

Unbiased Function Simulation Based on Good Lattice Points

Gregory M Duncan

Brattle Group

Department of Economics, University of California, Berkeley

Introduction:

In Duncan (2008) I showed how to simulate the values of analytic functions whose arguments are expectations which must be simulated. In this paper, I extend the results to quasi-random variables to reduce computational complexity and improve accuracy.

Setup:

Let $\ell(\bullet)$ is analytic with radius of convergence R and defined by the expansion $\ell(x) = \sum_{r=1}^{\infty} \lambda_r (x - x_0)^r$. $X(\theta)$ is a random function with expected value $E(X(\theta))$.

We desire unbiased simulators of $\ell(E(X(\theta)))$ and $\nabla_{\theta} \ell(E(X(\theta)))$ when

$$E(X(\theta)) = \int_0^1 k(z, \theta) dz \quad (1.1)$$

has no closed form and must be simulated, here by Quasi-Monte Carlo integration.

Transformation to Periodicity on the Unit Cube:

The periodicity of integrands in and on the unit cube plays an essential role in our solution. This is not a restrictive assumption however. With a change of variable, the domain of any function or the limits of any integral can be made the unit interval I or the unit cube. Similarly, any integrand on the unit cube, I , can be replaced by an integrand that is periodic with period 1 which has the same integral. For example, if, in (1.1), $k(z, \theta)$ is not periodic, apply the change in variable

$$z = \phi(t) = t - \frac{\sin[2\pi t]}{2\pi}, 0 \leq t \leq 1 \quad (1.2)$$

then $k(\phi(t), \theta)\phi'(t)$ is periodic with period 1 and

$$E(X(\theta)) = \int_0^1 k(\phi(t), \theta)\phi'(t) dt \quad (1.3)$$

Henceforth, $k(z, \theta)$ is assumed 1-periodic. In many dimensions one can apply the transformation one dimension at a time.

Unbiased Quasi-Monte Carlo Integration:

A lattice point in I is defined as follows. Let N be a prime number, let p be relatively prime with N .¹ Let where $\{x\}$ be the fractional part of x , then

$H = \left\{ \left\{ j \frac{p}{N} + z \right\}, j \in \square, z \in \square \right\}$ is the set of all lattice points in I . Let $k(t, \theta)$ be a periodic

function on I with Fourier expansion

$$k(t, \theta) = \sum_{h \in H} c_h \exp(2\pi i h t) \quad (1.4)$$

We know from Fourier analysis that

$$c_h = \int \exp(i h t) k(t, \theta) dt \quad (1.5)$$

Additionally if $k(t, \theta)$ is real then $c_h = \bar{c}_{-h}$, consequently, in (1.5) if $c_h = a_h + i b_h$, then

$c_h + c_{-h} = a_h$. Another well known result gives $a_h(\theta) = \int_0^1 \cos(ht) k(t, \theta) dt$. If

$u \sim U(0, 1)$, define $\hat{a}_h(\theta) = \cos(hu) k(u, \theta)$, then

$$\begin{aligned} E_U(\hat{a}_h(\theta)) &= E_U(\cos(hu) k(u, \theta)) \\ &= \int_0^1 \cos(ht) k(t, \theta) dt \quad . \\ &= a_h(\theta) \end{aligned}$$

Now let $\int_0^1 k(t, \theta) dt = \sum_{n=1}^m k\left(\frac{n}{m}, \theta\right) + \varepsilon$, where m is a large prime integer. A result due

to Haselgrove(1961) and Zaremba (1970) and proved in Sloan and Kachoyan (1987) states

¹ Two integers are relatively prime (or strangers or coprimes) if they share no common positive factors (divisors) except 1. Using the notation $GCD(m, n)$ to denote the greatest common divisor, two integers m and n are relatively prime if $GCD(m, n) = 1$; a relationship often denoted $m \perp n$.

$$\begin{aligned}
\sum_{n=1}^m k\left(\frac{n}{m}, \theta\right) - \int_0^1 k(t, \theta) dt &= \frac{1}{m} \sum_{h \neq 0} c_h \sum_{n=1}^m \exp\left(2\pi i \frac{nh}{m}\right) \\
&= \sum_{\substack{h \neq 0 \\ h=0 \pmod{m}}} c_h \\
&= \sum_{j=1}^{\infty} c_{h_j} + c_{-h_j}
\end{aligned}$$

