Guaranteed Approximate Fixed Width Confidence Intervals Via Monte Carlo Sampling *

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Summary. Monte Carlo methods are used to approximate the means, μ, of random variables Y, whose distributions are not known explicitly. This idea is to approximate μ by the average of a random sample, $Y_1, \ldots, Y_n$. This article explores how one can confidently construct a confidence interval for μ with a prescribed half-width ε. Our proposed two stage algorithm assumes that Y has bounded *kurtosis*. An initial independent and identically distributed (IID) sample is used to confidently estimate the variance of Y. A Berry-Esseen inequality then makes it possible to determine the size of the IID sample required to produce the desired confidence interval. We discuss the important case where $Y = f(\boldsymbol{X})$ and $\boldsymbol{X}$ is a random d-vector with probability density ρ. In this case μ can be interpreted as the integral $\int_{\mathbb{R}^d} f(\boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$, and the Monte Carlo method becomes a method for multidimensional cubature.

1 Introduction

Monte Carlo algorithms provide a flexible way to approximate $\mu = \mathbb{E}(Y)$ when one can generate samples of the random variable Y. For example, Y might be the discounted payoff of some financial derivative, which depends on the future performance of assets that are described by a stochastic model. Then μ is the fair option price. The goal is to obtain a *confidence interval*

$$\Pr[|\mu - \hat{\mu}| \le \varepsilon] \ge 1 - \alpha, \tag{1}$$

where

- μ is approximated by the sample average of n independent and identically distributed (IID) samples of Y,
$$\hat{\mu} = \hat{\mu}_n = \frac{1}{n}\sum_{i=1}^{n} Y_i, \tag{2}$$
- ε is the half-width of the confidence interval, which also serves as an *error tolerance*, and

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- α is the level of *uncertainty*, e.g., 1% or 0.1%, which is fixed in advance.

Often the sample size, n, is fixed in advance, and the central limit theorem (CLT) provides an approximate value for ε in terms of n and

$$\sigma^2 = \mathrm{Var}(Y) = \mathbb{E}[(Y-\mu)^2], \tag{3}$$

which itself may be approximated by the sample variance.

The goal here is somewhat different. We want to fix ε in advance and then determine how large the sample size must be to obtain a fixed width confidence intervals of the form (1). In this paper we present Algorithm 1 for obtaining such a fixed width confidence interval for the mean of a real random variable, which is suitable for Monte Carlo sampling.

Before presenting the method, we outline the reasons that existing fixed width intervals are not suitable. In summary, there are two drawbacks of existing procedures. Much existing theory is *asymptotic*, i.e., the proposed procedure attains the desired coverage level in the limit as $\varepsilon \to 0$ but does not provide coverage guarantees for fixed $\varepsilon > 0$. We want such fixed ε guarantees. A second drawback is that the theory may make distributional assumptions that are too strong. In Monte Carlo applications one typically does not have much information about the underlying distribution. The form of the distribution for Y is generally not known, $\mathrm{Var}(Y)$ is generally not known, and Y is not necessarily bounded. We are aiming to derive fixed-width confidence intervals that do not require such assumptions.

The width (equivalently length) of a confidence interval tends to become smaller as the number n of sampled function values increases. In special circumstances, we can choose n to get a confidence interval of at most the desired length and at least the desired coverage level, $1-\alpha$. For instance, if the variance, $\sigma^2 = \mathrm{Var}(Y)$, is known then an approach based on Chebychev's inequality is available, though the actual coverage will usually be much higher than the nominal level, meaning that much narrower intervals would have sufficed. Known variance in addition to a Gaussian distribution for Y supports a fixed width interval construction that is not too conservative. The CLT provides a confidence interval that is asymptotically correct, but our aim is for something that is definitely correct for finite sample sizes. Finally, conservative fixed width intervals for means can be constructed for bounded random variables, by appealing to exponential inequalities such as Hoeffding's or Chernoff's inequality. Unfortunately, Y is often unbounded, e.g., in the case where it represents the payoff of a call option.

If the relevant variance or bound is unknown, then approaches based on sequential statistics (Siegmund, 1985) may be available. In sequential methods one keeps increasing n until the interval is narrow enough. Sequential confidence intervals require us to take account of the stopping rule when computing the confidence level. Unfortunately, all existing sequential methods are lacking in some aspects.

Serfling and Wackerly (1976) consider sequential confidence intervals for the mean (alternatively for the median) in parametric distributions, symmetric about their center point. The symmetry condition is not suitable for general purpose Monte Carlo applications.

Chow and Robbins (1965) develop a sequential sampling fixed width confidence interval procedure for the mean, but its guarantees are only asymptotic. Mukhopadhyay and Datta (1996) give a procedure similar to Chow and Robbins', and it has similar drawbacks.

Bayesian methods can support a fixed width interval containing μ with $1-\alpha$ posterior probability, and Bayesian methods famously do not require one to account for stopping rules. They do however require strong distributional assumptions.

There is no assumption-free way to obtain exact confidence intervals for a mean, as has been known since (Bahadur and Savage, 1956, Corollary 2). Some kind of assumption is needed to rule out settings where the desired quantity is the mean of a heavy tailed random

variable in which rarely seen large values dominate the mean and spoil the estimates of the variance. The assumption we use is an upper bound on the modified kurtosis (normalized fourth moment) of the random variable Y:

$$\tilde{\kappa} = \frac{\mathbb{E}[(Y-\mu)^4]}{\sigma^4} \leq \tilde{\kappa}_{\max}. \tag{4}$$

(The quantity $\tilde{\kappa} - 3$ is commonly called the kurtosis.) Under such an assumption we present a two stage algorithm: the first stage generates a conservative variance estimate, and the second stage uses this variance estimate and a Berry-Esseen Theorem, which can be thought of as a non-asymptotic CLT, to determine how large n must be for the sample mean to satisfy the confidence interval (1). Theorem 5 then demonstrates the validity of the fixed-width confidence interval, and Theorem 6 demonstrates that the cost of this algorithm is reasonable. These are our main new theoretical results.

Our procedure is a two-stage procedure rather than a fully sequential one. In this it is similar to the method of Stein (1945, 1949), except that the latter requires normally distributed data.

One might question whether assumption (4), which involves fourth-order moments of Y, is more reasonable than an assumption involving only the second moment of Y. For example, using Chebychev's inequality with the assumption

$$\sigma^2 \leq \sigma^2_{\max} \tag{5}$$

also yields a fixed-width confidence interval of the form (1). We would argue that (4) is indeed more reasonable. First, if Y satisfies (4), then so does cY for any nonzero c, however, the analog does not hold for (5). In fact, if σ is nonzero (5) is violated by cY for c sufficiently large. Second, making $\tilde{\kappa}_{\max}$ a factor of 10 or 100 larger than $\tilde{\kappa}$ does not significantly affect the total cost (number of samples required) of our Monte Carlo Algorithm 1 for a large range of values of σ/ε. However, the cost of our Monte Carlo algorithm, and indeed any Monte Carlo algorithm is proportional to σ^2, so overestimating σ^2 by a factor of 10 or 100 to be safe, increases the cost of the algorithm by that factor.

