Discrepancy-based error estimates for Quasi-Monte Carlo.

II: Results in one dimension

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Abstract

The choice of a point set, to be used in numerical integration, determines, to a large extent, the error estimate of the integral. Point sets can be characterized by their discrepancy, which is a measure of its non-uniformity. Point sets with a discrepancy that is low with respect to the expected value for truly random point sets, are generally thought to be desirable. A low value of the discrepancy implies a negative correlation between the points, which may be usefully employed to improve the error estimate of a numerical integral based on the point set.

We apply the formalism developed in a previous publication to compute this correlation for one-dimensional point sets, using a few different definitions of discrepancy.
1 Introduction

In a previous publication [1], we have discussed the problem of computing a numerical integral estimate and its error, using a given set consisting of \(N\) points \(x_k, k = 1, 2, \ldots, N\) in the multi-dimensional hypercube \(K\). As is well known, in the Monte Carlo approach, where the points are chosen iid random with the uniform distribution, the expected error decreases as \(1/\sqrt{N}\). This can be improved upon by applying quasi-random point sets, that are, owing to some more or less sophisticated generation algorithm, more uniformly distributed than random ones. This is embodied in the notion of discrepancy \(D_N\), a measure of the deviation from uniformity. A very uniformly distributed point set will have a relatively low value \(s\) of this discrepancy, whereas very non-uniform ones will have a high value of \(s\). Obviously, different definitions of discrepancy are possible in addition to the best-known so-called star-discrepancy \(D^*_N\). Good uniformity implies, however, that the points are not independent, and in particular the distributions \(P_1(x_1)\) of a single point \(x_1\), and \(P_2(x_1, x_2)\), of a pair of points \(x_1, x_2\), will deviate from unity\(^3\). we can define

\[
P_1(x_1) = 1 - \frac{1}{N} F_1(s; x_1), \\
P_2(x_1, x_2) = 1 - \frac{1}{N} F_2(s; x_1, x_2). \tag{1}
\]

As discussed in [1], in order to talk sensibly about such distributions, we must have an underlying definition of an ensemble of point sets. In the truly random, Monte Carlo, case this is the ensemble of all sets of \(N\) points with the Cartesian product of \(N\) uniform one-point distributions: in the quasi-random case, we restrict this ensemble to all point sets having a fixed value \(s\) of the discrepancy. For truly random points, \(s\) is then a random variable, with a probability density \(H_0(s)\). In [1], we have developed a formalism that allows us to define a useful form for \(D_N\), and from that to compute a \(1/N\) expansion for \(H_0(s)\), \(F_1(s; x_1)\) and \(F_2(s; x_1, x_2)\). Let \(f(x)\) be a quadratically integrable function on \(K\). For a general integration error

\[
\eta = \frac{1}{N} \sum_{k=1}^{N} f(x_k) - \int_K dx f(x) \tag{2}
\]

we can then show that, averaged over the restricted ensemble (under our definition of discrepancy), the integral is unbiased, i.e. \(\langle \eta \rangle = 0\), and

\[
N \langle \eta^2 \rangle = \int_K dx (f(x))^2 - \left( \int_K dx f(x) \right)^2 - \left( 1 - \frac{1}{N} \right) \int_K dx_1 dx_2 f(x_1) f(x_2) F_2(s; x_1, x_2), \tag{3}
\]

\(^3\)These are the distributions obtained by integrating over the remaining points.
so that we may expect an improved error if $F_2$ is positive whenever $x_1$ and $x_2$ are close together. For truly random points, the term with $F_2$ drops out, and we recover the standard Monte Carlo result.

The treatment in [1] has been purely formal; if it is to be any good, we are obliged to show how it works out in practice. The present paper is the first step in that direction: we shall apply the formalism to a few particular definitions of $D_N$ in the case of one-dimensional point sets and integrals. Of course this is more or less academic since one-dimensional integrals can, in general, be approximated to extreme accuracy by other, non-stochastic methods. But, by keeping the extension to more dimensions in mind, we may hope to develop useful results and insights. The lay-out of this paper is as follows. In section 2, we briefly rehash the relevant results from [1]. In section 3, we present results for a very simple, and not altogether too useful, discrepancy. In section 4, we proceed to a more realistic definition of discrepancy, which will lead to a surprising connection with well-known results for the star-discrepancy. We conclude with some preliminary remarks on the extension to the case of more-dimensional point sets and integrals.