We can rewrite this as

$$\begin{aligned}
\int_0^1 k(t, \theta) dt &= \sum_{n=1}^m k\left(\frac{n}{m}, \theta\right) - \sum_{j=1}^{\infty} (c_{h_j} + c_{-h_j}) \\
&= \sum_{n=1}^m k\left(\frac{n}{m}, \theta\right) - \sum_{j=1}^{\infty} a_{h_j}(\theta)
\end{aligned} \tag{1.6}$$

Thus the integral on the left hand side is approximated by the sum involving k on the right and the sum involving the a gives the explicit error. The trick to the whole approach is the following lemma.

Lemma 1:

Let $S = \sum_{i=1}^{\infty} \alpha_i$ converge absolutely, and let J be a random variable on the natural

numbers, let $P(j) = \Pr[J = j]$ then $S = E_J\left(\frac{\alpha_j}{P(j)}\right)$.

Proof:

$E_J\left(\frac{\alpha_j}{P[j]}\right) = \sum_{j=1}^{\infty} \left(\frac{\alpha_j}{P[j]}\right) P[J] = \sum_{j=1}^{\infty} \alpha_j = S$. The validity of the exchange of limits

follows from the absolute convergence of S : if either limit exists (absolutely) both do and they are equal.

QED.

In our context then, $\frac{a_{h_j}(\theta)}{P[J]}$ is an unbiased estimator of the error in (1.6) where J is

chosen from \square with probability $P[J]$.

More generally, let N be a prime number and let $p \in \square^s$ be relatively prime with N . For $s \geq 2$ an s -dimensional lattice is the set of all linear combinations with integer coefficients of s linearly independent vectors in R^s . We only consider lattices which contain \square^s as a

sublattice. If L is such a lattice, then $S = L \cap [0, 1]^s$ is a finite set consisting, say, of the distinct points (x_1, \dots, x_N) . Now let $K(\theta) = \int_{I^s} k(x, \theta) dx$ where $k(x, \theta)$ is periodic with

period 1 on the unit cube. Approximate $K(\theta)$ by $\hat{K}(\theta) = \frac{1}{N} \sum_{j=0}^{N-1} k\left(\left\{j \frac{p}{N}\right\}, \theta\right)$ where

$\{x\} = x \bmod 1$, the fractional part of x . Define $S = \left\{j \frac{p}{N} + z, j \in \square, z \in \square^s\right\}$ and

$S^+ = \left\{m \in \square^s \mid m^T x \in \square, \forall x \in S\right\}$, if k has an absolutely convergent Fourier series representation

$$k(x, \theta) = \sum_{m \in \square^s} a(m, \theta) \exp(2\pi i m^T x) \quad x \in I^s \quad (1.7)$$

then the following theorem holds

Theorem 1:

Let M be a random element drawn from S^+ with probability $P(m)$

$$\tilde{\mu}(\theta) = \frac{1}{N} \sum_{j=0}^{N-1} k\left(\left\{j \frac{p}{N}\right\}, \theta\right) - \frac{a(M, \theta)}{P(M)} \quad (1.8)$$

is an unbiased estimator of $E(X(\theta))$.

Proof:

Apply Lemma 1. QED.

Variance:

The variance may or may not exist depending on the relationship between $P[M]$ and $a(M, \theta)$. However, if $k(t, \theta)$ in (1.7) is $m+1$ -times differentiable with m absolutely integrable derivatives, then from Fourier analysis we have $M^m a(M, \theta) \rightarrow 0$ and that $a(M, \theta)$ is bounded. Consequently if

$P[M] = \frac{M^{-q}}{\zeta(q)}, M = 1, \dots, \infty$, for some $q \in \{1, \dots, \infty\}$ then the second moment and hence

the variance will exist.

Theorem 2:

Let M be a random element drawn from S^+ with probability

$P[M] = \frac{M^{-q}}{\zeta(q)}, M = 1, \dots, \infty$, for some $q \in \{1, \dots, \infty\}$

$$V\left(\frac{a(M, \theta)}{P(M)}\right) \leq \infty \quad (1.9)$$

.