An important special case of computing $\mu = \mathbb{E}(Y)$ arises in the situation where $Y = f(\boldsymbol{X})$ for some function $f : \mathbb{R}^d \to \mathbb{R}$ and some random vector $\boldsymbol{X}$ with probability density $\rho : \mathbb{R}^d \to [0,\infty)$. One may then interpret the mean of Y as the multidimensional integral

$$\mu = \mathbb{E}(Y) = \mu(f) = \int_{\mathbb{R}^d} f(\boldsymbol{x})\rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}. \tag{6}$$

Given the problem of evaluating $\mu = \int_{\mathbb{R}^d} g(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$, one must choose a probability density ρ for which one can easily generate random vectors $\boldsymbol{X}$, and then set $f = g/\rho$. The quantities σ^2 and $\tilde{\kappa}$ defined above can be written in terms of weighted $\mathscr{L}_p$-norms of f:

$$\|f\|_p := \left\{ \int_{\mathbb{R}^d} |f(\boldsymbol{x})|^p \rho(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \right\}^{1/p}, \qquad \sigma^2 = \|f-\mu\|_2^2, \qquad \tilde{\kappa} = \frac{\|f-\mu\|_4^4}{\|f-\mu\|_2^4}. \tag{7}$$

For a given g, the choice of ρ is not unique, and making an optimal choice belongs to the realm of *importance sampling*. The assumption of bounded kurtosis, (4), required by Algorithm 1, corresponds to an assumption about the integrand f lying in the *cone* of functions

$$\mathscr{C}_{\tilde{\kappa}_{\max}} = \{ f \in \mathscr{L}_4 : \|f-\mu\|_4 \leq \tilde{\kappa}_{\max}^{1/4} \|f-\mu\|_2 \}. \tag{8}$$

From the perspective of numerical analysis, if ρ has independent marginals, one may apply a product form of a univariate quadrature rule to evaluate μ. However, this consumes a

geometrically increasing number of samples as d increases, and moreover, such methods often require rather strict smoothness assumptions on f. If f satisfies moderate smoothness conditions, then (randomized) quasi-Monte Carlo methods, or low discrepancy sampling (Niederreiter, 1992; Sloan and Joe, 1994; Lemieux, 2009; Dick and Pillichshammer, 2010) methods for evaluating μ that are more efficient than simple Monte Carlo. Unfortunately, practical error estimation remains a challenge for deterministic quasi-Monte Carlo methods, and randomized quasi-Monte Carlo methods do not yet yield guaranteed, fixed width confidence intervals.

Computational mathematicians have also addressed the problem of constructing automatic algorithms, i.e., given an error tolerance of ε, one computes an approximation, $\hat{\mu}$, based on n evaluations of the integrand f, such that $|\mu - \hat{\mu}| \le \varepsilon$. For example, MATLAB (The MathWorks, Inc., 2012), a popular numerical package, contains `quad`, an adaptive Simpson's rule for univariate quadrature routine developed by Gander and Gautschi (2000). Although `quad` and other automatic rules generally work well in practice, they do not have any rigorous guarantees that the error tolerance is met, and it is relatively simple to construct functions that fool them. This is discussed in Section 4. Since a random algorithm, like Monte Carlo, gives a random answer, any statements about satisfying an error criterion must be probabilistic. This leads us back to the problem of finding a fixed-width confidence interval, (1).

An outline of this paper follows. Section 2 defines key terminology and provides certain inequalities used to construct our fixed width confidence intervals. The new two-stage Algorithm 5 is described in Section 3, where theoretical guarantees of its success and its cost are provided. Section 4 illustrates the challenges of computing μ to a guaranteed precision through several numerical examples. This paper ends with a discussion of our results and further work to be done.

2 Background probability and statistics

In our Monte Carlo applications, a quantity of interest is written as an expectation: $\mu = \mathbb{E}(Y)$, where Y is a real valued random variable. As mentioned above, very often $Y = f(\boldsymbol{X})$ where $\boldsymbol{X} \in \mathbb{R}^d$ is a random vector with probability density function ρ. In other settings the random quantity $\boldsymbol{X}$ might have a discrete distribution or be infinite dimensional (e.g,. a Gaussian process) or both. For Monte Carlo estimation, we can work with the distribution of Y alone. The Monte Carlo estimate of μ is the sample mean, as given in (2), where the Y_i are IID random variables with the same distribution as Y.

2.1 Moments

Our methods require conditions on the first four moments of Y as described here. The variance of Y, as defined in (3), is denoted by σ^2, and its non-negative square root, σ, is the standard deviation of Y. Some of our expressions assume without stating it that $\sigma > 0$, and all will require $\sigma < \infty$. The skewness of Y is $\gamma = \mathbb{E}[(Y-\mu)^3]/\sigma^3$, and the kurtosis of Y is $\kappa = \tilde{\kappa} - 3 = \mathbb{E}((Y-\mu)^4)/\sigma^4 - 3$ (see (4)). The mysterious 3 in κ is there to make it zero for Gaussian random variables. Also, $\mu, \sigma^2, \gamma, \kappa$ are related to the first four cumulants (McCullagh, 1987, p.??) of the distribution of Y, meaning that

$$\log(\mathbb{E}[\exp(tY)]) = \mu t + \frac{\sigma^2 t^2}{2} + \frac{\sigma^3 \gamma t^3}{3!} + \frac{\sigma^4 \kappa t^4}{4!} + o(t^4).$$

Our main results require that $\kappa < \infty$, which then implies that σ and γ are finite.

2.2 CLT intervals

A random variable Z has the standard normal distribution, denoted by $\mathcal{N}(0,1)$, if

$$\Pr(Z \le z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{z} =: \Phi(z) \exp(-t^2/2)\,\mathrm{d}t.$$

Under the central limit theorem, the distribution of $\sqrt{n}(\hat{\mu}_n - \mu)/\sigma$ approaches $\mathcal{N}(0,1)$ as $n \to \infty$, where $\hat{\mu}_n$ denotes the sample mean of n IID samples. As a result

$$\Pr\big(\hat{\mu}_n - 2.58\sigma\sqrt{n} \le \mu \le \hat{\mu}_n + 2.58\sigma/\sqrt{n}\big) \to 0.99 \tag{9}$$

as $n \to \infty$. We write the interval in (9) as $\hat{\mu}_n \pm 2.58\sigma/\sqrt{n}$. Equation (9) is not usable when σ^2 is unknown, but the usual estimate

$$s_n^2 = \frac{1}{n-1} \sum_{i=1}^{n} (Y_i - \hat{\mu}_n)^2 \tag{10}$$

may be substituted, yielding the interval $\hat{\mu}_n \pm 2.58 s_n/\sqrt{n}$ which also satisfies the limit in (9) by Slutsky's theorem (**?**). For an arbitrary confidence level $1-\alpha \in (0,1)$, we replace the constant 2.58 by $z_{\alpha/2} = \Phi^{-1}(1-\alpha/2)$. The width of this interval is $2z_{\alpha/2}s_n/\sqrt{n}$, and when μ is in the interval then the absolute error $|\mu - \hat{\mu}_n| \le \varepsilon := z_{\alpha/2}s_n/\sqrt{n}$.

The coverage level of the CLT interval is only asymptotic. In more detail, (**?**, p. 948) shows that

$$\Pr\big(|\mu - \hat{\mu}_n| \le 2.58 s/\sqrt{n}\big) = 0.99 + \frac{1}{n}(A + B\gamma^2 + C\kappa) + O\Big(\frac{1}{n^2}\Big) \tag{11}$$

for constants A, B, and C that depend on the desired coverage level (here 99%). Hall's theorem requires only that the random variable Y has sufficiently many finite moments and is not supported solely on a lattice (such as the integers). It is interesting to note that the $O(1/n)$ coverage error in (11) is better than the $O(1/\sqrt{n})$ root mean squared error for the estimate $\hat{\mu}_n$ itself.

