Discrepancy-based error estimates for Quasi-Monte Carlo.

III: Error distributions and central limits

Jiri Hoogland
NIKHEF-H, Amsterdam, The Netherlands
and
Ronald Kleiss
University of Nijmegen, Nijmegen, The Netherlands

Abstract

In Quasi-Monte Carlo integration, the integration error is believed to be generally smaller than in classical Monte Carlo with the same number of integration points. Using an appropriate definition of an ensemble of quasi-random point sets, we derive various results on the probability distribution of the integration error, which can be compared to the standard Central Limit Theorem for normal stochastic sampling. In many cases, a Gaussian error distribution is obtained.

1e-mail: t96@nikhef.h nikhef.nl, research supported by Stichting FOM
2e-mail: kleiss@sci.kun.nl
1 Introduction

It is widely held that Quasi-Monte Carlo integration, in which the integration points are distributed more uniformly than in classical Monte Carlo integration which uses truly (or approximately) random points, can lead to potentially much smaller integration errors for the same amount of effort \textit{(i.e.} the same number of integrand evaluations). A number of theorems are known that relate information on the fluctuating behaviour of the integrand (such as variation, modulus of continuity, etc.) and information on the degree of uniformity of the point set employed (in terms of some quantitative notion of discrepancy) to the integration error \cite{1}. These results, however, do not easily lend themselves to practical error estimates and moreover, being usually upper limits, may be too pessimistic in many applications.

This situation is to be contrasted to that in classical Monte Carlo integration: there, one settles for a \textit{probabilistic} error estimate, which on the one hand does not give perfectly certain information but only confidence levels, but on the other hand can be easily computed by estimating not only the integral but at the same time the variance of the integrand. The essential point in this procedure is the existence of the Central Limit Theorem, which states that for a large number \( N \) of randomly chosen integration points, the integration error has an approximately Gaussian distribution with zero mean and a standard deviation related to the integrand’s variance. The estimation of this single parameter therefore suffices to determine the shape of the error distribution.

In this paper, we attempt to derive results similar to the Central Limit Theorem, for the case of Quasi-Monte Carlo. In previous publications \cite{2, 3} we have argued that such considerations require a definition of what constitutes an ensemble of \( N \)-point quasi-random point sets. For truly random points, this is an easy problem since we may simply assume the points to be iid uniformly over the integration region. For quasi-random points the situation is somewhat more subtle. We propose to use the fact that such more evenly distributed point sets are generally characterized by a low value of \textit{discrepancy}; given some definition of discrepancy (we shall specify one later on), we restrict ourselves to the set of \( N \)-point point sets in which the points are all uniformly iid, but with the additional condition that the discrepancy has a particular value \( s \) (by suitable integration over \( s \), we shall of course obtain again the classical results for truly random points). We can then study the distribution of the integration error over this ensemble of point sets.
The lay-out of this paper is as follows. In section 2 we establish some notation and define our point set ensemble. In section 3 we derive our main result on the distribution of the integration error, in terms of a single complex integral. In section 4, we present explicit results for a particular, simple definition of discrepancy. In section 5 we attempt to do the same for what we believe constitutes a realistic discrepancy. In each case we aim at arriving at an error distribution that depends on only a single parameter (so that confidence levels for the integration result can easily be computed), and ultimately, of course, the ideal Gaussian error distribution.

2 Notation and definitions

Our integration region will always be the $D$-dimensional hypercube $K = [0, 1)^D$, containing the point set $X_N = \{x_1, x_2, \ldots, x_N\}$. Where necessary, we shall denote the individual components of the vector $x_k$ with Greek indices:

$$x_k = x_k^\mu = (x_k^1, x_k^2, \ldots, x_k^D).$$

Let the integrand be denoted by $f(x)$; we assume, for simplicity, that the moments

$$J_p = \int_K dx \ f(x)^p$$

exist at least for the first few values of $p$. The numerical integral estimate is given by

$$S = \frac{1}{N} \sum_{k=1}^{N} f(x_k),$$

and the integration error $\eta$ is then, of course,

$$\eta = S - J_1.$$

It is the probability distribution of $\eta$ over the ensemble of point sets $X_N$ which is our object of concern here.