Proof:

The expectation exists by Theorem 1, hence the variance exists if $E\left(\left(\frac{a(M, \theta)}{P(M)}\right)^2\right) \leq \infty$

But

$$\begin{aligned} E\left(\left(\frac{a(M, \theta)}{P(M)}\right)^2\right) &= \sum_{m=1}^{\infty} \left(\frac{a(m, \theta)}{P(m)}\right)^2 P(m) \\ &= \sum_{m=1}^{\infty} \left(\frac{a(m, \theta)^2}{P(m)}\right) \\ &= \sum_{m=1}^{\infty} \xi(q) m^q a(m, \theta)^2 \\ &= \xi(q) \sum_{m=1}^{\infty} |a(m, \theta)| (m^q |a(m, \theta)|) \end{aligned}$$

Differentiability of order q implies $(m^q a(m, \theta))$ is bounded for finite m and converges

for infinite m , hence there is some $A^* < \infty$ such that $(m^q a(m, \theta)) < A^*$ so that

$$E\left(\left(\frac{a(M, \theta)}{P(M)}\right)^2\right) \leq \xi(q) A^* \sum_{m=1}^{\infty} |a(m, \theta)|, \text{ the result follows from the absolute}$$

convergence of the Fourier coefficients.

QED.

Unbiased Evaluation of Functions of Quasi-Monte Carlo Expectations:

Now consider an function of the expectation, $\ell(E(X(\theta)))$. Assume ℓ is analytic on I then,

$$\begin{aligned}
 \ell(X(\theta)) &= \ell\left(\int_0^1 k(z, \theta) dz\right) \\
 &= \ell\left(\sum_{n=1}^m k\left(\frac{n}{m}, \theta\right) - \sum_{m \in \mathcal{S}^+} a(m, \theta)\right) \\
 &= \ell\left(\sum_{n=1}^m k\left(\frac{n}{m}, \theta\right) + \varepsilon\right) \\
 &= \ell(\hat{K}(\theta) + \varepsilon)
 \end{aligned} \tag{1.10}$$

Now by Taylor's expansion,

$$\ell(\hat{K}(\theta) + \varepsilon) = \ell(\hat{K}(\theta)) - \sum_{r=1}^{\infty} \lambda_r \varepsilon^r$$

where $\varepsilon^r = \left(\left(\sum_{j=1}^{\infty} a_{h_j}(\theta)\right) - \hat{K}(\theta)\right)^r$. An unbiased estimator of $\sum_{r=1}^{\infty} \lambda_r \varepsilon^r$ can be gotten

by taking a random term and dividing by the probability. So $E_r \left[\frac{\lambda_r \varepsilon^r}{P[r]} \right] = \sum_{r=1}^{\infty} \lambda_r \varepsilon^r$ for

suitably defined $P[r]$. However ε^r involves an infinite number of terms and perhaps no closed form; an unbiased estimator of ε^r is the product of r unbiased estimators of $\varepsilon = \left(\sum_{j=1}^{\infty} a_{h_j}(\theta)\right) - \hat{K}(\theta)$, an unbiased estimator of which is obtained by choosing j at random with probability $Q[j]$ choosing the j th term in ε and dividing by the

probability. Thus $E_{rj} \left[\frac{\lambda_r}{P[r]} \prod_{s=1}^r \left(\frac{a_{h_{j_s}}(\theta)}{Q[j_s]} - \hat{K}(\theta) \right) \right] = \sum_{r=1}^{\infty} \lambda_r \varepsilon^r$ where the a and the j are

independently chosen.

Theorem 3:

Let T be a random integer drawn from the positive integers with probability $P[t]$, and let

I be drawn from the positive integers with probability $Q[i]$ and let $\hat{a}_h = \cos(hu) f(u)$,

where $u \sim U(0,1)$ and let

$$\ell(x) = \sum_{r=1}^{\infty} \lambda_r (x - x_0)^r, \text{ with } x_0 = \hat{K}(\theta) = \sum_{n=1}^m k\left(\frac{n}{m}, \theta\right)$$

$$\hat{A}_r = \prod_{s=1}^r \left(\frac{a_{h_s}(\theta)}{Q[j_s]} - \hat{K}(\theta) \right), \text{ with } h \text{ as above then}$$

$$\tilde{\ell} = \ell(\hat{K}(\theta)) - \frac{\lambda_r}{P(r)} \hat{A}_r \quad (1.11)$$

is an unbiased simulator of $\ell(E(X(\theta)))$.

