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ON THE CORNER AVOIDANCE PROPERTIES OF VARIOUS LOW-DISCREPANCY SEQUENCES

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Abstract

The minimum distance of QMC sample points to the boundary of the unit cube is an important quantity in the error analysis of QMC integration for functions with singularities. Sobol' and recently Owen show that the Sobol' and Halton sequences avoid a hyperbolically shaped region around the corners of the unit cube. We extend these results in two ways. First, we prove that generalized Niederreiter sequences possess similar properties as Sobol' and Halton sequences around the origin. Second, we show corner avoidance rates for the Halton and Faure sequence for corners different from the origin. While the all-corner avoidance of the Halton sequence is almost the same as its origin avoidance, the Faure sequence has a substantially smaller all-corner avoidance.

1. Introduction

Quasi-Monte Carlo (QMC) methods have been successfully deployed in various applications for the numerical evaluation of high dimensional integration problems. In contrast to Monte Carlo (MC) methods, the integration error can be bounded deterministically

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due to the famous Koksma-Hlawka Theorem [6] by the product of the discrepancy of the utilized sequences and the integrand's variation in the sense of Hardy and Krause.

Classical QMC theory – for a thorough introduction consult the monograph [11] – deals with functions of bounded variation and evinces that in terms of function evaluations the best known (and conjectured to be the best possible) QMC techniques using sequences yield an error bound of the order $\mathcal{O}(N^{-1}(\log N)^s)$ for s-dimensional integration problems. The convergence rate in the bound is solely induced by the uniformity of the sequence, measured by its discrepancy. The first construction of low-discrepancy sequences (LDS), i.e. sequences with this optimal order, is given by Halton [3]. Different LDS constructions are proposed by Sobol' [15], Faure [2] and Niederreiter [8, 10]. Tezuka and Tokuyama [19] show that these three approaches can be unified by a generalization of Niederreiter's principles.

A common phenomenon in applications are integrands that are unbounded at their domain boundaries. Such integrands are obviously not of bounded variation, so the superiority of QMC over MC, or even the convergence of QMC methods, is not guaranteed by Hlawka's theorem. It turns out that the additional error for the singularity depends on how far the sample points are away from the singularities. The first consideration of QMC methods for unbounded integrands can be found in an article by Sobol' [16], where he studies integrals with a power singularity at the origin, based on the fact that Sobol' sequences avoid a hyperbolic region around the origin. Klinger [7] investigates QMC integration for special classes of singular functions, numerical examples for Sobol' sequences are given by De Doncker and Guan [1]. QMC rules for weighted singular integration problems with emphasis on financial applications are considered by Hartinger, Kainhofer, and Tichy [5]. In a recent article [13], Owen extends Sobol's work, establishing a similar property for Halton sequences and convergence rates for functions with at most a power singularity at the integration boundaries. A generalization of these results to non-uniform integration is given by Hartinger and Kainhofer [4].

In this article, we distinguish two situations. After a review of the notation and some background in Section 2, we look at the case where the integrand has singularities only on boundaries of $\bar{U}^s$ that contain the origin. Hence we consider the origin avoidance of generalized Niederreiter sequences in Section 3. We show that the characteristics of Sobol' sequences also hold for generalized Niederreiter sequences. In particular, generalized Niederreiter sequences avoid the origin with an order of N^{-1}. In a second step the functions are allowed to be singular on all boundaries of $\bar{U}^s$, so the distance to any corner is investigated in Section 4. We look at the corner avoidance of Halton sequences in a rigorous way and prove that Halton sequences avoid all corners with an order of $N^{-1-\varepsilon}$. In addition we show first results on the corner avoidance properties of Faure sequences, proving that the Faure sequence approaches the other corners substantially faster than the origin.

2. Notation and background

We will denote by $\bar{U}^s = [0,1]^s$ the s-dimensional unit cube, and consider functions $f : \bar{U}^s \to \mathbb{R}$ such that $I = \int_{\bar{U}^s} f(\mathbf{x})d\mathbf{x}$ exists. Let furthermore $(\mathbf{x}_n)_{n>0}$ be a sequence with $\mathbf{x}_n = (x_n^{(1)}, \dots, x_n^{(s)}) \in [0,1)^s$. Then we define the *QMC estimator of I* as $\hat{I}_N = \frac{1}{N}\sum_{n=1}^{N} f(\mathbf{x}_n)$.

For a subset $B \subseteq \bar{U}^s$, denote by $\lambda(B)$ its Lebesgue measure and by χ_B its characteristic function, i.e. $\chi_B(\mathbf{x})$ equals 1 for $\mathbf{x} \in B$, and 0 otherwise.

The *star discrepancy* of the set $(\mathbf{x}_n)_{1\le n\le N}$, measuring its uniformness, is given by

$$D_N^*(\mathbf{x}_1, \dots, \mathbf{x}_N) = \sup_{J \in \mathcal{J}^*} \left| \frac{1}{N} \sum_{n=1}^{N} \chi_J(\mathbf{x}_n) - \lambda(J) \right|,$$

where $\mathcal{J}^*$ is the set of all subintervals of $\bar{U}^s$ of the form $\prod_{i=1}^{s} [0, u_i)$.

Hlawka's theorem [6] bounds the QMC integration error for a function with finite total variation in the sense of Hardy and Krause (see e.g. [12]), $V_{HK}(f) < \infty$, as follows:

$$\left| I - \hat{I}_N \right| \le V_{HK}(f) D_N^*(\mathbf{x}_1, \dots, \mathbf{x}_N).$$

Unbounded functions that approach $\pm\infty$ as the argument draws near the boundary clearly have unbounded variation. Owen [13] provides rates for the QMC convergence speed in this case, based on growth conditions on the integrand and its partial derivatives near the boundary, as well as on the speed the sequence approaches the boundary. The partial derivatives with respect to all variables x_i with $i \in u \subseteq \{1, \dots, s\}$ will be denoted by $\partial^u f$. For the origin case Owen's error bound is:

Theorem 1 ([13, Theorem 5.5]). *Let the function f satisfy the condition $|\partial^u f(\mathbf{x})| \le B\prod_{i=1}^{s}(x^{(i)})^{-A_i - \chi_u(i)}$ for some $A_i > 0$, $B < \infty$ and all $u \subseteq \{1, \dots, s\}$. Also suppose that for $N \ge 1$ and all $1 \le n \le N$ the sequence $(\mathbf{x}_n)_{1\le n}$ satisfies $\prod_{i=1}^{s} x_n^{(i)} \ge cN^{-r}$. Then for any $\eta > 0$ we have*

$$\left| I - \hat{I}_N \right| \le C_1 D_N^*(\mathbf{x}_1, \dots, \mathbf{x}_N) N^{\,\eta + r\ \max_i A_i} + C_2 N^{\,r\ (\max_i A_i - 1)}$$

with finite constants C_1 and C_2, that may depend on η. The estimate holds with $\eta = 0$, if there exists a unique maximum among $A_1, \dots, A_s$.