2.3 Standard Probability Inequalities

Here we present some well known inequalities that we will make use of. First, Chebychev's inequality ensures that a random variable (such as $\hat{\mu}_n$) is seldom too far from its mean.

Theorem 1 (Chebychev's Inequality). *(Lin and Bai, 2010, 6.1c, p. 52) Let Z be a random variable with mean μ and variance $\sigma^2 \ge 0$. Then for all $\varepsilon > 0$,*

$$\Pr[|Z - \mu| \ge \varepsilon] \le \frac{\sigma^2}{\varepsilon^2}.$$

In some settings we need a one sided inequality like Chebychev's. We will use this one due to Cantelli.

Theorem 2 (Cantelli's Inequality). *(Lin and Bai, 2010, 6.1e, p. 53) Let Z be any random variable with mean μ and finite variance σ^2. For any $a \ge 0$, it follows that:*

$$\Pr[Z - \mu \ge a] \le \frac{\sigma^2}{a^2 + \sigma^2}.$$

Berry-Esseen type theorems govern the rate at which a CLT takes hold. We will use the following one.

Theorem 3 (Non-uniform Berry-Esseen Inequality). *(Petrov, 1995, Theorem 5.16, p. 168) Let $Y_1,\ldots,Y_n$ be IID random variables with mean μ, variance $\sigma^2>0$, and third centered moment $M_3 = E\left|Y_i-\mu\right|^3/\sigma^3<\infty$. Then*

$$\left|\Pr\left[\frac{1}{\sigma\sqrt{n}}\sum_{i=1}^{n}(Y_i-\mu)<x\right]-\Phi(x)\right|\le\frac{AM_3}{\sqrt{n}(1+|x|)^3}\qquad\forall x\in\mathbb{R},$$

where A is some number satisfying $0.4097\le A\le 0.5600$.

Our method requires probabilistic bounds on the sample variance, s_n^2. For that, we will use some moments of the variance estimate.

Theorem 4. *(Miller, 1986, Eq. (7.16), p. 265) Let $Y_1,\ldots,Y_n$ be IID random variables with variance σ^2 and modified kurtosis $\tilde{\kappa}$ defined in* (4)*. Let s_n^2 be the sample variance as defined in* (10)*. Then the sample variance is unbiased, $\mathbb{E}(s_n^2)=\sigma^2$, and its variance is*

$$\mathrm{Var}(s_n^2)=\frac{\sigma^4}{n}\left(\tilde{\kappa}-\frac{n-3}{n-1}\right).$$

3 Two stage confidence interval

Our two stage procedure works as follows. In the first stage, we take a sample of independent values $Y_1,\ldots,Y_{n_\sigma}$ from the distribution of Y. From this sample we compute the sample variance, $s_{n_\sigma}^2$, according to (10) and estimate the variance of Y_i by $\hat{\sigma}^2=\mathfrak{C}^2\hat{v}_{n_\sigma}$, where $\mathfrak{C}^2>1$ is a "variance inflation factor" that will reduce the probability that we have underestimated $\sigma^2=\mathrm{Var}(Y)$. For the second stage, we use the estimate $\hat{\sigma}^2$ as if it were the true variance of Y_i and use Berry-Esseen theorem to obtain a suitable sample size, n_μ, for computing the sample average, $\hat{\mu}$, that satisfies the fixed with confidence interval (1).

The next two subsections give details of these two steps that will let us bound their error probabilities. Then we give a theorem on the method as a whole.

3.1 Conservative variance estimates

We need to ensure that our first stage estimate of the variance σ^2 is not too small. The following result bounds the probability of such an underestimate.

Lemma 1. *Let $Y_1,\ldots,Y_n$ be IID random variables with variance $\sigma^2>0$ and kurtosis κ. Let s_n^2 be the sample variance defined at* (10)*, and let $\tilde{\kappa}=\kappa+3$. Then*

$$\Pr\left[s_n^2<\sigma^2\left\{1+\sqrt{\left(\tilde{\kappa}-\frac{n-3}{n-1}\right)\left(\frac{1-\alpha}{\alpha n}\right)}\right\}\right]\ge 1-\alpha, \tag{12a}$$

$$\Pr\left[s_n^2>\sigma^2\left\{1-\sqrt{\left(\tilde{\kappa}-\frac{n-3}{n-1}\right)\left(\frac{1-\alpha}{\alpha n}\right)}\right\}\right]\ge 1-\alpha. \tag{12b}$$

Proof. Applying Theorem 4 and choosing

$$a = \sqrt{\mathrm{Var}(s_n^2)\frac{1-\alpha}{\alpha}} = \sigma^2\sqrt{\left(\kappa - \frac{n-3}{n-1}\right)\left(\frac{1-\alpha}{\alpha n}\right)} > 0,$$

it follows from Cantelli's inequality (Theorem 2) that

$$\begin{aligned}\Pr\left[s_n^2 - \sigma^2 \geq \sigma^2\sqrt{\left(\kappa - \frac{n-3}{n-1}\right)\left(\frac{1-\alpha}{\alpha n}\right)}\right] &= \Pr\left[s_n^2 - \sigma^2 \geq a\right] \\ &\leq \frac{\mathrm{Var}(s_n^2)}{a^2 + \mathrm{Var}(s_n^2)} = \frac{\mathrm{Var}(s_n^2)}{\mathrm{Var}(s_n^2)\frac{1-\alpha}{\alpha} + \mathrm{Var}(s_n^2)} = \frac{1}{\left(\frac{1-\alpha}{\alpha}\right)+1} = \alpha.\end{aligned}$$

Then (12a) follows directly. By a similar argument, applying Cantelli's inequality to the expression $\Pr\left[-s_n^2 + \sigma^2 \geq a\right]$ implies (12b). □

Using Lemma 1 we can bound the probability that $\hat{\sigma}^2 = \mathfrak{C}^2 s_{n_\sigma}^2 < \sigma^2$. Equation (12a) implies that

$$\Pr\left[\frac{s_{n_\sigma}^2}{1 - \sqrt{\left(\tilde{\kappa} - \frac{n_\sigma - 3}{n_\sigma - 1}\right)\left(\frac{1-\alpha}{\alpha n_\sigma}\right)}} > \sigma^2\right] \geq 1 - \alpha. \tag{13}$$

Thus, it makes sense for us to require the modified kurtosis, $\tilde{\kappa}$, to be small enough, relative to n_σ, α, and $\mathfrak{C}$, in order to ensure that (13) holds. Specifically, we require

$$\frac{1}{1 - \sqrt{\left(\tilde{\kappa} - \frac{n_\sigma - 3}{n_\sigma - 1}\right)\left(\frac{1-\alpha}{\alpha n_\sigma}\right)}} \leq \mathfrak{C}^2,$$

or equivalently,

$$\tilde{\kappa} \leq \frac{n_\sigma - 3}{n_\sigma - 1} + \left(\frac{\alpha n_\sigma}{1-\alpha}\right)\left(1 - \frac{1}{\mathfrak{C}^2}\right)^2 =: \tilde{\kappa}_{\max}(\alpha, n_\sigma, \mathfrak{C}). \tag{14}$$

This condition is the explicit version of (4) mentioned in the introduction.