Proof:

Apply Lemma 1. QED

Variance:

We show in the next theorem that the second moment and therefore the variance exists provided that certain moment and differentiability conditions obtain.

Theorem 4:

Let r be a random integer, with $P[r] > 0, r = 0, \dots, \infty$ and $rP[r] \rightarrow m > 0$ (so moments of no integral order exist), similarly, let j be a random integer, with $Q[j] > 0, j = 0, \dots, \infty$, and $jQ[j] \rightarrow n > 0$. Let $R_\varepsilon < R - \varepsilon$, with R the radius of convergence and let $\varphi(\square)$ be at least once differentiable, then $E|\tilde{f}(\theta)|^2$ exists and is bounded.

Proof:

$$E|\tilde{f}(\theta)|^2 = \left| \sum_{r=1}^{\infty} \left\{ \sum_{h_1=0}^{\infty} \dots \sum_{h_r=0}^{\infty} \left| \frac{\lambda_r R_\varepsilon^r}{P[r]} \prod_{j=1}^r \left(\frac{a_{h_j}}{Q[h_j]} - \hat{K} \right) / R_\varepsilon^r \prod_{j=1}^r Q[h_j] \right\}^2 P[r] \right|$$

We examine, first, $\frac{\lambda_r}{P[r]}$. Since f is analytic and differentiable $r\lambda_r R_\varepsilon^r \rightarrow 0$, also

$$rP[r] \rightarrow m > 0 \text{ so } \frac{\lambda_r R_\varepsilon^r}{P[r]} = \frac{r\lambda_r R_\varepsilon^r}{rP[r]} \rightarrow 0 \text{ so, in particular, } \left| \frac{\lambda_r R_\varepsilon^r}{P[r]} \right| \leq M_1 < \infty. \text{ By a similar}$$

logic, $\varphi(\)$ is (at least) once differentiable, $|h_j a_{h_j}| \rightarrow 0$ since $jQ[j] \rightarrow n > 0$,

$$\left| \frac{h_j a_{h_j}}{h_j Q[h_j]} \right| \rightarrow 0, \text{ hence for large enough } h_j \text{ and arbitrary } \eta > 0, \text{ we have } \left| \frac{a_{h_j}}{Q[h_j]} \right| < \eta,$$

for large enough h_j $\left| \frac{a_{h_j}}{Q[h_j]} - \hat{K} \right| / R_{\eta/2} \leq 1 < \infty$ (since \hat{K} is the middle of the circle of convergence.) Thus

$$\begin{aligned} E|\tilde{f}(\theta)|^2 &\leq \left| \sum_{r=1}^{\infty} \left\{ \sum_{h_1=0}^{\infty} \cdots \sum_{h_r=0}^{\infty} M_1^2 \prod_{j=1}^r Q[h_j] \right\} P[r] \right| \\ &= M_1^2 \end{aligned}$$

QED.

Gradients:

One of the results in Duncan (2008) is that the gradient of the unbiased simulator of $f(E(X(\theta)))$ is in turn an unbiased estimator of the $\nabla_{\theta} f(E(X(\theta)))$. The same result obtains here. This means that standard optimization software can be used to maximize the simulated functions.

Theorem 4:

Under the assumptions of the previous theorem, and the assumption that

$$\left| \nabla_{\theta} k\left(\frac{n}{m}, \theta\right) \right| \leq M < \infty \text{ then}$$

$$\begin{aligned} \nabla_{\theta} \tilde{\ell} &= \ell'(\hat{K}(\theta)) \sum_{n=1}^m \nabla_{\theta} k\left(\frac{n}{m}, \theta\right) - \frac{\lambda_r}{P(r)} \nabla_{\theta} \hat{A}_r \\ &= \ell'(\hat{K}(\theta)) \sum_{n=1}^m \nabla_{\theta} k\left(\frac{n}{m}, \theta\right) - \frac{\lambda_r}{P(r)} \nabla_{\theta} \prod_{s=1}^r \left(\frac{a_{h_s}(\theta)}{Q[j_s]} - \hat{K}(\theta) \right) \end{aligned} \quad (1.12)$$

is an unbiased simulator of $\nabla_{\theta} \ell(E(X(\theta)))$.