Thus, in order to get efficient QMC rules for these integrands one has to find point sets satisfying the condition

$$\prod_{i=1}^{s} x_n^{(i)} \ge cN^{-r}, \qquad (1 \le n \le N) \tag{1}$$

with small r. The bound $r \geq 1$ is obvious for (t, s)-nets and for Halton sequences. Sobol' [17] shows that $r = 1$ holds for Sobol' sequences, Owen [13] establishes $r \leq 1$ for Halton sequences. In Section 3 we show $r = 1$ for generalized Niederreiter sequences in the origin case.

The bound of Theorem 1 even holds for the general corner case, with similar conditions on the function and the sequence. The desired property for QMC sequences is a corner avoidance of the form

$$\min_{1 \leq n \leq N} \prod_{i=1}^{s} \min\{1 - x_n^{(i)}, x_n^{(i)}\} \geq cN^{-r}. \tag{2}$$

Owen [13] proves $r \leq 2$ for Halton sequences in this case. Section 4 will contain a proof for $r \leq 1 + \varepsilon$ for any $\varepsilon > 0$. Furthermore we show $r \geq 2$ for some subsequences of Faure sequences in the mixed-corner case, i.e. corners other than $\mathbf{0}$ and $\mathbf{1}$, and $r \geq \frac{3}{2}$ for some subsequences for the upper corner $\mathbf{1}$.

3. Generalized Niederreiter sequences and the origin

Most common low-discrepancy sequence construction schemes can be understood as Niederreiter's (t, s)-sequences, which were proposed in [9] and utilize the same ideas as Sobol' used for his net theory. For an integer base b, integers d_i and a_i for $i = 1, \ldots, s$ with $0 \leq a_i < b^{d_i}$, intervals of the form $\prod_{i=1}^{s} \left[a_i b^{-d_i}, (a_i + 1)b^{-d_i}\right)$ are called *elementary intervals*.

Furthermore, for $0 \leq t \leq m$, a (t, m, s)-*net in base* b is a point set of cardinality b^m in $[0, 1)^s$ such that every elementary interval of volume b^{t-m} contains exactly b^t points. A sequence of points $(\mathbf{x}_n)_{n \geq 0}$ is called (t, s)-*sequence in base* b if, for all $k \geq 0$ and $m > t$, the point set consisting of the $\mathbf{x}_n$ with $kb^m \leq n < (k + 1)b^m$ is a (t, m, s)-net in base b.

We will restrict us to prime power bases b and denote by $\mathbb{F}_b$ the corresponding finite field. For $r, j = 1, 2, \ldots$ and $1 \leq i \leq s$, we choose automorphisms ψ_r and η_{ij} with $\psi_r(0) = 0$ and $\eta_{ij}(0) = 0$. Then we define for $1 \leq i \leq s$ and $n \geq 0$ the i-th coordinate of the point $\mathbf{x}_n$ as

$$x_n^{(i)} = \sum_{j=1}^{\infty} v_{nj}^{(i)} b^{-j},$$

with the b-adic expansion $n = \sum_{r=1}^{\infty} a_r(n) b^{r-1}$ and, for $j \geq 1$,

$$v_{nj}^{(i)} = \eta_{ij} \left(\sum_{r=1}^{\infty} c_{jr}^{(i)} \psi_r(a_r(n)) \right).$$

The matrix $C^{(i)} = \left(c_{jr}^{(i)}\right)_{1\leq j,r}$ is called the generator matrix of the i-th coordinate. Let

$$\mathbf{c}_m^{(i)}(l) = \left(c_{m,1}^{(i)}, \ldots, c_{m,l}^{(i)}\right) \in \mathbb{F}_b{}^l,$$

and $C(d_1, \ldots, d_s; l) = \left\{\mathbf{c}_m^{(i)}(l) | 1 \leq m \leq d_i, 1 \leq i \leq s\right\}$. Furthermore, define $\rho(C; l)$ as the maximal integer d such that $C(d_1, \ldots, d_s; l)$ is linearly independent over $\mathbb{F}_b$ for all non-negative integers $d_1, \ldots, d_s$ satisfying $\sum_{1\leq i\leq s} d_i = d$. If, for an integer $t \geq 0$ and all integers $l > t$, the relation $t \geq l - \rho(C; l)$ holds, the constructed sequence is a (t, s)-sequence in base b.

