

On the Behavior of the Weighted Star Discrepancy Bounds for Shifted Lattice Rules

Vasile Sinescu and Pierre L'Ecuyer

Abstract We examine the question of constructing shifted lattice rules of rank one with an arbitrary number of points n , an arbitrary shift, and small weighted star discrepancy. An upper bound on the weighted star discrepancy, that depends on the lattice parameters and is easily computable, serves as a figure of merit. It is known that there are lattice rules for which this upper bound converges as $O(n^{-1+\delta})$ for any $\delta > 0$, uniformly over the shift, and lattice rules that achieve this convergence rate can be found by a component-by-component (CBC) construction. In this paper, we examine practical aspects of these bounds and results, such as: What is the shape of the probability distribution of the figure of merit for a random lattice with a given n ? Is the CBC construction doing much better than just picking the best out of a few random lattices, or much better than using a randomized CBC construction that tries only a small number of random values at each step? How does the figure of merit really behave as a function of n for the best lattice, and on average for a random lattice, say for n under a million? Do we observe a convergence rate near $O(n^{-1})$ in that range of values of n ? Finally, is the figure of merit a tight bound on the true discrepancy, or is there a large gap between the two?

1 Introduction and Background Results

We are concerned with the approximation of an integral over the d -dimensional unit cube,

Vasile Sinescu and Pierre L'Ecuyer
Département d'Informatique et de Recherche Opérationnelle, Université de Montréal,
C.P.6128 Succ. Centre-Ville, Montréal QC, H3C 3J7, Canada,
{sinescu, lecuyer}@iro.umontreal.ca

$$I_d(f) = \int_{[0,1]^d} f(\mathbf{u}) \, d\mathbf{u}$$

where $f : [0,1]^d \rightarrow \mathbb{R}$, by a shifted lattice rule of rank one with generating vector $\mathbf{z} \in \mathbb{Z}^d$ and arbitrary shift $\Delta \in [0,1]^d$, i.e., by the average

$$Q_{n,d}(f) = \frac{1}{n} \sum_{k=0}^{n-1} f\left(\left\{\frac{k\mathbf{z}}{n} + \Delta\right\}\right),$$

where n is the number of points in the rule [14, 22]. That is, the approximation is the average of the values of f over the set of quadrature points

$$P_n = \{\{k\mathbf{z}/n + \Delta\}, 0 \leq k \leq n-1\}. \quad (1)$$

We assume that each coordinate of \mathbf{z} is relatively prime to n . Thus, the set of admissible generating vectors \mathbf{z} is $(\mathbb{Z}'_n)^d$ where \mathbb{Z}'_n denotes the set of integers in $\{1, \dots, n-1\}$ that are relatively prime to n . This set has cardinality $|\mathbb{Z}'_n| = \varphi(n)$, where φ is Euler's totient function. When n is prime, we have $\varphi(n) = n-1$. (In this paper, $|\cdot|$ denotes the cardinality if the argument is a set and the absolute value if it is a real number.)

It is well known that the integration error $|Q_{n,d}(f) - I_d(f)|$ can be bounded in different ways by the product of a discrepancy measure of the point set used in the rule and the corresponding measure of variation $V(f)$ of the function f [5, 12, 14]. The discrepancy measure considered in this paper is the weighted star discrepancy, an L_∞ -type discrepancy defined below. This measure (with weights) was also used in [20], for example. The L_∞ -type discrepancies are of interest in particular because their corresponding $V(f)$ is finite under weaker smoothness assumptions than the other types of L_p discrepancies found in the literature.

For any $\mathbf{x} = (x_1, \dots, x_d) \in [0,1]^d$ and an arbitrary point set P_n , we define the local star discrepancy at \mathbf{x} by

$$\text{disc}(\mathbf{x}, P_n) := \frac{|[\mathbf{0}, \mathbf{x}) \cap P_n|}{n} - \prod_{j=1}^d x_j.$$

For any set of indices $\mathbf{u} \subseteq \mathcal{D} := \{1, \dots, d\}$, let $\mathbf{x}_{\mathbf{u}}$ denote the vector in $[0,1]^{|\mathbf{u}|}$ that contains the components of \mathbf{x} whose indices belong to \mathbf{u} , and let $(\mathbf{x}_{\mathbf{u}}, \mathbf{1}) \in [0,1]^d$ be the vector whose j -th component is x_j if $j \in \mathbf{u}$ and 1 if $j \notin \mathbf{u}$. The *weighted star discrepancy* of P_n is defined by

$$D_\gamma^*(P_n) := \max_{\mathbf{u} \subseteq \mathcal{D}} \gamma_{\mathbf{u}} \sup_{\mathbf{x}_{\mathbf{u}} \in [0,1]^{|\mathbf{u}|}} |\text{disc}((\mathbf{x}_{\mathbf{u}}, \mathbf{1}), P_n)|, \quad (2)$$

where $\gamma_{\mathbf{u}} > 0$ is the weight given to \mathbf{u} , for each $\mathbf{u} \subseteq \{1, \dots, d\}$. The weight $\gamma_{\mathbf{u}}$ should reflect the importance of the component that corresponds to the subset \mathbf{u} of coordinates, in the ANOVA decomposition of f [12, 13, 17]. Then

a weighted variant of the Koksma-Hlawka inequality [14, 20] gives

$$|Q_{n,d}(f) - I_d(f)| \leq D_{\gamma}^*(P_n) \times V(f) \quad (3)$$

if $V(f)$ exists, where

$$V(f) = \sum_{\mathbf{u} \subseteq \mathcal{D}} \gamma_{\mathbf{u}}^{-1} \int_{[0,1]^{|\mathbf{u}|}} \left| \frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{x}_{\mathbf{u}}} f(\mathbf{x}_{\mathbf{u}}, \mathbf{1}) \right| d\mathbf{x}_{\mathbf{u}}$$

measures the variation of f . Note that this variation, and the worst-case error bound (3), can be finite only for bounded integrands f .