Proof:

Assuming the proper domination conditions, if both $E\tilde{\ell}$, and $E(\nabla_{\theta} \tilde{\ell})$ exist, then

$E(\nabla_{\theta} \tilde{\ell}) = \nabla_{\theta} E(\tilde{\ell})$. $E\tilde{\ell}$ exists and is suitably dominated by dint of a the previous theorem.

$$\begin{aligned}
E(\nabla_{\theta} \tilde{\ell}) &= \ell'(\hat{K}(\theta)) \sum_{n=1}^m \nabla_{\theta} k\left(\frac{n}{m}, \theta\right) - E\left(\frac{\lambda_r}{P(r)} \nabla_{\theta} \hat{A}_r\right) \\
&= \ell'(\hat{K}(\theta)) \sum_{n=1}^m \nabla_{\theta} k\left(\frac{n}{m}, \theta\right) - E\left(\frac{\lambda_r}{P(r)} \nabla_{\theta} \prod_{s=1}^r \left(\frac{a_{h_{j_s}}(\theta)}{Q[j_s]} - \hat{K}(\theta)\right)\right)
\end{aligned}$$

Consider the term

$$\begin{aligned}
&E\left(\frac{\lambda_r}{P(r)} \nabla_{\theta} \prod_{s=1}^r \left(\frac{a_{h_{j_s}}(\theta)}{Q[j_s]} - \hat{K}(\theta)\right)\right) \\
&= E\left(\frac{\lambda_r}{P(r)} \sum_{s=1}^r \left(\nabla_{\theta} \left(\frac{a_{h_{j_s}}(\theta)}{Q[j_s]} - \hat{K}(\theta)\right) \prod_{\substack{k=1 \\ k \neq s}}^r \left(\frac{a_{h_{j_k}}(\theta)}{Q[j_k]} - \hat{K}(\theta)\right)\right)\right) \\
&= E\left(\frac{\lambda_r}{P(r)} \sum_{s=1}^r \left(\left(\frac{\nabla_{\theta} a_{h_{j_s}}(\theta)}{Q[j_s]} - \nabla_{\theta} \hat{K}(\theta)\right) \prod_{\substack{k=1 \\ k \neq s}}^r \left(\frac{a_{h_{j_k}}(\theta)}{Q[j_k]} - \hat{K}(\theta)\right)\right)\right) \\
&= E\left(\frac{\lambda_r}{P(r)} E_{|r} \left\{ \sum_{s=1}^r \left(\left(\frac{\nabla_{\theta} a_{h_{j_s}}(\theta)}{Q[j_s]} - \nabla_{\theta} \hat{K}(\theta)\right) \prod_{\substack{k=1 \\ k \neq s}}^r \left(\frac{a_{h_{j_k}}(\theta)}{Q[j_k]} - \hat{K}(\theta)\right)\right)\right\}\right) \quad (1.13)
\end{aligned}$$