We now turn to the definition of a discrepancy. We introduce the Fourier base of orthonormal function as follows. Starting with $D = 1$, we define

$$u_{2n-1}(x) = \sqrt{2} \sin(2\pi nx), \quad u_{2n}(x) = \sqrt{2} \cos(2\pi nx),$$

for $n = 1, 2, 3, \ldots$, and $u_0(x) = 1$. In more dimensions, we define vectors $\vec{n} = n^\mu = (n^1, n^2, \ldots, n^D)$ with integer, non-negative components, and write

$$u_{\vec{n}}(x) = \prod_{\mu=1}^{D} u_{n^\mu}(x^\mu).$$
We assume that the integrand $f$ can be decomposed into its various Fourier modes as follows:

$$f(x) = \sum_{\vec{n}} v_\vec{n} u_{\vec{n}}(x),$$

from which it immediately follows that

$$J_1 = v_{(0,0,\ldots,0)}, \quad V \equiv \sum_{\vec{n} > 0} v_\vec{n}^2 = J_2 - J_1^2.$$

Here and in the following, the notation $\vec{n} > 0$ means a sum over all vectors $\vec{n}$ except the null vector $(0,0,\ldots,0)$. Quadratic integrability of the integrand requires that the variance $V$, i.e. the sum of the $v_\vec{n}^2$, converges.

To each mode with wave vector $\vec{n}$ we associate a strength $\sigma_\vec{n}$. In [2] and [3] we relate these strengths to a definition of an ensemble of integrands, by letting every $v_\vec{n}$ be normally distributed with zero mean and width $\sigma_\vec{n}$, but here we do not have to assume a particular such ensemble. The definition of (quadratic) discrepancy that we propose to use is

$$D_N(X_N) = \frac{1}{N} \sum_{k,l=1}^N \beta(x_k, x_l), \quad \beta(x_k, x_l) = \sum_{\vec{n} > 0} \sigma_\vec{n}^2 u_{\vec{n}}(x_k) u_{\vec{n}}(x_l).$$

An essential property is that

$$\int_K dx_k \beta(x_k, x_l) = \int_K dx_l \beta(x_k, x_l) = 0.$$

Another important assumption is that of translational invariance, by which the sines and cosines of each particular wave component have equal strength:

$$\sigma_{(2n^1,2n^2,\ldots,2n^D)} = \sigma_{(2n^1-1,2n^2,\ldots,2n^D)} = \sigma_{(2n^1,2n^2-1,\ldots,2n^D)} = \cdots = \sigma_{(2n^1-1,2n^2-1,\ldots,2n^D-1)}.$$

One of the consequences of this choice is that $\beta(x_k, x_l)$ only depends on the difference $x_k - x_l$, and therefore

$$\beta(0) = \int_K dx \beta(x,x) = \sum_{\vec{n} > 0} \sigma_\vec{n}^2.$$

Hence, for truly random points the expected value of the discrepancy is

$$\langle D_N(X_N) \rangle = \sum_{\vec{n} > 0} \sigma_\vec{n}^2,$$
and of course we assume this sum to converge. For the particular point set \( X_N \) we are employing, we assume the discrepancy \( D_N(X_N) \) to have a known value \( s \), non-negative by construction. Super-uniform, or quasi-random, point sets are distinguished by the fact that \( s \) is small compared to its expectation for random point sets.

We now come to the definition of an ensemble of quasi-random point sets. We consider it to consist of all point sets \( X_N \) that have a value \( s \) of the above discrepancy, but are otherwise unrestricted. The combined probability density \( P_N \) for the \( N \) points \( x_k \) is then given by

\[
P_N(s; x_1, x_2, \ldots, x_N) = \frac{\delta(D_N(x_1, x_2, \ldots, x_N) - s)}{H_0(s)},
\]

\[
H_0(s) = \int_K dx_1 \cdots dx_N \delta(D_N(x_1, x_2, \ldots, x_N) - s) .
\] (13)

The number \( H_0(s) \) serves to normalize the probability density \( P_N \): it is nothing but the probability for a set of truly random points to attain the value \( s \) for its discrepancy. Indeed, we trivially have

\[
\int_0^\infty ds \, H_0(s) P_N(s; x_1, x_2, \ldots, x_N) = 1 .
\] (14)