Later in this paper we shall assume that the weights $\gamma_{\mathbf{u}}$ have the following product form, as was done in [4, 25] and several other places:

$$\gamma_{\mathbf{u}} = \prod_{j \in \mathbf{u}} \gamma_j, \quad (4)$$

where $\gamma_j > 0$ is the weight associated with coordinate j . We also assume that $\gamma_1 \geq \gamma_2 \geq \dots \geq \gamma_d$. We say that a family of lattice rules indexed by n and with point sets P_n has *low-discrepancy* if $D_{\gamma}^*(P_n) = O(n^{-1+\delta})$ for any $\delta > 0$.

The weight γ_j reflects the importance of coordinate j in the discrepancy measure. We should take it larger [smaller] if we believe that f depends more [less] on the j th coordinate of \mathbf{u} . For example, in situations where we have a low effective dimension in the truncation sense [2, 12], the first few random numbers have much more importance than the other ones for the realization of $f(\mathbf{u})$ and the importance decreases quickly with j . The weights should then decrease accordingly. In other applications where we have low effective dimension in the superposition sense [2, 12], all coordinates of \mathbf{u} have similar importance, but the importance of a subset \mathbf{u} in the ANOVA decomposition decreases quickly with the cardinality of \mathbf{u} . By taking equal weights $\gamma_j = \gamma < 1$, we assume implicitly that this decrease is geometric in $|\mathbf{u}|$.

Given that no efficient algorithm is available for computing $D_{\gamma}^*(P_n)$, we will follow the common practice of using an easily computable upper bound on $D_{\gamma}^*(P_n)$ as a figure of merit. This upper bound $\bar{D}_{\gamma}^*(P_n)$ will be written in terms of the generating vector \mathbf{z} and will be independent of the shift Δ .

Shifted lattice rules (often randomly shifted) for the approximation or estimation of integrals over the unit cube have been used for a long time [3, 13, 22]. Shifted lattice rules with low discrepancy have been constructed in [9, 10, 23, 24, 27], for example, under the assumption that n was prime, but with a different definition of discrepancy that required stronger smoothness assumptions on the integrands. Moreover, in [10, 23, 27] the authors considered the average discrepancy over all shifts, whereas in [24], the shift was optimized to minimize the discrepancy. In our case, the bounds are valid for an arbitrary (worst-case) shift. Under the additional condition that $\sum_{j=1}^{\infty} \gamma_j < \infty$

(the weights are summable), the $O(n^{-1+\delta})$ bound is also independent of the dimension d (we have strong tractability).

Rank-1 lattice rules that achieve this convergence rate can be found by a greedy-type component-by-component (CBC) construction. The CBC construction algorithm has been used by several authors recently, including [7, 9, 20, 24]. It defines the generating vector \mathbf{z} coordinate by coordinate. At the s th step, for $s = 2, \dots, d$, it selects the s th coordinate of \mathbf{z} as (one of) the integer(s) in \mathbb{Z}'_n for which the discrepancy bound $\bar{D}_\gamma^*(P_n)$ is minimized for the corresponding s -dimensional point set P_n . Once a coordinate is selected, it is never modified again. With this algorithm, one computes the discrepancy (2) for at most $|\mathbb{Z}'_n|d = \varphi(n)d$ generating vectors rather than for all $\varphi(n)^d$ possibilities, which would take an excessive amount of time when d is large.

When n is large, one could also think of sampling only a limited number of integers from \mathbb{Z}'_n and then picking the best one, at each step of the CBC algorithm, instead of trying all $\varphi(n)$ possibilities. This randomized CBC construction was already proposed in [26], where the authors also suggested to check if the retained rule had a figure of merit at least as small as the (known) average over all $\varphi^d(n)$ possibilities. This method is much simpler and can be faster than standard CBC when n is large. If it also provides a \mathbf{z} whose figure of merit is practically as good with high probability, then one might prefer it for its simplicity. Our empirical investigations indicate that this is indeed the case. They also indicate that we can do almost as well with a very naive method that just generates, say, r generating vectors \mathbf{z} randomly and uniformly in $(\mathbb{Z}'_n)^d$, and picking the best one. To get proper insight on those issues, we approximate (empirically) the distribution function of the figure of merit $\bar{D}_\gamma^*(P_n)$ for a random \mathbf{z} , and for a \mathbf{z} constructed from the randomized CBC construction, for given choices of r , n , d , and the weights.

We also examine the behavior of the figure of merit as a function of n , for the best lattice, and on average for a random lattice, for “reasonable” values of n (under a million). We see that unless d is very small or the weights γ_u converge very quickly as a function of $|u|$ (which is almost equivalent), the observed rate of decrease in that range of values of n is much slower than n^{-1} . This type of reality check for the behavior of the figure of merit is important from the practical viewpoint. Similar illustrations of the behavior as a function of n have been given earlier in [18, 19] for a bound on the classical (unweighted) star discrepancy for other types of low-discrepancy point sets, namely those produced by the Halton, Sobol', and Niederreiter-Xing sequences.

