$. Figure (b) shows the density, ρ , of $\delta = d/\sigma$. This figure shows that the density is bounded near 0, hence Assumption 2.1 is satisfied, even though ρ has an inverse-square root singularity near $\delta = 3.5$. For both figures, we use $\tau = 0.02$ and $L_\eta \approx 0.0805$ so that $\eta = 0.025$.

The cumulative distribution function (CDF) of the random variable, $\mathbb{E}[X|Y]$, is

$$\begin{aligned}
 \mathbb{P}[\mathbb{E}[X|Y] \leq x] &= \mathbb{P}\left[\mathbb{E}[P(\tilde{Y}, Z)] - \mathbb{E}[P(Y, Z)|Y] - L_\eta \leq x\right] \\
 &= \mathbb{P}\left[|Y| \leq \left(\frac{\tau + x + L_\eta}{\tau}\right)^{1/2}\right] \\
 &= 1 - 2\Phi\left(-\left(1 + \frac{x + L_\eta}{\tau}\right)^{1/2}\right),
 \end{aligned}
 \tag{3.3}$$

where Φ is the standard normal CDF, and where we substituted $\mathbb{E}[P(\tilde{Y}, Z)] = -1$ and $\mathbb{E}[P(Y, Z)|Y] = -\tau Y^2 - (1 - \tau)$. In particular,

$$\eta = \mathbb{P}[\mathbb{E}[X|Y] \geq 0] = 2\Phi\left(-\left(1 + \frac{L_\eta}{\tau}\right)^{1/2}\right).$$

The interested reader may refer to the supplementary material for more motivation and discussion regarding this model problem. Figure 2(a) shows the CDF of $\mathbb{E}[X|Y]$ and illustrates, as can be seen in the definition of the CDF in (3.3), its square-root behavior in the neighborhood of $x = -\tau - L_\eta$. This square root behavior results in an inverse-square root singularity in the density of $\mathbb{E}[X|Y]$ and also in ρ , the density of δ , which is illustrated in Figure 2(b).

Remark 3.1 (a simple model problem). By relying on the one-dimensional random variable δ and its approximation $\hat{\delta}$, our analysis in section 2.1 includes cases in which X is a function of many random variables and Y is multidimensional, e.g., X is the sum of losses at maturity from the options in a portfolio in excess of some threshold value, and Y is the value of the

underlying stocks. On the other hand, our constructed numerical example has Y being a simple one-dimensional normal random variable and X being a simple function of Y and hence easily sampled. This example is intentionally simplified and is meant to showcase the advantage of combining adaptive sampling with MLMC without the extra complications that dealing with a large portfolio would entail, e.g., the cost of evaluating X due to the large number of assets or the simulation cost of complicated assets.

Verifying the assumptions. As Figure 2(b) shows, despite the inverse square-root singularity near 3.5, the density ρ is bounded near 0, hence Assumption 2.1 is verified. On the other hand, to verify Assumption 2.4, we bound

$$\begin{aligned}\kappa_q &= \sup_y \left\{ \mathbb{E} \left[\frac{|X - \mathbb{E}[X | Y]|^q}{\sigma^q} \mid Y = y \right] \right\} \\ &= \sup_y \frac{\mathbb{E} \left[\left| 2\tau^{1/2}(1-\tau)^{1/2} Zy - \tau(\tilde{Y}^2 - 1) \right|^q \right]}{(2\tau^2 + 4\tau(1-\tau)y^2)^{q/2}} \\ &\leq \sup_y \frac{2^{q-1}2^q\tau^{q/2}(1-\tau)^{q/2}y^q \mathbb{E}[|Z|^q] + 2^{q-1}\tau^q\mathbb{E} \left[\left| \tilde{Y}^2 - 1 \right|^q \right]}{(4\tau(1-\tau)y^2 + 2\tau^2)^{q/2}} \\ &\leq 2^{q-1}\mathbb{E}[|Z|^q] + 2^{q/2-1}\mathbb{E} \left[\left| \tilde{Y}^2 - 1 \right|^q \right] \\ &< \infty\end{aligned}$$

for any $q > 0$.

Antithetic estimators. The MLMC estimator in (2.4) uses independent samples of X , conditioned on the same value of Y , for the fine and coarse estimators of the conditional inner expectation on each MLMC level. We can reduce the variance of the difference by a constant factor by using instead an antithetic estimator [9, 8]. The antithetic estimator uses the same set of independent samples to compute both the coarse and fine approximations. For a deterministic number of inner samples, $N_\ell = N_0 2^\ell$, we observe a variance reduction factor of approximately 3.5 compared to using separate independent samples for the fine and coarse estimators.