2 The formalism

Given a point set of $N$ points $x_1, x_2, \ldots, x_N$ in the unit interval $[0, 1)$, we define its discrepancy as

$$\quad D_N = \frac{1}{N} \sum_{n>0} \sigma_n^2 \sum_{k,l=1}^N u_n(x_k)u_n(x_l),$$

where $u_{2n}(x) = \sqrt{2}\cos(2\pi nx)$, $u_{2n-1}(x) = \sqrt{2}\sin(2\pi nx)$, and the numbers $\sigma_n$ depend on the class of integrands that our particular integrand is thought to be a member of. In the present model of integration, a typical integrand $f(x)$ is of the form

$$f(x) = v_0 + \sum_{n>0} v_n u_n(x),$$

where the coefficients $v_n$ are distributed independently and normally around zero with standard deviation $\sigma_n$. We shall always assume translational invariance, that is, $\sigma_{2n-1} = \sigma_{2n}$. This implies that $F_2(s; x_1, x_2)$ only depends on $x_1 - x_2$, so that we may as well write it as $F_2(s; x_1 - x_2)$. Moreover, for the integrands to be quadratically integrable, the sum $\sum_{n>0} \sigma_n^2$ must converge. We define

$$G_0(z) = \exp \left( -\frac{1}{2} \sum_{n>0} (1 - 2z\sigma_n^2) \right),$$

$$\phi(z; x) = \sum_{n>0} \frac{2z\sigma_n^2}{1 - 2z\sigma_n^2} u_n(x)u_n(0).$$
Let now the value of $D_N$ equal $s$ for our point set. Then, we may compute $H_0$ and $F_2$ to leading order in $1/N$ as follows:

$$
H_0(s) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dz \, e^{-zs} G_0(z),
$$

$$
R_2(s; x) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dz \, e^{-zs} \phi(z; x) G_0(z),
$$

$$
F_2(s; x) = -\frac{R_2(s; x)}{H_0(s)},
$$

(7)

where the integration contours run to the left of all singularities. Hence, both $H_0$ and $R_2$ vanish trivially whenever $s < 0$. Owing to the translational invariance in our model, the function $F_1$ vanishes to all orders in $1/N$, making the integration unbiased. Moreover, the average value of $D_N$ for truly random point sets is

$$
\langle D_N \rangle = \sum_{n>0} \sigma_n^2.
$$

(8)

Finally, from the definitions (6,7), we may immediately infer that

$$
F_2(s; 0) = 2 \frac{\partial}{\partial s} \left( s H_0(s) \right),
$$

(9)

which may serve as a check on the computations, and – since $F_2$ may be supposed to reach a maximum for $x_1 = x_2$, at least for small $s$ – can yield an approximation to a lower bound on $s$, simply by putting $F_2(s; x, x) = N$.

3 A simple model

The first, and simplest model, of integrands is obtained by taking

$$
\sigma_{2n}^2 = \frac{1}{2M}, \quad n = 1, 2, \ldots, M
$$

(10)

and zero for higher values of $n$. This means that our typical integrand has all Fourier components up to frequency $M$ occurring with equal strength on the average, higher modes being absent. Note that this gives $\langle s \rangle = 1$ for truly random point sets. In this case, we have

$$
G_0(z) = \left(1 - \frac{z}{M}\right)^{-M}, \quad H_0(s) = \frac{M}{\Gamma(M)} s^{-M-1} e^{-sM},
$$

(11)

where the last result (for $s > 0$) follows when we close the integral by a contour to the right. Note that, for large $M$, $H_0(s)$ approximates a Gaussian with unit
mean and width $1/\sqrt{M}$. The discrepancy is given by

$$D_N = \frac{1}{N} \sum_{k,l=1}^{N} [\xi_M(x_k - x_l) - 1] ,$$

$$\xi_M(x) = \sum_{n=0}^{M} \cos(2\pi nx) = \frac{\cos(M\pi x) \sin((M+1)\pi x)}{\sin(\pi x)} .$$

(12)

A particularly interesting point set is the one with minimal discrepancy, namely

$$x_k = \left\{ x_0 + \frac{k}{N} \right\} , \quad k = 1, 2, \ldots, N ,$$

(13)

where $x_0$ is arbitrary, and \{x\} denotes $x \mod 1$. The discrepancy depends, in this case, only on $N$ and $M$:

$$D_N = 1 - \frac{M \mod N}{M} .$$

(14)