Another important reality check, given the slow decrease of the bound in the practical range of values of n , is to see how close is the bound from the true discrepancy. We provide a partial answer by computing the true discrepancy for the cases where we can (for $d = 2$ for all n , and for $d = 3$ with small n) and comparing it with the bound. The gap turns out to be significant, and

seems to increase with the dimension. Our conclusion discusses the practical meaning of this fact.

2 Bounds on the Weighted Star Discrepancy

Proposition 1 below provides a conveniently computable bound on the discrepancy (2) for any given \mathbf{z} . This proposition puts together some known results to provide a bound for a discrepancy with general weights and arbitrary shift of the lattice.

Proposition 1. *For any $n > 1$, any $\mathbf{z} \in (\mathbb{Z}'_n)^d$, arbitrary weights $\gamma_{\mathbf{u}}$, and point set P_n defined in (1), we have*

$$D_{\gamma}^*(P_n) \leq \bar{D}_{\gamma}^*(P_n) := \sum_{\mathbf{u} \subseteq \mathcal{D}} \gamma_{\mathbf{u}} \left(1 - (1 - 1/n)^{|\mathbf{u}|} \right) + \frac{1}{2} e_{n,d}^2(\mathbf{z}), \quad (5)$$

where the sum on the right does not depend on \mathbf{z} ,

$$e_{n,d}^2(\mathbf{z}) = \sum_{\mathbf{u} \subseteq \mathcal{D}} \gamma_{\mathbf{u}} \left(\frac{1}{n} \sum_{k=0}^{n-1} \prod_{j \in \mathbf{u}} \left(1 + \sum'_{-n/2 < h \leq n/2} \frac{e^{2\pi i h k z_j / n}}{|h|} \right) - 1 \right),$$

and \sum' denotes the sum over the nonzero integers h .

For the case of product weights of the form (4), we can also write

$$\sum_{\mathbf{u} \subseteq \mathcal{D}} \gamma_{\mathbf{u}} \left(1 - (1 - 1/n)^{|\mathbf{u}|} \right) = \prod_{j=1}^d \beta_j - \prod_{j=1}^d (\beta_j - \gamma_j/n) = O(n^{-1}) \quad (6)$$

and

$$e_{n,d}^2(\mathbf{z}) = \frac{1}{n} \sum_{k=0}^{n-1} \prod_{j=1}^d \left(\beta_j + \gamma_j \sum'_{-n/2 < h \leq n/2} \frac{e^{2\pi i h k z_j / n}}{|h|} \right) - \prod_{j=1}^d \beta_j, \quad (7)$$

where $\beta_j = 1 + \gamma_j$.

Proof. The inequality (5) is obtained by applying Lemma 6 of [4] to bound the maximum in (2) for each \mathbf{u} , and then bounding the maximum over \mathbf{u} by the sum over \mathbf{u} . Then it suffices to note that $e_{n,d}^2(\mathbf{z})$ is the same as $\sum_{\mathbf{u} \subseteq \mathcal{D}} \gamma_{\mathbf{u}} R_1(\mathbf{h}, \mathbf{1}, n, \mathbf{u})$, where R_1 is defined in Lemma 6 of [4]. We recognize that bounding the max by the sum is likely to give a loose bound, but this is the standard approach used by other authors [4, 7, 21]. The second part follows by identical arguments as in [7].

For the remainder of the paper, we assume that the weights have the product form (4). Observe that the term (6) decays linearly with n for any

choice of weights. It does not depend on \mathbf{z} , so it is just a constant part in the figure of merit $\bar{D}_\gamma^*(P_n)$. In fact, the bound in (5) depends essentially on the quantity $e_{n,d}^2(\mathbf{z})$. We will now focus on this quantity. We compute it as explained in [21, page 657], via asymptotic expansions from [8] and by storing the products during the construction.

The average of this quantity over all admissible generating vectors is

$$M_{n,d,\gamma} = \frac{1}{\varphi^d(n)} \sum_{\mathbf{z} \in (\mathbb{Z}'_n)^d} e_{n,d}^2(\mathbf{z}).$$

The corresponding average value of $\bar{D}_\gamma^*(P_n)$ is

$$T_{n,d,\gamma} = \prod_{j=1}^d \beta_j - \prod_{j=1}^d (\beta_j - \gamma_j/n) + \frac{M_{n,d,\gamma}}{2}.$$

If n is prime, we have the following explicit formula [7]:

$$M_{n,d,\gamma} = \frac{1}{n} \prod_{j=1}^d (\beta_j + \gamma_j S_n) + \frac{n-1}{n} \prod_{j=1}^d \left(\beta_j - \gamma_j \frac{S_n}{n-1} \right) - \prod_{j=1}^d \beta_j, \quad (8)$$

where $S_n = \sum'_{-n/2 < h \leq n/2} 1/|h|$. For the general case where n can be composite, we do not have an explicit formula for $M_{n,d,\gamma}$, but an upper bound is given in [21]. In any case, regardless of n (unless it is very small), $M_{n,d,\gamma}$ is well approximated by its dominant term

$$M_{n,d,\gamma} \approx T_{n,d,\gamma} := \frac{1}{n} \prod_{j=1}^d (\beta_j + \gamma_j S_n) = O(n^{-1+\delta}),$$

with an approximation error of $O((\log \log(n+1))/n)$. In numerical experiments with small values of n , in which the average was computed explicitly, it has been observed that $T_{n,d,\gamma}$ was actually always larger than $M_{n,d,\gamma}$. For the case where n is prime, it is easy to prove that $T_{n,d,\gamma}$ is always larger [7].