To present the antithetic estimator when using an adaptive number of inner samples, as returned by Algorithm 1, first note that since Algorithm 1 returns N_ℓ that is a multiple of $N_{\ell-1}$ or vice versa, then both $\max(N_\ell, N_{\ell-1})/N_\ell$ and $\max(N_\ell, N_{\ell-1})/N_{\ell-1}$ are integers. The antithetic estimator can then be written as

$$(3.4) \quad \hat{\eta} := \sum_{\ell=0}^L \frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \hat{H}_{\ell, N_\ell}^{(\ell, m)}(y^{(\ell, m)}) - \hat{H}_{\ell, N_{\ell-1}}^{(\ell, m)}(y^{(\ell, m)}),$$

where the $\max(N_\ell, N_{\ell-1})$ samples for the level ℓ correction are split into subsets of size N_ℓ and $N_{\ell-1}$ to give the estimator

$$\hat{H}_{\ell, N}^{(\ell, m)}(y) := \frac{N}{\max(N_\ell, N_{\ell-1})} \sum_{i=1}^{\max(N_\ell, N_{\ell-1})/N} H(\hat{E}_{N, i}^{(\ell, m)}(y)).$$

With $\hat{H}_{0,N-1}(\cdot) := 0$, similarly to (2.5), we define

$$(3.5) \quad \hat{E}_{N,i}^{(\ell,m)}(y) := \frac{1}{N} \sum_{n=1}^N x^{(\ell,m,(i-1)N+n)}(y).$$

Here $\{x^{(\ell,m,n)}(y)\}_{n=1}^{\max(N_\ell, N_{\ell-1})}$ are i.i.d. samples of X conditioned on $Y = y$. Moreover, these samples are independent from $x^{(\tilde{\ell}, \tilde{m}, n)}$ for $(\ell, m) \neq (\tilde{\ell}, \tilde{m})$ and any n .

Starting MLMC level. The MLMC estimator in (3.4) includes the levels $0, 1, \dots, L$. However, this might be suboptimal in some cases. To see this, denote

$$G_\ell(y) = \hat{H}_{\ell, N_\ell}(y) - \hat{H}_{\ell, N_{\ell-1}}(y),$$

and let $V_\ell = \text{Var}[G_\ell(Y)]$ and $V_\ell^f = \text{Var}[\hat{H}_{\ell, N_\ell}(Y)]$. Moreover, let $W_\ell = \mathbb{E}[N_\ell]$ denote the expected number of inner samples, which in our case, is the average work required to compute a sample of G_ℓ . Recall that, to approximate a quantity of interest with RMS error ε , the total work of MLMC is approximately [8]

$$\varepsilon^{-2} \left(\sqrt{V_{\ell_0}^f W_{\ell_0}} + \sum_{\ell=\ell_0+1}^L \sqrt{V_\ell W_\ell} \right)^2$$

for $0 \leq \ell_0 < L$. Here, we are assuming that we only include the levels ℓ_0, \dots, L in the MLMC estimator. Then including the level ℓ_0 in the MLMC estimator is optimal if

$$(3.6) \quad R_{\ell_0} := \frac{\sqrt{V_{\ell_0}^f W_{\ell_0}} + \sqrt{V_{\ell_0+1} W_{\ell_0+1}}}{\sqrt{V_{\ell_0+1}^f W_{\ell_0+1}}} \leq 1.$$

Otherwise, discarding that level and starting from $\ell_0 + 1$ would yield less computational work. Note that if $V_\ell^f = V^f$ and $W_\ell \propto 2^{\gamma\ell}$ for all ℓ , then the previous inequality simplifies to

$$V_{\ell_0+1} \leq \left(1 - 2^{-\gamma/2}\right)^2 V^f.$$

For example, for $\gamma = 1$, the variance of the first level-difference, V_{ℓ_0+1} , to be included in the MLMC estimator should be more than 11 times smaller than the variance of the quantity of interest.

To deal with this issue, our MLMC algorithm starts from some level, ℓ_0 , and approximates the variance estimates and average work for levels ℓ_0 and $\ell_0 + 1$ using some small number of outer samples. Then if (3.6) is not satisfied, level ℓ_0 is discarded, and the MLMC algorithm is restarted with the first level being $\ell_0 + 1$. This process is repeated until (3.6) is satisfied.

Results. We apply MLMC with deterministic and adaptive sampling. The deterministic sampling algorithm is run with either $N_\ell = N_0 2^\ell$ or $N_\ell = N_0 4^\ell$ for $N_0 = 32$. On the other hand, the adaptive sampling algorithm is run with different values of $r = 1.25, 1.5$, and 1.75 , the same value of N_0 , and the confidence constant $C = 3$. On every iteration of the adaptive

algorithm, we use the same estimator for d and σ as defined in (2.19) and (2.20), respectively. Our theory on the adaptive sampling method requires bounded q normalized moments, κ_q , for $q > 2r/(2-r)^2$; recall (2.18) in Theorem 2.7. In our tests, we use $r = 1.25, 1.5$, and 1.75 , which requires $q > 4.45, 12$, and 56 , respectively, but recall that for our model problem, κ_q is bounded for all $q \geq 2$. As with Figure 2, we set $\tau := 0.02$ and $L_\eta \approx 0.0805$ so that our goal is to estimate $\eta = 0.025$.

Figure 3(a) shows the average number of used inner samples per level for the different methods. For the adaptive algorithm, the average number of inner samples is around ten times larger than $N_0 2^\ell$, which is used in the deterministic algorithm, but grows at the same rate with respect to ℓ , as proved in Theorem 2.7.

On the other hand, Figure 3(b) plots $V_\ell := \text{Var}[G_\ell]$ and $V_\ell^f := \text{Var}[\hat{H}_{\ell, N_\ell}(Y)]$ versus ℓ . This figure shows that the variance of the MLMC levels with adaptive sampling is the same as the variance when using deterministic sampling with $N_\ell = N_0 4^\ell$, i.e., the variance converges like $\mathcal{O}(2^{-\ell})$ in both cases as proved in Theorem 2.7, even though MLMC with adaptive sampling uses on average fewer inner samples per level. The variance convergence rate of the deterministic algorithm with $N_\ell = N_0 2^\ell$ is shown to be $\mathcal{O}(2^{-\ell/2})$, as proved in Proposition 2.2. Note also that the variance of the quantity of interest, V_ℓ^f , decreases slightly as ℓ increases but converges to the same value for all methods for sufficiently large ℓ .

