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1 **ADAPTIVE MULTILEVEL MONTE CARLO FOR PROBABILITIES***

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3 **Abstract.** We consider the numerical approximation of $\mathbb{P}[G \in \Omega]$ where the d -dimensional
4 random variable G cannot be sampled directly, but there is a hierarchy of increasingly accurate
5 approximations $\{G_\ell\}_{\ell \in \mathbb{N}}$ which can be sampled. The cost of standard Monte Carlo estimation scales
6 poorly with accuracy in this setup since it compounds the approximation and sampling cost. A direct
7 application of Multilevel Monte Carlo improves this cost scaling slightly, but returns sub-optimal
8 computational complexities since estimation of the probability involves a discontinuous functional of
9 G_ℓ . We propose a general adaptive framework which is able to return the MLMC complexities seen
10 for smooth or Lipschitz functionals of G_ℓ . Our assumptions and numerical analysis are kept general
11 allowing the methods to be used for a wide class of problems. We present numerical experiments on
12 nested simulation for risk estimation, where $G = \mathbb{E}[X|Y]$ is approximated by an inner Monte Carlo
13 estimate. Further experiments are given for digital option pricing, involving an approximation of a
14 d -dimensional SDE.

15 **AMS subject classifications.** 65C05, 62P05

16 **Key words.** Multilevel Monte Carlo, Nested simulation, Risk estimation

17 **1. Introduction.** This paper proposes general, efficient numerical methods to
18 compute

19 (1.1)
$$\mathbb{P}[G \in \Omega] = \mathbb{E}[\mathbb{I}_{G \in \Omega}], \quad \mathbb{I}_{G \in \Omega} := \begin{cases} 1 & G \in \Omega \\ 0 & G \notin \Omega \end{cases},$$

20 within an error tolerance ε , where G is a d -dimensional random variable which cannot
21 be sampled directly and $\mathbb{I}_{G \in \Omega}$ is the indicator of the set Ω . In Subsection 1.1, we
22 relate (1.1) to the one-dimensional problem

23 (1.2)
$$\mathbb{P}[g > 0] = \mathbb{E}[\mathbb{H}(g)],$$

24 where $\mathbb{H}(g)$ is the Heaviside function, equal to 1 when $g \geq 0$ and to 0 otherwise. In
25 most problems of interest, g requires approximate sampling. We assume access to
26 a hierarchy of increasingly accurate approximations $\{g_\ell\}_{\ell \in \mathbb{N}}$ converging to g almost
27 surely as $\ell \rightarrow \infty$. Approximate simulation of g induces a bias in typical Monte Carlo
28 methods for (1.2), increasing the cost of standard Monte Carlo averages. In such
29 situations, Multilevel Monte Carlo (MLMC) [6, 11, 12] is often able to reduce the
30 cost, but is known to suffer when the observable is discontinuous as in (1.1) or (1.2)
31 [9, 10, 13]. Adaptive sampling techniques [5, 9, 13] have proven successful in reducing
32 the cost of Monte Carlo and MLMC for specific instances of (1.2). This paper builds
33 upon such methods to establish a general framework for this problem with an emphasis
34 on ensuring applicability to wide ranging problems. Examples are discussed below.

35 **EXAMPLE 1.1 (Nested Simulation).** *Equation (1.2) often arises in financial risk*
36 *estimation. For example, many risk measures involve conditional expectations of the*
37 *form $g = \mathbb{E}[X|Y]$ for some random variables X, Y [13, 14, 18, 19]. Approximation of*
38 *g by g_ℓ is possible using an inner Monte Carlo average with $N_\ell \in \mathbb{N}$ samples.*

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39 EXAMPLE 1.2 (Digital Option Pricing). *Let S satisfy the d -dimensional SDE*

$$40 \quad dS(t) = a(t, S(t))dt + b(t, S(t))dW(t),$$

41 *for sufficiently smooth functions a and b , and Brownian motion W . For a (European-*
 42 *type) digital option with deterministic maturity $T > 0$, we set $G \equiv S(T)$ and return a*
 43 *unit payoff if $G \in \Omega$ and no payoff otherwise. The (non-discounted) value at time 0*
 44 *of this option is of the form (1.1), where G can be approximately sampled using SDE*
 45 *discretisation methods [21].*

46 A related setup is discussed in [9] and applied in [8] to compute failure properties of
 47 systems governed by PDEs. In [9], the idea of selective refinement is used to adaptively
 48 refine MLMC samples based on the uncertainty of $g > 0$. Selective refinement aims to
 49 reduce the cost of sampling level ℓ without affecting the approximation error of $\mathbb{H}(g)$.
 50 There, it is assumed that the error $|g - g_\ell|$ is bounded when g_ℓ is near zero, excluding
 51 applications like Examples 1.1 and 1.2.

52 There is extensive research into Monte Carlo approximation of nested simulation
 53 problems as in Example 1.1. Analysis of standard Monte Carlo methods for nested
 54 simulation is discussed in [18]. Adaptivity is then combined with standard Monte
 55 Carlo methods for this problem in [5]. Moreover, in [13, 14] adaptive MLMC methods
 56 for nested simulation are discussed. Contrary to the selective refinement algorithm
 57 in [9], these methods aim to improve the approximation error of $\mathbb{H}(g)$ at level ℓ while
 58 the average work of sampling at level ℓ is relatively unaffected. This approach forms
 59 the basis for the present work. Similar results are obtained in [24], where the authors
 60 approximate the inner expectation $\mathbb{E}[X|Y]$ using Quasi-Monte Carlo techniques.

61 An alternative approach to compute (1.2) via MLMC is to approximate $\mathbb{H}(g)$ by a
 62 Lipschitz function. This idea of smoothing the Heaviside function has been employed
 63 successfully in [2, 15, 23]. See also [3], where a polynomial chaos expansion is used to
 64 approximate the indicator function of a random variable. These approaches require an
 65 explicit smoothing step, which the work presented here removes by using adaptivity.

66 The key contributions of this paper are as follows:

- 67 • A generalisation of the adaptive MLMC sampling scheme for nested simula-
 68 tion [13, 14] is presented in Algorithm 3.1. The new procedure requires less
 69 restrictive moment bounds on g and is formulated in a general framework
 70 allowing for applications beyond nested simulation.
- 71 • By reformulating the ideas in [13], we are able to significantly simplify the
 72 analysis compared with the previous work.
- 73 • Numerical experiments show the adaptive MLMC scheme introduced here re-
 74 mains effective for nested simulation, with a slight relaxation of the sampling
 75 process used in [13, 14]. Additional results show the scheme has an equally
 76 strong impact when applied to digital option pricing as in Example 1.2.

77 Subsection 1.1 outlines the problem setup and necessary assumptions for this
 78 analysis, before discussing the link between problems (1.1) and (1.2). We describe
 79 the MLMC approach to (1.2) in Section 2 and show how the complexity of MLMC
 80 suffers because $\mathbb{H}(g)$ is discontinuous. We show how the results can be improved
 81 slightly under stronger assumptions. In Section 3, we introduce the adaptive MLMC
 82 procedure and analyse its benefits to the MLMC complexity. Numerical results are
 83 then presented in Section 4.

84 **1.1. Problem Setup.** For the majority of this paper, we focus on the problem
 85 (1.2). At the end of this section, we discuss how to extend the methods to general
 86 problems of the form (1.1). As is typical for MLMC, we assume the expected sampling

87 cost of g_ℓ , denoted W_ℓ , increases geometrically with ℓ . For ease of notation we use the
 88 operator $f_0 \lesssim f_1$ throughout this paper to denote $f_0 \leq C \cdot f_1$, where C is independent
 89 of ℓ and the error tolerance ε . In particular,

$$90 \quad (1.3) \quad W_\ell \lesssim 2^{\gamma\ell}, \quad \text{for some } \gamma > 0.$$

91 The following assumption controls the strong approximation error of g_ℓ .

92 ASSUMPTION 1.3. *For some $2 < q, \beta > 0$ and positive valued random variable σ_ℓ ,*
 93 *define*

$$94 \quad (1.4) \quad Z_\ell := \frac{g_\ell - g}{\sigma_\ell 2^{-\beta\ell/2}},$$

95 *and assume $\mathbb{E}[|Z_\ell|^q]$ is uniformly bounded in $\ell \geq 0$.*

96 In this context, σ_ℓ represents fluctuations in the approximation uncertainty for a
 97 given instance of g_ℓ . In practice, σ_ℓ will typically form an estimate of the variability
 98 of g_ℓ . For example, in the nested simulation problem (Example 1.1), where $g =$
 99 $\mathbb{E}[X|Y]$, we can take σ_ℓ to be the sample standard deviation of X given Y , as in [13].
 100 Assumption 1.3 allows us to use Markov's inequality to bound

$$101 \quad (1.5) \quad \mathbb{P}[|Z_\ell| \geq x] \leq x^{-q} \mathbb{E}[|Z_\ell|^q]$$

102 for all $x > 0$. This result is used in many proofs within this paper.

103 To implement MLMC successfully, we control the probability of sampling g_ℓ close
 104 to 0. In doing so, we introduce the parameter

$$105 \quad (1.6) \quad \delta_\ell := \frac{g_\ell}{\sigma_\ell},$$

106 which models the sample specific uncertainty in the sign of g_ℓ and thus $\mathbb{H}(g_\ell)$.

107 ASSUMPTION 1.4. *There exists $\delta, \rho_0 > 0$ such that for all $0 < x \leq \delta$ we have*

$$108 \quad \mathbb{P}[|\delta_\ell| < x] \leq \rho_0 x$$

109 *for all $\ell \geq 0$.*

110 Assumptions 1.3 and 1.4 are enough to bound the strong error of approximations
 111 $\mathbb{H}(g_\ell)$, which underpin the complexity theory for MLMC approximation of (1.2).
 112

113 It is important to remark here that the assumptions above allow for the simple
 114 extension to the general problem (1.1) under equivalent assumptions. To see this,
 115 assume that (for $\|\cdot\|$ being the Euclidean norm)

$$116 \quad d_\Omega(G) := \min_{\omega \in \partial\Omega} \{\|G - \omega\|\}$$

117 exists. Here, we are assuming the minimum distance to the boundary of Ω is attained
 118 by a point on the boundary. Then, (1.1) is equivalent to (1.2) when

$$119 \quad g = \bar{d}_\Omega(G) := \begin{cases} d_\Omega(G) & G \in \Omega \\ -d_\Omega(G) & G \notin \Omega \end{cases}$$

120 is a signed distance. If we denote approximations of G at level $\ell \in \mathbb{N}$ by G_ℓ then we
 121 have approximations $g_\ell := \bar{d}_\Omega(G_\ell)$ of g . Assumption 1.3 then holds provided

$$122 \quad \mathbb{E} \left[\left(\frac{\|G - G_\ell\|}{\sigma_\ell 2^{-\beta\ell/2}} \right)^q \right]$$

123 is uniformly bounded in ℓ , since the Euclidean norm is Lipschitz continuous. Assump-
124 tion 1.4 becomes an equivalent condition on the distribution of $|\delta_\ell| = d_\Omega(G_\ell)/\sigma_\ell$.