### 3 The error distribution

We now start to work our way towards a Central Limit Theorem for Quasi-Monte Carlo, assuming the point set \( X_N \) to be a member of the ensemble constructed above. Let \( P(s; \eta) \) be the probability density of the integration error \( \eta \) over the ensemble of possible point sets \( X_N \). We may write

\[
P(s; \eta) = \int_K dx_1 \cdots dx_N \, P_N(s; x_1, \ldots, x_N) \delta(\eta - S + J_1) .
\] (15)

Using the definition of the Dirac delta distributions in Eqs. (13,15) as Fourier integrals, we may write this as

\[
P(s; \eta) = \frac{1}{H_0(s)} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} \frac{dz}{2\pi i} e^{z\eta-\zeta J_1-ts} M(z, t) ,
\]
\[ M(z, t) = \int dx_1 \cdots dx_N \exp \left( \frac{z}{N} \sum_{k=1}^N f(x_k) + \frac{t}{N} \sum_{k,l=1}^N \beta(x_k, x_l) \right) \]
\[ = \sum_{m \geq 0} \frac{t^m}{m!} M_m(z) , \quad (16) \]

where the integration contours for \( t \) and \( z \) run to the left of any singularities.

In the spirit of the classical Central Limit Theorem, we must now proceed to take the asymptotic limit \( N \to \infty \) in a careful manner, taking into account that the dominant part of the \( z \) integral comes from the region where \( z \) is of order \( O\left(\sqrt{N}\right) \). The procedure is most easily illustrated by considering the first few powers of \( t \). To start, we have
\[ M_0(z) = \int dx_1 \cdots dx_N e^{z \sum_k f(x_k)/N} = \left< e^{zf(x)/N} \right>^N \]
\[ = \left( 1 + \frac{z}{N} J_1 + \frac{z^2}{2N^2} J_2 + \mathcal{O} \left( \frac{z^3}{N^3} \right) \right)^N \]
\[ = \exp \left( z J_1 + \frac{z^2}{2N} (J_2 - J_1^2) + \mathcal{O} \left( \frac{z^3}{N^2} \right) \right) . \quad (17) \]

Due to Eq.(9), the next contribution evaluates as follows:
\[ M_1(z) = \int dx_1 \cdots dx_N e^{z \sum_k f(x_k)/N} \frac{1}{N} \sum_{k,l} \beta(x_k, x_l) \]
\[ = \left< e^{zf(x)/N} \right>^{N-1} = \frac{N(N-1)}{2N} \int_K dx_1 dx_2 e^{z(f(x_1)+f(x_2))/N} \beta(x_1, x_2) \]
\[ + \left< e^{zf(x)/N} \right>^{N-1} \frac{1}{N} \int_K dx e^{zf(x)/N} \beta(x, x) \]
\[ \sim M_0(z) \left( \int_K dx \beta(x, x) + \frac{z^2}{2N} \int_K dx_1 dx_2 f(x_1) \beta(x_1, x_2) f(x_2) \right) , \quad (18) \]

where we have suppressed all subleading terms. The higher-order terms can easily be worked out: the only combinations that survive in the limit \( N \to \infty \)
are
\[ C_k = \int_k dx_1 dx_2 \cdots dx_k \beta(x_1, x_2)\beta(x_2, x_3) \cdots \beta(x_{k-1}, x_k)\beta(x_k, x_1) \]
\[ = \sum_{\vec{n} > 0} \sigma_{\vec{n}}^{2k}, \]  
(19)
and
\[ F_k = \int_k dx_1 dx_2 \cdots dx_k dx_{k+1} f(x_1)\beta(x_1, x_2) \cdots \beta(x_k, x_{k+1})f(x_{k+1}) \]
\[ = \sum_{\vec{n} > 0} v_{\vec{n}}^2 \sigma_{\vec{n}}^{2k}. \]  
(20)