Figure 3(c) plots $E_\ell := |\mathbb{E}[G_\ell]|$ and $E_\ell^f := |\mathbb{E}[\hat{H}_{\ell, N_\ell}(Y)]|$ versus ℓ . The plot paints the same relative picture as the variance plot Figure 3(b). However, recall that the complexity of MLMC when using adaptive sampling, $\mathcal{O}(\varepsilon^{-2} |\log \varepsilon|^2)$, does *not* depend on the convergence rate of E_ℓ since the variance, V_ℓ , converges at the same rate that the average number of inner samples, $\mathbb{E}[N_\ell]$, increases. For the deterministic algorithm, on the other hand, since $N_\ell = N_0 2^\ell$, $V_\ell = \mathcal{O}(2^{-\ell/2})$, and $E_\ell = \mathcal{O}(2^{-\ell})$, the complexity of MLMC is $\mathcal{O}(\varepsilon^{-5/2})$. When using $N_\ell = N_0 4^\ell$, MLMC has the same complexity.

Figure 3(d) plots the ratio R_ℓ , as defined in (3.6), versus ℓ . This figure shows the first level, ℓ_0 , that should be included in the MLMC estimator for the different methods, namely the first level for which $R_{\ell_0} < 1$. Hence, for the adaptive method, $\ell_0 = 4$ is optimal, while for the deterministic algorithm, $\ell_0 = 2$ when $N_\ell = N_0 4^\ell$ and $\ell_0 = 7$ when $N_\ell = N_0 2^\ell$ are optimal.

Finally, Figure 4(a) shows the total number of used inner samples for the different methods for multiple tolerances. This number corresponds to the total work of each method and includes both the samples that are used to compute the MLMC estimator and the samples that were used in the adaptive algorithm (as detailed in Algorithm 1). This figure, and Figure 4(b), which shows the total running time, verify that the actual work follows the predicted work complexities for each of the considered methods. The running times of the simulations were obtained using a C++ implementation of the adaptive algorithm and the samplers of Y and X . Moreover, CUDA was used to parallelize the computation of the inner and outer samples on a Tesla P100 GPU with 3584 cores.

4. Beyond probabilities. Using the adaptive method that we developed in the previous section and denoting the random variable $L := \mathbb{E}[X | Y]$, for