125 **2. Multilevel Monte Carlo for Probabilities.** In this section, we outline the
126 use of standard MLMC methods [6, 11, 12] for approximating (1.2). In particular,
127 we show that the discontinuity at 0 in the Heaviside function limits the effectiveness
128 of standard MLMC for this problem. Similar arguments from the context of nested
129 simulation can be found in [13, 16, 18]. We begin by approximating $\mathbb{P}[g > 0]$ by
130 $\mathbb{P}[g_L > 0]$, where L should be chosen large enough to control the approximation bias.
131 Sampling g at large levels L is typically expensive. The key idea of MLMC is to split
132 this computation over levels $0 \leq \ell \leq L$ using a telescopic sum. Specifically, using
133 $\mathbb{H}(g_{-1}) := 0$

$$134 \quad (2.1) \quad \begin{aligned} \mathbb{E}[\mathbb{H}(g)] &\approx \mathbb{E}[\mathbb{H}(g_L)] = \sum_{\ell=0}^L \mathbb{E}[\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})] \\ &\approx \sum_{\ell=0}^L \left(\frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \left(\mathbb{H}(g_\ell^{(f,m)}) - \mathbb{H}(g_{\ell-1}^{(c,m)}) \right) \right), \end{aligned}$$

135 where we approximate each expectation in the telescopic sum by an independent
136 Monte Carlo sum with samples $\mathbb{H}(g_\ell^{(f,m)}) - \mathbb{H}(g_{\ell-1}^{(c,m)}) \stackrel{\text{i.i.d.}}{\sim} \mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})$. Samples
137 $g_\ell^{(f,m)}$ and $g_{\ell-1}^{(c,m)}$ should be closely correlated to reduce $\text{Var}[\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})]$, lower-
138 ing the number of samples, M_ℓ required at level ℓ . The following result bounds the
139 total work of sampling (2.1) within a given error tolerance.
140

141 **PROPOSITION 2.1** ([6, 12]). *Let $\{\Delta\mathbb{H}_\ell\}_{\ell=0}^\infty$ be a sequence of random variables*
142 *with $\mathbb{P}[g > 0] = \sum_{\ell=0}^\infty \mathbb{E}[\Delta\mathbb{H}_\ell]$. Assume the following rates of convergence for some*
143 *$\gamma, \beta_{\text{ind}} > 0$, $\alpha_{\text{ind}} \geq \frac{\min(\gamma, \beta_{\text{ind}})}{2}$:*

- 144 • *The expected work of sampling $\Delta\mathbb{H}_\ell$ is $W_\ell \lesssim 2^{\gamma\ell}$.*
- 145 • *The mean and variance of $\Delta\mathbb{H}_\ell$ converge to 0 with the following rates*

$$146 \quad (2.2) \quad E_\ell := |\mathbb{E}[\Delta\mathbb{H}_\ell]| \lesssim 2^{-\alpha_{\text{ind}}\ell}.$$

$$147 \quad (2.3) \quad V_\ell := \text{Var}[\Delta\mathbb{H}_\ell] \lesssim 2^{-\beta_{\text{ind}}\ell},$$

149 *Then, there is optimal L and $\{M_\ell\}_{0 \leq \ell \leq L}$ such that the total work of computing the*
150 *MLMC estimator*

$$151 \quad (2.4) \quad \mathcal{M}_{M_0, \dots, M_L}^L := \sum_{\ell=0}^L \left(\frac{1}{M_\ell} \sum_{m=1}^{M_\ell} \Delta\mathbb{H}_\ell^{(m)} \right), \quad \Delta\mathbb{H}_\ell^{(m)} \stackrel{\text{i.i.d.}}{\sim} \Delta\mathbb{H}_\ell$$

152 *with mean square error satisfying $\mathbb{E}[(\mathbb{P}[g > 0] - \mathcal{M}_{M_0, \dots, M_L}^L)^2] \leq \varepsilon^2$ is*

$$153 \quad \text{Work}(\mathcal{M}_{M_0, \dots, M_L}^L, \varepsilon) \lesssim \begin{cases} \varepsilon^{-2} & \beta_{\text{ind}} > \gamma \\ \varepsilon^{-2} (\log \varepsilon)^2 & \beta_{\text{ind}} = \gamma \\ \varepsilon^{-2 - (\gamma - \beta_{\text{ind}})/\alpha_{\text{ind}}} & \beta_{\text{ind}} < \gamma \end{cases}$$

154 *We will denote the estimator (2.4) with optimal L and $\{M_\ell\}_{0 \leq \ell \leq L}$ by \mathcal{M}^* .*

155 **REMARK 2.2.** *Proposition 2.1 can be applied to the MLMC estimator (2.1) by tak-*
156 *ing $\Delta\mathbb{H}_\ell := \mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})$. In Section 3 we see $\Delta\mathbb{H}_\ell$ take a slightly different form to*

157 accommodate adaptive approximation of g . E_ℓ in (2.2) and V_ℓ in (2.3) are the bias and
 158 variance of the multilevel correction, respectively. Rather than prove convergence rates
 159 for these terms directly, we provide stronger results on $\mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_\ell))^2]$, $|\mathbb{E}[\mathbb{H}(g) -$
 160 $\mathbb{H}(g_\ell)]|$. The bound on $\text{Work}(\mathcal{M}^*; \varepsilon)$ is sometimes referred to as the complexity of
 161 \mathcal{M}^* , since it describe how the total work scales as the error decreases. Replacing $\mathbb{H}(\cdot)$
 162 with a smooth/Lipschitz functional, a similar result to Proposition 2.1 holds [6, 12]
 163 for $\beta_{\text{ind}} = \beta$ and we see ε^{-2} complexity for $\beta > \gamma$, up to an additional bias induced
 164 by the smoothing. In this paper, we refer to ε^{-2} as the ‘canonical’ complexity since it
 165 is the same as seen for standard Monte Carlo with exact sampling of g .

166 The following result provides a bound on $\mathbb{E}[(\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1}))^2]$ under the assump-
 167 tions in Subsection 1.1. The rate is worse than that of smooth/Lipschitz functionals
 168 mentioned in Remark 2.2, since we make an $\mathcal{O}(1)$ approximation error in $\mathbb{H}(g) - \mathbb{H}(g_\ell)$
 169 whenever g, g_ℓ lie on opposite sides of 0.

170 **PROPOSITION 2.3** (Variance With General Assumptions). *By Assumptions 1.3*
 171 *and 1.4 we have $\mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_\ell))^2] \lesssim 2^{-(\frac{q}{q+1})\ell\beta/2}$.*

172 *Proof.* We compute

$$173 \quad \begin{aligned} \mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_\ell))^2] &\leq \mathbb{E}[\mathbb{I}_{|g-g_\ell| \geq |g_\ell|}] \\ &= \mathbb{E}[\mathbb{I}_{|Z_\ell| \geq 2^{\ell\beta/2} |\delta_\ell|}], \end{aligned}$$

174 where Z_ℓ and δ_ℓ are as in (1.4) and (1.6). It follows from Markov’s inequality (1.5)
 175 that, for any $\psi > 0$

$$176 \quad \begin{aligned} \mathbb{E}[\mathbb{I}_{|Z_\ell| \geq 2^{\ell\beta/2} |\delta_\ell|}] &= \mathbb{E}[\mathbb{I}_{|Z_\ell| \geq 2^{\ell\beta/2} |\delta_\ell|} \mathbb{I}_{|\delta_\ell| \leq \psi}] + \mathbb{E}[\mathbb{I}_{|Z_\ell| \geq 2^{\ell\beta/2} |\delta_\ell|} \mathbb{I}_{|\delta_\ell| \geq \psi}] \\ &\leq \mathbb{E}[\mathbb{I}_{|\delta_\ell| \leq \psi}] + \mathbb{E}[\mathbb{I}_{|Z_\ell| \geq 2^{\ell\beta/2} \psi}] \\ &\leq \rho_0 \psi + (2^{\ell\beta/2} \psi)^{-q} \mathbb{E}[|Z_\ell|^q], \end{aligned}$$

177 where we have used Assumption 1.4. Then we set $\psi = \min(1, \delta) 2^{-(\frac{q}{q+1})\ell\beta/2}$ to get the
 178 previous two terms of equal rate, which is the variance convergence rate. \square

179 **REMARK 2.4.** *Proposition 2.3 also proves an upper bound on E_ℓ for $\Delta\mathbb{H}_\ell =$*
 180 *$\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})$ (2.2) since we have $|\mathbb{E}[\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})]| \leq \mathbb{E}[|\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})|] \leq$*
 181 *$\mathbb{E}[(\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1}))^2]$.*

182 **REMARK 2.5.** *All even moments of $\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})$ are equal, thus Proposition 2.3*
 183 *actually proves a bound for all absolute moments of $\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})$. This leads to a*
 184 *large kurtosis of the multilevel correction which can impact the robustness of MLMC*
 185 *and is discussed further in Section 4.*

186 In the context of Proposition 2.1, Proposition 2.3 shows $\beta_{\text{ind}} = (\frac{q}{q+1})\frac{\beta}{2}$ and we
 187 only observe ε^{-2} complexity when $\beta > 2(\frac{q+1}{q})\gamma$. In many examples, including those
 188 discussed here, $\beta \leq 2\gamma$ and we need tight bounds on E_ℓ (2.2) to state accurate com-
 189 plexities. To derive tighter bounds than Remark 2.4 we require further assumptions.

190 **ASSUMPTION 2.6** ([18]). *Let $\rho_\ell(y, z)$ be the joint density of δ_ℓ (1.6) and Z_ℓ (1.4),*
 191 *defined for some $\beta > 0$. Assume that for all ℓ , ρ_ℓ is twice differentiable in y and there*
 192 *exists $p_{i,\ell}(\cdot)$ such that*

$$193 \quad \left| \frac{\partial^i}{\partial y^i} \rho_\ell(y, z) \right| \leq p_{i,\ell}(z), \quad \sup_\ell \int_{\mathbb{R}} |z|^j p_{i,\ell}(z) dz < \infty,$$

194 for $i = 0, 1, 2$ and $0 \leq j \leq q + 2$ for some $q > 2$.

195 ASSUMPTION 2.7. For Z_ℓ, β as in Assumption 1.3, we have $|\mathbb{E}[Z_\ell]| \lesssim 2^{\ell(\beta/2-\alpha)}$,
 196 for some $\frac{\beta}{2} \leq \alpha \leq \beta$.

197 From (1.4) we see that Assumption 2.7 bounds $\mathbb{E}[\sigma_\ell^{-1}(g - g_\ell)] \lesssim 2^{-\alpha\ell}$. Assump-
 198 tion 2.7 is instead expressed in terms of Z_ℓ to align with the analysis in Section 3 (see
 199 Assumption 3.8). We stress that these assumptions are required only to obtain better
 200 convergence rates of E_ℓ . Reasonable results can still be obtained using Remark 2.4
 201 when they are false. Nonetheless, Assumption 2.6 also provides slightly better bounds
 202 for $\mathbb{E}[(\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1}))^2]$. For completeness, we state this result below.

203 PROPOSITION 2.8 (Variance With Strict Assumptions). Under Assumption 2.6
 204 it follows that $\mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_\ell))^2] \lesssim 2^{-\ell\beta/2}$.

205 *Proof.* By Assumption 2.6, we have

$$\begin{aligned} \mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_\ell))^2] &\leq \mathbb{E}[\mathbb{I}_{|Z_\ell| \geq b|\delta_\ell|}] \\ &= \int_{\mathbb{R}} \int_{-2^{-\ell\beta/2}|z|}^{2^{-\ell\beta/2}|z|} \rho_\ell(y, z) dy dz \\ 206 &\leq \int_{\mathbb{R}} \int_{-2^{-\ell\beta/2}|z|}^{2^{-\ell\beta/2}|z|} p_{0,\ell}(z) dy dz \\ &\leq 2 \times 2^{-\ell\beta/2} \int_{\mathbb{R}} |z| p_{0,\ell}(z) dz \\ &\lesssim 2^{-\ell\beta/2}, \end{aligned}$$

207 where we use Assumption 2.6 to bound $\int_{\mathbb{R}} |z| p_{0,\ell}(z) dz$ uniformly in ℓ . \square

208 The stricter conditions also give a tighter bound on the E_ℓ than Remark 2.4, and
 209 hence better MLMC complexity when $\beta < 2\gamma$.

210 PROPOSITION 2.9 ([18, Proposition 1]). Let Assumptions 2.6 and 2.7 hold for
 211 some $\beta > 0$, $\frac{\beta}{2} \leq \alpha \leq \beta$. Then, $|\mathbb{E}[\mathbb{H}(g) - \mathbb{H}(g_\ell)]| \lesssim 2^{-\alpha\ell}$.