3.2 Conservative interval widths

Here we consider how to choose the sample size n to get the desired coverage level from an interval with half-length at most ε. We suppose here that σ is known. In practice we will use a conservative (biased high) estimate for σ.

First, if the CLT held exactly and not just asymptotically, then we could use a CLT sample size of

$$N_{\mathrm{CLT}}(\varepsilon, \sigma, \alpha) = \left\lceil \left(\frac{z_{\alpha/2}\sigma}{\varepsilon}\right)^2 \right\rceil$$

independent values of Y_i in an interval like the one in (9).

Given knowledge of σ, but no assurance of a Gaussian distribution for $\hat{\mu}_n$, we could instead select a sample size based on Chebychev's inequality (Theorem 1). Taking

$$N_{\mathrm{Cheb}}(\varepsilon, \sigma, \alpha) = \left\lceil \frac{\sigma^2}{\alpha\varepsilon^2} \right\rceil \tag{15}$$

IID observations of Y gives the confidence interval (1). Naturally $N_{\text{Cheb}} \geq N_{\text{CLT}}$.

Finally, we could use the non-uniform Berry-Esseen inequality from Theorem 3. This inequality requires a finite scaled third moment $M_3 = E\left|Y_i - \mu\right|^3/\sigma^3$. If The non-uniform Berry-Esseen inequality implies that

$$\begin{aligned}\Pr\left[|\mu - \hat{\mu}_n| \leq \frac{\sigma}{\sqrt{n}}x\right] &= \Pr\left[\hat{\mu}_n - \mu \leq \frac{\sigma}{\sqrt{n}}x\right] - \Pr\left[\hat{\mu}_n - \mu < -\frac{\sigma}{\sqrt{n}}x\right] \\ &\geq \left[\Phi(x) - \frac{0.56M_3}{\sqrt{n}(1+|x|)^3}\right] - \left[\Phi(-x) + \frac{0.56M_3}{\sqrt{n}(1+|x|)^3}\right] \\ &= 1 - 2\left(\frac{0.56M_3}{\sqrt{n}(1+|x|)^3} + \Phi(-x)\right). \end{aligned} \tag{16}$$

Letting $x = \varepsilon\sqrt{n}/\sigma$, the probability of making an error no greater than ε is bounded below by $1-\alpha$, i.e., the fixed width confidence interval (1) holds, provided $n \geq N_B(\varepsilon/\sigma, \alpha, M_3)$, where the Berry-Esseen sample size is

$$N_{\text{BE}}(\varepsilon, \sigma, \alpha, M) := \min\left\{n \in \mathbb{N} : \Phi\left(-\sqrt{n}\varepsilon/\sigma\right) + \frac{0.56M}{\sqrt{n}\left(1+\sqrt{n}\varepsilon/\sigma\right)^3} \leq \frac{\alpha}{2}\right\}. \tag{17}$$

To compute this value, we need to know M_3. In practice, substituting an upper bound on M_3 yields an upper bound on the necessary sample size.

It is possible that in some situations $N_{\text{BE}} > N_{\text{Cheb}}$ might hold. In such cases we could use N_{Cheb} instead.

3.3 Algorithm and Proof of Its Success

In detail, the two stage algorithm works as described below.

Algorithm 1 (Two Stage). The user specifies four quantities:

- an initial sample size for variance estimation, $n_\sigma \in \{2, 3, \ldots\}$,
- a variance inflation factor $\mathfrak{C}^2 \in (1, \infty)$,
- an uncertainty tolerance $\alpha \in (0, 1)$, and,
- an error tolerance or confidence interval width, $\varepsilon > 0$.

At the first stage of the algorithm, $Y_1, \ldots, Y_{n_\sigma}$ are sampled independently from the same distribution as Y. Then the conservative variance estimate, $\hat{\sigma}^2 = \mathfrak{C}^2 s_{n_\sigma}^2$ is computed in terms of the sample variance, $s_{n_\sigma}^2$, defined by (10).

To prepare for the second stage of the algorithm we compute $\tilde{\alpha} = 1 - \sqrt{1-\alpha}$ and then $\tilde{\kappa}_{\max} = \tilde{\kappa}_{\max}(\tilde{\alpha}, n_\sigma, \mathfrak{C})$ using equation (14). The sample size for the second stage is

$$n_\mu = N_\mu(\varepsilon, \hat{\sigma}, \tilde{\alpha}, \tilde{\kappa}_{\max}^{3/4}), \tag{18}$$

where

$$N_\mu(\varepsilon, \sigma, \alpha, M) := \max\bigl(1, \min\bigl(N_{\text{Cheb}}(\varepsilon, \sigma, \alpha), N_{\text{BE}}(\varepsilon, \sigma, \alpha, M)\bigr)\bigr). \tag{19}$$

Recall that N_{Cheb} is defined in (15) and N_{BE} is defined in (17).

After this preparation, the second stage is to sample $Y_{n_\sigma+1}, \ldots, Y_{n_\sigma+n}$ independently from the distribution of Y and compute the sample mean,

$$\hat{\mu} = \frac{1}{n_\mu}\sum_{i=n_\sigma+1}^{n_\sigma+n_\mu} Y_i. \tag{20}$$

The success of this algorithm is guaranteed in the following theorem. The main assumption needed is bounded kurtosis.

Theorem 5. *Let Y be a random variable with mean μ, and either zero variance or positive variance with modified kurtosis $\tilde{\kappa} \leq \tilde{\kappa}_{\max}(\tilde{\alpha}, n_\sigma, \mathfrak{C})$. It follows that Algorithm 1 above yields an estimate $\hat{\mu}$ given by* (20) *which satisfies the fixed width confidence interval condition*

$$\Pr(|\hat{\mu} - \mu| \leq \varepsilon) \geq 1 - \alpha.$$

Proof. If $\sigma^2 = 0$, then $s^2_{n_\sigma} = 0$, $n_\mu = 1$ and $\hat{\mu} = \mu$ with probability one. Now consider the case of positive variance. The first stage yields a variance estimate satisfying $\Pr(\hat{\sigma}^2 > \sigma^2) \geq 1 - \tilde{\alpha}$ by (14) applied with uncertainty tolerance $\tilde{\alpha}$. The second stage yields $\Pr(|\hat{\mu} - \mu| \leq \varepsilon) \geq 1 - \tilde{\alpha}$ by the Berry-Esseen result (16), so long as $\hat{\sigma} \geq \sigma$ and $M_3 \leq \tilde{\kappa}_{\max}(\tilde{\alpha}, n_\sigma, \mathfrak{C})^{3/4}$. The second condition holds because $M_3 \leq \tilde{\kappa}^{3/4}$ by Jensen's Inequality (Lin and Bai, 2010, 8.4.b). Thus, in the two stage algorithm we have

$$\begin{aligned}
\Pr(|\hat{\mu} - \mu| \leq \varepsilon) &= \mathbb{E}\big(\Pr(|\hat{\mu} - \mu| \leq \varepsilon \mid \hat{\sigma})\big) \\
&\geq \mathbb{E}\left((1 - \tilde{\alpha}) 1_{\sigma \leq \hat{\sigma}}\right) \\
&\geq (1 - \tilde{\alpha})(1 - \tilde{\alpha}) = 1 - \alpha. \qquad \square
\end{aligned}$$