Tezuka [18] proposes to construct generator matrices in the following way: Let the polynomials $p_1(z), \ldots, p_s(z) \in \mathbb{F}_b[z]$ be pairwise coprime and $e_i = deg(p_i) \geq 1$ their degrees. Furthermore consider polynomials $y_{im}(z)$ for $m \geq 1$, $1 \leq i \leq s$, such that for any $j > 0$ the family

$$\{y_{im}(z) \bmod p_i(z) \;\mid\; (j-1)e_i \leq m - 1 < je_i\}$$

is linearly independent over $\mathbb{F}_b$. If elements $a^{(i)}(j, m, r)$ are defined by the expansion

$$\frac{y_{im}(z)}{p_i(z)^j} = \sum_{r=w}^{\infty} a^{(i)}(j, m, r) z^{-r} \tag{3}$$

with an integer $w \leq 0$, then the generator matrices are given by

$$c_{mr}^{(i)} = a^{(i)}(m_i + 1, m, r), \tag{4}$$

for $1 \leq i \leq s$, $m \geq 1$ and $r \geq 1$, where $m_i = [(m-1)/e_i]$ and $[\cdot]$ denotes the integer part. Observe that w in (3) may depend on i, j, and m. This construction yields a (t, s)-sequence with $t = \sum_{i=1}^{s}(e_i - 1)$, called generalized Niederreiter sequence. In particular, for each integer $l > \sum_{i=1}^{s}(e_i - 1)$ and all integers $d_1, \ldots, d_s \geq 0$ with

$$1 \leq \sum_{i=1}^{s} d_i \leq l - \sum_{i=1}^{s}(e_i - 1),$$

the vectors $C(d_1, \ldots, d_s; l)$ are linearly independent over $\mathbb{F}_b$. Sobol', Faure and Niederreiter sequences are special cases of this construction (see [18]).

Observe, that for $(0, s)$-sequences, the definition already provides elementary intervals containing only one point, which simplifies the considerations significantly.

Theorem 2. *Let $(\mathbf{x}_n)_{n\geq 1}$ be a generalized Niederreiter $(0, s)$-sequence in base b (sometimes called generalized Faure sequence) and $0 < n < b^l$. Then $\prod_{i=1}^{s} x_n^{(i)} \geq b^{-l-s}$.*

Proof. Let d_i be the number of leading zeros in the b-adic expansion of $x_n^{(i)}$. For all $d_1, \ldots, d_s$ with $\sum_{i=1}^{s} d_i = l$, the homogeneous equation $C\,(d_1, \ldots, d_s; l)\,\mathbf{z} = \mathbf{0}$ has only the trivial solution $\mathbf{z} = \mathbf{0}$. This corresponds to the point $\mathbf{x}_0 = \mathbf{0}$, which is left out of our considerations. Thus, for the product of the coordinates we have

$$\prod_{i=1}^{s} x_n^{(i)} \geq \prod_{i=1}^{s} b^{-d_i-1} \geq b^{-l-s}. \qquad \square$$

For generalized Niederreiter (t, s)-sequences, the ideas of the proof are similar to Sobol's ideas [17]. There exist special elementary intervals with volume b^{-l}, such that just one point among the first b^l elements of the sequence lies in any such interval. Using formal Laurent series, we will show that the whole region $\left\{\mathbf{x} \in \bar{U}^s : \prod_{i=1}^{s} x^{(i)} < b^{-l-t-s}\right\}$ can be covered by such special intervals that contain the point $\mathbf{x}_0 = \mathbf{0}$. Consequently, no other points may lie in this region.

A formal Laurent series $S(z)$ over $\mathbb{F}_b$ is given by $S(z) = \sum_{j=w}^{\infty} a_j z^{-j}$, where w is an integer and all $a_j \in \mathbb{F}_b$. The discrete exponential valuation ν is defined by $\nu(S(z)) = -w$ if $S(z) \neq 0$ and w is the least integer with $a_w \neq 0$, and by $\nu(0) = -\infty$.
For $S(z)$ we define the polynomial part by $[S(z)] = \sum_{j=\min\{w,0\}}^{0} a_j z^{-j}$. Furthermore we use the notation $[S(z)]_{p_i(z)} = [S(z)] \bmod (p_i(z))$. Define

$$y_{im}^{(q)}(z) = \begin{cases} \left[y_{im}/p_i(z)^{m_i+1}\right] & \text{for } q = 0, \\ \left[y_{im}/p_i(z)^{m_i+1-q}\right]_{p_i(z)} & \text{for } 0 < q \leq m_i + 1, \\ 0 & \text{for } q > m_i + 1. \end{cases}$$

Then we have the representation

$$y_{im}(z) = \sum_{q=0}^{m_i+1} y_{im}^{(q)}(z) p_i(z)^{m_i+1-q} = p_i(x)^{m_i+1} \sum_{q=0}^{m_i+1} \frac{y_{im}^{(q)}(z)}{p_i(z)^q}.$$

Lemma 1. *Let the elements $c_{mr}^{(i)} \in \mathbb{F}_b$ be defined by Tezuka's construction (4). Choose any integers $d_1, \ldots, d_s \geq 0$ and $l > \sum_{i=1}^{s}(e_i - 1)$ with $1 \leq \sum_{i=1}^{s} d_i \leq l$ and $e_i | d_i$. Then the vectors $\mathbf{c}_m^{(i)} = \left(c_{m1}^{(i)}, \ldots, c_{ml}^{(i)}\right) \in \mathbb{F}_b{}^l$ with $1 \leq m \leq d_i$, $1 \leq i \leq s$, are linearly independent over $\mathbb{F}_b$.*

Proof. Suppose that the family of vectors $\mathbf{c}_m^{(i)}$, $1 \leq m \leq d_i$, $1 \leq i \leq s$, satisfies the linear dependence relation

$$\sum_{i=1}^{s} \sum_{m=1}^{d_i} f_m^{(i)} \mathbf{c}_m^{(i)} = \mathbf{0} \in \mathbb{F}_b{}^l.$$

Componentwise, this relation reads $\sum_{i=1}^{s} \sum_{m=1}^{d_i} f_m^{(i)} a^{(i)}(m_i + 1, m, r) = 0$ for $1 \leq r \leq l$. Now consider for $1 \leq i \leq s$ the integers $q_i = d_i/e_i - 1$ and define for $1 \leq q \leq q_i + 1$ the polynomials

$$f_{iq}(z) = \sum_{m=1}^{d_i} f_m^{(i)} y_{im}^{(q)}(z).$$

¿From this, define the rational function

$$\begin{aligned}
L &= \sum_{i=1}^{s}\sum_{q=1}^{q_i+1} \frac{f_{iq}(z)}{p_i(z)^q} = \sum_{i=1}^{s}\sum_{q=1}^{m_i+1} \frac{f_{iq}(z)}{p_i(z)^q} = \sum_{i=1}^{s}\sum_{q=1}^{m_i+1}\sum_{m=1}^{d_i} f_m^{(i)} \frac{y_{im}^{(q)}(z)}{p_i(z)^q} \\
&= \sum_{i=1}^{s}\sum_{m=1}^{d_i} f_m^{(i)} \frac{y_{im}(z) - y_{im}^{(0)} p_i(z)^{m_i+1}}{p_i(z)^{m_i+1}} = \sum_{i=1}^{s}\sum_{m=1}^{d_i} f_m^{(i)} \sum_{r=1}^{\infty} a^{(i)}(m_i+1, m, r) z^{-r} \\
&= \sum_{r=1}^{\infty}\left(\sum_{i=1}^{s}\sum_{m=1}^{d_i} f_m^{(i)} c_{mr}^{(i)}\right) z^{-r}.
\end{aligned}$$