It is also known (see Lemma 3 in [4]) that $T_{n,d,\gamma} = O(n^{-1+\delta})$ for any $\delta > 0$ when d is fixed and $n \rightarrow \infty$, and uniformly over d when the weights γ_j are summable. Then a simple argument that the best is at least as good as the average leads to the following result (see also [4, Theorem 7]):

Proposition 2. *For any n there is a generating vector \mathbf{z} such that the weighted star discrepancy of the corresponding shifted lattice rule satisfies*

$$D_\gamma^*(P_n) = O(n^{-1+\delta})$$

for any $\delta > 0$, where the implied constant depends on δ and the weights, but does not depend on n and on the shift. If the weights are summable, then the implied constant can also be taken independent of the dimension d .

3 The CBC Construction and Random Search Methods

The CBC algorithm constructs the generating vector $\mathbf{z} = (z_1, z_2, \dots, z_d)$ as follows. We suppose that $n \geq 2$, and that d and the weights are fixed.

CBC construction algorithm:

Let $z_1 := 1$;

For $s = 2, 3, \dots, d$, find $z_s \in \mathbb{Z}'_n$ that minimizes $e_{n,s}^2(z_1, z_2, \dots, z_s)$, defined in (7), while z_1, \dots, z_{s-1} remain unchanged.

The following result, proved in [21, Theorem 2], combined with Proposition 1, implies that the algorithm produces a generating vector \mathbf{z} whose corresponding weighted star discrepancy (2) has the same order of magnitude as the bound provided by Proposition 2.

Proposition 3. *This CBC algorithm returns a vector \mathbf{z} for which*

$$e_{n,d}^2(\mathbf{z}) \leq \frac{1}{n} \prod_{j=1}^d (\beta_j + \alpha \gamma_j \ln n) = O(n^{-1+\delta}),$$

where $\alpha > 0$ is an absolute constant.

This bound implies that for a fixed d , we have $e_{n,d}^2(\mathbf{z}) = O(n^{-1+\delta})$. And if the weights are summable, then this holds uniformly in d . The costs for the CBC construction algorithm using the fast implementation of [15, 16], is $O(nd \log n)$ computing time and $O(n)$ space for storage (see also [21] for further details). A more straightforward implementation requires $O(dn^2)$ time. The fast CBC construction is actually based on the fast Fourier transform, allowing to reduce the typical $O(n^2)$ operations required by a matrix-vector multiplication to $O(n \log n)$. However, the $O(n \log n)$ term has a larger hidden constant, which depends on the respective implementations. We did not use the fast Fourier transform in our implementation; it would have taken much more time to implement it than what we were ready to spend, and our goal was not really to compare speeds.

The following randomized CBC construction algorithm is simpler to implement and can reduce the computing cost by examining only a small number of integers $z_s \in \mathbb{Z}'_n$ (chosen at random) at each step.

Randomized CBC construction algorithm (R-CBC):

Let $z_1 := 1$;

For $s = 2, 3, \dots, d$,

choose r integers z_s at random in \mathbb{Z}'_n , and select the one that minimizes $e_{n,s}^2(z_1, z_2, \dots, z_s)$, while z_1, \dots, z_{s-1} remain unchanged.

A similar algorithm was proposed in [26], with the additional feature that for any given s , new integers z_s are examined until $e_{n,s}^2(z_1, \dots, z_s)$ is less than the average $M_{n,d,\gamma}$. An even simpler (and more naive) algorithm is a

uniform random search in $(\mathbb{Z}'_n)^d$, as follows (we can also stop only when $e_{n,d}^2(\mathbf{z}) \leq M_{n,d,\gamma}$):

Uniform random search algorithm:

Choose r vectors \mathbf{z} at random in $(\mathbb{Z}'_n)^d$, and select the one that minimizes $e_{n,d}^2(\mathbf{z})$.

In the next section, we compare empirically the performance of these three algorithms, in terms of the figures of merit of the returned vectors \mathbf{z} . We know a priori that the CBC construction should provide better figures of merit, but is the difference really significant?

4 Empirical Assessments

Our aim in this section is to explore the behavior of the discrepancy bound (or figure of merit) $\bar{D}_\gamma^*(P_n)$ defined in (5), empirically, from various angles, for n not exceeding one million. We first examine its distribution function when \mathbf{z} is drawn uniformly from $(\mathbb{Z}'_n)^d$ (so the figure of merit is a random variable). This distribution function F is defined by $F(x) = \mathbb{P}[\bar{D}_\gamma^*(P_n) \leq x]$. We find that typically, this distribution is positively skewed, and the median is smaller than the mean $\Gamma_{n,d,\gamma}$, so the probability $q_{n,d,\gamma}$ of a value smaller than the mean is more than 1/2 (often more than 0.75). This implies that a vector \mathbf{z} whose figure of merit is smaller than the mean (and thus satisfies the bound in Proposition 2) is easy to find by uniform random search. By applying this algorithm with r trials, the probability of finding such a vector is $1 - (1 - q_{n,d,\gamma})^r$. With $q_{n,d,\gamma} = 0.75$, this probability is approximately $1 - 9.5 \times 10^{-7}$ for $r = 10$, and $1 - 6.2 \times 10^{-61} \approx 1$ for $r = 100$, for example. That is, finding a \mathbf{z} smaller than the mean is very easy, even with the most naive method.