$$X := \frac{1}{2} \left(P(\tilde{Y}, Z) + P(-\tilde{Y}, Z) \right) - P(Y, Z),$$

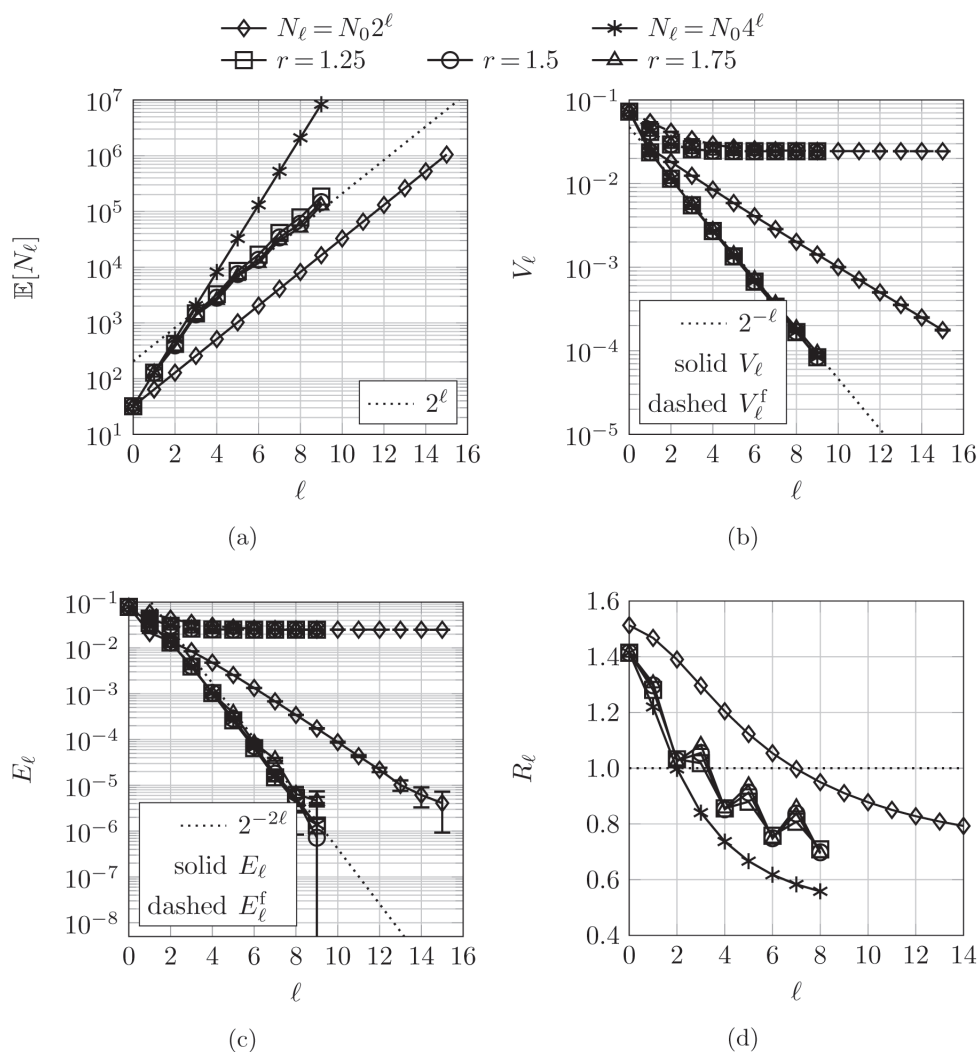


Figure 3. (a) The average number of samples, (b) variance, and (c) absolute error per level for the MLMC estimator of $\mathbb{E}[\mathbb{H}(\mathbb{E}[X|Y])]$ for the model problem described in section 3 using deterministic and adaptive sampling with different values of r . Note that the average number of samples in the adaptive method increases like $\mathcal{O}(2^\ell)$ while the variance decreases like $\mathcal{O}(2^{-\ell})$.

we can estimate

$$\eta = \mathbb{P}[L > L_\eta] = \mathbb{E}[\mathbb{H}(L - L_\eta)]$$

for a given L_η up to an error tolerance ε with complexity $\mathcal{O}(\varepsilon^{-2}|\log \varepsilon|^2)$. Using these estimates, we can solve the inverse problem to find L_η for a given η , i.e., compute the $(1-\eta)$ -quantile. In the context of financial applications, L_η is called the Value-at-Risk (VaR) of a financial portfolio. Finding L_η can be formulated as finding the root of $\hat{f}(L_\eta) = \eta - \mathbb{P}[L > L_\eta]$. To that end, we can use a stochastic root finding algorithm such as the stochastic approximation method [15, 1] and its multilevel extensions [6, 5]. Instead, since X is one-dimensional and since $\mathbb{P}[L > L_\eta]$ is monotonically decreasing with respect to L_η , we use in the current work

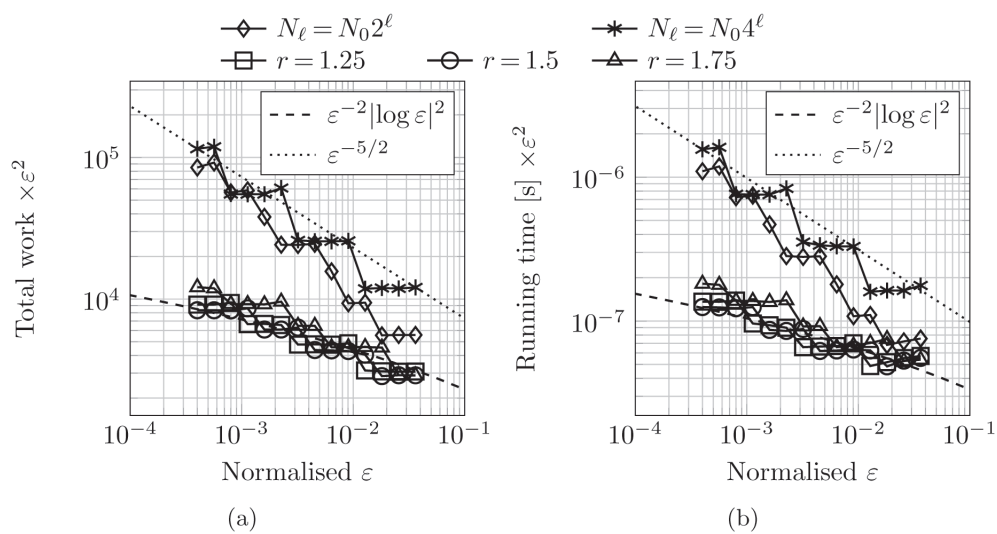


Figure 4. The (a) total work and (b) total running time for the MLMC estimator of $\mathbb{E}[\mathbb{H}(\mathbb{E}[X|Y])]$ versus multiple error tolerances, normalized by the exact value, i.e., η , with deterministic and adaptive sampling. We also plot the expected work complexities in each case, as predicted in theory.

Algorithm 2 Stochastic root-finding algorithm.

Data: $\eta, \varepsilon, \lambda_0, L_0, h_0 > \varepsilon/2$

Result: \hat{L}_η such that $|\hat{L}_\eta - L_\eta| \leq \varepsilon$

$\hat{L}_\eta := L_0$ $\lambda := \lambda_0$ Compute $\hat{\eta} \approx \mathbb{P}[L > \hat{L}_\eta]$ with RMS error λ $h := h_0 \text{ sign}(\hat{\eta} - \eta)$

while $2|h| > \varepsilon$ **do**

$\hat{L}_\eta := \hat{L}_\eta + h$ Compute $\hat{\eta} \approx \mathbb{P}[L > \hat{L}_\eta]$ with RMS error λ

if $h \text{ sign}(\hat{\eta} - \eta) < 0$ **then**

$h := -h/2$

end

if $|\hat{\eta} - \eta| < 3\lambda$ **then**

 set $\lambda := \lambda/2$

end

end

return \hat{L}_η

the simplified algorithm listed in Algorithm 2. The algorithm starts with an estimate of L_η , denoted by \hat{L}_η , then depending on where $\hat{\eta} := \mathbb{P}[L > \hat{L}_\eta]$ lies with respect to η , \hat{L}_η is adjusted. To account for the fact that $\hat{\eta}$ can only be estimated with a specified RMS error tolerance, whenever $\hat{\eta}$ is close to η , the RMS error tolerance is halved. We leave the analysis of the root-finding algorithm and comparison to other algorithms in the literature to future work. Numerically, the complexity of the algorithm seems to be close to $\mathcal{O}(\varepsilon^{-2} |\log \varepsilon|^2)$; see Figure 5.