The fact that L has no polynomial part follows readily from the construction, since $y_{im}^{(0)}(z)$ is exactly the polynomial part of $y_{im}(z)/p_i(z)^{m_i+1}$. Thus, r only assumes positive values in the second line.
Hence, the discrete exponential valuation $\nu(L)$ is less than $-l$. Now let $g = \prod_{i=1}^{s} p_i(z)^{q_i+1}$, then Lg is a polynomial. On the other hand,

$$\nu(Lg) < -l + \deg(g) = -l + \sum_{i=1}^{s}(q_i+1)e_i = -l + \sum_{i=1}^{s} d_i \le 0.$$

Therefore $Lg = 0$, thus $L = 0$. Like in [18, Lemma 6.1] and [11, Theorem 4.49], one can also understand L as a partial fraction decomposition of a rational function, and so the uniqueness of the partial fraction decomposition gives us

$$f_{iq} = 0 \text{ for } 1 \le q \le q_i + 1, 1 \le i \le s.$$

First consider the case $q = q_i + 1$. We have $q > m_i + 1$, whenever $m \le (q-1)e_i$. Thus $y_{im}^{(q)} = 0$ for $1 \le m \le (q-1)e_i$, or equivalently

$$f_{iq}(z) = \sum_{m=(q-1)e_i+1}^{qe_i} f_m^{(i)} y_{im}^{(q)}(z) = 0.$$

For $m = (q-1)e_i + 1, \ldots, qe_i$, we have $q = m_i + 1$ and therefore by construction the $y_{im}^{(q)}(z)$, $(q-1)e_i < m \le qe_i$, are linearly independent. In particular, $f_m^{(i)} = 0$ for $(q-1)e_i + 1 \le m \le qe_i$.
By repeating the last argument for $q = q_i, \ldots, 1$, it follows that all $f_m^{(i)} = 0$. □

Theorem 3. *Each point $\mathbf{x}_n$, $1 \le n < b^l$, of a generalized Niederreiter (t,s)-sequence in base b fulfills*

$$\prod_{i=1}^{s} x_n^{(i)} \ge b^{-l-t-s}.$$

Proof. We fix $1 \leq n < b^l$ and consider the b-adic expansions $n = \sum_{r=1}^{l} a_r(n) b^{r-1}$ and

$$x_n^{(i)} = \sum_{r=1}^{l} v_{nr}^{(i)} b^{-r}$$

for $1 \leq i \leq s$. Define d_i by $v_{n1}^{(i)} = \cdots = v_{nd_i}^{(i)} = 0$ and $v_{nd_i+1}^{(i)} \neq 0$. Consequently, $x_n^{(i)} \geq b^{-d_i-1}$ and

$$\prod_{i=1}^{s} x_n^{(i)} \geq b^{-s-\sum_{i=1}^{s} d_i}.$$

If $\sum_{i=1}^{s} d_i \leq l+t$, the theorem holds. Otherwise we assume that there is a solution $\hat{a}_r(n)$, $1 \leq r \leq l$, to the system of linear equations

$$\sum_{r=1}^{l} c_{jr}^{(i)} \psi_r\left(a_r(n)\right) = 0, \tag{5}$$

$1 \leq j \leq d_i$, $1 \leq i \leq s$. Every d_i can be written as $d_i = \hat{d}_i e_i + \rho_i$ with $\rho_i \leq e_i - 1$. It follows, that $\sum_{i=1}^{s} \rho_i \leq \sum_{i=1}^{s} e_i - s = t$ and

$$\sum_{i=1}^{s} \hat{d}_i e_i \geq \sum_{i=1}^{s} d_i - t \geq l.$$

Consider only the first $\hat{d}_i e_i$, $1 \leq i \leq s$, equations in (5) and append $\sum_{i=1}^{s} \hat{d}_i e_i - l$ variables. Then

$$\left(\hat{a}_1(n), \ldots, \hat{a}_l(n), \underbrace{0, \ldots, 0}_{\sum_{i=1}^{s} \hat{d}_i e_i - l}\right)$$

is a nontrivial solution to the homogeneous system

$$\sum_{r=1}^{\sum_{i=1}^{s} \hat{d}_i e_i} c_{mr}^{(i)} \psi_r\left(a_r(n)\right) = 0,$$

$1 \leq m \leq \hat{d}_i e_i$, $1 \leq i \leq s$, which is a contradiction to Lemma 1. $\square$

Corollary 1. *For $b^{l-1} \leq n < b^l$ with arbitrary $l > 1$ we have $\prod_{i=1}^{s} x_n^{(i)} \geq b^{-l-t-s} \geq b^{-t-s+1} n^{-1}$. Thus, for generalized Niederreiter sequences (and the special cases of Sobol', Faure and Niederreiter's (t, s) sequences) condition (1) is fulfilled with $r = 1$ and we have a hyperbolic origin avoidance of order $r = 1$.*

4. Avoiding all corners

For the numerical evaluation of functions with singularities on all boundaries of the unit cube, one is interested in the minimal volume of the intervals defined by a given corner

$\mathbf{h} = (h_1, \ldots, h_s) \in \{0,1\}^s$ of the unit cube and the used QMC points $\mathbf{x}_n$, also called the minimal hyperbolic distance of the points $\mathbf{x}_n$ to the corner $\mathbf{h}$:

$$M_N(\mathbf{h}) = \min_{1 \le n \le N} \prod_{i=1}^{s} \left| h_i - x_n^{(i)} \right|.$$

The left term of the corner avoidance condition (2) may then be written as $M_N(\min) = \min_{\mathbf{h}} M_N(\mathbf{h})$. One also has to notice that $M_N(\mathbf{0})$ was the quantity considered in the previous section. In the following we will use the notations $J = \{i \in \{1, \ldots, s\} : h_i = 0\}$ and $K = \{i \in \{1, \ldots, s\} : h_i = 1\}$. Corners different from $\mathbf{0}$ and $\mathbf{1}$ will be called mixed corners.