212 *Proof.* For $\rho_\ell(y, z)$ given by Assumption 2.6 we have

$$213 \quad \mathbb{E}[\mathbb{H}(g)] = \int_{\mathbb{R}} \int_{2^{-\beta\ell/2}z}^{\infty} \rho_\ell(y, z) dy dz.$$

214 Thus

$$\begin{aligned} |\mathbb{E}[\mathbb{H}(g) - \mathbb{H}(g_\ell)]| &= |\mathbb{E}[\mathbb{H}(g_\ell)] - \mathbb{E}[\mathbb{H}(g)]| \\ 215 &= \left| \int_{\mathbb{R}} \int_0^{2^{-\beta\ell/2}} \rho_\ell(y, z) dy dz \right|. \end{aligned}$$

216 A Taylor expansion gives

$$217 \quad (2.5) \quad \rho_\ell(y, z) = \rho_\ell(0, z) + y \frac{\partial}{\partial y} \rho_\ell(0, z) + \frac{y^2}{2} \frac{\partial^2}{\partial y^2} \rho_\ell(\hat{y}, z),$$

218 for some $\hat{y} \in [0, y]$. Inserting this into the double integral above and using Assump-

219 tions 2.6 and 2.7 gives

$$\begin{aligned}
E_\ell &\leq \left| 2^{-\beta\ell/2} \int_{\mathbb{R}} z \rho_\ell(0, z) dz \right| + 2^{-\beta\ell} \int_{\mathbb{R}} |z|^2 p_{1,\ell}(z) dz \\
&\quad + 2^{-3\beta\ell/2} \int_{\mathbb{R}} |z|^3 p_{2,\ell}(z) dz \\
&\lesssim 2^{-\beta\ell/2} |\mathbb{E}[Z_\ell \mid \delta_\ell = 0]| + \mathcal{O}(2^{-\beta\ell}) \\
&\lesssim 2^{-\alpha\ell},
\end{aligned}$$

221 where we used Assumption 2.7 and the definition of Z_ℓ to bound $\mathbb{E}[Z_\ell \mid \delta_\ell = 0] \lesssim$
222 $2^{\ell(\beta/2-\alpha)}$ and assume $\int_{\mathbb{R}} \rho_\ell(0, z) dz > 0$ as in the proof of Proposition 2.8. \square

223 The discussion above proves the following complexity results.

224 **COROLLARY 2.10.** *Under Assumptions 1.3 and 1.4, the total work required for*
225 *the MLMC estimator (2.1) with mean square error ε^2 can be bounded by*

$$\text{Work}(\mathcal{M}^*; \varepsilon) \lesssim \begin{cases} \varepsilon^{-2} & \beta > 2(\frac{q+1}{q})\gamma \\ \varepsilon^{-2}(\log \varepsilon)^2 & \beta = 2(\frac{q+1}{q})\gamma \\ \varepsilon^{-1-2(\frac{q+1}{q})\gamma/\beta} & \beta < 2(\frac{q+1}{q})\gamma \end{cases}$$

227 *Proof.* The result follows by combining Proposition 2.3 and Remark 2.4 with
228 Proposition 2.1 for $\Delta\mathbb{H}_\ell = \mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})$. \square

229 **COROLLARY 2.11.** *Under Assumption 2.6 and, when $\beta < 2\gamma$, also under Assump-*
230 *tion 2.7 the total work required for the MLMC estimator (2.1) with mean square error*
231 *ε^2 can be bounded by*

$$\text{Work}(\mathcal{M}^*; \varepsilon) \lesssim \begin{cases} \varepsilon^{-2} & \beta > 2\gamma \\ \varepsilon^{-2}(\log \varepsilon)^2 & \beta = 2\gamma \\ \varepsilon^{-2-(\gamma-\beta/2)/\alpha} & \beta < 2\gamma \end{cases}$$

233 *Proof.* The result follows by combining Proposition 2.3 and Proposition 2.9 with
234 Proposition 2.1 for $\Delta\mathbb{H}_\ell = \mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})$. \square

235 In some applications, Assumption 1.3 holds for all $q < \infty$. Under the conditions
236 of Corollary 2.10 and by considering arbitrarily large values of q we then bound the
237 total work by

$$\text{Work}(\mathcal{M}^*; \varepsilon) \lesssim \begin{cases} \varepsilon^{-2} & \beta > 2\gamma \\ \varepsilon^{-1-\nu-2\gamma/\beta} & \beta \leq 2\gamma \end{cases},$$

239 for any $\nu > 0$.

240 For Examples 1.1 and 1.2 with Euler-Maruyama simulation of the SDE, we can
241 show (under certain assumptions on the underlying SDE [21]) that $\alpha = \beta = \gamma$ and the
242 complexity is at best $\varepsilon^{-5/2}$, a significant increase over the canonical ε^{-2} complexity.
243 For SDE simulation we can replace the $\varepsilon^{-\nu}$ term appearing in the complexity in the
244 limit $q \rightarrow \infty$ with a logarithmic factor using the analysis in [1].

245 **3. Adaptive Multilevel Monte Carlo.** In the previous section, we described
246 how the complexity of MLMC calculations for the problem (1.2) is affected by the
247 discontinuous observable $\mathbb{H}(g)$. To improve the performance of MLMC we replace

248 the approximation g_ℓ at level ℓ with $g_{\ell+\eta_\ell}$. Where we introduce the random, non-
 249 negative, integer η_ℓ which should reflect the uncertainty in the sign of $g_{\ell+\eta_\ell}$. The
 250 MLMC estimator (2.4) then uses the multilevel correction term $\Delta\mathbb{H}_\ell$ given by

$$251 \quad (3.1) \quad \Delta\mathbb{H}_\ell := \begin{cases} \mathbb{H}(g_{\ell+\eta_\ell}) - \mathbb{H}(g_{\ell-1+\eta_{\ell-1}}) & \ell > 0 \\ \mathbb{H}(g_{\eta_0}) & \ell = 0 \end{cases}$$

252 Heuristically, approximations which are close to zero with high variability should be
 253 refined further (have larger values of η_ℓ) than approximations which lie far away
 254 from zero with low variability. The chosen approach for sampling $g_{\ell+\eta_\ell}$ is detailed
 255 in Algorithm 3.1. We refine between levels $\ell \leq \ell + \eta_\ell \leq \ell + \lceil\theta\ell\rceil$, for a supplied
 256 parameter θ , based on the value of $|\delta_{\ell+\eta_\ell}|$ (1.6). Algorithm 3.1 also has the parameter
 257 r , determining how strict we are with the refinement, and a confidence constant $c > 0$.
 258 Algorithm 3.1 implies that we refine by η_ℓ levels, where

$$259 \quad (3.2) \quad \eta_\ell = k \iff \begin{cases} |\delta_{\ell+m}| < c2^{\gamma(\theta\ell(1-r)-m)/r} & \forall m \leq k-1 \\ |\delta_{\ell+k}| \geq c2^{\gamma(\theta\ell(1-r)-k)/r} & \text{if } k < \theta\ell \end{cases},$$

260 for $0 \leq k \leq \lceil\theta\ell\rceil$. For small values of r we refine samples to higher levels than for
 261 large r . Ideally, we want to allow the refinement procedure to take r as large as
 262 possible while observing maximum benefit to the MLMC complexity. For the MLMC
 263 computation to converge to the correct mean, it is important that the method of
 264 refining $g_{\ell+k}$ to $g_{\ell+k+1}$ does not affect the almost sure convergence of $g_{\ell+\eta_\ell}$ to g .
 265 To ensure the cost of computing $\sigma_{\ell+k}$ does not dominate the refinement, we assume
 266 throughout that the cost of computing $\sigma_{\ell+k}$ is of order $2^{\gamma(\ell+k)}$.

267 **EXAMPLE 3.1.** *For the nested simulation problem (Example 1.1), we can refine*
 268 *$g_{\ell+k}$ to $g_{\ell+k+1}$ by sampling an additional $N_{\ell+k+1} - N_{\ell+k}$ samples of X given Y to*
 269 *use in the refined Monte Carlo average. Alternatively, we may sample $N_{\ell+k+1}$ new,*
 270 *independent samples of X given the same value of Y to compute $g_{\ell+k+1}$. $\sigma_{\ell+k}$ may*
 271 *be computed as the sample standard deviation of $N_{\ell+k}$ samples.*

272 **EXAMPLE 3.2.** *For digital option pricing (Example 1.2), the underlying Brownian*
 273 *path of the SDE can be refined using the Brownian Bridge construction, and $\sigma_{\ell+k}$ can*
 274 *be chosen to be a constant. See Subsection 4.2 for more details.*

Algorithm 3.1 Adaptive sampling at level ℓ

Input: $\ell, r, \theta, c > 0, \gamma, \beta$
Output: Adaptively refined sample $g_{\ell+\eta_\ell}$
 Set $k = 0$
 Sample (g_ℓ, σ_ℓ)
 Compute δ_ℓ given (g_ℓ, σ_ℓ)
while $|\delta_{\ell+k}| < c2^{\gamma(\theta\ell(1-r)-k)/r}$ and $k < \lceil\theta\ell\rceil$ **do**
 Refine $(g_{\ell+k}, \sigma_{\ell+k})$ to $(g_{\ell+k+1}, \sigma_{\ell+k+1})$
 Compute $\delta_{\ell+k+1}$ given $(g_{\ell+k+1}, \sigma_{\ell+k+1})$
 Set $k = k + 1$
end while
 Set $\eta_\ell = k$
return $g_{\ell+\eta_\ell}$

275 Algorithm 3.1 has many similarities to the adaptive nested simulation algorithm
 276 in [13, 14], which considers the specific case $g = \mathbb{E}[X|Y]$ approximated by an inner

277 Monte Carlo sampler. However, besides being applicable to a wider class of problems,
 278 the present algorithm has some key differences: The nested simulation algorithm in
 279 [13, 14] requires that each refined value $g_{\ell+k+1}$ is independent of the previous term
 280 $g_{\ell+k}$ conditioned on Y , which is not required here. This accelerates the refinement
 281 procedure since one can reuse all terms from the computation of $g_{\ell+k}$ in the refinement
 282 to $g_{\ell+k+1}$. Moreover, in [13] the adaptive algorithm returns only the number of inner
 283 samples one should use to approximate $\mathbb{E}[X|Y]$, given Y , and the estimate of g
 284 should then be computed independently. In contrast, Algorithm 3.1 requires that the
 285 estimate of g matches the output of the refinement process. The parameter θ is also
 286 a novel introduction to Algorithm 3.1. In [13], the nested simulation application has
 287 $\beta = \gamma$ for which the value $\theta = 1$ is optimal (see Lemma 3.7). For $\beta \neq \gamma$ it can
 288 be optimal to refine over a wider or narrower range of levels, see Lemma 3.4 and
 289 Remark 3.5. In [13], the theory requires the stronger assumption that

$$290 \quad \sup_y \mathbb{E} \left[\text{Var}[X|Y]^{-q/2} |X - \mathbb{E}[X|Y]|^q \mid Y = y \right] < \infty,$$

291 for some $2 < q < \infty$ which results in a different analysis to that presented below.
 292 However, for most practical examples the key results are similar.

293 To satisfy (2.2) and (2.3), one must typically correlate the fine and coarse com-
 294 ponents of $\Delta\mathbb{H}_\ell$. The adaptivity introduced in Algorithm 3.1 does not impact this
 295 correlation. In fact, the algorithm can be modified naturally to compute $g_{\ell+\eta_\ell}$ and
 296 $g_{\ell-1+\eta_{\ell-1}}$ simultaneously using correlated noise, provided that $\eta_{\ell-1}$ is also chosen ac-
 297 cording to Algorithm 3.1 with $\ell - 1 \leftarrow \ell$. Since η_ℓ and $\eta_{\ell-1}$ are both chosen according
 298 to Algorithm 3.1, it is worth noting whether it is possible that in some circumstances
 299 the ‘coarse’ estimator $g_{\ell-1+\eta_{\ell-1}}$ is in fact refined further by Algorithm 3.1 than the
 300 ‘fine’ estimator $g_{\ell+\eta_\ell}$. We consider the case where the refinement of the fine esti-
 301 mator $g_{\ell+\eta_\ell}$ is correlated to that of the coarse estimator $g_{\ell-1+\eta_{\ell-1}}$ such that when
 302 $\eta_{\ell-1} = \eta_\ell + 1$ we have $\delta_{\ell+\eta_\ell} = \delta_{\ell-1+\eta_{\ell-1}}$. For example, this is false in the nested
 303 simulation problem discussed in Example 3.1 if one uses independent samples of X
 304 given Y for the fine and coarse estimator, but is true for the digital option problem
 305 considered in Example 3.2 when the fine and coarse estimator use the same underlying
 306 Brownian path. In this case, when $r \leq \theta^{-1} + 1$ it follows from (3.2) that $\eta_{\ell-1} \leq \eta_\ell + 1$.
 307 However, when $r > \theta^{-1} + 1$ there is a small chance that the ‘coarse’ sample, $g_{\ell-1+\eta_{\ell-1}}$,
 308 is actually refined to greater accuracy than the ‘fine’ estimator, $g_{\ell+\eta_\ell}$. Proposition 3.3
 309 below assures that on average $g_{\ell+\eta_\ell}$ has greater accuracy than $g_{\ell-1+\eta_{\ell-1}}$.

310 **3.1. Work Analysis.** In the context of Proposition 2.1, using $\Delta\mathbb{H}_\ell$ as in (3.1)
 311 we wish to improve upon the convergence rate of V_ℓ seen for the estimator (2.1) in
 312 Proposition 2.3. Proposition 2.1 implies that for this to be effective the expected cost
 313 of computing $g_{\ell+\eta_\ell}$ and g_ℓ must be similar. The following result ensures the expected
 314 cost of sampling $g_{\ell+\eta_\ell}$ is also $\mathcal{O}(2^{\gamma\ell})$.