To approximate the distribution function F and the density f of $\bar{D}_\gamma^*(P_n)$ for a random \mathbf{z} , we generated a sample of $r = 10^5$ generating vectors \mathbf{z} and computed the empirical distribution function \hat{F} of the r realizations. We also computed a kernel estimator \hat{f} of the corresponding density, using a Gaussian kernel, with the bandwidth selected as suggested in [6, pages 308–309]. Note that these density estimates inflate the tails (compare with the empirical distribution). This tail inflation can be reduced by reducing the bandwidth, but then the curve becomes less smooth. Thus, the empirical distribution seems to give a better idea of the distribution. The computations and plots were made with SSJ [11]. We did this with various choices of n , d , and the weights, and the shape of the empirical distribution (with proper scaling) was very much the same in all cases.

Figure 1 (upper panel) gives an illustration with $n = 32749$ (a prime number), $d = 10$, and weights $\gamma_j = 1/j^2$ for all j . Here the figure of merit obtained via the CBC construction was 0.14996, while the best one among

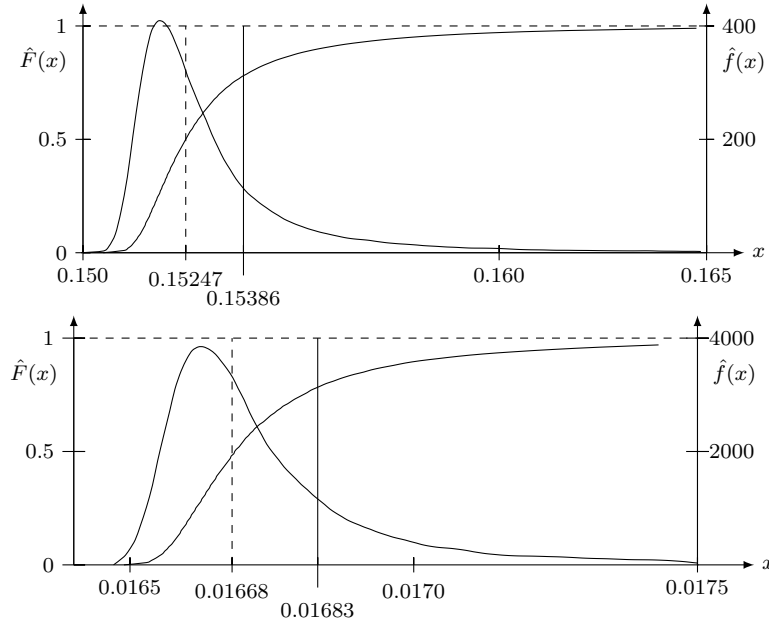


Fig. 1 Estimated distribution function \hat{F} (increasing curve) and density \hat{f} (other curve) of the figure of merit $\bar{D}_{\gamma}^*(P_n)$ defined in (5). Above: $n = 32749$, $d = 10$, and $\gamma_j = 1/j^2$. Below: $n = 1048573$, $d = 5$, and $\gamma_j = 1/4$. The solid and dashed vertical lines indicate the mean and the median, respectively.

the 10^5 random z was 0.15048, the median was 0.15247 (indicated by the leftmost vertical line), the empirical mean was 0.15367, and theoretical mean $\Gamma_{n,d,\gamma}$ is 0.15386 (the rightmost vertical line). Here the probability $q_{n,d,\gamma}$ is slightly more than 0.75.

The lower panel of the same figure provides another illustration with $n = 1048573$, $d = 5$, and weights $\gamma_j = 1/4$ for all j . Here, we know a priori that the weighted discrepancy cannot exceed $1/4$. The CBC construction gave a figure of merit of 0.01646, the best random vector had 0.01649, the median was 0.01668, and both the empirical and theoretical means were 0.01683. The probability $q_{n,d,\gamma}$ is again very close to 0.75.

Table 1 summarizes the figures of merit obtained for other values of n , d , and the weights. The CBC algorithm usually returned a value slightly smaller than the best values from the two randomized methods. However, in absolute terms, the values returned by all three algorithms are typically very close to each other. The difference between the corresponding error bounds can be deemed negligible. Moreover, those best values are not much smaller than the median and the mean. We also observe that unless the weights decrease very quickly with j or are all small, the discrepancy bounds become larger than the trivial bound of $\gamma_{\max} = \max_j \gamma_j$ already in 5 dimensions, even for

Table 1 Values of the figure of merit obtained by the CBC algorithm (CBC), the randomized CBC construction with $r = 5$ (R-CBC), and uniform random search with $r = 10^5$ (Best-R), for various choices of weights, d , and n . The last three columns also provide the median and the mean of the empirical distribution (Median and Mean), and the exact mean $\Gamma_{n,d,\gamma}$, for comparison.