4.1 Halton sequences

For integers p and n with p-adic expansion $n = \sum_{r=1}^{l} a_r(n) p^{r-1}$ define the radical inverse function by $\Phi_p(n) = \sum_{r=1}^{l} a_r(n) p^{-r}$. The n-th element of the s-dimensional Halton sequence [3] in relatively coprime bases $p_1, \ldots, p_s$ (typically the first s primes) is then given by $\mathbf{x_n} = (\Phi_{p_1}(n), \ldots, \Phi_{p_s}(n))$.

Owen [13] shows $M_N(\mathbf{0}) \ge c_1 N^{-1}$, $M_N(\mathbf{1}) \ge c_2 (N+1)^{-1}$, and $M_N(\min) \ge c_3 (N(N+1))^{-1}$, for suitable constants $c_1, c_2, c_3 > 0$.

A simple argument shows the converse, namely that $M_N(\mathbf{0}) \le c_2 N^{-1}$ for Halton sequences. To see this, first consider integers of the form $\tilde{n} = \prod_{i=1}^{s} p_i^{\alpha_i}$. Then

$$M_{\tilde{n}}(\mathbf{0}) \le \prod_{1 \le i \le s} x_{\tilde{n}}^{(i)} \le \prod_{1 \le i \le s} p_i^{-\alpha_i} = \frac{1}{\tilde{n}}.$$

Using $\bar{p} = \min_{i \in \{1, \ldots, s\}} p_i$, the inequality $\bar{p}^{[\log_{\bar{p}} n]} \ge n/\bar{p}$ holds for all $n > 0$ and therefore also

$$M_n(\mathbf{0}) \le M_{\bar{p}^{[\log_{\bar{p}} n]}}(\mathbf{0}) \le \frac{1}{\bar{p}^{[\log_{\bar{p}} n]}} \le \frac{\bar{p}}{n}.$$

A similar argument can be formulated to show $M_N(\mathbf{1}) \le c_2 (N+1)^{-1}$.

The following theorem proves that – for infinitely many N – the mixed-corner avoidance is of the form $M_N(\min) \le c_2 (N \log N)^{-1}$.

Theorem 4. *For $n \ge 1$ let $\mathbf{x}_n$ be the n-th point of the Halton sequence in distinct prime bases $p_1, \ldots, p_s$. Then there exist subsequences $\mathbf{y}_n = \mathbf{x}_{N(n)}$ for which the minimum distance $M_{N(n)}(\mathbf{h})$ to any mixed corner $\mathbf{h}$ is bounded by*

$$M_{N(n)}(\mathbf{h}) = \mathcal{O}\left(\frac{1}{N(n) \log N(n)} \right).$$

In particular, the Halton sequence tends to the mixed corners faster than it tends towards the origin.

Proof. For all numbers a, b with $gcd(a,b) = 1$, according to Euler's Theorem, we have $a^{\varphi(b)} \equiv 1 \mod (b)$. Let $a = \prod_{k\in K} p_k^{\alpha_k}$ and $b = \prod_{j\in J} p_j^{\beta_j}$, with $\alpha_j, \beta_k \in \mathbb{N}$. Then clearly $gcd(a,b) = 1$. Furthermore $\varphi(b) = b\prod_{j\in J}(1 - 1/p_j)$.
Fix an $a > 1$ as above and let the β_i and thus b vary. Consider the subsequences with indices $N(a,b) = a^{\varphi(b)} - 1$, then $b|N(a,b)$ and $a^{\varphi(b)}|N(a,b)+1$. Thus

$$\prod_{j\in J} x_{N(a,b)}^{(j)} \prod_{k\in K}\left(1 - x_{N(a,b)}^{(k)}\right) \le \frac{1}{a^{\varphi(b)}b} \le$$

$$\frac{(\log a)\prod_{j\in J}(1-1/p_j)}{(N(a,b)+1)\log(N(a,b)+1)} = \mathcal{O}\left(\frac{1}{N(a,b)\log N(a,b)}\right).$$

□

Remark 2. *For the Halton sequence in relatively prime bases $p_i = \prod_g q_{ig}^{\gamma_{ig}}$, $1 \le i \le s$, the same argument holds, with $\varphi(b) = b\prod_{j\in J}\prod_g\left(1 - \frac{1}{q_{jg}}\right)$ and thus a similar change in the constant of the last inequality.*

Next we are looking for a better lower bound for $M_N(\min)$. We will restrict our investigations to prime bases $p_1, \ldots, p_s \in \mathbb{P}$. Observe that if we could find n with $n = \prod_{j\in J} p_j^{\alpha_j}$ and $n+1 = \prod_{k\in K} p_k^{\beta_k}$, then the following bounds would hold

$$\prod_{i=1}^{s} p_i^{-1} \prod_{j\in J} p_j^{-\alpha_j} \prod_{k\in K} p_k^{-\beta_k} \le M_n(\mathbf{h}) = \prod_{j\in J} x_n^{(j)} \prod_{k\in K}\left(1 - x_n^{(k)}\right) \le \prod_{j\in J} p_j^{-\alpha_j} \prod_{k\in K} p_k^{-\beta_k}.$$

Generally, finding such an n will not be possible. However, to find points with a small hyperbolic distance, the conditions are $n \equiv 0 \mod p_i^{\alpha_i}$ for all $j \in J$, and $n \equiv -1 \mod p_k^{\beta_k}$ for all $k \in K$. Alternatively, this family of s congruences may be written as

$$n = C\prod_{j\in J} p_j^{\alpha_j} \quad \text{and} \quad n+1 = \tilde{C}\prod_{k\in K} p_k^{\beta_k} \tag{6}$$

with some unknown constants C and $\tilde{C}$. Subtracting these equations we get the Diophantine equation

$$1 = \tilde{C}\prod_{k\in K} p_k^{\beta_k} - C\prod_{j\in J} p_j^{\alpha_j} \tag{7}$$

with unknown integers C, $\tilde{C}$, β_k, and α_j. We now need to find numbers n of the form (6) with minimal constants C and $\tilde{C}$ in terms of n, and thus minimal $d = \prod_{j\in J} p_j^{-\alpha_j} \prod_{k\in K} p_k^{-\beta_k}$.