Another important quantity to compute is $\mathbb{E}[L | L > L_\eta]$ for a given η . In the context of finance application, this quantity is the Conditional Value-at-Risk (CVaR), also known

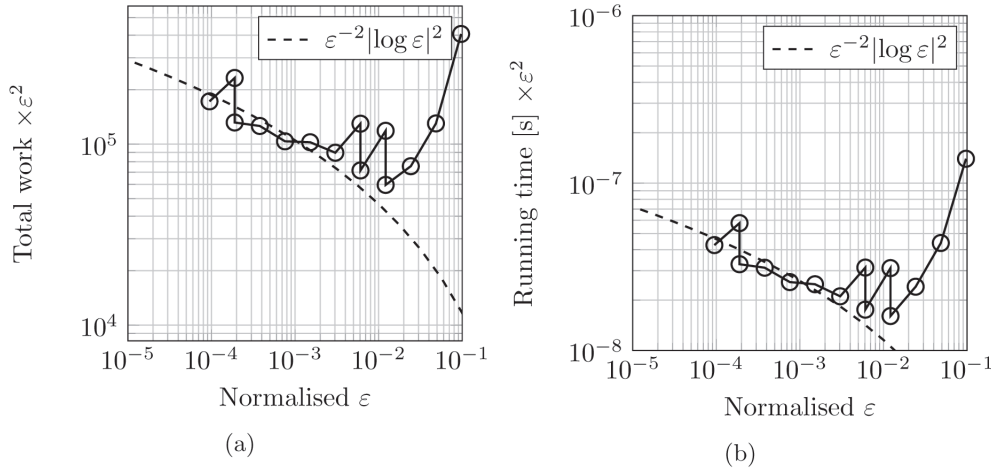


Figure 5. The complexity of [Algorithm 2](#) to compute the L_η that satisfies $\eta = \mathbb{P}[L > L_\eta]$ for a given η . In (a) the total work is the total number of generated samples of X .

as the expected shortfall, which is the expected loss from a portfolio given that the loss exceeds the $(1 - \eta)$ -quantile for a given η . In [16], it was shown that by denoting $f(x) := x + \frac{1}{\eta} \mathbb{E}[\max(L - x, 0)]$, CVaR can be written as $\mathbb{E}[L | L > L_\eta] = f(L_\eta) = \inf_x f(x)$ since, for the cumulative distribution function, $F(x) := \mathbb{P}[L < x]$, and the corresponding probability density function, $\varrho := \frac{dF}{dx}$, we have

$$\begin{aligned} \frac{df(x)}{dx} &= 1 - \frac{1}{\eta} \mathbb{E}[H(L - x)] = 1 - \frac{1 - F(x)}{\eta}, \\ \frac{d^2 f(x)}{dx^2} &= \frac{d}{dF(x)} \left(1 - \frac{1 - F(x)}{\eta} \right) \frac{dF(x)}{dx} = \frac{1}{\eta} \varrho(x) \geq 0, \end{aligned}$$

and $\frac{df(x)}{dx} \big|_{x=L_\eta} = 0$. Hence if L_η is approximated with \hat{L}_η , using, for example, [Algorithm 2](#), and the CVaR value, $f(L_\eta)$, is approximated with $f(\hat{L}_\eta)$, then the error is

$$|f(L_\eta) - f(\hat{L}_\eta)| = \mathcal{O}\left((L_\eta - \hat{L}_\eta)^2\right).$$

That is, an $\mathcal{O}(\varepsilon^{1/2})$ error in the approximation of the VaR, L_η , with $\mathcal{O}(\varepsilon^{-1} |\log \varepsilon|^2)$ complexity yields an $\mathcal{O}(\varepsilon)$ error in the approximation of the CVaR $f(L_\eta) = \mathbb{E}[L | L > L_\eta]$.

To approximate CVaR given \hat{L}_η by computing $f(\hat{L}_\eta)$, we still need to approximate the expectation $\mathbb{E}[\max(\mathbb{E}[X | Y] - \hat{L}_\eta, 0)]$, where the outer expectation is with respect to Y , while the inner conditional expectation is with respect to X . Without loss of generality, we can set $\hat{L}_\eta := 0$ by defining $X_{\text{new}} := X_{\text{old}} - \hat{L}_\eta$. The resulting problem, to compute $\mathbb{E}[\max(\mathbb{E}[X | Y], 0)]$, is similar to (1.1) but with a maximum function instead of a step function. Hence, we can again use the MLMC method, as described [section 2.2](#), with an antithetic sampler, as mentioned in