γ_j	d	n	CBC	R-CBC	Best-R	Median	Mean	$\Gamma_{n,d,\gamma}$
$1/j^2$	5	8009	0.0719	0.0729	0.0723	0.0759	0.0787	0.0792
		32749	0.0292	0.0294	0.0293	0.0306	0.0317	0.0318
		131071	0.0114	0.0115	0.0115	0.0119	0.0123	0.0123
		1048573	0.0026	0.0026	0.0026	0.0027	0.0028	0.0028
"	10	8009	0.3125	0.3135	0.3137	0.3192	0.3223	0.3229
		32749	0.1499	0.1500	0.1504	0.1524	0.1536	0.1538
		131071	0.0689	0.0691	0.0691	0.0698	0.0702	0.0703
		1048573	0.0198	0.0198	0.0199	0.0200	0.0201	0.0201
"	20	8009	0.7315	0.7347	0.7337	0.7400	0.7432	0.7439
		32749	0.3934	0.3943	0.3943	0.3967	0.3980	0.3981
		131071	0.2021	0.2025	0.2025	0.2033	0.2039	0.2039
		1048573	0.0686	0.0686	0.0687	0.0688	0.0689	0.0689
$1/j$	3	8009	0.0733	0.0762	0.0735	0.0802	0.0874	0.0881
		32749	0.0266	0.0270	0.0266	0.0290	0.0317	0.0319
		131071	0.0093	0.0095	0.0093	0.0101	0.0111	0.0112
		1048573	0.0018	0.0018	0.0018	0.0020	0.0022	0.0022
"	5	32749	1.1037	1.1078	1.1044	1.1179	1.1249	1.1252
		131071	0.4728	0.4759	0.4732	0.4782	0.4811	0.4811
		1048573	0.1206	0.1211	0.1207	0.1217	0.1222	0.1222
1	3	8009	0.4036	0.4206	0.4033	0.4349	0.4659	0.4682
		32749	0.1480	0.1498	0.1476	0.1590	0.1712	0.1718
		131071	0.0526	0.0536	0.0522	0.0562	0.0608	0.0610
		1048573	0.0096	0.0107	0.0103	0.0111	0.0120	0.0120
$1/4$	3	8009	0.0081	0.0083	0.0081	0.0090	0.0100	0.0102
		32749	0.0029	0.0029	0.0029	0.0032	0.0036	0.0036
		131071	0.0010	0.0010	0.0010	0.0011	0.0012	0.0012
"	5	32749	0.1568	0.1583	0.1572	0.1601	0.1617	0.1618
		131071	0.0660	0.0663	0.0662	0.0671	0.0678	0.0678
		1048573	0.0165	0.0166	0.0165	0.0167	0.0168	0.0168

$n = 1048573 \approx 2^{20}$. For $\gamma_j = 1$, $d = 10$ and $n = 131071$, the best bound is approximately 4.15×10^8 . Any discrepancy bound (or figure of merit) larger than γ_{\max} is in fact totally useless, because the discrepancy itself is never larger than $\sup_j \gamma_j \leq 1$.

We made some experiments to estimate the distribution function of the (random) figure of merit returned by the randomized CBC algorithm. The minimal value was usually slightly larger than that returned by the CBC algorithm, but on rare occasions the R-CBC algorithm did a bit better. The

latter can happen in situations where the CBC path is not optimal and the randomized method finds a better one by chance. As an illustration, for $n = 32749$, $d = 10$ and weights $\gamma_j = 1/j^2$ (as in the upper panel of Figure 1 and in row 6 of the table), the CBC construction gave a figure of merit of 0.1499629, and the randomized CBC algorithm gave figures of merit between 0.1500882 and 0.1504918 (from 1000 independent runs of the algorithm), with a median of 0.1502565 and a mean of 0.1502607. Figure 2 shows the estimated distribution function and density of the value returned by the R-CBC algorithm, from the 1000 runs. The density is slightly asymmetric and is concentrated in a narrow interval.

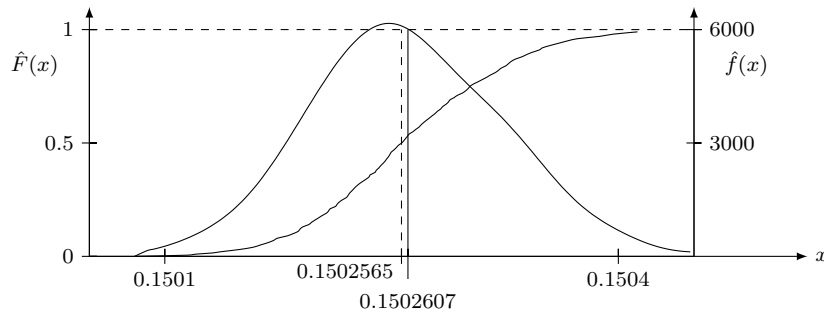


Fig. 2 Empirical distribution \hat{F} and density estimate \hat{f} of $\bar{D}_\gamma^*(P_n)$ for the point set P_n returned by the R-CBC algorithm with $r = 5$, when $n = 32749$, $d = 10$, and $\gamma_j = 1/j^2$ (based on 1000 replicates). The vertical lines indicate the median (dashed) and the mean.

Figure 3 shows the best figure of merit obtained by the CBC construction, as a function of n , in a log-log scale, for various choices of the weights and dimension. These plots provide good insight on how the best bound behaves as a function of n in general. We see that unless the dimension is very small (e.g., 2 or 3, as in the upper panel) or the weights converge extremely fast (as in the bottom panel), the observed convergence rate for n up to one million is much slower than $O(1/n)$. That is, we know that the slope of all the curves in the figure converges to -1 , asymptotically, when $n \rightarrow \infty$, but for the observed values of n , the curves have a concave shape and the slope is often much less than -1 . This behavior is typical and was observed in our plots for several other parameters as well.