315 **PROPOSITION 3.3** ([13, Theorem 2.7]). *Define η_ℓ as in (3.2) and assume As-*
 316 *sumption 1.4 holds for fixed $\rho_0, \delta > 0$. Provided $r > 1$, we have*

$$317 \quad \mathbb{E} \left[2^{\gamma(\ell+\eta_\ell)} \right] \lesssim 2^{\gamma\ell}.$$

318 *Proof.* We start with

$$\begin{aligned}
\mathbb{E}[2^{\gamma(\ell+\eta_\ell)}] &= \sum_{k=0}^{\lceil \theta \ell \rceil} 2^{\gamma(\ell+k)} \mathbb{P}[\eta_\ell = k] \\
319 \quad &\leq 2^{\gamma \ell} + \sum_{k=1}^{\lceil \theta \ell \rceil} 2^{\gamma(\ell+k)} \mathbb{P}[|\delta_{\ell+k-1}| < c 2^{\gamma(\theta \ell(1-r)-k+1)/r}],
\end{aligned}$$

320 where we used (3.2) to bound the probabilities. Provided $r > 1$, for large enough ℓ
321 we have $c 2^{\gamma(\theta \ell(1-r)-k+1)/r} < \delta$ for all $k \geq 0$. Using Assumption 1.4

$$\begin{aligned}
\mathbb{E}[2^{\gamma(\ell+\eta_\ell)}] &\leq 2^{\gamma \ell} + \rho_0 c 2^{\gamma/r} 2^{\gamma \ell(1+\theta(1-r)/r)} \sum_{k=1}^{\lceil \theta \ell \rceil} 2^{\gamma k(r-1)/r} \\
322 \quad &\leq 2^{\gamma \ell} + c_0 2^{\gamma \ell} 2^{\gamma \ell \theta(1-r)/r} 2^{\gamma \lceil \theta \ell \rceil (r-1)/r} \\
&\lesssim 2^{\gamma \ell},
\end{aligned}$$

323 since $r > 1$. □

324 Note that the above proof emphasises that a larger r value results in a lower
325 sampling cost.

326 **3.2. Analysis of the Variance.** The following results highlight improvements
327 to the convergence of $\mathbb{E}[(\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1}))^2]$ to 0 under the adaptive sampling pro-
328 cedure in Algorithm 3.1. As with the non-adaptive case, we obtain slightly better
329 results using the stronger Assumption 2.6. However, this condition is not essential
330 and we still see an improvement under the general Assumptions 1.3 and 1.4, as seen
331 below.

332 **LEMMA 3.4.** *Let Assumptions 1.3 and 1.4 hold for some $\beta > 0$ and $q > 2$. As-*
333 *sume:*

- 334 • For $\beta \leq (\frac{q+1}{q})\gamma$ we take

$$335 \quad (3.3) \quad \theta = \left(2 \left(\frac{q+1}{q} \right) \frac{\gamma}{\beta} - 1 \right)^{-1},$$

336 and $r < 2\frac{\gamma}{\beta}$.

- 337 • For $\beta > (\frac{q+1}{q})\gamma$ we take $\theta = 1$ and

$$338 \quad (3.4) \quad \begin{cases} r \leq \left(1 - \frac{(q-1)\beta}{2(q+1)\gamma} \right)^{-1} & \text{when } \beta < 2 \left(\frac{q+1}{q-1} \right) \gamma \\ r < \infty & \text{when } \beta \geq 2 \left(\frac{q+1}{q-1} \right) \gamma \end{cases}.$$

339 Then, for $g_{\ell+\eta_\ell}$ given by Algorithm 3.1,

$$340 \quad (3.5) \quad \mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+\eta_\ell}))^2] \lesssim 2^{-(\frac{q}{q+1})\ell\beta(1+\theta)/2}.$$

341 *Proof.* As with the work analysis, we split the calculation across possible values

342 of η_ℓ

$$\begin{aligned}
\mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+\eta_\ell}))^2] &= \sum_{k=0}^{\lceil \theta \ell \rceil} \mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+\eta_\ell}))^2 \mathbb{I}_{\eta_\ell=k}] \\
343 \quad (3.6) \quad &\leq \underbrace{\sum_{k=0}^{\lceil \theta \ell \rceil - 1} \mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+k}))^2 \mathbb{I}_{\eta_\ell=k}]}_{=:\Sigma_0} \\
&\quad + \underbrace{\mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+\lceil \theta \ell \rceil}))^2]}_{=:\Sigma_1}
\end{aligned}$$

344 By Proposition 2.3 we have

$$345 \quad \Sigma_1 \lesssim 2^{-(\frac{q}{q+1})\ell\beta(1+\theta)/2}.$$

346 We now turn our attention to terms for which $k < \lceil \theta \ell \rceil$. Using (3.2) to relate the
347 condition $\eta_\ell = k$ to the value of $\delta_{\ell+k}$ we have

$$\begin{aligned}
\Sigma_0 &\leq \sum_{k=0}^{\lceil \theta \ell \rceil - 1} \mathbb{E}[\mathbb{I}_{|g - g_{\ell+k}| \geq |g_{\ell+k}|} \mathbb{I}_{\eta_\ell=k}] \\
348 \quad &\leq \sum_{k=0}^{\lceil \theta \ell \rceil - 1} \mathbb{E}[\mathbb{I}_{|g - g_{\ell+k}| \geq |g_{\ell+k}|} \mathbb{I}_{|\delta_{\ell+k}| \geq c2^{(\theta\ell(1-r)-k)\gamma/r}}] \\
&\leq \sum_{k=0}^{\lceil \theta \ell \rceil - 1} \mathbb{E}[\mathbb{I}_{a_k \leq |Z_{\ell+k}| b_k^{-1}}]
\end{aligned}$$

349 where $Z_{\ell+k}$ is as in (1.4) and we introduce the terms

$$\begin{aligned}
350 \quad a_k &:= c2^{(\theta\ell(1-r)-k)\gamma/r} \\
b_k &:= 2^{(\ell+k)\beta/2}.
\end{aligned}$$

351 Using Assumption 1.3 and Markov's inequality (1.5) we obtain

$$352 \quad \Sigma_0 \leq \sum_{k=0}^{\lceil \theta \ell \rceil - 1} a_k^{-q} b_k^{-q} \mathbb{E}[|Z_{\ell+k}|^q].$$

353 Thus we restrict our attention to the term

$$354 \quad (3.7) \quad a_k^{-q} b_k^{-q} = 2^{-q(\beta/2 - \gamma/r)(k+\ell)} 2^{-q\gamma\ell(1+\theta - \theta r)/r}.$$

355 Suppose first that $\beta \leq (\frac{q+1}{q})\gamma$. Using the assumption that $r < 2\frac{\gamma}{\beta}$ in this case,
356 (3.7) is an increasing function of k . It follows that

$$\begin{aligned}
357 \quad (3.8) \quad \sum_{k=0}^{\lceil \theta \ell \rceil - 1} a_k^{-q} b_k^{-q} \mathbb{E}[|Z_{\ell+k}|^q] &\lesssim a_{\theta\ell}^{-q} b_{\theta\ell}^{-q} \\
&\lesssim 2^{q\ell(\gamma\theta - \beta(1+\theta)/2)}.
\end{aligned}$$

358 In order to ensure the above term is of the same order as Σ_1 we take θ as in (3.3).

359 Now suppose $\beta > (\frac{q+1}{q})\gamma$ and consider first $r < 2\frac{\gamma}{\beta}$ so that (3.8) holds. Note that
 360 taking $\theta = 1$ is enough to guarantee $\Sigma_1 \lesssim 2^{-(\frac{q}{q+1})\beta\ell}$ and, by (3.8), $\Sigma_0 \lesssim 2^{q\ell(\gamma-\beta)} \leq$
 361 $2^{-(\frac{q}{q+1})\beta\ell}$ since $\beta \geq (\frac{q+1}{q})\gamma$. Since $\beta > (\frac{q+1}{q})\gamma$ this is enough to guarantee ε^{-2}
 362 complexity. If $r = 2\frac{\gamma}{\beta}$ the bound (3.8) becomes (again taking $\theta = 1$)

$$363 \quad \Sigma_0 \leq \sum_{k=0}^{\ell-1} a_k^{-q} b_k^{-q} \mathbb{E}[|Z_{\ell+k}|^q] = \sum_{k=0}^{\ell-1} 2^{q\ell(\gamma-\beta)} \\ \lesssim \ell 2^{q\ell(\gamma-\beta)} \lesssim 2^{-(\frac{q}{q+1})\beta\ell}.$$

364 On the other hand, for $r > \frac{2\gamma}{\beta}$, (3.7) is a decreasing function of k and we have

$$\Sigma_0 \leq \sum_{k=0}^{\ell-1} a_k^{-q} b_k^{-q} \mathbb{E}[|Z_{\ell+k}|^q] \lesssim a_0^{-q} b_0^{-q} \\ 365 \quad \lesssim 2^{q(\gamma(r-1)/r-\beta/2)\ell} \lesssim 2^{-(\frac{q}{q+1})\beta\ell}, \quad \square$$

366 provided we take r as in (3.4), completing the proof.

367 **REMARK 3.5.** *The proof of Lemma 3.4 allows (3.5) to hold for certain values*
 368 *$\theta > 1$ provided $\beta > (\frac{q+1}{q})\gamma$ and under tighter upper bounds for r . However, for such*
 369 *values of β we are already in the ε^{-2} complexity regime of MLMC at $\theta = 1$, thus any*
 370 *increase in θ can improve the MLMC cost by a constant at best. Moreover, tighter*
 371 *bounds on r will increase the expected cost of sampling $g_{\ell+\eta_\ell}$, limiting the value of any*
 372 *constant reduction in the MLMC cost.*

373 **REMARK 3.6.** *As with the non-adaptive MLMC, the absolute moments of $\mathbb{H}(g_\ell) -$*
 374 *$\mathbb{H}(g_{\ell-1})$ are equal, thus Lemma 3.4 actually proves a bound for all even moments of*
 375 *$\mathbb{H}(g_\ell) - \mathbb{H}(g_{\ell-1})$.*

376 Below, we state an extension to Lemma 3.4 under the stricter assumptions re-
 377 quired for the bias analysis.

378 **LEMMA 3.7.** *Let Assumption 2.6 hold for some $\beta > 0$ and $q > 2$. Assume:*

379 • For $\beta \leq \gamma$ we take

$$380 \quad (3.9) \quad \theta = \left(2\frac{\gamma}{\beta} - 1\right)^{-1}, \\ 381 \quad r < 2\frac{\gamma}{\beta} \left(1 - \frac{1}{q}\right).$$

383 • For $\beta > \gamma$ we take $\theta = 1$ and

$$384 \quad (3.10) \quad \begin{cases} r \leq \left(1 - \frac{(q-2)\beta}{2(q-1)\gamma}\right)^{-1} & \text{when } \beta < 2\left(\frac{q-1}{q-2}\right)\gamma \\ r < \infty & \text{when } \beta \geq 2\left(\frac{q-1}{q-2}\right)\gamma \end{cases}.$$

385 Then, for $g_{\ell+\eta_\ell}$ as in Algorithm 3.1

$$386 \quad (3.11) \quad \mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+\eta_\ell}))^2] \lesssim 2^{-\beta\ell \cdot (1+\theta)/2}.$$

387 *Proof.* As in the previous result, we split the calculation across all refined levels as
 388 in (3.6). By Proposition 2.8, it follows that $\Sigma_1 \lesssim 2^{-\beta(1+\theta)\ell/2}$. Moreover, for $k < \lceil \theta \ell \rceil$
 389 and defining a_k, b_k as in the proof of Lemma 3.4 we have

$$\begin{aligned}
 & \mathbb{E} \left[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+k}))^2 \mathbb{I}_{\eta_\ell=k} \right] \\
 &= \mathbb{E} \left[\left(\mathbb{I}_{0 > \delta_{\ell+k} > b_k^{-1} Z_{\ell+k}} + \mathbb{I}_{b_k^{-1} Z_{\ell+k} > \delta_{\ell+k} > 0} \right) \mathbb{I}_{|\delta_{\ell+k}| \geq c \cdot a_k} \right] \\
 390 &= \mathbb{E} \left[\left(\mathbb{I}_{0 > \delta_{\ell+k} > b_k^{-1} Z_{\ell+k}} + \mathbb{I}_{b_k^{-1} Z_{\ell+k} > \delta_{\ell+k} > 0} \right) \mathbb{I}_{b_k^{-1} |Z_{\ell+k}| \geq |\delta_{\ell+k}| \geq c \cdot a_k} \right] \\
 &\leq a_k^{1-q} b_k^{1-q} \mathbb{E} \left[|Z_{\ell+k}|^{q-1} \left(\mathbb{I}_{0 > \delta_{\ell+k} > b_k^{-1} Z_{\ell+k}} + \mathbb{I}_{b_k^{-1} Z_{\ell+k} > \delta_{\ell+k} > 0} \right) \right] \\
 &= a_k^{1-q} b_k^{1-q} \left(\int_0^\infty \int_0^{b_k^{-1} z} |z|^{q-1} \rho_{\ell+k}(y, z) dy dz + \int_{-\infty}^0 \int_{-b_k^{-1} z}^0 |z|^{q-1} \rho_{\ell+k}(y, z) dy dz \right).
 \end{aligned}$$