These objects come with topological symmetry factors of \(2^k/(2k)\) and \(2^k/2\), respectively [2]. To leading order in \(N\), we can therefore write
\[ M(z, t) \sim M_0(z) \exp \left( \sum_{k \geq 0} C_k \frac{(2t)^k}{2k} + \frac{z^2}{N} \sum_{k > 0} F_k \frac{(2t)^k}{2} \right) \]
\[ = M_0(z) \exp \left( \sum_{k \geq 0} \sum_{\vec{n} > 0} \frac{(2t\sigma_{\vec{n}}^2)^k}{2k} + \frac{z^2}{N} \sum_{k > 0} \sum_{\vec{n} > 0} \frac{(2t\sigma_{\vec{n}}^2)^k v_{\vec{n}}^2}{2} \right) \]
\[ = M_0(z) \exp \left( -\frac{1}{2} \sum_{\vec{n} > 0} \log(1 - 2t\sigma_{\vec{n}}^2) + \frac{z^2}{2N} \sum_{\vec{n} > 0} \frac{2t\sigma_{\vec{n}}^2 v_{\vec{n}}^2}{1 - 2t\sigma_{\vec{n}}^2} \right) \]  
(21)

Combining everything, we have
\[ P(s; \eta) = \frac{1}{H_0(s)} \int_{-i\infty}^{i\infty} \frac{dz}{2\pi i} \frac{dt}{2\pi i} \]
\[ \times \exp \left( -z\eta - ts - \frac{1}{2} \sum_{\vec{n} > 0} \log(1 - 2t\sigma_{\vec{n}}^2) + \frac{z^2}{2N} B(t) \right), \]
\[ B(t) = \sum_{\vec{n} > 0} \frac{v_{\vec{n}}^2}{1 - 2t\sigma_{\vec{n}}^2}. \]  
(22)

The \(z\) integral converges provided Re\(B(t) > 0\), which certainly holds if \(1 - 2\sigma_{\vec{n}}^2\)Re\(t > 0\) for all \(\vec{n}\). Performing the \(z\) integration, we arrive at our master
We see that, for the types of discrepancy discussed here, the error distribution is symmetric around $\eta = 0$. Its precise form, however, will depend on our choice for the $\sigma_{\vec{n}}$. As we have said, a particular such choice reflects our belief about which kind of function class our actual integrand is a typical member of: but it must be realized that we are, in fact, allowed to take any choice for the $\sigma_{\vec{n}}$ that satisfies $\sum \sigma_{\vec{n}}^2 < \infty$. A choice that does not ‘fit’ the behaviour of $f(x)$ too well will just result in a somewhat worse error estimate: but the error distribution itself is only based on our assumption on the ensemble of point sets $X_N$, and not on any assumption about the integrand apart from its quadratic integrability.

From Eq. (23) a number of results immediately follow. In the first place, we can recover the case of truly random point sets by simply averaging over all possible values of $s$, with the appropriate probability distribution $H_0(s)$: this immediately leads to

$$\int_0^{\infty} ds \ H_0(s) \ P(s; \eta) = \frac{\sqrt{N}}{2\pi V} \exp \left( -\frac{\eta^2 N}{2V} \right), \tag{24}$$

which is the standard Central Limit Theorem. Another result comes from the normalization of $P(s; \eta)$: upon integrating over $\eta$ we find

$$H_0(s) = \int_{-\infty}^{\infty} \frac{dt}{2\pi i} \ \exp \left( -ts - \frac{1}{2} \sum_{\vec{n}>0} \log \left( 1 - 2t\sigma_{\vec{n}}^2 \right) \right), \tag{25}$$

in accordance with Ref. [3]. A final observation to be made is that the error $\eta$ only occurs in the combination $\eta^2 N$. From this it immediately follows that, all other things being equal, the error will only decrease as $1/\sqrt{N}$. Any improved rate of convergence is therefore solely due to a decrease of the discrepancy value $s$ with $N$. 

7
4 A simple model: uniform strengths

The first, and simplest, model that we shall consider is that where $2M$ of the $\sigma_{\vec{n}}^2$ are equal to $1/2M$, and all the other ones vanish. It is natural to take for the nonzero modes the ones with the lowest frequencies (i.e. small values of the components of $\vec{n}$), but this is not necessary. As mentioned above, the choice of $\sigma_{\vec{n}}$ only establishes which modes are covered, that is, enter in the computation of the discrepancy: a general integrand will, of course have modes with different frequencies, which are not covered. We therefore write