In the case of the fast-decaying weights $\gamma_j = 1/2^j$ (bottom panel), increasing the dimension has eventually almost no visible effect: the upper curve appears a bit thicker because it contains the curves for $d = 10, 20$, and 40 , which almost overlap. The reason is simple: the weights decrease so fast that the high-dimensional coordinates have a negligible contribution to the discrepancy. This effect also appears to a lesser extent for $\gamma_j = 1/j^2$ (middle panel).

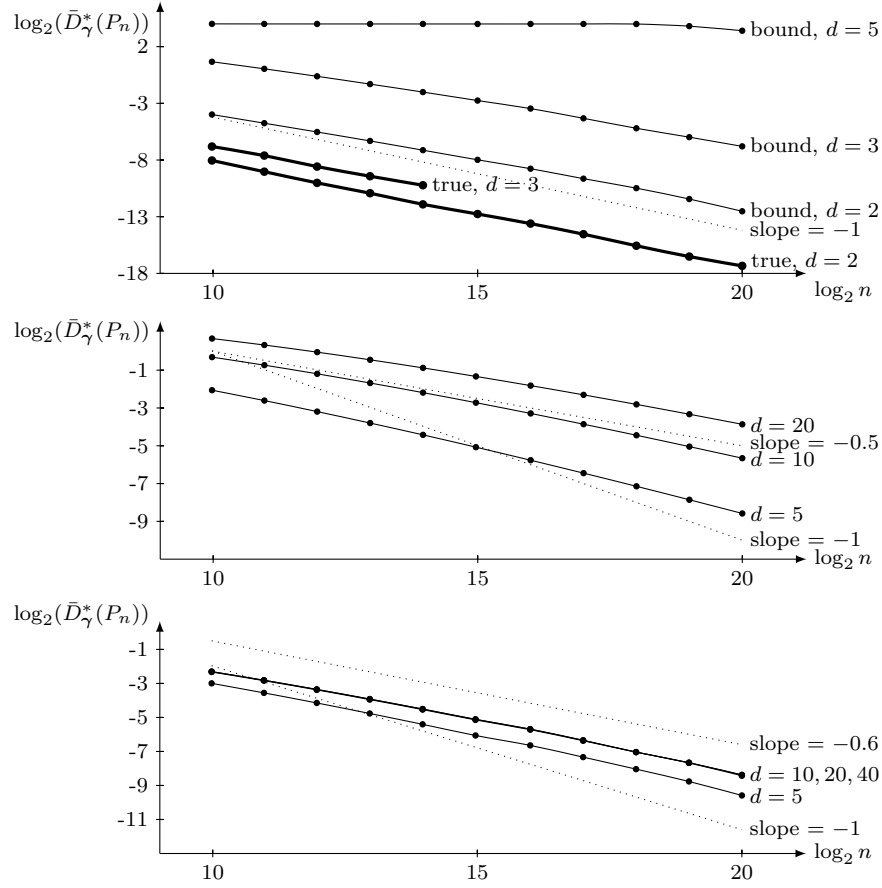


Fig. 3 The best bound $\bar{D}_\gamma^*(P_n)$ obtained with the CBC construction as a function of n , in a log-log scale, in d dimensions, when $\gamma_j = 1$ for all j (upper panel), $\gamma_j = 1/j^2$ (middle panel), and $\gamma_j = 1/2^j$ (lower panel). In the upper panel, we also have the true weighted star discrepancy $D_\gamma^*(P_n)$ (the thick lines) for the cases where we were able to compute it (for $d = 2$ and for $d = 3$ with small n). Selected slopes are shown for reference. All these functions have a slope of -1 asymptotically when $n \rightarrow \infty$.

In the upper panel, we also show the true value of the discrepancy $D_\gamma^*(P_n)$ for the same point sets P_n , for $\gamma_j = 1$, for the cases where we have been able to compute it, namely for $d = 2$ and for $d = 3$ with small n . For this, we implemented the algorithm given in [1] (the required work increases as $O(n^d)$). One can see that the upper bound $\bar{D}_\gamma^*(P_n)$ (the figure of merit) is much larger than the true discrepancy $D_\gamma^*(P_n)$, and the gap seems to increase rapidly with the dimension d . As an illustration, when $d = 2$ and $n = 32749$, the true discrepancy is 0.00014 and the bound is 0.00382. For $d = 3$ and $n = 8009$, the true discrepancy is 0.0017, whereas the bound is 0.4036, which

is about 240 times larger! This gap is orders of magnitude larger than the gain of the CBC algorithm over the two randomized methods (see Table 1), even with small r .

Conclusion

We have provided a reality check on the practical meaning of known upper bounds on the weighted star discrepancy, the convergence rate of these bounds for the best rank-1 lattices, the distribution of the value of the bound for a random rank-1 lattice, and the behavior of the CBC construction algorithm as well as randomized algorithms based on these bounds. We saw that the best achievable value of the upper bound is typically not much smaller than the average value over all admissible generating vectors, and that a value close to the minimum can easily be found by a simple randomized algorithm and even by naive random search. Our experiments confirm the popular belief that these discrepancy bounds are not always tight and that they may converge rather slowly. Even though the best achievable value of the bound decreases as $O(n^{-1+\delta})$ for any $\delta > 0$ asymptotically, its rate of decrease is typically slower than this asymptotic rate for reasonable values of n . For n less than a million (say), the bound turns out to be practically useless unless the dimension d is very small or the weights converge very quickly. One implication might be that other types of discrepancies, which can be computed exactly and converge faster than the bounds considered here [5, 12], provide more appropriate figures of merit from the practical viewpoint.