We see that, for $M < N$, the discrepancy actually vanishes. This is reasonable, since an integrand that only has Fourier modes of frequency $N - 1$ or lower is indeed integrated with zero error by $N$ equidistant points. For large $M$, the value of $D_N$ lies generally quite close to one. The function $F_2(s; x)$ can easily be constructed in this case: since all the nonzero $\sigma_n$ are equal, it must be proportional to $\xi_M(x) - 1$, and from Eq.3 we can immediately find its normalization, to arrive at

$$F_2(s; x) = 2(1 - s) [\xi_M(x) - 1] .$$

(15)

In Fig. 1, we present $\xi_M(x)$ as a function of $x$ for a few values of $M$. As $M$ increases, $\xi_M$ approaches $1/2 + 1/2\delta(\{x\})$, where $\delta(x)$ is the Dirac delta function. Finally, the requirement $F_2(s; 0) < N$ leads to $s > 1 - N/(2M)$, which is a quite useless bound if $N \gg M$, but is reasonable if $M \gg N$.

The main attraction of this model is its simplicity. The extension to more dimensions is straightforward. Also, as proven in the appendix to [1], one can indeed show that, relative to the expected error from classical Monte Carlo, the expected error obtained with a point set of discrepancy $s$ is indeed reduced by a factor $s$. On the other hand, functions that have only a finite number of modes, and all equally strong at that, do not really form a good model for integrands likely to be encountered in practice. We therefore move, now, to a more realistic model.

### 4 A non-simple model

The next model we shall study is characterized by

$$\sigma_{2n} = \frac{1}{n} , \quad n = 1, 2, 3, \ldots .$$

(16)
Therefore, all Fourier modes can occur in the integrand, the higher modes being typically smaller than the lowest ones. Note that, with respect to the summability requirement on the $\sigma_n$, this is not the slowest possible behaviour: we are, in principle, allowed to take $\sigma_{2n} \sim n^{\epsilon-1/2}$, with any positive $\epsilon$: but the above choice appears to be the most manageable. In fact, integrands with discontinuities typically have Fourier coefficients decreasing like $1/n$, so that the above choice for $\sigma$ appears to be justified for integrands that may be discontinuous but in which quadratically integrable singularities have been mapped away. This is precisely the usual situation in, e.g., particle phenomenology.

We may now reapply the formalism of section 2. In the first place, the discrepancy is given by

$$D_N = \frac{1}{N} \sum_{k,l=1}^{N} \beta_1(x_k - x_l) ,$$

$$\beta_1(x) = \sum_{n>0} \frac{2}{n^2} \cos(2\pi nx) = \frac{\pi^2}{3} [1 - 6\{x\}(1 - \{x\})] ,$$

which follows trivially from the properties of Bernouilli polynomials. Some special cases are of interest.

- The most non-uniform point set, in which all points coincide, has discrepancy $D_N = \pi^2 N/3$.
- For truly random points, the expected discrepancy is $\langle D_N \rangle = \pi^2/3$. 

Figure 1: The function $\xi_M(x)$ for various values of $M$. 

![Graph showing the function $\xi_M(x)$ for various values of $M$.](image)
• Generalized Richtmeyer sequences, defined by
\[ x_k = \{ x_0 + k\alpha \} , \]
with arbitrary \( x_0 \) and non-integer \( \alpha \), lead to a discrepancy
\[ D_N = \frac{\pi^2}{3N} \left[ N + 2 \sum_{m=1}^{N-1} (N-m)(1-6\{m\alpha\}(1-\{m\alpha\})) \right] , \]
which can conveniently be computed in time \( \mathcal{O}(N) \).

• The most uniform point set, that of Eq.13, has a discrepancy
\[ D_N = \frac{\pi^2}{3N} . \]

The least and most uniform point sets are in fact, special cases of the generalized
Richtmeyer sequence with \( \alpha = 0 \) and \( \alpha = 1/N \), respectively. A nice illustration
is the following. We consider generalized Richtmeyer sequences, starting with
\( \alpha = 0 \). We then iterate \( \alpha \leftarrow 1/(1+\alpha) \), which gives us a series of rational
(Fibonacci) approximants to the golden ratio. For each \( \alpha \) we then compute the
discrepancy, for several values of \( N \). The results are given in table 1. We see that
the discrepancy decreases as the approximation improves: however, for every fixed
\( N \) there are some lower approximants that give a better discrepancy than some
higher approximants: the phenomenon of irregularity of distribution. Similarly,
with increasing \( N \), the discrepancy decreases somewhat slower than with \( 1/N \).