Remark 2.3 and explained in section 3. Using the notation in section 3, we set

$$(4.1) \quad \hat{H}_{\ell,N}^{(\ell,m)}(y) := \frac{N}{\max(N_\ell, N_{\ell-1})} \sum_{i=1}^{\max(N_\ell, N_{\ell-1})/N} \max(\hat{E}_{N,i}^{(\ell,m)}(y), 0).$$

Note that, for a given y , whenever the estimates $\hat{E}_{N_\ell,i}^{(\ell,m)}(y)$ and $\hat{E}_{N_{\ell-1},i}^{(\ell,m)}(y)$ are positive for all i , then (cf. (3.5))

$$\hat{H}_{\ell,N_\ell}^{(\ell,m)}(y) = \frac{1}{\max(N_\ell, N_{\ell-1})} \sum_{n=1}^{\max(N_\ell, N_{\ell-1})} x^{(\ell,m,n)}(y) = \hat{H}_{\ell,N_{\ell-1}}^{(\ell,m)}(y)$$

and hence the difference $\hat{H}_{\ell,N_\ell}^{(\ell,m)}(y) - \hat{H}_{\ell,N_{\ell-1}}^{(\ell,m)}(y)$ is zero. Similarly, if $\hat{E}_{N_\ell,i}^{(\ell,m)}(y)$ and $\hat{E}_{N_{\ell-1},i}^{(\ell,m)}(y)$ are negative for all i , then the difference is trivially zero. Using a deterministic number of samples $N_\ell = N_0 2^\ell$ results in an error $\mathcal{O}(2^{-\ell/2})$ in estimating the inner expectation, $\mathbb{E}[X|Y]$. Therefore, the two estimates, $\hat{E}_{N_\ell,i}^{(\ell,m)}(y)$ and $\hat{E}_{N_{\ell-1},i}^{(\ell,m)}(y)$, might have different signs whenever the exact value, $\mathbb{E}[X|Y]$, is $\mathcal{O}(2^{-\ell/2})$. Hence the variance of the MLMC difference is $\mathcal{O}(2^{-3\ell/2})$ and its absolute expectation is $\mathcal{O}(2^{-\ell})$. This is made more precise in the following theorem.

Theorem 4.1. Assume that Assumptions 2.1 and 2.4 hold, and assume further that $\mathbb{E}[\sigma^2] < \infty$ and that there exists σ_0 such that $\sigma \leq \sigma_0$ given $\delta < \delta_0$. Then denoting

$$G_\ell := \hat{H}_{\ell,N_\ell}(Y) - \hat{H}_{\ell,N_{\ell-1}}(Y),$$

where $\hat{H}_{\ell,N}$ is defined as in (4.1) and $N_\ell = N_0 2^\ell$, we have

$$\mathbb{E}[|G_\ell|] = \mathcal{O}(N_\ell^{-1}) \quad \text{and} \quad \mathbb{E}[G_\ell^2] = \mathcal{O}(N_\ell^{-\min(3,q)/2}).$$

Comment. The proof follows the same ideas as in [9, Theorem 5.2], where a similar result was derived for an antithetic estimator with respect to time-discretization. The same proof idea was also employed in [3, Theorem 2.3], where the result was shown for the same antithetic estimator considered here, a more generic piecewise linear function, and X being a Bernoulli random variable.

Proof. Since $N_\ell = 2N_{\ell-1}$, the antithetic estimator is

$$G_\ell = \max\left(0, \frac{1}{2} \sum_{i=1}^2 \hat{E}_{N_{\ell-1},i}(Y)\right) - \frac{1}{2} \sum_{i=1}^2 \max(0, \hat{E}_{N_{\ell-1},i}(Y)).$$

For a given Y , define the Bernoulli random variable

$$B = \mathbf{1}_{|\hat{E}_{N_{\ell-1},1}(Y) - \mathbb{E}[X|Y]| \geq |\mathbb{E}[X|Y]| \vee |\hat{E}_{N_{\ell-1},2}(Y) - \mathbb{E}[X|Y]| \geq |\mathbb{E}[X|Y]|},$$

i.e., $B = 1$ whenever $|\hat{E}_{N_{\ell-1},i}(Y) - \mathbb{E}[X|Y]| \geq |\mathbb{E}[X|Y]|$ for $i = 1$ or 2 and zero otherwise. Then for $p = 1$ or 2 ,

$$\mathbb{E}[|G_\ell|^p] = \mathbb{E}[|G_\ell|^p B] + \mathbb{E}[|G_\ell|^p (1 - B)].$$

Considering the second term, when $B = 0$, we have that both $\widehat{\mathbb{E}}_{N_{\ell-1},1}$ and $\widehat{\mathbb{E}}_{N_{\ell-1},2}$ share the same sign. Therefore, in this case, $G_\ell = 0$, and the expected value is zero. On the other hand, for the first term, using Hölder's inequality gives

$$(4.2) \quad \mathbb{E}[G_\ell^p B] = \mathbb{E}\left[\mathbb{E}[G_\ell^p B \mid Y]\right] \leq \mathbb{E}\left[\mathbb{E}[|G_\ell|^q \mid Y]^{p/q} \mathbb{E}[B \mid Y]^{1-p/q}\right],$$

where using (2.12) yields

$$\begin{aligned} \mathbb{E}[B \mid Y] &\leq \sum_{i=1}^2 \mathbb{P}[|\widehat{\mathbb{E}}_{N_{\ell-1},i}(Y) - \mathbb{E}[X \mid Y]| \geq |\mathbb{E}[X \mid Y]|] \\ &\leq 2 \min\left(1, C_q \kappa_q \delta^{-q} N_{\ell-1}^{-q/2}\right). \end{aligned}$$