391 By Assumption 2.6 we can bound $\rho_{\ell+k}(y, z)$ from above by $p_{0, \ell+k}(z)$ and obtain

$$\begin{aligned}
 392 \quad \mathbb{E} \left[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+k}))^2 \mathbb{I}_{\eta_\ell=k} \right] &\lesssim a_k^{1-q} b_k^{-q} \\
 &= 2^{\frac{\gamma}{r}(\ell + \theta \ell(1-r))(1-q)} 2^{((q-1)\gamma/r - q\beta/2)(\ell+k)}.
 \end{aligned}$$

393 When $r < \frac{2\gamma}{\beta}(1 - 1/q)$, this above term is dominant when $k = \lceil \theta \ell \rceil$. It follows that
 394 one can make the orders of Σ_0 and Σ_1 equal as $\ell \rightarrow \infty$ in (3.6) by taking θ as in (3.9).
 395 When $\beta \geq \gamma$, instead we fix $\theta = 1$. A similar calculation to Lemma 3.4 then shows
 396 the result holds provided r satisfies (3.10). \square

397 **3.3. Analysis of the Bias.** In the context of Lemma 3.7, Proposition 2.1 implies
 398 the complexity of (adaptive) MLMC is affected by the convergence rate of $E_\ell =$
 399 $|\mathbb{E}[\mathbb{H}(g) - \mathbb{H}(g_{\ell+\eta_\ell})]|$ whenever $\beta < \gamma$. To improve the rate given by Proposition 2.9
 400 due to adaptive sampling, we make a further assumption.

401 **ASSUMPTION 3.8.** Define $Z_\ell, \beta > 0$ as in Assumption 1.3 and $\frac{\beta}{2} \leq \alpha \leq \beta$ as in
 402 Assumption 2.7. Then, for $j = 0, 1$ and all $\ell \in \mathbb{N}, x \geq 0$ we have

$$403 \quad \left| \mathbb{E} \left[\text{sign}(Z_\ell) |Z_\ell|^j \mid |Z_\ell| \geq x \right] \right| \lesssim 2^{\ell(\beta/2 - \alpha)}.$$

404 By Assumptions 2.6 and 2.7 we know that this condition holds for $j = 1$ and
 405 $x = 0$. Assumption 3.8 ensures that the mean of Z_ℓ converges at the same rate even
 406 when conditioned on taking large values. When $j = 0$ the assumption implies that
 407 the probability of observing large positive Z_ℓ is reasonably close to the probability of
 408 observing large negative Z_ℓ . The necessity for this assumption arises since the refined
 409 samples are only accepted before the maximum level if $|\delta_\ell|$ is sufficiently large. As
 410 such, the error $\mathbb{H}(g) - \mathbb{H}(g_\ell)$ is non-zero only for suitably large values of Z_ℓ . The
 411 resulting improvement to E_ℓ is discussed below.

412 **LEMMA 3.9.** Let Assumptions 2.6 and 3.8 hold for $\beta > 0$ and $\frac{\beta}{2} \leq \alpha \leq \beta$. For
 413 $\beta \leq \gamma$, if we tighten the bound on r in Lemma 3.7 to $r < 2^{\frac{\gamma}{\beta}} \left(\frac{q-2}{q} \right)$, then for $g_{\ell+\eta_\ell}$ as
 414 in Algorithm 3.1 and θ as in (3.9) we have

$$415 \quad |\mathbb{E}[\mathbb{H}(g) - \mathbb{H}(g_{\ell+\eta_\ell})]| \lesssim 2^{-\alpha(1+\theta)\ell}.$$

416 *Proof.* We bound

$$417 \quad |\mathbb{E}[\mathbb{H}(g) - \mathbb{H}(g_{\ell+\eta_\ell})]| \leq \sum_{k=0}^{\lceil \theta \ell \rceil - 1} |\mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+k}))\mathbb{I}_{\eta_\ell=k}]| \\ + |\mathbb{E}[\mathbb{H}(g) - \mathbb{H}(g_{\ell+\lceil \theta \ell \rceil})]|.$$

418 By Proposition 2.9 we know that the final term satisfies

$$419 \quad (3.12) \quad |\mathbb{E}[\mathbb{H}(g) - \mathbb{H}(g_{\ell+\lceil \theta \ell \rceil})]| \lesssim 2^{-\alpha(1+\theta)\ell}.$$

420 By expanding the difference $\mathbb{H}(g) - \mathbb{H}(g_{\ell+k})$ according to when the difference is either
421 ± 1 and considering the event $\eta_\ell = k$ we arrive at

$$\begin{aligned} & |\mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+k}))\mathbb{I}_{\eta_\ell=k}]| \\ &= \left| \mathbb{E} \left[\left(\mathbb{I}_{b_k^{-1}Z_{\ell+k} < \delta_{\ell+k} < 0} - \mathbb{I}_{0 < \delta_{\ell+k} < b_k^{-1}Z_{\ell+k}} \right) \mathbb{I}_{|\delta_{\ell+k}| \geq c \cdot a_k} \right] \right| \\ 422 \quad &= \left| \mathbb{E} \left[\left(\mathbb{I}_{b_k^{-1}Z_{\ell+k} < \delta_{\ell+k} < a_k} - \mathbb{I}_{a_k < \delta_{\ell+k} < b_k^{-1}Z_{\ell+k}} \right) \right] \right| \\ &= \left| \int_{-\infty}^{-b_k a_k} \int_{b_k^{-1}z}^{-a_k} \rho_{\ell+k}(y, z) dy dz - \int_{b_k a_k}^{\infty} \int_{a_k}^{b_k^{-1}z} \rho_{\ell+k}(y, z) dy dz \right|, \end{aligned}$$

423 where a_k, b_k are as in the proof of Lemma 3.4. We again use the Taylor expansion
424 (2.5) on the density $\rho_{\ell+k}(y, z)$. The absolute value of the zero'th-order term is

$$\begin{aligned} & \left| \int_{-\infty}^{-b_k a_k} (-a_k - b_k^{-1}z) \rho_{\ell+k}(0, z) dz + \int_{b_k a_k}^{\infty} (a_k - b_k^{-1}z) \rho_{\ell+k}(0, z) dz \right| \\ & \leq a_k |\mathbb{E}[\text{sign}(Z_{\ell+k})\mathbb{I}_{|Z_{\ell+k}| \geq a_k b_k} |\delta_{\ell+k} = 0]| + b_k^{-1} |\mathbb{E}[Z_{\ell+k}\mathbb{I}_{|Z_{\ell+k}| \geq b_k a_k} |\delta_{\ell+k} = 0]| \\ 425 \quad & \lesssim \mathbb{P}[|Z_{\ell+k}| \geq b_k a_k] \left(a_k \left| \mathbb{E}[\text{sign}(Z_{\ell+k}) \mid |Z_{\ell+k}| \geq b_k a_k, \delta_{\ell+k} = 0] \right| \right. \\ & \quad \left. + b_k^{-1} \left| \mathbb{E}[Z_{\ell+k} \mid |Z_{\ell+k}| \geq b_k a_k, \delta_{\ell+k} = 0] \right| \right) \\ & \lesssim a_k^{1-q} b_k^{-q} 2^{(\ell+k)(\beta/2-\alpha)} \end{aligned}$$

426 where we used Assumption 3.8 and bounded $\mathbb{P}[|Z_{\ell+k}| \geq b_k a_k] \leq a_k^{-q} b_k^{-q} \mathbb{E}[|Z_k|^q]$. For
427 the first-order term, we obtain

$$\begin{aligned} & \left| a_k^2 \int_{-\infty}^{\infty} \mathbb{I}_{|z| \geq b_k a_k} \frac{\partial}{\partial y} \rho_{\ell+k}(0, z) dz - b_k^{-2} \int_{-\infty}^{\infty} \mathbb{I}_{|z| \geq b_k a_k} z^2 \frac{\partial}{\partial y} \rho_{\ell+k}(0, z) dz \right| \\ 428 \quad & \leq \left| b_k^{-q} a_k^{2-q} \int_{-\infty}^{\infty} |z|^q \frac{\partial}{\partial y} \rho_{\ell+k}(0, z) dz - b_k^{-2-q} a_k^{-q} \int_{-\infty}^{\infty} |z|^{2+q} \frac{\partial}{\partial y} \rho_{\ell+k}(0, z) dz \right| \\ & \lesssim b_k^{-q} a_k^{2-q} \end{aligned}$$

429 by Assumption 2.6. Similarly, we can bound the second-order term up to a constant
430 by $a_k^{3-q} b_k^{-q}$. Consequently, we have

$$431 \quad \sum_{k=0}^{\lceil \theta \ell \rceil - 1} |\mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+k}))\mathbb{I}_{\eta_\ell=k}]| \lesssim \sum_{k=0}^{\lceil \theta \ell \rceil - 1} a_k^{1-q} b_k^{-q} 2^{(\ell+k)(\beta/2-\alpha)} + \sum_{k=0}^{\lceil \theta \ell \rceil - 1} a_k^{2-q} b_k^{-q}.$$

432 Provided $r < \frac{2\gamma}{\beta} \frac{q-2}{q}$, the dominant cost of each sum on the right hand side occurs at
 433 $k = \lceil \theta \ell \rceil - 1$, giving

$$434 \quad \sum_{k=0}^{\lceil \theta \ell \rceil - 1} |\mathbb{E}[(\mathbb{H}(g) - \mathbb{H}(g_{\ell+k}))\mathbb{I}_{\eta_{\ell}=k}]| \lesssim a_{\theta \ell}^{1-q} b_{\theta \ell}^{-q} 2^{\ell(1+\theta)(\beta/2-\alpha)} + a_{\theta \ell}^{2-q} b_{\theta \ell}^{-q} \\ \lesssim 2^{-\alpha(1+\theta)\ell} + 2^{-\beta(1+\theta)\ell},$$

435 for θ as in (3.9). □

436 Numerical tests suggest that the previous result does not hold when Assump-
 437 tion 3.8 is false, see Appendix A. However, one can still obtain reasonable convergence
 438 rates of E_{ℓ} without this result by Remark 2.4.

439 **3.4. Bounds on $\text{Work}(\mathcal{M}^*; \varepsilon)$.** We conclude this section with a discussion on
 440 how the improved variance rate given by Lemma 3.4 affects the work bounds of
 441 MLMC. We begin by discussing the impact of adaptive sampling under the weaker
 442 assumptions.

443 **THEOREM 3.10.** *Under the assumptions of Lemma 3.4, the total work of MLMC*
 444 *using adaptive sampling as in Algorithm 3.1 with $\Delta \mathbb{H}_{\ell}$ given by (3.1) is*

$$445 \quad \text{Work}(\mathcal{M}^*; \varepsilon) \lesssim \begin{cases} \varepsilon^{-2} & \beta > (\frac{q+1}{q})\gamma \\ \varepsilon^{-2}(\log \varepsilon)^2 & \beta = (\frac{q+1}{q})\gamma \\ \varepsilon^{-2(\frac{q+1}{q})\gamma/\beta} & \beta < (\frac{q+1}{q})\gamma \end{cases}$$

446 *Proof.* The result follows from applying Proposition 3.3, Lemma 3.4 to Proposi-
 447 tion 2.1, with $\Delta \mathbb{H}_{\ell}$ given by (3.1). Similar to Remark 2.4 we can bound E_{ℓ} using
 448 Lemma 3.4. □

449 This result should be contrasted with Corollary 2.10. In particular, note how
 450 the canonical ε^{-2} complexity is obtained when $\beta > (\frac{q+1}{q})\gamma$ as opposed to when
 451 $\beta > 2(\frac{q+1}{q})\gamma$ for non-adaptive sampling. Moreover, even in the sub-optimal case
 452 when $\beta < (\frac{q+1}{q})\gamma$ the complexity is improved by a factor of ε^{-1} over the non-adaptive
 453 case. Often Assumption 1.3 holds for arbitrary $q < \infty$, in which case one can remove
 454 the q -dependence in Theorem 3.10 by adding a factor $\varepsilon^{-\nu}$ for any $\nu > 0$ to the
 455 complexity whenever $\beta \leq \gamma$. When the assumptions of Lemma 3.9 hold, we obtain a
 456 slightly stronger result.