In order to find a lower bound for d we use the following variant of the Subspace Theorem (cf. [14]).

Theorem 5 (Subspace Theorem)**.** *Let K be an algebraic number field and let $S \subset M(K) = \{$canonical absolute values of $K\}$ be a finite set of absolute values which contains all of the Archimedean ones. For each $\nu \in S$ let $L_{\nu,1}, \cdots, L_{\nu,n}$ be n linearly independent linear forms in n variables with coefficients in K. Then for given $\delta > 0$, the* *solutions of the inequality*

$$\prod_{\nu\in S}\prod_{i=1}^{n}|L_{\nu,i}(\mathbf{x})|_{\nu}^{n_\nu} < \overline{|\mathbf{x}|}^{-\delta}$$

with $\mathbf{x}\in\mathfrak{a}_K^n$ *and* $\mathbf{x}\neq\mathbf{0}$, *where*

$$\overline{|\mathbf{x}|} = \max_{\substack{1\le i\le n\\ 1\le j\le \deg K}} |x_i^{(j)}|,$$

$|\cdot|_\nu$ *denotes valuation corresponding to* ν, n_ν *is the local degree and* $\mathfrak{a}_K$ *is the maximal order of* K, *lie in finitely many proper subspaces of* K^n.

We can now prove that asymptotically $M_N(\min) > cN^{-1-\varepsilon}$ for all $\varepsilon > 0$.

Theorem 6. *If* C, $\tilde{C}$, α_j, *and* β_k *satisfy equation* (7), *then for every* $\varepsilon > 0$ *we have* $d^{-1} = \prod_{j\in J} p_j^{\alpha_j}\prod_{k\in K} p_k^{\beta_k} < cN^{1+\varepsilon}$, *where* c *depends only on* s *and* ε. *In particular* $M_N(\min) > \mathcal{O}(N^{-1-\varepsilon})$.

Proof. Let us write $x_1 = \tilde{C}\prod_{k\in K} p_k^{\beta_k} = N+1$ and $x_2 = C\prod_{j\in J} p_j^{\alpha_j} = N$. Assume first $\frac{\tilde{C}C}{x_2} \ge N^{-\varepsilon}$. Then

$$\begin{aligned}
\tilde{C}N^{\varepsilon} &\ge \frac{x_2}{C} = \prod_{j\in J} p_j^{\alpha_j},\\
x_1 N^{\varepsilon} &\ge \prod_{j\in J} p_j^{\alpha_j}\prod_{k\in K} p_k^{\beta_k},\\
(N+1)^{1+\varepsilon} &\ge \prod_{j\in J} p_j^{\alpha_j}\prod_{k\in K} p_k^{\beta_k},
\end{aligned}$$

hence we are done in this case. It remains to show that the converse, $\frac{\tilde{C}C}{x_2} < N^{-\varepsilon}$, holds only for finitely many N and its effects can thus be included in the constant. We want to use the Subspace Theorem stated above. Our field are the rationals $\mathbb{Q}$, and the set S consists of the valuations corresponding to the primes $p_1,\ldots,p_s$ and the usual Archimedean valuation. We define our linear forms $L_{\nu,1}(x,y) = x$ for all $\nu\in S$ and $L_{\nu,2}(x,y) = y$ for all non-Archimedean valuations of S and $L_{\infty,2}(x,y) = x-y$. We have:

$$\overline{|(x_1,x_2)|}^{-\varepsilon} \ge N^{-\varepsilon} > \frac{\tilde{C}C}{x_2} = \frac{x_1}{\prod_{j\in J} p_j^{\alpha_j}}\cdot\frac{1}{\prod_{k\in K} p_k^{\beta_k}} = \prod_{i=1}^{2}\prod_{\nu\in S}|L_{\nu,i}(x_1,x_2)|_\nu^{n_\nu}.$$

By the Subspace Theorem all solutions to this inequality lie in finitely many proper subspaces of $\mathbb{Q}^2$. Let T be such a subspace. Then we have

$$\begin{aligned}
x_1 a + x_2 b &= 0 \quad \text{(Subspace } T\text{)}\\
x_1 - x_2 &= 1
\end{aligned} \tag{8}$$

The linear System (8) has at most one solution, hence the inequality has only finitely many solutions and we have proved our theorem. ∎

Remark 3. *Theorem 6 also proves that* $M_N(\min) > cN^{-1-\varepsilon}$ *if we consider bases* $p_i = \prod_g q_{ig}^{\gamma_{ig}}$, $1 \leq i \leq s$, *that are "only" relatively prime. In this case, the products in* (7) *contain all prime factors of the bases, and the* α_j *and* β_k *are restricted to multiples of the corresponding* γ_{ig}.