Remark 1. In this algorithm it is possible to choose n_μ much smaller than n_σ if the sample variance is small. As a practical matter we suggest that if one is willing to invest n_σ samples to estimate the variance then one should be willing to invest at least that many additional samples to estimate the mean. Therefore, in the numerical examples of Section 4 we use

$$N_\mu(\varepsilon, \sigma, \alpha, M) := \max\big(n_\sigma, \min\big(N_{\text{Cheb}}(\varepsilon, \sigma, \alpha), N_{\text{BE}}(\varepsilon, \sigma, \alpha, M)\big)\big) \tag{21}$$

to determine the sample size for the sample mean. By the error bound following from Chebychev's inequality (Theorem 1), this means that the probabilistic absolute error bound in Theorem 5 also holds for random variables, Y, with $\sigma^2 \leq \varepsilon^2 \alpha n_\sigma$.

$$N_\mu(\varepsilon, \sigma, \alpha, M) := \max\big(n_\sigma, \min\big(N_{\text{Cheb}}(\varepsilon, \sigma, \alpha), N_{\text{BE}}(\varepsilon, \sigma, \alpha, M)\big)\big). \tag{22}$$

As mentioned in the introduction, one frequently encountered case occurs when Y is a d-variate function of a random vector $\boldsymbol{X}$. Then μ corresponds to the multivariate integral in (6) and Theorem 5 may be interpreted as below:

Corollary 1. *Suppose that $\rho : \mathbb{R}^d \to \mathbb{R}$ is a probability density, $f : \mathbb{R}^d \to \mathbb{R}$ has finite $\mathscr{L}_4$ norm as defined in* (7)*, and furthermore f lies in the cone $\mathscr{C}_{\tilde{\kappa}_{\max}}$ defined in* (8)*, where $\tilde{\kappa}_{\max} = \tilde{\kappa}_{\max}(\tilde{\alpha}, n_\sigma, \mathfrak{C})$. It follows that Algorithm 1 yields an estimate, $\hat{\mu}$, of the multidimensional integral μ defined in* (6)*, which satisfies the fixed width confidence interval condition*

$$\Pr(|\hat{\mu} - \mu| \leq \varepsilon) \geq 1 - \alpha.$$

3.4 Cost of the Algorithm

The number of function values required by the two-stage Algorithm 1 is $n_\sigma + n_\mu$, the sum of the initial sample size used to estimate the variance of Y and the sample size used to estimate the mean of Y. Although n_σ is deterministic, n_μ is a random variable, and so the cost of this algorithm might best be defined probabilistically. Moreover, the only random quantity in the formula for n_μ in (18) is $\hat{\sigma}^2$, the upper bound on variance. Clearly this depends on the unknown population variance, σ^2, and we expect $\hat{\sigma}^2$ not to overestimate σ^2 by much. Thus, the algorithm cost is defined below in terms of σ^2 and the error tolerance (interval width), ε. An upper bound on the cost is then derived in Theorem 6.

Let A be any random algorithm that takes as its input, a method for generating random samples, $Y_1, Y_2, \ldots$ with common distribution function F having variance σ^2 and modified kurtosis $\tilde{\kappa}$. Additional algorithm inputs are an error tolerance, ε, an uncertainty tolerance, α, and a maximum modified kurtosis, $\tilde{\kappa}_{\max}$. The algorithm then computes $\hat{\mu} = A(F, \varepsilon, \alpha, \tilde{\kappa}_{\max})$, an approximation to $\mu = \mathbb{E}(Y)$, based on a total of $N_{\text{tot}}(\varepsilon, \alpha, \tilde{\kappa}_{\max}, F)$ samples. The probabilistic cost of the algorithm, with uncertainty β, for integrands of variance no greater than $\sigma_{\max}^2$ and modified kurtosis no greater than $\tilde{\kappa}_{\max}$ is defined as

$$N_{\text{tot}}(\varepsilon, \alpha, \beta, \tilde{\kappa}_{\max}, \sigma_{\max}) := \sup_{\substack{\tilde{\kappa} \le \tilde{\kappa}_{\max} \\ \sigma \le \sigma_{\max}}} \min\{N : \Pr[N_{\text{tot}}(\varepsilon, \alpha, \tilde{\kappa}_{\max}, F) \le N] \ge 1 - \beta\}. \tag{23}$$

Note that $\tilde{\kappa}_{\max}$ is an input to the algorithm, but $\sigma_{\max}$ is not.

The cost of the particular two-stage Monte Carlo algorithm defined in Algorithm 1 is

$$\sup_{\substack{\tilde{\kappa} \le \tilde{\kappa}_{\max} \\ \sigma \le \sigma_{\max}}} \min\left\{N : \Pr(n_\sigma + N_\mu(\varepsilon, \hat{\sigma}, \tilde{\alpha}, \tilde{\kappa}_{\max}^{3/4}) \le N) \ge 1 - \beta\right\}. \tag{24}$$

Since n_σ is fixed, bounding this cost depends on bounding $N_\mu(\varepsilon, \hat{\sigma}, \tilde{\alpha}, \tilde{\kappa}_{\max}^{3/4})$, which depends on $\hat{\sigma}$ as given by Algorithm 1. Moreover, $\hat{\sigma}$ can be bounded above using (12b) in Lemma 1. For $\tilde{\kappa} \le \tilde{\kappa}_{\max}$,

$$\begin{aligned}
1 - \beta &\le \Pr\left[s_{n_\sigma}^2 < \sigma^2 \left\{1 + \sqrt{\left(\tilde{\kappa} - \frac{n_\sigma - 3}{n_\sigma - 1}\right)\left(\frac{1-\beta}{\beta n_\sigma}\right)}\right\}\right] \\
&\le \Pr\left[\hat{\sigma}^2 = \mathfrak{C}^2 s_{n_\sigma}^2 < \mathfrak{C}^2 \sigma^2 \left\{1 + \sqrt{\left(\tilde{\kappa}_{\max}(n_\sigma, \tilde{\alpha}, \mathfrak{C}) - \frac{n_\sigma - 3}{n_\sigma - 1}\right)\left(\frac{1-\beta}{\beta n_\sigma}\right)}\right\}\right] \\
&= \Pr\left[\hat{\sigma}^2 < \sigma^2 v^2(\tilde{\alpha}, \beta, \mathfrak{C})\right],
\end{aligned}$$

where

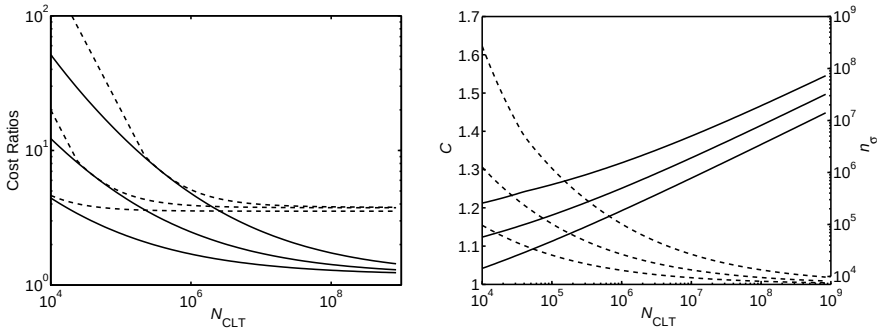
$$v^2(\tilde{\alpha}, \beta, \mathfrak{C}) := \mathfrak{C}^2 + \left(\mathfrak{C}^2 - 1\right)\sqrt{\frac{\tilde{\alpha}(1-\beta)}{(1-\tilde{\alpha})\beta}} > 1.$$

Noting that $N_\mu(\varepsilon, \cdot, \tilde{\alpha}, \tilde{\kappa}_{\max}^{3/4})$ is a non-decreasing function allows one to derive the following upper bound on the cost of the adaptive Monte Carlo algorithm.