457 **THEOREM 3.11.** *Under the assumptions of Lemma 3.7 and, when $\beta < \gamma$, under*
 458 *the additional assumptions of Lemma 3.9, the total work of MLMC using adaptive*
 459 *sampling as in Algorithm 3.1 with $\Delta \mathbb{H}_{\ell}$ given by (3.1) is*

$$460 \quad \text{Work}(\mathcal{M}^*; \varepsilon) \lesssim \begin{cases} \varepsilon^{-2} & \beta > \gamma \\ \varepsilon^{-2}(\log \varepsilon)^2 & \beta = \gamma \\ \varepsilon^{-2-(1-\beta/(2\gamma))(\gamma-\beta)/\alpha} & \beta < \gamma \end{cases}$$

461 *Proof.* The result follows by combining Proposition 3.3 and Lemma 3.7 with
 462 Proposition 2.1 for $\Delta \mathbb{H}_{\ell}$ given by (3.1). When $\beta < \gamma$ we use Lemma 3.9 to obtain a
 463 rate for E_{ℓ} . □

464 The previous result should be compared with Corollary 2.11. Again, we can see
 465 optimal complexities for β half as large as in the non-adaptive case. When $\beta < \gamma$ and
 466 $\alpha = \beta$ we can observe an improvement of order $\varepsilon^{-1/2}$ in the complexity.

467 **4. Numerical Experiments.** This section presents several numerical experi-
 468 ments to highlight the preceding theory¹. We begin with some remarks on the tech-
 469 nical components of MLMC.

470 **Optimal Starting Level.** In Section 2 we consider the MLMC estimator start-
 471 ing at level $\ell = 0$. When the approximations g_ℓ have pre-asymptotic behavior at
 472 small levels, it may be more efficient to start from some level $\ell_0 > 0$. For adaptive
 473 sampling, this is not the same as simply adjusting the work required at level $\ell = 0$
 474 by a constant to account for a more accurate starting estimator. To see this, observe
 475 from Algorithm 3.1 that samples at level $\ell = 0$ cannot be refined further. In contrast,
 476 at level $\ell_0 > 0$ samples can be refined to maximum level $\ell_0 + \lceil \theta \ell_0 \rceil$. A heuristic
 477 approach for estimating the optimal starting level by a small computation is given in
 478 [13, Section 3]. We use optimal starting levels to obtain all MLMC estimates in the
 479 following sections.

480 **Error Estimation.** We illustrate the results of previous sections using the av-
 481 erage work of sampling the multilevel correction term, W_ℓ , and the multilevel cor-
 482 rection variance V_ℓ (2.3) and bias E_ℓ (2.2). Typically, V_ℓ and E_ℓ must be estimated
 483 using Monte Carlo sampling within MLMC. The robustness and accuracy of standard
 484 MLMC algorithms [11, 12] depends on reliable estimates of V_ℓ and E_ℓ to determine
 485 the optimal final level L and number of samples per level $\{M_\ell\}_{\ell_0 \leq \ell \leq L^*}$ required to
 486 have mean square error ε^2 . Estimates of V_ℓ using a sample of size M_ℓ have standard
 487 deviation approximately given by $\sqrt{M_\ell^{-1}(\kappa_\ell - 1)\text{Var}[\Delta\mathbb{H}_\ell^2]}$, where κ_ℓ is the kurtosis
 488 of $\Delta\mathbb{H}_\ell$ [12, Section 3.3]. Thus we need $M_\ell \geq \kappa_\ell$ samples to obtain a reliable esti-
 489 mate for V_ℓ . From Remarks 2.5 and 3.6 it follows that $\kappa_\ell \approx V_\ell^{-1}$. Thus, we require
 490 more samples to reliably estimate V_ℓ as ℓ increases, which contradicts the intuition
 491 that MLMC aims to reduce the number of samples required at the finest levels. As a
 492 result, the robustness of MLMC can be affected by poor parameter estimation at the
 493 finest levels. One solution is detailed in [9], where E_ℓ and V_ℓ are approximated by
 494 Bayesian estimation with a beta prior distribution. An alternative solution, and the
 495 one used for the results stated here, is to estimate the proportionality constants in
 496 the bounds on V_ℓ and E_ℓ . We estimate these constants using the continuation MLMC
 497 approach discussed in [7].

498 **4.1. Nested Expectation.** The first numerical experiment is concerned with
 499 multilevel nested simulation [4, 13, 16, 24]. We take $g = \mathbb{E}[X|Y]$ so that (1.2) becomes
 500 $\mathbb{E}[\mathbb{H}(\mathbb{E}[X|Y])]$. Approximations of g at a level ℓ are given by an inner Monte Carlo
 501 estimator

$$502 \quad (4.1) \quad g_\ell = \frac{1}{N_\ell} \sum_{n=1}^{N_\ell} X^{(n)}(Y), \quad X^{(n)}(Y) \stackrel{\text{i.i.d.}}{\sim} X|Y$$

503 using $N_\ell = N_0 2^{\gamma \ell}$ samples. When refining from level $\ell+k$ to $\ell+k+1$ in Algorithm 3.1
 504 we take the $N_{\ell+k}$ samples used to sample $g_{\ell+k}$ and add another $N_{\ell+k}(2^\gamma - 1)$ inde-
 505 pendent samples to form the sample of $g_{\ell+k+1}$. We assume σ_ℓ^2 is given by the sample
 506 variance of the samples used to generate g_ℓ , other choices of σ_ℓ are discussed in Ap-
 507 pendix B. Using this choice of σ_ℓ , we can write Z_ℓ in (1.4) as

$$508 \quad (4.2) \quad Z_\ell = \sqrt{\frac{N_0 N_\ell}{N_\ell - 1}} T_{N_\ell},$$

¹The code used for these experiments is written in Python, and can be found at <https://github.com/JSpence97/mlmc-for-probabilities>.

509 where T_{N_ℓ} is Student's t -statistic with samples $\{X^{(n)}(Y) - \mathbb{E}[X|Y]\}_{n=1}^{N_\ell}$. If the joint
 510 density $\hat{\rho}(x, y)$ of $X - \mathbb{E}[X|Y]$ and Y is bounded and monotone decreasing (increasing)
 511 for large positive (large negative) values of x , it follows from [20, Proposition 5.1,
 512 Theorem 6.2] that for each Y , $\mathbb{E}[|Z_\ell|^q | Y]$ is uniformly bounded in ℓ provided $N_\ell \geq$
 513 $q + 1$. For reasonable X and Y we can extend this to a uniform bound in Y as well as
 514 ℓ , thus proving Assumption 1.3 for $q < N_\ell - 1$ using the Tower Property. By taking
 515 $q < N_\ell - 1$ we recover optimal results from the limit $q \rightarrow \infty$ only as $\ell \rightarrow \infty$. However,
 516 by taking a large enough number of inner samples at level 0, say $N_0 = 32$, we observe
 517 near asymptotic performance even at small levels.

518 Assumption 1.4 would follow by showing that $\delta_\infty := |g|/\sqrt{\text{Var}[X|Y]}$ has a den-
 519 sity which is bounded in some open interval containing 0, as in [13]. We leave a
 520 more rigorous discussion of exact conditions required for the validity of these assump-
 521 tions, and the effect of having $q < N_\ell - 1$ on the complexity of MLMC, to future work.

522

523 For comparison with [13] we consider the model problem used there, given by

$$524 \quad X = \frac{2}{100}(Y^2 - Y_0^2) + \frac{7\sqrt{2}}{25}YY_1 - 0.0805$$

525 for $Y, Y_0, Y_1 \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$. For this problem, one has $\mathbb{E}[\mathbb{H}(\mathbb{E}[X|Y])] \approx 0.025$. In [13]
 526 the use of additional measures such as antithetic sampling of $\Delta\mathbb{H}_\ell$ [4, 13] is considered
 527 to reduce the total cost of MLMC by a constant factor independent of the error bound
 528 ε . Such approaches can easily be altered to suit the present setup. We emphasize
 529 that the key difference between Algorithm 3.1 and the adaptive scheme in [13] for this
 530 setup is that here we do not re-sample all values of $X^{(n)}(Y)$ when refining to higher
 531 levels and the samples generated in Algorithm 3.1 are used to form our estimate of
 532 $g_{\ell+\eta_\ell}$, in contrast to [13, 14].

533 The MLMC estimator is computed using non-adaptive sampling with $\gamma = 1, 2$ and
 534 adaptive sampling as in Algorithm 3.1 with $\gamma = 1$ and $r = 1.95, \theta = 1$ to fulfill the
 535 assumptions of Proposition 3.3 and Lemma 3.4 in the limit $q \rightarrow \infty$. The confidence
 536 constant is taken to be $c = 3/\sqrt{N_0}$, which aligns with the corresponding parameter
 537 in [13]. For each method, we plot W_ℓ, V_ℓ and E_ℓ versus ℓ .

538

539 Results are shown in Figure 4.1. The top left plot shows W_ℓ vs ℓ . By construction,
 540 the work per level for the non-adaptive schemes is a deterministic term proportional to
 541 2^ℓ . For the adaptive scheme and $\ell > 2$, we observe $W_\ell \propto 2^\ell$, increased by a constant
 542 factor over the non-adaptive sampler with $\gamma = 1$. This agrees with Proposition 3.3,
 543 which states that adaptive sampling does not affect the rate at which W_ℓ increases.
 544 The variance V_ℓ per level is shown in the top right plot of Figure 4.1. Following from
 545 Proposition 2.3 with $q \rightarrow \infty$, the non-adaptive samplers have variance decreasing at
 546 rate $\beta/2 \approx \gamma/2$. Instead, the adaptive sampler matches the variance seen for the
 547 non-adaptive method with $\gamma = 2$, as predicted by Lemma 3.4. Moreover, in the
 548 bottom left plot of Figure 4.1, we see that the bias reduction rates guaranteed from
 549 Proposition 2.9 and Lemma 3.9 with $\alpha = \beta$. In other words, the adaptive scheme
 550 exhibits the same variance and bias reduction rate as the non-adaptive method with
 551 $\gamma = 2$, but has expected work per level comparable to the non-adaptive method with
 552 $\gamma = 1$.

553 In the bottom right plot of Figure 4.1, we display the total work of sampling
 554 \mathcal{M}^* multiplied by ε^2 against the accuracy ε , normalised according to the true value
 555 0.025. The total work is taken as the number of inner samples generated from X

556 for a given Y . For each method, we run the algorithm from an estimated optimal
 557 starting level as in [13]. The theoretical complexity rates given by Corollary 2.11 and
 558 Theorems 3.10 and 3.11 for $q \rightarrow \infty$ are plotted as dashed and dotted lines, highlighting
 559 the applicability of the preceding theory to this example. The adaptive approach is
 560 able to reduce the complexity from order $\varepsilon^{-5/2}$ to order $\varepsilon^{-2}(\log \varepsilon)^2$. This is equivalent
 to the performance in [13] and the observed numerical results are similar.