4.2 Faure Sequences

Let p be the least prime larger or equal to the dimension s, and let x be a p-adic rational in $[0,1)$ with expansion $x = \sum_{i=0}^{\infty} x_{(i)} p^{-i-1}$, for which we will use the short notation $x = (x_{(0)}, x_{(1)}, x_{(2)}, \ldots)$. For $m \geq 1$ define

$$B_m(k) = \begin{pmatrix} \binom{0}{0}k^0 & \binom{1}{0}k^1 & \cdots & \binom{m}{0}k^m \\ \binom{0}{1}k^{-1} & \binom{1}{1}k^0 & \cdots & \binom{m}{1}k^{m-1} \\ \vdots & & \ddots & \vdots \\ \binom{0}{m}k^{-m} & \binom{1}{m}k^{1-m} & \cdots & \binom{m}{m}k^0 \end{pmatrix} \text{ if } k \neq 0$$

and let $B_m(0)$ be the $(m+1) \times (m+1)$ unit matrix.
Further, define $P(x) = B_m(1)(x_{(0)}, \ldots, x_{(m)})^T \bmod p$ for a sufficiently large m. The n-th point of the Faure sequence [2] is given by $(\Phi_p(n), P(\Phi_p(n)), \ldots, P^{s-1}(\Phi(n))$, where $\Phi_p(n)$ is again the radical inverse function defined in Section 4.1.

Observe that for $l, k \in \mathbb{R}$ we have $B_m(k)B_m(l) = B_m(l+k)$, in particular $B_m(k)^{-1} = B_m(-k)$, and that the function P is nilpotent, i.e. $P^p = \mathrm{id}$ or equivalently $B_m(p) = I \pmod p$. Furthermore, the n-th point of the Faure sequence can also be written as $(B(0)\Phi_p(n), B(1)\Phi_p(n), \ldots, B(s-1)\Phi_p(n))$.

Remark 4. *The shift of coordinates in the Faure sequence corresponds to a permutation of the Faure sequence. Let* s *be prime,* $\mathbf{x}$ *be an* s*-tuple, and* $S(\mathbf{x}) = S(x^{(1)}, \ldots, x^{(s)}) = (x^{(s)}, x^{(1)}, \ldots, x^{(s-1)})$. *Consider an* $n \in \mathbb{N}$ *with* $p^l \leq n < p^{l+1}$ *and* $\mathbf{x}_n$ *the* n*-th element of the Faure sequence. Then* $S(\mathbf{x}_n) = \mathbf{x}_m$ *for some* m *with* $p^l \leq m < p^{l+1}$, *which is an immediate consequence of the aforementioned properties.*

As the Faure sequence is a generalized Niederreiter $(0,s)$-sequence, Theorem 2 already proves an origin avoidance $M_N(\mathbf{0}) > cN^{-1}$. Now we consider mixed corners.

Lemma 5. *Let* s *be prime. There exists a subsequence* $\mathbf{y}_n = \mathbf{x}_{N(n)}$ *of the Faure sequence such that* $\prod_{i=1}^{s} \left| h_i - y_n^{(i)} \right| \leq \frac{p^3}{N(n)^2}$.

Proof. Consider the subsequence with indices $N(n) = (p-1)p^{p^n-1}$. By shifting the coordinates we may assume $s = p$ and $h_1 = 0, h_p = 1$.

It is sufficient to show that $y_n^{(p)} = (p-1, p-1, \ldots, p-1)^T$. We know

$$y_n^{(p)} = B(p-1)y_n^{(1)} = B(-1)(0, \ldots, 0, p-1)^T,$$

hence we have to prove

$$\binom{p^n - 1}{j} = \prod_{i=1}^{j} \frac{p^n - i}{i} = (-1)^j \text{ over } \mathbb{F}_p. \tag{9}$$

Every $i = 1, \ldots, j$ can be written as $i = lp^k$ with $0 \leq k < n$ and $p \nmid l$. Then $\frac{p^n - i}{i} = \frac{p^{n-k}}{l} - 1 = -1$ in $\mathbb{F}_p$. Adding an additional factor p in the bound for the case when we need to shift the coordinates completes the proof. □

Remark 6. *The previous lemma holds even for non-prime s, if the vector $\mathbf{h}$ contains the pattern $(\ldots, 1, 0, \ldots)$.*

Finally, we consider the upper corner $\mathbf{1}$. Let us start with two-dimensional Faure sequences.

Lemma 7. *Let $s = 2$. There exists a subsequence $\mathbf{y}_n = \mathbf{x}_{N(n)}$ of the Faure sequence such that $\prod_{i=1}^{2} \left(1 - y_n^{(i)}\right) \leq \frac{p^2}{N(n)^2}$.*

Proof. Consider the subsequence with indices $N(n) = 2^{2^n - 1} - 1$. We have to prove that $y_n^{(2)} = B(1)y_n^{(1)} = (1, \ldots, 1)$, or equivalently

$$\sum_{i=0}^{2^n - 2} \binom{i}{j} = \binom{2^n - 1}{j} = 1$$

over $\mathbb{F}_2$. This, however, can be easily seen by the same arguments used for equation (9) with $p = 2$ and by the fact that $-1 = 1$ over $\mathbb{F}_2$. □

In higher dimensions, only a slower upper bound of order $N^{-3/2}$ for the corner approach rate of the upper corner $\mathbf{1}$ can be shown.

Lemma 8. *Let $s > 2$. There exists a subsequence $\mathbf{y}_n = \mathbf{x}_{N(n)}$ of the Faure sequence such that*

$$\prod_{i=1}^{s} \left(1 - y_n^{(i)}\right) \leq \frac{p^3}{(N(n))^{3/2}}.$$

Proof. Let us consider the subsequence with indices $N(n) = p^{2p^n - 1} - 1$. Since $y_n^{(1)} = (p-1, \ldots, p-1)$, it is sufficient to prove $y_n^{(s)} = (\eta_{(0)}, \ldots, \eta_{(2p^n - 2)})$ with $\eta_{(j)} = p - 1$ for $0 \leq j \leq p^n$. We may assume that the dimension $s = p$ is a prime. Otherwise we consider the p-dimensional Faure sequence (where p is the smallest prime larger than s) and shift

the coordinates accordingly.
We compute

$$B(p-1)y_n^{(1)} = B(-1)y_n^{(1)} = y_n^{(p)}.$$

Since $y_n^{(1)} = (p-1,\dots,p-1)$, we have to prove

$$F(n,j) = \sum_{k=0}^{2p^n-2} (-1)^{k-j}\binom{k}{j} = 1$$

for $0 \le j \le p^n-1$ over $\mathbb{F}_p$. For $j=0$, we have $F(n,0) = \sum_{k=0}^{2p^n-2}(-1)^k = 1-1+1-\cdots+1 = 1$, and for $j=1$, we have

$$F(n,1) = \sum_{k=0}^{2p^n-2}(-1)^{k-1}k = -0+1-2+3-4+-\cdots-(2p^n-2) = -(p^n-1) = 1.$$