On the other hand, since $2 \max(0, x) = x + |x|$, we have that

$$\begin{aligned} f(x_1, x_2) &:= \max\left(0, \frac{x_1 + x_2}{2}\right) - \frac{1}{2} \max(0, x_1) - \frac{1}{2} \max(0, x_2) \\ &= \frac{1}{4}(|x_1 + x_2| - |x_1| - |x_2|) \end{aligned}$$

and $f(x_1, x_2) \leq 0$ by the triangular inequality, while

$$\begin{aligned} 4f(x_1, x_2) &= |2x_1 - (x_1 - x_2)| - |x_1| - |x_1 + (x_2 - x_1)| \\ &\geq 2|x_1| - |x_1 - x_2| - |x_1| - |x_1| - |x_2 - x_1| \\ &= -2|x_1 - x_2|. \end{aligned}$$

Therefore,

$$|f(x_1, x_2)| \leq \frac{1}{2}|x_1 - x_2| \leq \frac{1}{2}(|x_1 - x| + |x_2 - x|)$$

for any x . Using this and Jensen's inequality yields

$$\begin{aligned} \mathbb{E}[|G_\ell|^q \mid Y]^{p/q} &\leq \mathbb{E}\left[2^{-q} \left(\sum_{i=1}^2 |\widehat{\mathbb{E}}_{N_{\ell-1},i}(Y) - \mathbb{E}[X \mid Y]|\right)^q \mid Y\right]^{p/q} \\ &\leq 2^{-p/q} \sum_{i=1}^2 \mathbb{E}\left[|\widehat{\mathbb{E}}_{N_{\ell-1},i}(Y) - \mathbb{E}[X \mid Y]|^q \mid Y\right]^{p/q}. \end{aligned}$$

Finally, using Lemma 2.5 yields

$$\mathbb{E}[|G_\ell|^q \mid Y]^{p/q} \leq 2^{1-p/q} C_q^{p/q} \kappa_q^{p/q} \sigma^p N_{\ell-1}^{-p/2} = 4^{1-1/q} C_q^{p/q} \kappa_q^{p/q} \sigma^p N_\ell^{-p/2}.$$

Substituting back into (4.2), there exist constants c_1 , c_2 , and $q' = q(1 - p/q)$, independent of

ℓ , such that

$$\begin{aligned}
 \mathbb{E}[\mathbb{E}[G_\ell^p B \mid Y]] &\leq c_1 \mathbb{E}\left[\sigma^p N_\ell^{-p/2} \min\left(1, c_2 \delta^{-q'} N_\ell^{-q'/2}\right)\right] \\
 &\leq c_1 N_\ell^{-p/2} \mathbb{E}\left[\sigma^p \min\left(1, c_2 \delta^{-q'} N_\ell^{-q'/2}\right) \mathbf{1}_{\delta < \delta_0}\right] \\
 &\quad + c_1 N_\ell^{-p/2} \mathbb{E}\left[\sigma^p \min\left(1, c_2 \delta^{-q'} N_\ell^{-q'/2}\right) \mathbf{1}_{\delta > \delta_0}\right] \\
 &\leq c_1 N_\ell^{-p/2} \sigma_0^p \mathbb{E}\left[\min\left(1, c_2 \delta^{-q'} N_\ell^{-q'/2}\right) \mathbf{1}_{\delta < \delta_0}\right] \\
 &\quad + c_1 c_2 \delta_0^{-q'} N_\ell^{-1-q'/2} \mathbb{E}[\sigma^p \mathbf{1}_{\delta > \delta_0}] \\
 &\leq c_1 N_\ell^{-p/2} \rho_0 \sigma_0^p \int_0^\infty \min\left(1, c_2 \delta^{-q'} N_\ell^{-q'/2}\right) d\delta \\
 &\quad + c_1 c_2 \delta_0^{-q'} N_\ell^{-1-q'/2} \mathbb{E}[\sigma^p] \\
 &\leq \frac{q'}{q'-1} c_1 c_2^{1/q'} \rho_0 \sigma_0^p N_\ell^{-(p+1)/2} + c_1 c_2 \delta_0^{-q'} N_\ell^{-1-q'/2} \mathbb{E}[\sigma^p].
 \end{aligned}$$

Substituting q' and assuming that $\mathbb{E}[\sigma^p]$ is bounded yields

$$\mathbb{E}[G_\ell^p B] \leq \mathcal{O}(N^{-\min(p+1, 2-p+q)/2}),$$

which gives the two results for $p = 1$ or 2 and $q > 2$. ■

Hence, for $q > 2$, the complexity of the resulting MLMC method is then $\mathcal{O}(\varepsilon^{-2})$ since $\alpha = 1$ and $\beta > \gamma = 1$, using the notation of [8]. This complexity was also shown in [3]. This is also the optimal complexity of MLMC. Therefore, using adaptive sampling does not improve the complexity. Nevertheless, we can use exactly the same adaptive [Algorithm 1](#) to select a random number of samples, N_ℓ , depending on Y . We omit the analysis of the resulting MLMC method and refer instead to the numerical results in [Figure 6](#). This figure shows that the variance and absolute errors converge like $\mathcal{O}(2^{-3\ell})$ and $\mathcal{O}(2^{-2\ell})$, respectively, when using an adaptive number of samples. Even though this is faster than $\mathcal{O}(2^{-3\ell/2})$ and $\mathcal{O}(2^{-\ell})$, respectively, that are observed when using a deterministic number of samples (and proved in [Theorem 4.1](#)), the overall complexity of the MLMC is the same when using the two sampling methods, as shown in [Figure 6\(d\)](#).