$$V = \sum_{\vec{n} > 0} v_{\vec{n}}^2 = V_1 + V_2 ,$$

where $V_1$ contains the $2M$ covered modes, for which $\sigma_{\vec{n}} \neq 0$, and $V_2$ contains all the other, uncovered, ones. The larger $V_1$ is with respect to $V_2$, the better our discrepancy model ‘fits’ the integrand. We immediately have

$$\frac{1}{2} \sum_{\vec{n} > 0} \log \left(1 - 2t\sigma_{\vec{n}}^2\right) = M \log \left(1 - \frac{t}{M}\right) ,$$

$$B(t) = V_1 / \left(1 - \frac{t}{M}\right) + V_2 ,$$

$$H_0(s) = \frac{M^M}{\Gamma(M)} s^{M-1} e^{-Ms}$$

$$\sim \sqrt{\frac{M}{2\pi}} \exp \left(-\frac{M(s-1)^2}{2}\right) ,$$

where the last line holds for large $M$. Both the form of $H_0(s)$ and that of $\beta(x_k, x_l)$ for this model are given in [3]; by construction, the expected discrepancy for truly random points is $\langle s \rangle = 1$. The master formula now becomes

$$P(s; \eta) = \frac{\Gamma(M)}{M^{M-1}} \int_{-\infty}^{\infty} \frac{dx}{2\pi i} \sqrt{\frac{N}{2\pi \left(V_2 + sV_1 / x\right)}}$$

$$\times \exp \left(Mx - M \log x - \frac{\eta^2 N}{2(V_2 + sV_1 / x)}\right) ,$$

where we have written $x \equiv s(1-t/M)$. Consequently the integration contour must cross the positive real axis. Two special cases can immediately be
derived from this. In the first place, suppose that we had chosen the nonzero \( \sigma_{\vec{n}} \) in a very bad way, such that \( V_1 = 0 \): that is, the integrand consists only of uncovered modes. It then follows immediately that

\[
P(s; \eta)\big|_{V_1=0} = \sqrt{\frac{N}{2\pi V_2}} \exp \left( -\frac{\eta^2 N}{2V_2} \right),
\]

which is the standard Central Limit Theorem. In this case, nothing is really lost, and the error estimate is just as good (or bad) as in classical Monte Carlo. On the other hand, if the integrand consists only of covered modes, so that \( V_2 = 0 \), we find after some straightforward manipulations:

\[
P(s; \eta) = \xi(M) \sqrt{\frac{N}{2\pi V_1 s}} \left( 1 - \frac{\eta^2 N}{2V_1 s M} \right)^{M-3/2},
\]

\[
\xi(M) = \frac{4^{M-1}}{\sqrt{M\pi}} \frac{\Gamma(M)^2}{\Gamma(2M-1)} = 1 + \mathcal{O}\left( \frac{1}{M} \right),
\]

with the strict constraint \( \eta^2 N < 2V_1 s M \). This follows from the fact that, if this inequality is violated, the complex integration contour for \( x \) can be closed to the right, where the integrand has no singularities; for the same reason [3], \( H_0(s) \) vanishes for \( s < 0 \). Note that, for this particular discrepancy, \( s \) can actually vanish: this happens in one dimension, if the point set is equidistant and \( N > M \). In that case, \( \eta \) is always zero, so that the function is integrated exactly. This is just another instance of the Nyqvist theorem [4].

For general \( V_1 \) and \( V_2 \), we may consider the case where \( M \) becomes large. The integral can then be approximated by the saddle-point method. The saddle point is located at \( x = 1 + \mathcal{O}(1/M) \), and we find

\[
P(s; \eta) \sim \sqrt{\frac{N}{2\pi (V_1 s + V_2)}} \exp \left( -\frac{\eta^2 N}{2(V_1 s + V_2)} \right).
\]