Theorem 6. *The two stage Monte Carlo algorithm for fixed width confidence intervals based on IID sampling described in Algorithm 1 has a probabilistic cost bounded above by*

$$\begin{aligned}
&N_{\text{tot}}(\varepsilon, \alpha, \beta, \tilde{\kappa}_{\max}, \sigma_{\max}) \\
&\qquad \le N_{\text{up}}(\varepsilon, \alpha, \beta, \tilde{\kappa}_{\max}, \sigma_{\max}) := n_\sigma + N_\mu(\varepsilon, \sigma_{\max} v(\tilde{\alpha}, \beta, \mathfrak{C}), \tilde{\alpha}, \tilde{\kappa}_{\max}^{3/4}).
\end{aligned}$$

Note that the Chebychev sample size, N_{Cheb}, defined in (15), the Berry-Esseen sample size, N_{BE}, defined in (17), and thus N_μ all depend on σ and ε through their ratio, σ/ε. Thus, ignoring the initial sample used to estimate the variance, $N_{\text{tot}}(\varepsilon, \alpha, \beta, \mathscr{C}_{\kappa_{\max}}, \sigma_{\max})$ is roughly proportional to $\sigma_{\max}^2/\varepsilon^2$, even though $\sigma_{\max}$ is not a parameter of the algorithm. Algorithm 1 *adaptively* determines the sample size and thus the cost to fit the unknown variance of Y. Random variables, Y, with small variances will require a lower cost to estimate μ with a given error tolerance than random variables with large variances.



(a) (b)

Fig. 1. (a) The cost ratios of $N_{\text{up}}(\varepsilon, 0.01, 0.01, \tilde{\kappa}_{\max}, \sigma)/N_{\text{CLT}}(\varepsilon, \sigma, 0.01)$ for $\tilde{\kappa}_{\max} = 10, 100,$ and 1000 with $n_\sigma = 1000\tilde{\kappa}_{\max}$ (dashed) and n_σ optimized (solid); (b) the optimal values of n_σ (solid) and $\mathfrak{C}$ (dashed).

Figure 1a shows the ratio of upper bound of the cost, $N_{\text{up}}(\varepsilon, 0.01, 0.01, \tilde{\kappa}_{\max}, \sigma)$, to the ideal CLT cost, $N_{\text{CLT}}(\varepsilon, \sigma, 0.01) = \lceil (2.58\sigma/\varepsilon)^2 \rceil$, for a range of σ/ε ratios for $\tilde{\kappa}_{\max} = 10, 100,$ and 1000. The formula defining N_{up} in Theorem 6 uses the alternative and somewhat costlier formula for N_μ in (21). The dashed curves in Figure 1a show these cost ratios with $n_\sigma = 1000\tilde{\kappa}_{\max}$, which corresponds to $\mathfrak{C} \approx 1.2$. The solid curves denote the case where n_σ and $\mathfrak{C}$ vary with σ/ε to minimize N_{up}. Figure 1b displays the optimal values of n_σ (solid) and $\mathfrak{C}$ (dashed). In both figures, higher curves correspond to higher values of $\tilde{\kappa}_{\max}$.

Here N_{CLT} denotes the ideal cost if one knew the variance of Y a priori and knew that the distribution of the sample mean was close to Gaussian. The cost ratio is the penalty for having a guaranteed fixed-width confidence interval in the absence of this knowledge about the distribution of Y. For smaller values of N_{CLT}, equivalently smaller σ/ε, this cost ratio can be rather large. However the absolute effect of this large penalty is mitigated by the fact that the total number of samples needed is not much. For larger N_{CLT}, equivalently smaller σ/ε, the cost ratio approaches somewhat less than 1.5 in the case of optimal n_σ and $\mathfrak{C}$, and somewhat less than 4 for $n_\sigma = 1000\tilde{\kappa}_{\max}$.

The ideal case of optimizing n_σ and $\mathfrak{C}$ with respect to σ/ε is impractical, since σ is not known in advance. Our suggestion is to choose $\mathfrak{C}$ around 1.2–1.5, and then choose n_σ as large as needed to ensure that $\tilde{\kappa}_{\max}$ is as large as desired. For example with $\mathfrak{C} = 1.5$ and $\tilde{\kappa} = 10, 100, 1000$ we get $n_\sigma = 2888$, 31755, and 320440 respectively.

4 Numerical Examples

4.1 Illustrative Univariate Examples of Automatic Algorithms

Several commonly used software packages have automatic algorithms for integrating functions of a single variable. These include

- `quad` in MATLAB (The MathWorks, Inc., 2012), adaptive Simpson's rule based on `adaptsim` by Gander and Gautschi (2000),
- `quadgk` in MATLAB (The MathWorks, Inc., 2012), adaptive Gauss-Kronrod quadrature based on `quadva` by Shampine (2008), and
- the `chebfun` (Hale et al, 2012) toolbox for MATLAB (The MathWorks, Inc., 2012), which approximates integrals by integrating interpolatory Chebychev polynomial series for the integrands.

For these three automatic algorithms one can easily probe where they sample the integrand, feed the algorithms zero values, and then construct fooling functions for which the automatic algorithms will return a zero value for the integral. Figure 2 displays these fooling functions for the problem $\mu = \int_0^1 f(x)\,\mathrm{d}x$ for these three algorithms. Each of these algorithms is asked to provide an answer with an absolute error no greater than 10^{-14}, but in fact the the absolute error is 1 for these fooling functions. The algorithms `quad` and `chebfun` sample only about a dozen points before concluding that the function is zero, whereas the algorithm `quadgk` samples a much larger number of points (only those between 0 and 0.01 are shown in the plot).

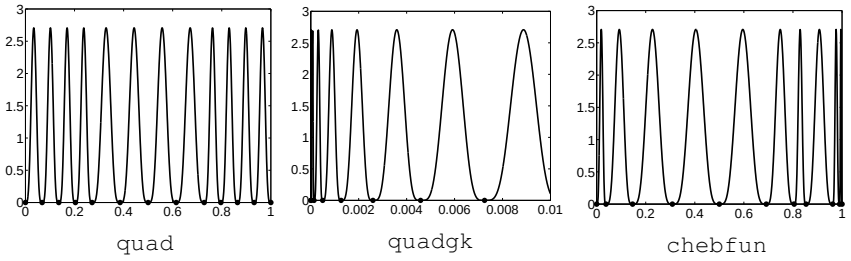


Fig. 2. Plots of fooling functions, f, with $\mu = \int_0^1 f(x)\,\mathrm{d}x = 1$, but for which the corresponding algorithms return values of $\hat{\mu} = 0$.