Acknowledgments

This research has been supported by NSERC-Canada grant No. ODGP0110050 and a Canada Research Chair to P. L'Ecuyer. The authors are grateful to Richard Simard who helped with the computations.

References

1. Bunschuh, P., Zhu, Y.: A method for exact calculation of the discrepancy of low-dimensional finite point sets I. *Abh. Math. Sem. Univ. Hamburg* **63**, 115–133 (1993)
2. Caffisch, R.E., Morokoff, W., Owen, A.: Valuation of mortgage-backed securities using Brownian bridges to reduce effective dimension. *The Journal of Computational Finance* **1**(1), 27–46 (1997)
3. Cranley, R., Patterson, T.N.L.: Randomization of number theoretic methods for multiple integration. *SIAM Journal on Numerical Analysis* **13**(6), 904–914 (1976)

4. Hickernell, F., Niederreiter, H.: The existence of good extensible rank-1 lattices. *J. Complexity* **19**, 286–300 (2003)
5. Hickernell, F.J.: What affects the accuracy of quasi-Monte Carlo quadrature? In: H. Niederreiter, J. Spanier (eds.) *Monte Carlo and Quasi-Monte Carlo Methods 1998*, pp. 16–55. Springer-Verlag, Berlin (2000)
6. Hörmann, W., Leydold, J., Derflinger, G.: *Automatic Nonuniform Random Variate Generation*. Springer-Verlag, Berlin (2004)
7. Joe, S.: Construction of good rank-1 lattice rules based on the weighted star discrepancy. In: H. Niederreiter, D. Talay (eds.) *Monte Carlo and Quasi-Monte Carlo Methods 2004*, pp. 181–196. Springer (2006)
8. Joe, S., Sloan, I.: On computing the lattice rule criterion *R. Math. Comp* **59**, 557–568 (1992)
9. Kuo, F.Y.: Component-by-component constructions achieve the optimal rate of convergence for multivariate integration in weighted Korobov and Sobolev spaces. *Journal of Complexity* **19**(3), 301–320 (2003)
10. Kuo, F.Y., Wasilkowski, G.W., Waterhouse, B.J.: Randomly shifted lattice rules for unbounded integrands. *Journal of Complexity* **22**(5), 630–651 (2006)
11. L'Ecuyer, P.: *SSJ: A Java Library for Stochastic Simulation* (2008). Software user's guide, available at <http://www.iro.umontreal.ca/lecuyer>
12. L'Ecuyer, P.: *Quasi-Monte Carlo methods with applications in finance*. *Finance and Stochastics* (2009). To appear
13. L'Ecuyer, P., Lemieux, C.: Variance reduction via lattice rules. *Management Science* **46**(9), 1214–1235 (2000)
14. Niederreiter, H.: *Random Number Generation and Quasi-Monte Carlo Methods*. SIAM, Philadelphia (1992)
15. Nuyens, D., Cools, R.: Fast algorithms for component-by-component construction of rank-1 lattice rules in shift-invariant reproducing kernel Hilbert spaces. *Math. Comp* **75**, 903–920 (2006)
16. Nuyens, D., Cools, R.: Fast component-by-component construction of rank-1 lattice rules with a non-prime number of points. *J. Complexity* **22**, 4–28 (2006)
17. Owen, A.B.: Latin supercube sampling for very high-dimensional simulations. *ACM Transactions on Modeling and Computer Simulation* **8**(1), 71–102 (1998)
18. Schlier, C.: Discrepancy behaviour in the non-asymptotic regime. *Appl. Numer. Math.* **50**, 227–238 (2004)
19. Schlier, C.: Error trends in Quasi-Monte Carlo integration. *Comp. Phys. Comm.* **159**, 93–105 (2004)
20. Sinescu, V., Joe, S.: Good lattice rules based on the general weighted star discrepancy. *Mathematics of Computation* **76**(258), 989–1004 (2007)
21. Sinescu, V., Joe, S.: Good lattice rules with a composite number of points based on the product weighted star discrepancy. In: A. Keller, S. Heinrich, H. Niederreiter (eds.) *Monte Carlo and Quasi-Monte Carlo Methods 2006*, pp. 645–658. Springer (2008)
22. Sloan, I.H., Joe, S.: *Lattice Methods for Multiple Integration*. Clarendon Press, Oxford (1994)
23. Sloan, I.H., Kuo, F.Y., Joe, S.: Constructing randomly-shifted lattice rules in weighted Sobolev spaces. *SIAM Journal on Numerical Analysis* **40**, 1650–1665 (2002)
24. Sloan, I.H., Kuo, F.Y., Joe, S.: On the step-by-step construction of quasi-Monte Carlo rules that achieve strong tractability error bounds in weighted Sobolev spaces. *Mathematics of Computation* **71**, 1609–1640 (2002)
25. Sloan, I.H., Woźniakowski, H.: When are quasi-Monte Carlo algorithms efficient for high-dimensional integrals. *Journal of Complexity* **14**, 1–33 (1998)
26. Wang, X., Sloan, I.H.: Efficient weighted lattice rules with applications to finance. *SIAM Journal on Scientific Computing* **28**(2), 728–750 (2006)
27. Waterhouse, B.J., Kuo, F.Y., Sloan, I.H.: Randomly shifted lattice rules on the unit cube for unbounded integrands in high dimensions. *Journal of Complexity* **22**(1), 71–101 (2006)