Again, we recover a Gaussian limiting distribution; its width is no longer parameterized by \( V = V_1 + V_2 \) but rather by \( V_1 s + V_2 \): the information we have gathered by computing the discrepancy \( s \) is seen to result in a reduced error, depending on how much of the fluctuating behaviour of the integrand is actually covered by the modes entering in the discrepancy. The limit of large \( M \) is actually justified by a self-consistency argument: the error distribution [31] heavily suppresses the region \( \eta^2 N \gg 2(V_1 s + V_2) \), so that (as can also be gleaned from Eq.(30)) \( M \) does not actually have to be a huge number.
for the saddle-point approximation to work. Note, moreover, that if we only allow the lowest frequency mode in each dimension, that is, only \( n^\mu = 0, 1, 2 \) for each component of \( \vec{n} \), \( M \) already equals \((3^D - 1)/2\) which grows very rapidly with increasing \( D \). The upshot of this (admittedly simple-minded, but nevertheless possible) model is: first, that we may hope for an error distribution which tends to a Gaussian (especially in high dimension), and, secondly, the width of this distribution depends on the discrepancy \( s \) in a manner which depends on the degree in which the relevant modes of the integrand correspond to those used in the evaluation of the discrepancy. We conjecture that these two conclusions will persist in more realistic models of discrepancy.

5 A more realistic model: one dimension

The model of discrepancy discussed above has the advantages both of simplicity and dimensionality-independence: but it may not be altogether too realistic, in particular because covered modes with high frequency are assumed to have the same strength as those with low frequency. An alternative, which we discuss now, covers all modes, but with strengths that decrease with increasing frequency. For simplicity, we start with \( D = 1 \). We shall take

\[
\sigma_{2n} = \sigma_{2n-1} = \frac{1}{n}, \quad n = 1, 2, 3, \ldots,
\]

just the same as in [3]. For truly random points we have, then, \( \langle s \rangle = \pi^2/3 \), and we shall assume that we have at our disposal a point set with a discrepancy value \( s \) much lower than this average. First of all, we compute \( H_0(s) \) for this small \( s \). In Ref.[3], we performed an exact calculation, but here we shall settle for a more simple-minded saddle-point approximation. We assume that the \( t \) integral in Eq.(25) is saturated by a saddle-point lying at \( t = -a^2/2 \), that is,

\[
H_0(s) = \int_{-i\infty}^{i\infty} \frac{dt}{2\pi i} e^{\phi(t)}
\sim \frac{\exp(\phi(-a^2/2))}{\sqrt{2\pi \phi''(-a^2/2)}},
\]

10
\[ \phi(t) = -st - \sum_{n>0} \log \left(1 - \frac{2t}{n^2}\right), \]

\[ \phi(-a^2/2) = \frac{sa^2}{2} - \pi a + \log(2\pi a) + O\left(\frac{1}{a}\right), \]

\[ \phi'(-a^2/2) = -s + \frac{\pi}{a} + O\left(\frac{1}{a^2}\right) \equiv 0, \]

\[ \phi''(-a^2/2) = \frac{\pi}{a^3} + O\left(\frac{1}{a^4}\right). \]  

\text{(33)}

The saddle point is seen to correspond to \( a \sim \pi/s \) which is large for small values of \( s \), thus justifying the neglect of higher orders in \( 1/a \). The resulting form for \( H_0 \) is (\( s \ll \pi^2/3 \))

\[ H_0(s) \sim \frac{\pi^2\sqrt{2\pi}}{s^{3/2}} \exp\left(-\frac{\pi^2}{2s}\right), \]  

\text{(34)}

in agreement with the corresponding limit of the exact result from [3].

For the evaluation of the error distribution \( P(s;\eta) \) we must now also compute \( B(t) \), which involves the unknown coefficients \( v_n \) of the integrand. It is certainly too crude, but nonetheless instructive, to study the simple case where

\[ v_n^2 = \sigma_n^2, \quad n = 1, 2, 3, \ldots. \]

In that case, we have

\[ B(t) = 2 \sum_{n>0} \frac{1}{n^2 - 2t} = 2 \sum_{n>0} \frac{1}{n^2 + a^2} = \frac{\pi}{a} + O\left(\frac{1}{a^2}\right), \]  

\text{(35)}

where \( a \) has now to be determined anew for the saddle point in the \( t \) integration of Eq.(23). It is seen to be equal to

\[ a \sim \frac{\pi \gamma}{s}, \quad \gamma = 1 + \frac{\eta^2 N}{2\pi^2}. \]  

\text{(36)}

Performing the saddle integral we arrive at

\[ P(s;\eta) \sim \sqrt{\frac{N}{2\pi s}} \gamma^{5/2} \exp\left(-\frac{\pi^2}{2s}(\gamma^2 - 1)\right) \]

\[ \sim \sqrt{\frac{N}{2\pi s}} \exp\left(-\frac{\eta^2 N}{2s}\right). \]  