Accuracy and timing results have been recorded integration problem $\mu = \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$ for a single hump test integrand

$$f(\boldsymbol{x}) = a_0 + b_0 \prod_{j=1}^{d} \left[1 + b_j \exp\left(-\frac{(x_j - h_j)^2}{c_j^2} \right) \right]. \tag{25}$$

Here $\boldsymbol{x}$ is a d dimensional vector, and $a_0, b_0, \ldots, b_d, c_1, \ldots, c_d, h_1, \ldots, h_d$ are parameters. Figure 3 shows the results of different algorithms being used to integrate 500 different instances of f. For each instance of f, the parameters are chosen as follows:

- $b_1, \ldots, b_d \in [0.1, 10]$ with $\log(b_j)$ being i.i.d. uniform,
- $c_1, \ldots, c_d \in [10^{-6}, 1]$ with $\log(c_j)$ being i.i.d. uniform,

- $h_1,\ldots,h_d \in [0,1]$ with h_j being i.i.d. uniform,
- b_0 chosen in terms of the $b_1,\ldots,b_d,c_1,\ldots,c_d,h_1,\ldots,h_d$ to make $\sigma^2 = \|f-\mu\|_2^2 \in [10^{-2},10^2]$, with $\log(\sigma)$ being i.i.d. uniform for each instance, and
- a_0 chosen in terms of the $b_0,\ldots,b_d,c_1,\ldots,c_d,h_1,\ldots,h_d$ to make $\mu = 1$.

These ranges of parameters are chosen so that the algorithms being tested fail to meet the error tolerance a significant number of times.

These 500 random constructions of f with $d = 1$ are integrated using `quad`, `quadgk`, `chebfun`, and Algorithm 1, and an automatic quasi-Monte Carlo algorithm that uses scrambled Sobol' sampling (Owen, 1995, 1997a,b; Matoušek, 1998; Hong and Hickernell, 2003; Dick and Pillichshammer, 2010) and quasi-standard error (Halton, 2005; Owen, 2006) to determine the sample size. We do not yet have a theorem providing sufficient conditions under which this quasi-Monte Carlo algorithm is guaranteed to provide the answer within the specified error tolerance, and so we do not describe this algorithm in detail.

For all but `chebfun`, the specified absolute error tolerance is $\varepsilon = 0.001$. The algorithm `chebfun` attempts to do all calculations to near machine precision. The observed error and execution times are plotted in Figure 3. Whereas `chebfun` uses a minimum of $2^3+1 = 9$ function values, the figure labeled "`chebfun` (heavy duty)" displays the results of requiring chebfun to use at least $2^{10}+1 = 1025$ function values. Algorithm 1 takes $\alpha = 0.01$, and $\mathfrak{C} = 1.5$. For the plot on the left, $n_\sigma = 2^{10} = 1024$, which corresponds to $\tilde{\kappa}_{\max} = 2.59$. For the heavy duty plot on the right, $n_\sigma = 2^{17} = 131\,072$, which corresponds to $\kappa_{\max} = 205$. The same initial sample sizes are used for the Sobol' sampling algorithm.

Figure 3 shows that `quad` and `quadgk` are quite fast, nearly always providing an answer in less that 0.01 seconds. Unfortunately, they successfully meet the error tolerance only about 30% of the time for `quad` and 50–60% of the time for `quadgk`. The difficult cases are those where c_1 is quite small, and these algorithms miss the sharp peak. The performance of `chebfun` is similar to that of `quad` and `quadgk`. The heavy duty version of `chebfun` fares somewhat better.

In the plots for Algorithm 1 those points where the integrands satisfy $\tilde{\kappa}(f) \le \tilde{\kappa}_{\max}$ are labeled *, and all such points fall within the prescribed error tolerance. For Algorithm 1 (heavy duty) $\kappa_{\max}$ is larger, so there are more points for which the guarantee holds. Those points labeled with a dot, are those for which $\tilde{\kappa}(f) > \tilde{\kappa}_{\max}$, and so no guarantee holds. The points labeled with a diamond are those for which Algorithm 1 attempts to exceed the cost budget that we set, i.e., it wants to choose n such that $(n_\sigma+n)d > N_{\max} = 10^9$. Algorithm 1 performs somewhat more robustly than `quad`, `quadgk`, and `chebfun`, because it requires only a low degree of smoothness and takes a fairly large minimum sample. The more important point is that Algorithm 1 has a guarantee, where to our knowledge, the other routines do not.

From Figure 3, the Sobol' sampling algorithm is more reliable and takes less time than Algorithm 1. This is due primarily to the fact that in dimension one, Sobol' sampling is equivalent to stratified sampling, where the points are more evenly spread.

Figure 5 repeats the simulation shown in Figure 3 for the same test function (25), but now with $d = 2,\ldots,8$ chosen randomly and uniformly. For this case the univariate integration algorithms are inapplicable, but the two multidimensional routines can be used. There are more cases where the Algorithm 1 tries to exceed the maximum sample size allowed, but the behavior seen for $d = 1$ still generally apply.

We will put one more finance example here.