The evaluation of \( H_0 \) and \( F_2 \) is somewhat more complicated than in the previous model. In the first place, we have
\[ G_0(z) = \prod_{n>0} \frac{n^2}{n^2 - 2z} = \frac{\sqrt{2\pi^2 z}}{\sin \sqrt{2\pi^2 z}} . \]
The simplest way to compute \( H_0(s) \) is, then, to close the complex contour of the
\( z \) integral to the right and contract it to run around all the poles at \( z = m^2/2, \)
\( m = 1, 2, \ldots \) : this immediately gives us
\[ H_0(s) = \sum_{m>0} (-)^{m-1} m^2 e^{-sm^2/2} . \]
This result is, in some sense, surprising, since it is essentially identical to that of
the star-discrepancy \( D^*_N \): by comparison with the Kolmogorov-Smirnov law, we have
\[ \text{Prob} (D_N < s) = \text{Prob} \left( D^*_N < \sqrt{s/(16N)} \right) . \]
It is not completely clear why there should be such a simple relation between
the two cases, as they are based on quite different models of the underlying class
| iter. | α         | $N = 100$ | $N = 1000$ | $N = 10000$ |
|-------|-----------|-----------|------------|-------------|
| 1     | 1.00000000 | 328.98681 | 3289.86813 | 32898.68134 |
| 2     | .50000000  | 82.24670  | 822.46703  | 8224.67033  |
| 3     | .66666667  | 36.58333  | 365.54383  | 3655.40933  |
| 4     | .60000000  | 13.15947  | 131.59473  | 1315.94725  |
| 5     | .62500000  | 5.18977   | 51.40419   | 514.04190   |
| 6     | .61538462  | 1.99806   | 19.46995   | 194.66713   |
| 7     | .61904762  | .78420    | 7.46330    | 74.60073    |
| 8     | .61764706  | .32284    | 2.85192    | 28.45961    |
| 9     | .61818182  | .16748    | 1.09343    | 10.87618    |
| 10    | .61797753  | .10234    | .41917     | 4.15401     |
| 11    | .61805556  | .09481    | .16257     | 1.58743     |
| 12    | .61802575  | .09296    | .06628     | .60668      |
| 13    | .61803714  | .09298    | .02975     | .23233      |
| 14    | .61803279  | .09287    | .01554     | .08931      |
| 15    | .61803445  | .09290    | .00732     | .03473      |
| 16    | .61803381  | .09288    | .00832     | .01404      |
| 17    | .61803406  | .09289    | .00763     | .00604      |
| 18    | .61803396  | .09289    | .00784     | .00303      |
| 19    | .61803400  | .09289    | .00775     | .00206      |
| 20    | .61803399  | .09289    | .00779     | .00146      |
| 21    | .61803399  | .09289    | .00777     | .00155      |
| 22    | .61803399  | .09289    | .00778     | .00149      |
| 23    | .61803399  | .09289    | .00778     | .00150      |
| 24    | .61803399  | .09289    | .00778     | .00151      |
| 25    | .61803399  | .09289    | .00778     | .00151      |

Table 1: Discrepancies for generalized Richtmeyer point sets with $N = 10^2, 10^3, 10^4$ points, with for $\alpha$ successive Fibonacci approximations to the golden ratio.
of typical integrands. The result of Eq. (22) is useful for large $s$ values, but for small values another approach is more efficient. In it, we write $z = -u^2/2$, with $u = a + iv$, where $a$ is fixed and $v$ runs over the real axis. This gives us

\begin{align*}
G_0(z) &= \frac{i\pi u}{\sin i\pi u} = 2\pi u \sum_{m>0} e^{-(2m-1)i\pi u}, \\
H_0(s) &= \sum_{m>0} H_0(2m-1; s), \\
H_0(y; s) &= \int_{-\infty}^{\infty} dv \left( a^2 - v^2 + 2iav \right) e^{\frac{1}{2} s((a+iv)^2 - \pi y(a+iv))}.
\end{align*}

(24)

We can now choose $a = y\pi/s$, independently for each $m$, and so end up with

\begin{equation}
H_0(s) = \sum_{m>0} \frac{\sqrt{2\pi}}{s^{5/2}} \left( \pi^2 (2m-1)^2 - s \right) e^{-\frac{\pi^2(2m-1)^2}{2s}},
\end{equation}

(25)

which converges very rapidly for small $s$. This is of course the essence of the Poisson summation formula. In Fig. 2 we plot $H_0(s)$ as a function of $s$. The distribution is seen to be considerably skewed, with the maximum around $s \sim 1.8$ occurring a good deal before $\langle s \rangle \sim 3.28$. 

Figure 2: The function $H_0(s)$ as a function of $s$. 