5. Conclusions. In this work, we presented an MLMC method for nested expectations with a step function, in which deeper levels use more samples for a Monte Carlo estimator of the inner conditional expectation. We also presented an adaptive algorithm that selects the number of inner samples given a sample of the outer random variable. We showed that under certain assumptions, the variance of the MLMC levels decreases at the same rate that the work increases, and hence the MLMC method achieves a near-optimal $\mathcal{O}(\varepsilon^{-2} |\log \varepsilon|^2)$ complexity for an RMS error tolerance ε . We also showed how our methods can be combined with a root-finding algorithm to compute more complicated risk measures, namely, the VaR and the CVaR, the latter obtained with $\mathcal{O}(\varepsilon^{-2})$ complexity.

The next step in our work is to apply MLMC with adaptive sampling to the problem of estimating the probability of large loss from a financial portfolio consisting of many financial options based on underlying assets described by general SDEs. Using unbiased MLMC,

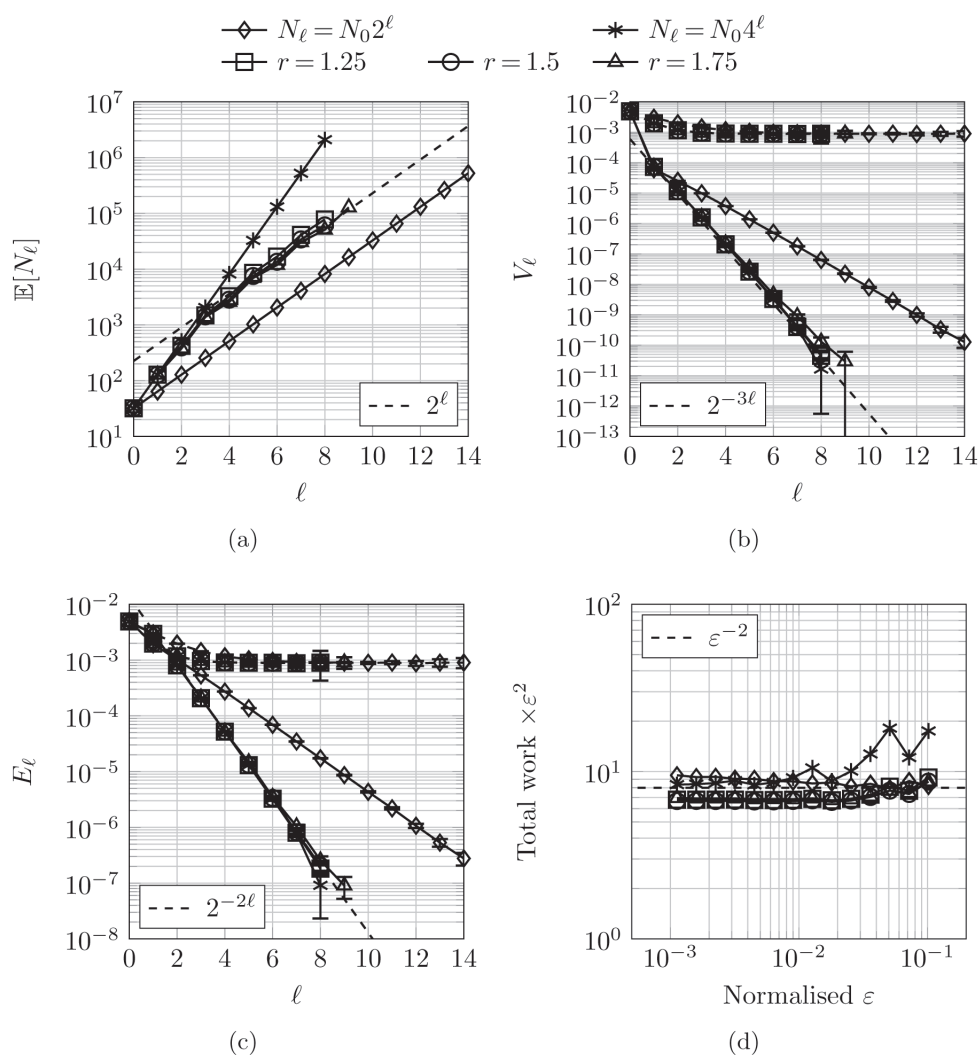


Figure 6. (a) The average number of samples, (b) variance, and (c) absolute error per level for the MLMC estimator of $\mathbb{E}[\max(\mathbb{E}[X|Y, 0])]$ using antithetic deterministic and adaptive sampling with different values of r . Also, (d) shows the total work of the MLMC estimator. We also plot the predicted rates, as discussed in section 4.

this probability can be written as a nested expectation even in the case when paths of the underlying stochastic differential equation must be estimated using a time-stepping scheme. Moreover, various control variates and sampling strategies make computing this probability more efficient. The result is that the complexity of computing CVaR is also $\mathcal{O}(\varepsilon^{-2})$, independent of the number of options in the portfolio.

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