Quasi-Monte Carlo Algorithms for unbounded, weighted integration problems

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Abstract

In this article we investigate Quasi-Monte Carlo methods for multidimensional improper integrals with respect to a measure other than the uniform distribution. Additionally, the integrand is allowed to be unbounded at the lower boundary of the integration domain. We establish convergence of the Quasi-Monte Carlo estimator to the value of the improper integral under conditions involving both the integrand and the sequence used. Furthermore, we suggest a modification of an approach proposed by Hlawka and Mück for the creation of low-discrepancy sequences with regard to a given density, which are suited for singular integrands.

Key words: Quasi-Monte Carlo integration, weighted integration, non-uniformly distributed low-discrepancy sequences

This paper is devoted to Quasi-Monte Carlo (QMC) techniques for weighted integration problems of the form

$$I = \int_{[\mathbf{a},\mathbf{b}]} f(\mathbf{x}) dH(\mathbf{x}), \tag{1}$$

where H denotes a s-dimensional distribution with support $K = [\mathbf{a}, \mathbf{b}] \subseteq \mathbb{R}^s$ and f is a function with singularities on the left boundary of K.

Numerical integration problems of this form frequently occur in practice, e.g. in the field of computational finance. A typical example is the estimation of the mean of a random variate X with support $\mathbb{R}^s$. In case of variates with

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unbounded variance Monte Carlo simulation is inapplicable, but (after a transformation) QMC algorithms might be available.

Let $H(J)$ denote the probability of $J \subseteq K$ under H. A sequence $\omega = (y_1, y_2, \dots)$ is defined to be H-distributed if for all intervals $\tilde{K} \subseteq K$ the following condition holds:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \chi_{\tilde{K}}(y_n) = H(\tilde{K}).$$

For Riemann integrable (thus bounded) functions it is well known that the integral (1) can be approximated by

$$\int_K f(\mathbf{x})dH(\mathbf{x}) = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(y_n),$$

where $(y_n)_{n>0}$ denotes an H-distributed sequence. The aim is to establish conditions on integrands and sequences to guarantee the convergence of QMC techniques for unbounded weighted problems and to justify the commonly used strategy of

ignoring the singularity.

Furthermore techniques proposed by Hlawka and Mück for bounded, weighted integration problems are adapted for the unbounded case.

1 Preliminaries and basic definitions

Hlawka [1] established the first quantitative error bound for QMC-algorithms on the s-dimensional unit cube, where H equals the uniform distribution U. To gain a deep insight in the classical QMC theory we refer to the monographs of Kuipers and Niederreiter [2] or Niederreiter [3]. Quasi-Monte Carlo algorithms for (Riemann) improper integrals with regard to the uniform distribution ($H = U\,[0,1]^s$) were first investigated by Sobol. In [4] he dealt with integrands, which are unbounded for $x_1 x_2 \cdots x_s \to 0$. Asymptotic error estimates, as well as numerical examples for some special functions were presented by Klinger [5], De Doncker and Guan [6].

We consider integration problems, which have the following properties

- The improper integral (1) on a compact subinterval of $\mathbb{R}^s$ exists in the sense that the limes

$$\lim_{\substack{\mathbf{c}\to\mathbf{a}\\ \mathbf{c}>\mathbf{a}}} \int_{[\mathbf{c},\mathbf{b}]} f(\mathbf{x})dH(\mathbf{x}) \qquad (2)$$

exists independent of the $\mathbf{c}$, where $\mathbf{c} > \mathbf{a}$ should be understood componentwise. We will define this limes as the value of the improper integral.

- If the integration domain is not a compact subinterval of $\mathbb{R}^s$, i.e. at least one coordinate is unbounded ($a_i = -\infty$ or $b_i = \infty$ for a $1 \leq i \leq s$), the limes

$$\lim_{\mathbf{c} \to \mathbf{a}^+} \int_{[\mathbf{c},\mathbf{d}]} f(\mathbf{x}) dH(\mathbf{x})$$

has to exist for every finite fixed upper boundary $\mathbf{d} \in (\mathbf{a}, \mathbf{b})$, $\|\mathbf{d}\| < \infty$. Independently, for any fixed $\mathbf{c} \in [\mathbf{a}, \mathbf{b}]$ as lower integration boundary with $\mathbf{c} > \mathbf{a}$ componentwise, the limes