The computation of $R_2(s; x)$ runs along the same lines. We may use the properties of Bernoulli polynomials to write
\[ \phi(z; x) = \sum_{n>0} \frac{4z}{n^2 - 2z} \cos(2\pi nx) = 1 - G_0(z) \cos\left(\xi \sqrt{2\pi^2 z}\right), \] (26)
with $\xi = 1 - 2x$. Therefore, we may write
\[ R_2(s; x) = H_0(s) - T(s; \xi), \]
\[ T(s; \xi) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dz \, e^{-zs} \cos\left(\xi \sqrt{2\pi^2 z}\right) \frac{2\pi^2 z}{(\sin(\sqrt{2\pi^2 z}))^2}; \] (27)
by closing the contour around the (double) poles, we obtain after some delicate but straightforward algebra:
\[ R_2(s; \xi) = \sum_{m>0} (-)^{m+1} m^2 e^{-s m^2 / 2} \left[ 1 + (m^2 s - 3) \cos(2\pi m x) + \pi m (2x - 1) \sin(2\pi m x) \right]; \] (28)
It is easily checked that $R_2$ vanishes upon integration over either $x$ or $s$, as it should. The form for small $s$ can be obtained along the same lines as above, where we may use
\[ \phi(-u^2/2; x)G_0(z) = G_0(z) - 2\pi^2 u^2 \left( e^{\pi u \xi} + e^{-\pi u \xi} \right) \sum_{m>0} m e^{-2\pi um}, \] (29)

\[
\text{to arrive at}
\begin{align*}
R_2(s; x) &= H_0(s) - \sum_{m>0} m \left[ T(2m + \xi) + T(2m - \xi) \right], \\
T(y) &= \frac{\sqrt{2\pi}}{s^{7/2}} \pi^2 y (\pi^2 y^2 - 3s) e^{-\frac{\pi^2 y^2}{2s}}. \quad (30)
\end{align*}
\]
Again, also this form can, in principle, be obtained from Eq.28 by means of the Poisson summation formula. In Fig.3 we show the resulting forms for $F_2(s; x)$ for a number of different values for $s$. We see that, for small $s$, this quantity indeed peaks at $\{x\} \sim 0$. For large $s$, on the other hand, it is actually negative for small $x$, implying that an anomalously large discrepancy occurs when the points are positively correlated, that is, clumped together. Finally, for small $s$, it is easily shown that $F_2(s; 0) \sim \pi^2 / s$. This gives us an approximate lower bound of $\pi^2 / N$ on $s$, which should be compared to Eq.20. The bound is quite reasonable, given that all our results are obtained in the large-$N$ limit, where we have assumed $sN \gg 1$. Including more terms ought to enable us to improve on this limit.

Concerning the low-$s$ approximation, we want to remark the following. We can, in principle, also obtain a similar result by a straightforward saddle-point
approximation, in which the integration over $z$ runs parallel to the imaginary axis, with a large negative real part. That this approach must work well is already evident from Eq. 29, in which the leading term is supplemented by exponentially small corrections. For large $s$, a similar saddle-point approximation, where the real part of $z$ is close to $1/2$, is not so good, since the sub-leading corrections are of the same order as the leading term: this yields the correct behaviour with $s$, but with an erroneous normalization. However, we are mainly interested in point-sets with low $s$, so that we may hope to at least approximate $H_0(s)$ and $F_2(s; x)$ by similar saddle-point approximations [2]. This however will depend sensitively on the multi-dimensional generalization of $\sigma_n$. 

Figure 3: The function $F_2(s; x)$ for various $s$. 

5 Conclusions

In this paper, we have presented, for the first time, expressions for the two-point correlation function $F_2(s; x_1 - x_2)$ for point sets, that are restricted to have a certain value $s$ of the discrepancy. These results will be employed to study the improvement in integration error for Quasi-Monte Carlo [2]. A number of points remains to be more fully understood.

On the one hand, there is the similarity between our form of $H_0(s)$ and the Kolmogorov-Smirnov distribution. This is surprising, since they are based on quite different discrepancies.

On the other hand, our ‘simple’ model lends itself to a generalization to more dimensions, but lacks realism. It remains to be seen whether there exists a discrepancy-definition, that combines simplicity of results with an easy extension to higher dimensions.

References

[1] J. Hoogland and R. Kleiss, Discrepancy-based error estimates for Quasi-Monte Carlo. I: General formalism, preprint NIKHEF 96-02, e-Print archive: http://xxx.lanl.gov/hep-ph/9601270

[2] J. Hoogland and R. Kleiss, in preparation.