\text{(37)}
This last, Gaussian, central limit is self-consistently justified from the fact that it implies $\eta^2 N = \mathcal{O}(s)$ which is indeed small by assumption. Note that we may write for this case (see Eq. (31)):

$$s = V \frac{s}{\langle s \rangle} .$$

What, now, happens for more general $v_n$? One answer is to assume that, since the integrand must be quadratically integrable, the sum $\sum v_n^2$ must converge; if we also assume that it has no exceptionally strong higher modes, it is reasonable to write

$$v_{2n-1}^2 + v_{2n}^2 = \frac{C\omega_n}{n^2} ,$$

where $C$ is a constant, and the $\omega_n$ are numbers that are not too different from unity. Not rigorously, but at least reasonably, we may then write

$$B(t) = \sum_{n>0} \frac{C\omega_n}{n^2 + a^2} \sim \frac{C\pi}{a} + \mathcal{O}\left(\frac{1}{a^2}\right) ,$$

leading to

$$P(s;\eta) \sim \sqrt{\frac{N}{2\pi sC}} \exp\left(-\frac{\eta^2 N}{2sC}\right) .$$

The essential point here is that the deviations of the individual $\omega_n$ from unity can give rise, in $B(t)$ to contributions that are of order $\mathcal{O}(1/a^2)$, and not of order $\mathcal{O}(1/a)$. Another argument leading to the same conclusion is to compute the moments of $B(t)$ over the ensemble of integrands described in Refs. [2, 3]: the $v_n$ are assumed to be normally distributed around zero with standard deviation $\sigma_n$. The expectation of $B(-a^2/2)$ is then, of course, just the result of Eq. (33), but its variance goes as $\mathcal{O}(1/a^3)$. If $a$ increases (for decreasing $s$), the probable values for $B(t)$ therefore cluster together more and more closely around the expectation value, again justifying our approximations.

A last example in this context is that of an integrand that has only a single mode, with frequency $k$, so that only $v_{2k}$ and $v_{2k-1}$ are non-vanishing, and we have

$$B(t) = \frac{V k^2}{k^2 - 2t} .$$
We immediately find that
\[ \hat{s} \equiv s - \frac{\eta^2 N}{V k^2} > 0 , \] (41)
by the same arguments as above; and, for \( \eta \) values smaller than this limit, we may again apply the saddle-point method to find
\[
P(s; \eta) \sim \sqrt{\frac{N}{2\pi V}} \left( \frac{s}{\hat{s}} \right)^{5/2} \sqrt{1 + \frac{\pi^2}{s^2 k^2}} \exp \left( -\frac{\eta^2 N}{2V} + \frac{\pi^2}{2s} - \frac{\pi^2}{2\hat{s}} \right) \]
\[
\sim \sqrt{\frac{N}{2\pi V}} \left( 1 + \frac{\pi^2}{k^2 s^2} \right) \exp \left( -\frac{\eta^2 N}{2V} \left( 1 + \frac{\pi^2}{k^2 s^2} \right) \right) , \] (42)
where the last line holds if \( \hat{s} \) and \( s \) are close in value. In this limit, again a Gaussian distribution is obtained, with variance \( V/(1 + \pi^2/k^2 s^2) \). Note that the error improvement now not only depends on the smallness of \( s \) but also on the number \( k \); this is reasonable because the mode with frequency \( k \) enters in this particular discrepancy with a factor \( 1/k^2 \) so that, when \( k \) is large, a small value of \( s \) does not tell us too much about how well the \( k \)th mode is integrated by the point set.

6 Conclusions and outlook

We have shown that we can define a Central Limit for the case of Quasi-Monte Carlo using a suitable definition of the discrepancy. A master-formula was derived for the error-distribution density over point sets with a fixed discrepancy.

We have given two simple examples of problem classes and their error-distribution densities. These results indicate that the expected error will improve if low-discrepancy point sets are used to evaluate integrals.

We would like to extend these results to more realistic and more dimensional cases. An explicit result seems to be too far-fetched, at the moment, but it might be possible to use saddle-point methods to derive similar results for more realistic cases.
References