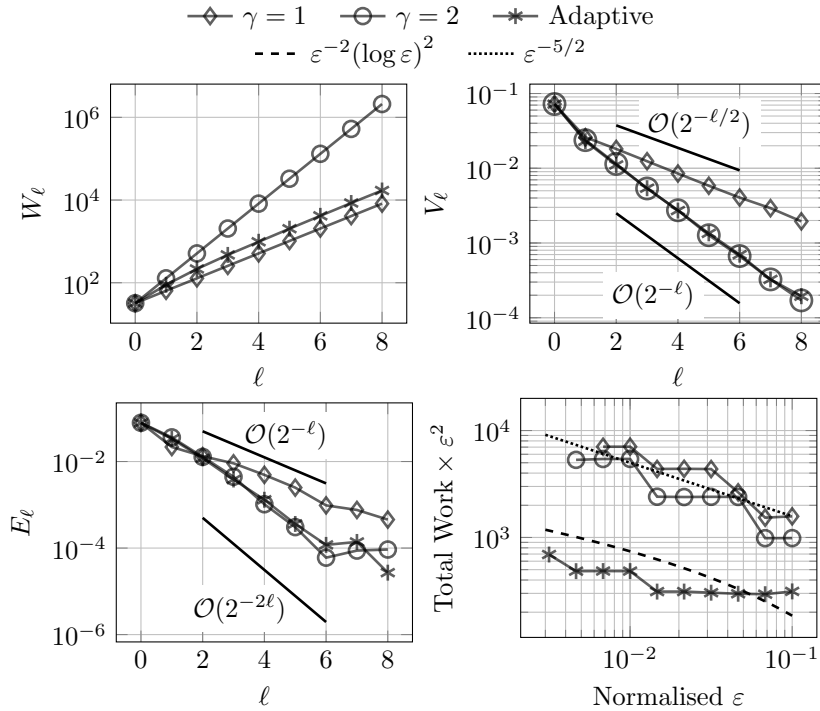


FIG. 4.1. Results for the nested simulation model problem: Expected work per level W_ℓ (top left) taken as expected number of required inner samples from $X|Y$, multilevel correction variance V_ℓ (top right) and bias E_ℓ (bottom left) versus ℓ . The total work of MLMC times ε^2 versus ε , normalised by the true value of the solution (bottom right). Results are given for non-adaptive schemes with $\gamma = 1, 2$ and the adaptive scheme with $r = 1.95$.

561

562 **4.2. Stochastic Differential Equations.** We now consider a setup where g is
 563 determined by d stock prices modeled by the geometric Brownian motions

$$564 \quad (4.3) \quad dS^{(i)}(t) = a_i S^{(i)}(t) dt + b_i S^{(i)}(t) dW^{(i)}(t), \quad 1 \leq i \leq d,$$

565 for constants $a_i, b_i \in \mathbb{R}$ and where the one-dimensional Brownian motions take the
 566 form

$$567 \quad W^{(i)}(t) = \rho W_{\text{com}}(t) + \sqrt{1 - \rho^2} W_{\text{ind}}^{(i)}(t),$$

568 for a correlation coefficient $\rho \in [0, 1]$ and independent Brownian motions $W_{\text{com}}(t)$ and
 569 $\{W_{\text{ind}}^{(i)}(t)\}_{i=1}^d$. Here, $W_{\text{com}}(t)$ models common market noise shared by all of the stocks
 570 whereas $W_{\text{ind}}^{(i)}(t)$ represents idiosyncratic noise of stock i only. Specifically, we set

$$571 \quad (4.4) \quad g = \frac{1}{d} \sum_{i=1}^d S^{(i)}(1) - K,$$

572 so that $\mathbb{P}[g > 0]$ reflects the non-discounted price of a so-called digital option, a
 573 financial derivative which pays a unit price at time 1 if the mean value of the stocks
 574 exceeds K , and nothing otherwise.

575 The approximate samples, g_ℓ , are computed using either Euler-Maruyama or Mil-
 576 stein discretisation of the underlying SDEs with step size $h_\ell = 2^{-\gamma\ell}$. When adaptively
 577 refining samples of g_ℓ we use the Brownian Bridge construction to refine the sampled
 578 Brownian paths conditioned on their existing points [21, Section 1.8]. Specifically,
 579 given W_{nh_ℓ} and $W_{(n+1)h_\ell}$ we can sample the Brownian motion at time $(n + 1/2)h_\ell$
 580 using

$$581 \quad W_{(n+1/2)h_\ell} \stackrel{d}{=} \frac{W_{nh_\ell} + W_{(n+1)h_\ell}}{2} + \sqrt{\frac{h_\ell}{4}} \zeta_n, \quad \text{for } \zeta_n \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1).$$

582 This procedure can be used recursively within Algorithm 3.1 to refine from step-size
 583 $h_{\ell+k}$ to $h_{\ell+k+1} = 2^{-\gamma}h_{\ell+k}$. It follows from the strong convergence results of each
 584 method that Assumption 1.3 holds for all $q < \infty$ using deterministic, constant σ_ℓ and
 585 $\beta = \gamma$ for Euler-Maruyama [21, Theorem 10.2.2] and $\beta = 2\gamma$ for the Milstein scheme
 586 [21, Theorem 10.3.5]. That Assumption 1.4 holds for constant $\sigma_\ell = \sigma$ can be shown
 587 for Euler-Maruyama using [17, Theorem 2.3] to bound the difference in the densities
 588 of g_ℓ and g . The result then follows since g has a bounded density [22, Theorem
 589 10.9.11]. Moreover, from the weak convergence results in [21], we know that Assump-
 590 tion 2.7 holds for both SDE schemes with $\alpha = \beta$. Bounding the variance of $S^{(i)}(1)$
 591 for all instances of $a_i, b_i, S^{(i)}(0)$ we see that $\text{Var}[g] \propto d^{-1}$. Consequently, we choose
 592 $\sigma_\ell = \sigma = d^{-1/2}$.

593

594 We first consider (4.4) for a single stock, $d = 1$. In (4.3), we take $a_1 = 0.05, b_1 =$
 595 0.4 and K is chosen such that $\mathbb{E}[\mathbb{H}(g)] = 0.025$. The terms W_ℓ, V_ℓ, C_ℓ of the MLMC
 596 estimator is shown in Figure 4.2 for Euler and Milstein approximation of g , using
 597 non-adaptive and adaptive simulation. For non-adaptive sampling we consider the
 598 cases $h_\ell = 2^{-\gamma\ell}$ for $\gamma = 1, 2$. The adaptive samplers take $\gamma = \theta = c = 1$. For the
 599 Euler-Maruyama scheme we take $r = 1.95$. Since $\beta = 2\gamma$ for the Milstein scheme,
 600 Lemma 3.4 allows us to take larger values of r and we set $r = 10$ here. W_ℓ is taken
 601 as the expected number of SDE steps required from the fine and coarse estimator
 602 at level ℓ . By construction, the work for both non-adaptive samplers is proportional
 603 to $2^{\gamma\ell}$. The adaptive schemes have $W_\ell \lesssim 2^\ell$ following Proposition 3.3. Note that
 604 the expected work per sample is slightly lower at each level for adaptive sampling
 605 using the Milstein scheme, as the larger value $r = 10$ requires fewer refinements to
 606 be made. For the Euler-Maruyama samplers we see $V_\ell \lesssim 2^{-\gamma\ell/2}$ for the non-adaptive
 607 and $V_\ell \lesssim 2^{-\ell}$ for the adaptive sampler, as expected for $\beta = \gamma$. These bounds are
 608 all squared when using the Milstein scheme since $\beta = 2\gamma$ in this case. Moreover,
 609 we observe $E_\ell \lesssim 2^{-\gamma\ell}$ for the non-adaptive sampler for both SDE schemes, with
 610 $E_\ell \lesssim 2^{-2\ell}$ for the adaptive samplers. This provides evidence that the stronger results
 611 following from Assumptions 2.6, 2.7 and 3.8 hold for the Euler-Maruyama scheme. For
 612 the Milstein scheme, the observed rates of E_ℓ follow immediately from the equivalent
 613 rates on V_ℓ and Remark 2.4.

614 For the non-adaptive schemes with $\gamma = 2$ and the adaptive samplers, we compute
 615 \mathcal{M}^* for various error tolerances ε . In Figure 4.3, we plot the total work (taken as
 616 overall number of SDE time-steps) times ε^2 versus ε , normalized by the true solution.
 617 For the non-adaptive, Euler-Maruyama sampler, we observe a rate close to $\varepsilon^{-5/2}$ as
 618 predicted by Corollary 2.10. This is reduced to $\varepsilon^{-2}(\log \varepsilon)^2$ using adaptive sampling
 619 with the Euler-Maruyama scheme as in Theorem 3.10 for $q \rightarrow \infty$. Note that we

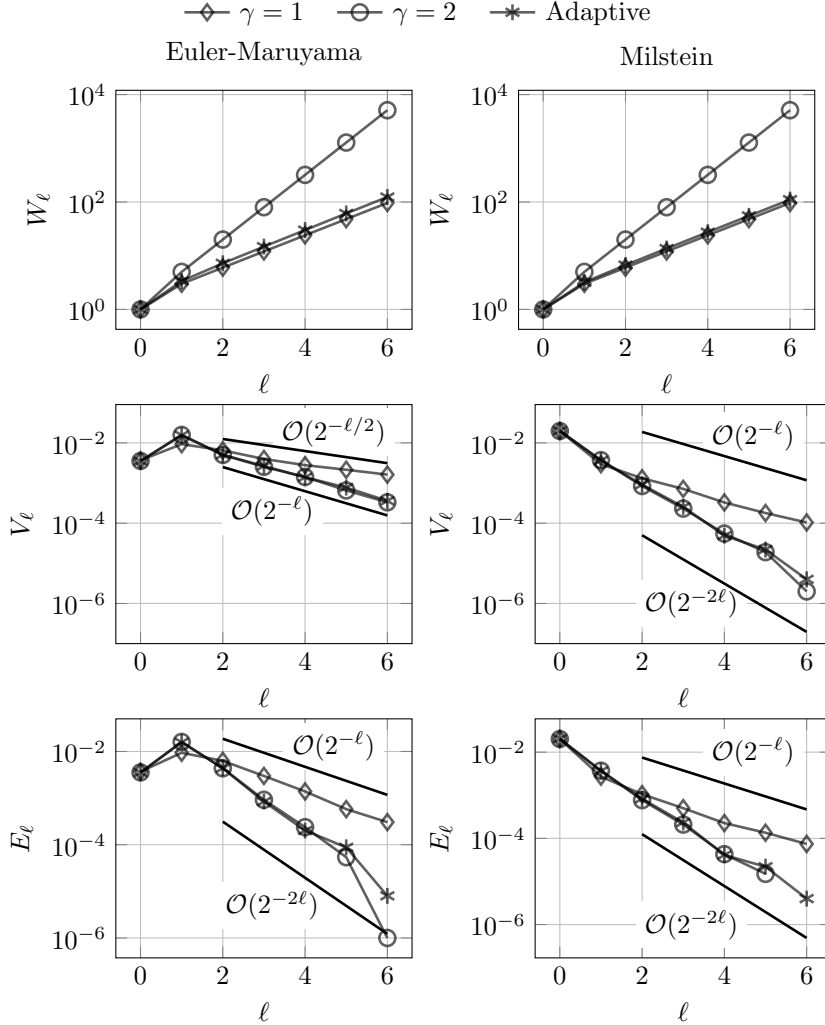


FIG. 4.2. W_ℓ (top), V_ℓ (middle) and E_ℓ (bottom) vs ℓ for the one dimensional SDE problem using Euler-Maruyama (left) and Milstein (right) simulation of the underlying SDE. We consider non-adaptive samplers with $\gamma = 1, 2$ and adaptive sampling with $r = 1.95$ for the Euler scheme and $r = 10$ for Milstein simulation.

620 observe the same rate without adaptive sampling when using the Milstein scheme,
 621 by Corollary 2.10 since $\beta = 2\gamma$. The cost is slightly lower for the non-adaptive Mil-
 622 stein scheme than for adaptive Euler-Maruyama, since the variance rate $V_\ell \lesssim 2^{-\gamma\ell}$
 623 is observed without refining the samples beyond level ℓ at all. However, we obtain the
 624 best results by combining the Milstein scheme with adaptive MLMC. In this case we
 625 observe complexity very close to ε^{-2} as in Theorem 3.10.

626

627 To illustrate how this performance translates to higher dimensional problems we
 628 consider the case $d = 10$, with correlation coefficient $\rho = 0.2$. We assume that
 629 $0.05 \leq a_i \leq 0.15$, $0.01 \leq b_i \leq 0.4$ and $0.9 \leq S^{(i)}(0) \leq 1.1$, where the drift and
 630 diffusion coefficients a_i and b_i are uniformly sampled along with the initial values

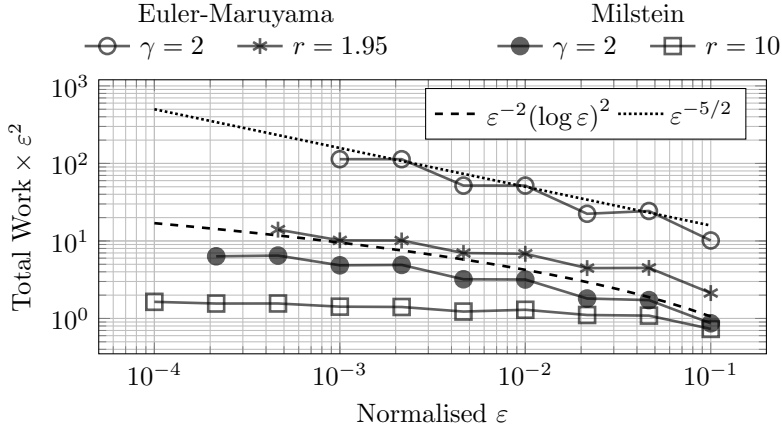


FIG. 4.3. The total work times ε^2 of MLMC for the one-dimensional SDE problem versus ε , normalised by the true value of the solution. Results are shown for both Euler-Maruyama and Milstein simulation of the underlying SDE. For each method we show results for non-adaptive sampling with $\gamma = 2$ and adaptive sampling with $r = 1.95$ for the Euler scheme and $r = 10$ for Milstein simulation.