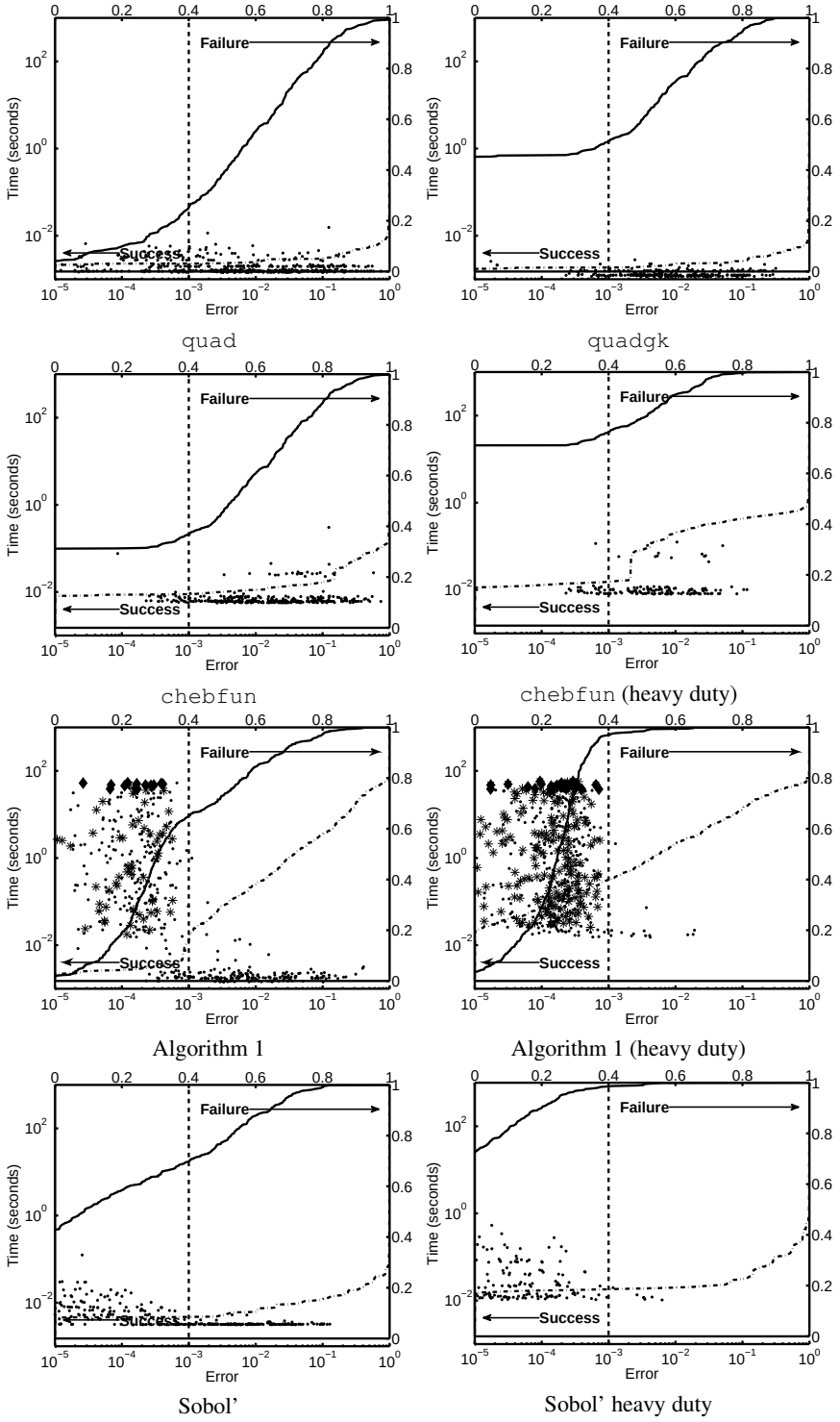


Fig. 3. Execution times and errors for test function (25) for $d = 1$ and $\varepsilon = 10^{-3}$, and a variety of parameters giving a range of $\sigma(f)$ and $\kappa(f)$. The solid line shows that cumulative distribution of actual errors, and the dot-dashed line shows the cumulative distribution of execution times. For the Algorithm 1 the points labeled * are those for which the Theorem 5 guarantees the error tolerance.

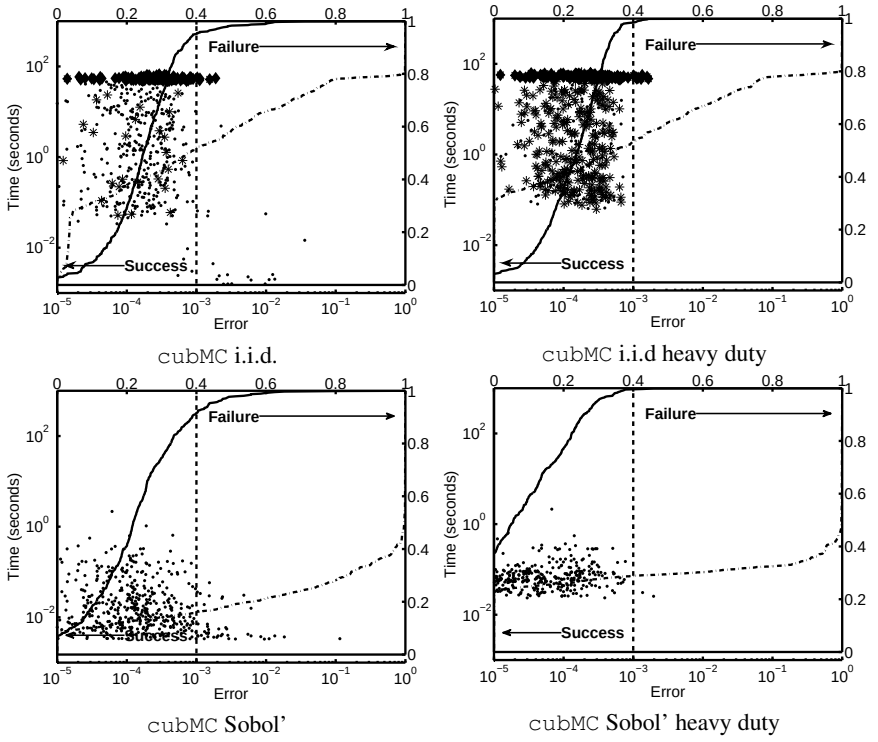


Fig. 4. Execution times and errors for test function (25) for $d = 2, \ldots, 8$ and $\varepsilon = 10^{-3}$, with the rest of the parameters as in Figure 3.

5 Discussion

Put something here.

Looking for algorithms that work well for cones of integrands, $\mathcal{C}_{\mathbf{K}_{\max}}$, leads one to *adaptive* algorithms. The sample size used to estimate the integral is determined adaptively by first computing an upper bound on $\|f - \mu(f)\|_2$. In information-based complexity theory it is known that adaptive information does not help for convex sets of integrands in the worst case and probabilistic settings (Traub et al, 1988, Chapter 4, Theorem 5.2.1; Chapter 8, Corollary 5.3.1). Here, the cone, $\mathcal{C}_{\mathbf{K}_{\max}}$ is not a convex set, so adaption can help.

Again, it should be stressed that the algorithm to be presented here is automatic. It does not require information about $\|f - \mu(f)\|_2 = \sigma$, but this quantity needs to be reliably estimated by the algorithm. Thus, the sample size needed, and consequently the time required, to estimate μ to within the prescribed error tolerance depends on how large $\|f - \mu(f)\|_2 = \sigma$ is estimated to be. The algorithm is adaptive, and its cost depends on the integrand.

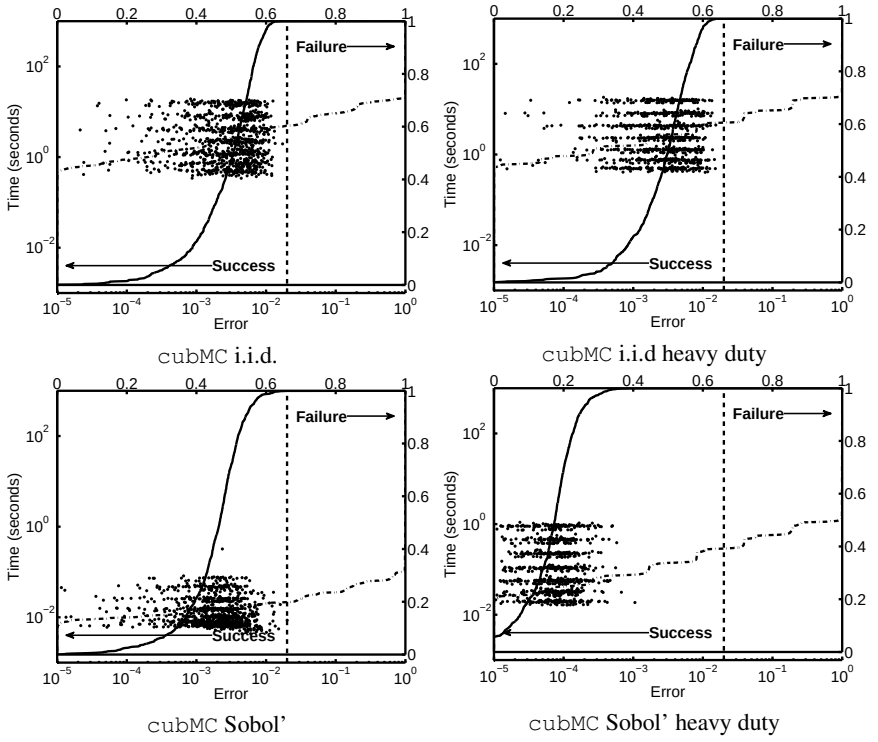


Fig. 5. Execution times and errors for the geometric mean Asian call option for $d = 2, 4, \ldots, 64$ and $\varepsilon = 0.02$, with the rest of the parameters as in Figure 3.

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