Note the term in braces

$$\begin{aligned}
&E_{|r} \left\{ \sum_{s=1}^r \left(\left(\frac{\nabla_{\theta} a_{h_{j_s}}(\theta)}{Q[j_s]} - \nabla_{\theta} \hat{K}(\theta)\right) \prod_{\substack{k=1 \\ k \neq s}}^r \left(\frac{a_{h_{j_k}}(\theta)}{Q[j_k]} - \hat{K}(\theta)\right)\right)\right\} = \\
&\sum_{j_1, \dots, j_r} \left\{ \sum_{s=1}^r \left(\left(\frac{E(\nabla_{\theta} \hat{a}_{h_{j_s}}(\theta))}{Q[j_s]} - \nabla_{\theta} \hat{K}(\theta)\right) \prod_{\substack{k=1 \\ k \neq s}}^r \left(\frac{E(\hat{a}_{h_{j_k}}(\theta))}{Q[j_k]} - \hat{K}(\theta)\right)\right)\right\} \prod_{k=1}^r Q[j_k] \\
&= \sum_{j_1, \dots, j_r} \left\{ \sum_{s=1}^r \left(\frac{\nabla_{\theta} a_{h_{j_s}}(\theta)}{Q[j_s]} - \nabla_{\theta} \hat{K}(\theta)\right) \left(\prod_{\substack{k=1 \\ k \neq s}}^r \left(\frac{a_{h_{j_k}}(\theta)}{Q[j_k]} - \hat{K}(\theta)\right)\right)\right\} \prod_{k=1}^r Q[j_k] \\
&= r \left(\left(\sum_{j=1}^{\infty} \nabla_{\theta} a_{h_j}(\theta)\right) - \nabla_{\theta} \hat{K}(\theta)\right) \left(\left(\sum_{j=1}^{\infty} a_{h_j}(\theta)\right) - \nabla_{\theta} \hat{K}(\theta)\right)^{r-1}
\end{aligned}$$

Substituting into (1.13) gives

$$\begin{aligned}
E(\nabla_{\theta} \tilde{\ell}) &= \ell'(\hat{K}(\theta)) \nabla_{\theta} \hat{K}(\theta) - \sum_{r=0}^{\infty} \frac{\lambda_r}{P(r)} r \left(\left(\sum_{j=1}^{\infty} \nabla_{\theta} a_{h_j}(\theta) \right) - \nabla_{\theta} \hat{K}(\theta) \right) \left(\left(\sum_{j=1}^{\infty} a_{h_j}(\theta) \right) - \nabla_{\theta} \hat{K}(\theta) \right)^{r-1} P(r) \\
&= \ell'(\hat{K}(\theta)) \nabla_{\theta} \hat{K}(\theta) - \sum_{r=0}^{\infty} r \lambda_r \left(\left(\sum_{j=1}^{\infty} \nabla_{\theta} a_{h_j}(\theta) \right) - \nabla_{\theta} \hat{K}(\theta) \right) \left(\left(\sum_{j=1}^{\infty} a_{h_j}(\theta) \right) - \nabla_{\theta} \hat{K}(\theta) \right)^{r-1} \\
&= \ell'(\hat{K}(\theta)) \nabla_{\theta} \hat{K}(\theta) - \sum_{r=0}^{\infty} r \lambda_r \nabla_{\theta} \varepsilon(\theta) \varepsilon(\theta)^{r-1}
\end{aligned}$$

which is the term by term gradient of the Taylor's expansion of $\ell(\theta)$, domination and absolute convergence of which follow from analyticity and absolute convergence of Fourier coefficients.

Comparison with Alternative Approach:

One could also take an approach that used Duncan (2008). Calculate $\hat{K}_0(\theta)$ using the original lattice. Randomly shift the lattice L by adding a uniform random variable, then the resulting $\hat{K}_i(\theta)$ is a random variable with expectation $K(\theta)$. Randomly choose an integer from \square using a distribution with survivor function $G(i) = \Pr[I \geq i]$. Expand $\ell(\theta)$ around the initial $\hat{K}(\theta)$ and truncate the expansion at I terms. Generate I unbiased estimates of $K(\theta)$, $\{\hat{K}_i(\theta)\}$ and calculate the U-statistics of $\hat{K}_i(\theta) - \hat{K}(\theta)$ up to order I . Then the estimator

$$\tilde{\ell}(\theta) = \ell(\hat{K}(\theta)) + \sum_{i=1}^I \frac{\lambda_i}{G(i)} U_i$$

is unbiased. The problem with this estimator is that each $\hat{K}_i(\theta)$ is computationally expensive and so is computing the ensemble of U-statistics up to order I . The estimator proposed here is computationally simpler. I have not yet compared variances between the two. Clearly the version in this paper can be replicated a number of times and averaged to obtain any variance desired. I speculate that the number of simulations in current version will be far smaller the estimator in Duncan(2008) for comparable variances. So this estimator will likely dominate that. Also in the approach in this paper, each simulation is associated with a much smaller computational burden and so would be preferred simply on those grounds.

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