For the general case $1 < j \le p^n-1$, we will first rewrite the sum. Therefore we recall the relation $\binom{k}{j} = \sum_{l=0}^{k-1}\binom{l}{j-1}$ to obtain

$$\begin{aligned} F(n,j) = \sum_{k=0}^{2p^n-2}(-1)^{k-j}\binom{k}{j} &= \sum_{k=0}^{2p^n-2}\sum_{l=0}^{k-1}(-1)^{k-j}\binom{l}{j-1} \\ &= \sum_{l=0}^{2p^n-3}\binom{l}{j-1}\sum_{k=l+1}^{2p^n-2}(-1)^{k-j} = (-1)^j\sum_{l=0}^{p^n-2}\binom{2l+1}{j-1}. \end{aligned}$$

Furthermore we consider for $1 \le j \le p^n-2$

$$\begin{aligned} 2F(n,j+1)-F(n,j) =&(-1)^{j+1}\left(2\sum_{l=0}^{p^n-2}\binom{2l+1}{j} + \sum_{l=0}^{p^n-2}\binom{2l+1}{j-1}\right) \\ =&(-1)^{j+1}\left(\sum_{l=0}^{p^n-2}\binom{2l+1}{j} + \sum_{l=0}^{p^n-2}\left(\binom{2l+1}{j-1}+\binom{2l+1}{j}\right)\right) \\ =&(-1)^{j+1}\left(\sum_{l=0}^{p^n-2}\binom{2l+1}{j} + \sum_{l=0}^{p^n-2}\binom{2l+2}{j}\right) \\ =&(-1)^{j+1}\sum_{l=1}^{2p^n-2}\binom{l}{j} = (-1)^{j+1}\binom{2p^n-1}{j+1}. \end{aligned}$$

By a similar argument as for equation (9) we have $\binom{2p^n-1}{j+1} = (-1)^{j+1}$, hence

$$2F(n,j+1)-F(n,j) = 1 \qquad (1 \le j \le p^n-2).$$

By induction on j it follows that $F(n,j)=1$ for all $0 \le j \le p^n-1$. This implies

$$\prod_{i=1}^{s}\left(1-y_n^{(i)}\right) \le \frac{1}{p^{2p^n-2}}\frac{1}{p^{p^n-1}} = \frac{p^{3/2}}{\left((N(n)+1)/p\right)^{3/2}} < \frac{p^3}{\left(N(n)\right)^{3/2}},$$

where the additional factor p for $N(n)$ stems from a possible coordinate shift in the case when s is not prime. $\square$

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References

[1] E. de Doncker and Y. Guan. Error bounds for the integration of singular functions using equidistributed sequences. *J. Complexity*, 19(3):259–271, 2003.

[2] H. Faure. Discrépance de suites associées à un système de numération (en dimension un). *Bull. Soc. Math. France*, 109:143–182, 1981.

[3] J. H. Halton. On the efficiency of certain quasi-random sequences of points in evaluating multidimensional integrals. *Numer. Math.*, 2:84–90, 1960.

[4] J. Hartinger and R. Kainhofer. Non-uniform low-discrepancy sequence generation and integration of singular integrands. Submitted, 2004.

[5] J. Hartinger, R. Kainhofer, and R. Tichy. Quasi-Monte Carlo algorithms for unbounded, weighted integration problems. *Journal of Complexity*, 20(5):654–558, 2004.

[6] E. Hlawka. Uniform distribution modulo 1 and numerical analysis. *Compositio Math.*, 16:92–105, 1964.

[7] B. Klinger. Numerical integration of singular integrands using low-discrepancy sequences. *Computing*, 59(3):223–236, 1997.

[8] H. Niederreiter. Point sets and sequences with small discrepancy. *Monatsh. Math.*, 104:273–337, 1987.

[9] H. Niederreiter. Quasi-Monte Carlo methods and pseudo-random numbers. *Bulletin of the AMS*, 84(6):957–1029, 1987.

[10] H. Niederreiter. Low-discrepancy and low-dispersion sequences. *Journal of Number Theory*, 30(1):51–70, 1988.

[11] H. Niederreiter. *Random number generation and Quasi-Monte Carlo methods*, volume 63 of *SIAM Conf. Ser. Appl. Math.* SIAM, Philadelphia, 1992.

[12] A. B. Owen. Multidimensional variation for Quasi-Monte Carlo. *In J. Fan and G. Li, editors,* International Conference on Statistics in Honour of Professor Kai-Tai Fang's 65th Birthday, 2005.

[13] A. B. Owen. Halton sequences avoid the origin. *SIAM Review*, 48, 2006, (to appear).

[14] W. M. Schmidt. *Diophantine approximations and Diophantine equations*, volume 1467 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 1991.

[15] I. M. Sobol'. On the distribution of points in a cube and the approximate evaluation of integrals. *USSR Comput. Math. Math. Phys.*, 7:86–112, 1967.

[16] I. M. Sobol'. Computation of improper integrals by means of equidistributed sequences. *Dokl. Akad. Nauk SSSR*, 210:278–281, 1973.

[17] I. M. Sobol'. Использование равноиерно распределенных Последовательностей для приближенного вычислеия Несобственных интегралов (On the use of uniformly distributed sequences for approximate computations of improper integrals). In S. Sobolev, editor, *Теория кубатуриых формул и приложения функциональиого анализа к некоторым задачам математической физики (Theory of cubature formulas and applications to certain problems in mathematical physics)*, pages 62–66. Novosibirsk Nauka, 1973.

[18] S. Tezuka. *Uniform Random Numbers: Theory and Practice*. Kluwer Academic Publishers, Norwell, Mass, 1995.

[19] S. Tezuka and T. Tokuyama. A note on polynomial arithmetic analogue of halton sequences. *ACM Trans. Model. Comput. Simul.*, 4(3):279–284, 1994.