631 $S^{(i)}(0)$. Euler-Maruyama simulation of g is used in non-adaptive MLMC for $\gamma = 1, 2$
 632 and adaptive sampling with $\gamma = 1$ and $r = 1.95$. The parameter K is again tuned
 633 so that $\mathbb{E}[\mathbb{H}(g)] \approx 0.025$. The values of W_ℓ, V_ℓ, E_ℓ for each method are plotted
 634 against ℓ in Figure 4.4. We observe a slight increase to each term. However, the
 635 rates of each parameter are all equivalent to those seen before, and the complexity
 636 of MLMC is unaffected by the increased dimensionality. To emphasize this point,
 637 Figure 4.4 also displays the total work ($\times \varepsilon^2$) against ε . In particular, we again
 638 observe $\varepsilon^{-2}(\log \varepsilon)^2$ complexity for the adaptive sampler, as opposed to $\varepsilon^{-5/2}$ for the
 639 non-adaptive samplers.

640 **5. Conclusion.** We presented an efficient, general, MLMC framework for computing
 641 probabilities as in (1.2). The inherent discontinuity in the problem leads to
 642 high complexities for standard MLMC methods. We are able to improve the performance
 643 of MLMC using adaptive sampling based on the methods for nested simulation
 644 in [13]. The approach used is applicable to a wide class of problems and is often able
 645 to recover the canonical ε^{-2} MLMC complexity. The theory is supported by numerical
 646 experiments for nested simulation and SDEs.

647 The adaptive algorithm is limited by a high kurtosis of the multilevel correction
 648 terms $\Delta \mathbb{H}_\ell$ caused by the discontinuous observable. This makes estimates of E_ℓ and V_ℓ
 649 unreliable for a small number of samples at larger levels. Smoothing methods [2, 3, 15]
 650 can control the kurtosis by removing the discontinuity. For the present work, Bayesian
 651 estimation [7, 9] of E_ℓ and V_ℓ is used to improve the robustness of MLMC. Since a
 652 high kurtosis can have a large impact on the robustness of MLMC, the next step is
 653 to explore additional methods to reduce the kurtosis or obtain reliable estimates for
 654 E_ℓ and V_ℓ in this setup.

655 It is straightforward to extend the methods considered here to compute expectations
 656 of discontinuous functionals other than $\mathbb{I}_{G \in \Omega}$ or $\mathbb{H}(g)$. For example, in barrier
 657 option pricing, the payoff can be written as a product of a smooth/Lipschitz function
 658 with an indicator function. We will consider applications to other financial derivatives
 659 and risk measures in future work.

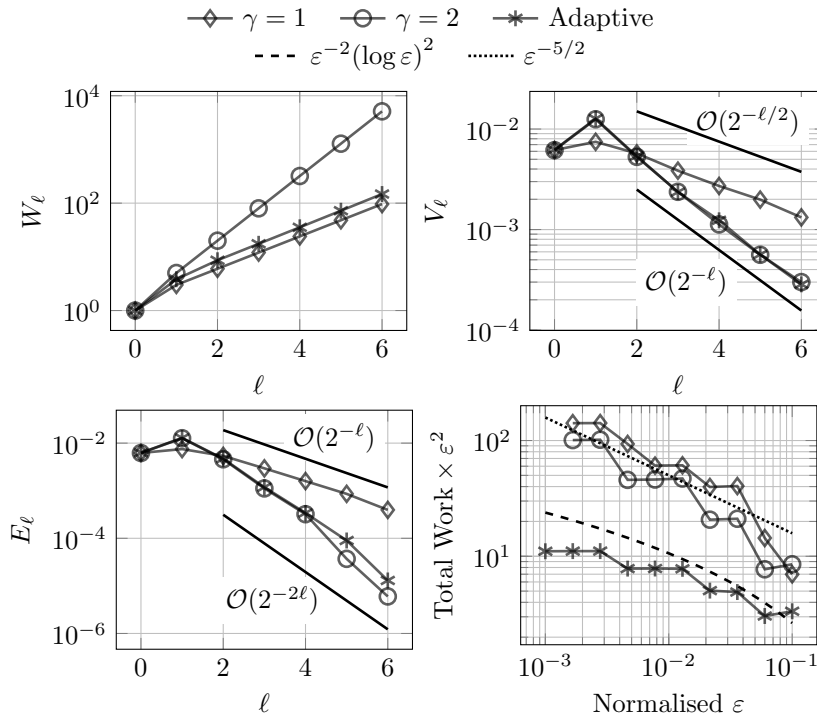


FIG. 4.4. Results for 10-dimensional digital option: Expected work per level W_ℓ (top left) taken as expected number of time-steps required to sample g_ℓ and $g_{\ell-1}$, V_ℓ (top right) and E_ℓ (bottom left) versus ℓ . The total work of MLMC times ϵ^2 against ϵ , normalised by the true value of the solution is shown (bottom right). Results are given for non-adaptive schemes with $\gamma = 1, 2$ and the adaptive scheme with $r = 1.95$.

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665

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727 **Appendix A. Discussion of Assumption 3.8.** This appendix discusses
728 the necessity of Assumption 3.8 to observe better convergence rates for E_ℓ due to
729 adaptive sampling. Evidence is given in the form of a numerical experiment when
730 Assumption 3.8 is false. In particular, we consider (1.2) where $g \sim \mathcal{N}(-\mu, 1)$ for
731 $\mu > 0$ chosen such that $\mathbb{P}[g > 0] = 0.025$. Approximations g_ℓ are artificially sampled
732 through

$$733 \quad g_\ell = g + 2^{-\ell\gamma/2} \left(2^{-\ell\gamma/2} + \zeta^2 - 1 \right), \quad \zeta \sim \mathcal{N}(0, 1).$$

734 We assume an artificial cost of $2^{\gamma\ell}$ in sampling g_ℓ . It follows that Assumptions 1.3
735 and 1.4 hold for $\beta = \gamma$, $\sigma_\ell \equiv \sigma$ constant and any $q < \infty$. From (1.4),

$$736 \quad Z_\ell = \frac{2^{-\ell\gamma/2} + \zeta^2 - 1}{\sigma},$$

737 and so Assumption 2.7 holds for $\beta = \gamma$. However, Assumption 3.8 is false since

738 $\mathbb{P}[Z_\ell > 0] \rightarrow 1$ as $\ell \rightarrow \infty$. Thus, the hypothesis of Lemma 3.9 is false.
739

740 Figure A.1 plots E_ℓ as in (2.2) for non-adaptive sampling with $\gamma = 1, 2$ and for
741 adaptive sampling with $r = 1.95, \gamma = \theta = c = 1$ and $\sigma_\ell = \sigma = \sqrt{3}$. We use the
742 same sample of ζ for the fine and coarse levels in each MLMC correction term, and
743 when adaptively refining samples. For all methods we see $E_\ell \lesssim 2^{-\gamma\ell}$. Since $\beta = \gamma$ this
744 agrees with Proposition 2.9 for the non-adaptive samplers. If Assumption 3.8 holds, we
745 expect that the adaptive refinement would provide $E_\ell \lesssim 2^{-2\ell}$ by Lemma 3.9. However,
746 we observe a worse rate numerically, which provides evidence that Assumption 3.8 is
747 crucial to improve the bias convergence rate using adaptive sampling.

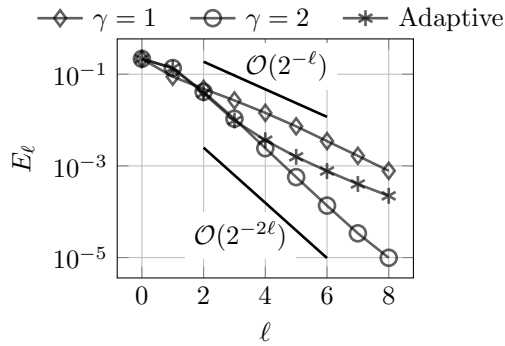


FIG. A.1. E_ℓ versus ℓ for the artificial problem considered in Appendix A used as evidence of worse weak error rates for adaptive sampling when Assumption 3.8 is false.

748 **Appendix B. Different values of σ_ℓ .** In Subsection 4.1 we assumed σ_ℓ^2 was
749 the sample conditional variance of X given Y . However, the other examples consid-
750 ered all use constant values $\sigma_\ell \equiv \sigma$. In this appendix we discuss other choices of σ_ℓ for
751 the nested simulation problem and the impact on the work of MLMC. One option is to
752 take $\sigma_\ell^2 = \text{Var}[X|Y]$. However, this information is likely unavailable for all practical
753 applications. Thus, we consider instead the approximation $\sigma_\ell \equiv \sigma$, for some constant
754 $\sigma > 0$. For Assumption 1.3 to hold for $\sigma_\ell \equiv \sigma$, we now require bounded moments
755 of $g - g_\ell$, opposed to the t -statistic appearing in (4.2), which is a more restrictive
756 condition.

757

758 We present results using adaptive sampling for the model problem presented in
759 Subsection 4.1. Specifically, we estimate the total work of MLMC with several error
760 tolerances ε and optimal starting levels as in Subsection 4.1 but with constant $\sigma_\ell = \sigma$.
761 The total work required with constant $\sigma_\ell = \sigma$ divided by the work when using the
762 sample standard deviation is shown in Figure B.1. The solid markers show the value
763 σ^2 estimating the value $\mathbb{E}[\text{Var}[X|Y]]$. When $\sigma \rightarrow 0$, the term $|\delta_\ell|$ in Algorithm 3.1
764 tends to ∞ and we instead use deterministic sampling with $N_\ell = N_0 2^\ell$ inner samples
765 per level in the limiting case. Conversely, when $\sigma \rightarrow \infty$, $|\delta_\ell| \rightarrow 0$ and the adaptive
766 algorithm reverts to deterministic sampling with $N_\ell = N_0 2^{2\ell}$ inner samples per level.
767 This leads to expensive pre-asymptotic regimes for large and small σ and we observe
768 worse performance as ε decreases. The work is typically lower for large σ opposed to
769 small σ is consistent with results showing MLMC is more effective when the approx-
770 imations are refined by a factor of around 7 per level in this application ($W_\ell \propto 7^\ell$)
771 [11]. The only value of σ for which we consistently observe equal performance using

772 constant σ_ℓ , opposed to the sample variance, is $\sigma^2 \approx \mathbb{E}[\text{Var}[X|Y]]$. MLMC actually
 773 has slightly lower cost for constant σ_ℓ in this instance, likely due to statistical errors
 774 in the sample variance impacting the refinement of certain samples, whereas taking
 775 constant $\sigma^2 \approx \mathbb{E}[\text{Var}[X|Y]]$ refines samples enough on average to observe the benefits
 776 of adaptive sampling. To draw further conclusions, more rigorous justification of
 Assumptions 1.3 and 1.4 is required.

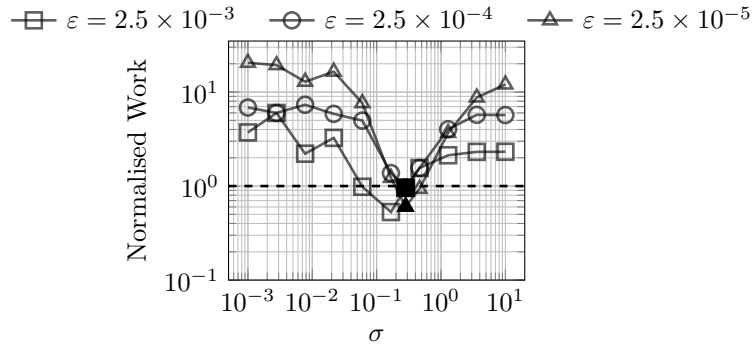


FIG. B.1. The work required for the model problem in Subsection 4.1 using adaptive MLMC with constant $\sigma_\ell = \sigma$, normalised by the work when σ_ℓ is the sample standard deviation. The solid markers show $\sigma = \sqrt{\mathbb{E}[\text{Var}[X|Y]]} \approx 0.28$.

777