$$\lim_{\mathbf{d} \to \mathbf{b}^-} \int_{[\mathbf{c},\mathbf{d}]} f(\mathbf{x}) dH(\mathbf{x})$$

needs to exists. Then we let the lower and upper integration bounds independently tend to the boundaries of the integration domain K and define the value of the improper integral as

$$\lim_{\mathbf{d} \to \mathbf{b}^-} \lim_{\mathbf{c} \to \mathbf{a}^+} \int_{[\mathbf{c},\mathbf{d}]} f(\mathbf{x}) dH(\mathbf{x}) .$$

- The integrand $f(\mathbf{x})$ possibly has singularities at the left boundary of the integration domain, i.e. $\lim_{x_i \to a_i} |f(x)| = \infty$ for some $i \in \{1, \ldots, s\}$.
- These singularities are the only singularities of $f(\mathbf{x})$. In particular this means that for all $\varepsilon > 0$ there exists some $M < \infty$, such that $|f(x)| < M$ for all $x \in [a + \varepsilon, b]$.

Before we recall Hlawka's integration error bound (respectively a slight generalization for weighted integration) some more definitions are required:

Definition 1.1 *The H-discrepancy of $\omega = (y_1, y_2, \dots)$ measures the distribution properties of the sequence. It is defined as*

$$D_{N,H}(\omega) = \sup_{J \subseteq K} \left| \frac{1}{N} A_N(J, \omega) - H(J) \right| , \tag{3}$$

where A_N counts the number of elements in $(y_1, \dots, y_N)$ falling into the interval J, i.e.

$$A_N(J, \omega) = \sum_{n=1}^{N} \chi_J(y_n).$$

Definition 1.2 *By a partition P of K we mean a set of s finite sequences $(j = 1, \dots, s)$,*

$$a_j = \nu_0^{(j)} \leq \nu_1^{(j)} \leq \dots \leq \nu_{m_j}^{(j)} = b_j.$$

In connection with such a partition one defines for each j two operators by

$$\Delta_j f(x^{(1)},\dots,x^{(j-1)},\nu_i^{(j)},x^{(j+1)},\dots,x^{(s)}) = \\ f(x^{(1)},..,x^{(j-1)},\nu_{i+1}^{(j)},x^{(j+1)},..,x^{(s)}) - f(x^{(1)},..,x^{(j-1)},\nu_i^{(j)},x^{(j+1)},..,x^{(s)})$$

for $0 \leq i < m_j$ and

$$\Delta_j^* f(x^{(1)},\dots,x^{(j-1)},1,x^{(j+1)},\dots,x^{(s)}) = \\ f(x^{(1)},..,x^{(j-1)},\nu_{i+1}^{(j)},x^{(j+1)},..,x^{(s)}) - f(x^{(1)},..,x^{(j-1)},0,x^{(j+1)},..,x^{(s)}).$$

Definition 1.3 *For a function f on K, we set the variation in the sense of Vitali as follows*

$$V^{(l)}(f) = \sup_P \sum_{i_1=0}^{m_1-1} \cdots \sum_{i_l=0}^{m_l-1} \left| \Delta_{1,\dots,l} f(\nu_{i_1}^{(1)},\dots,\nu_{i_l}^{(l)}) \right|,$$

where the supremum is extended over all partitions P of K. The variation of f restricted to an interval $[\mathbf{a},\mathbf{b}]$ will be denoted $V_{[\mathbf{a},\mathbf{b}]}(f)$.

Finally let $1 \leq l \leq s$, $1 \leq i_1 < \cdots < i_l \leq s$ and $V^{(l)}(f; i_1,\dots,i_l)$ be the Vitali variation of the restriction of f to the l-dimensional face

$$\{(u_1,\dots,u_s) \in K : u_j = b_j \text{ for } j \neq i_1,\dots,i_l\}.$$

The variation in the sense of Hardy and Krause is defined by

$$V(f) = \sum_{l=1}^{s} \sum_{1\leq i_1<\cdots<i_l\leq s} V^{(l)}(f; i_1,\dots,i_l). \tag{4}$$

Naturally f is called of bounded variation on K, when $V(f) < \infty$.

Theorem 1.4 (Koksma-Hlawka Inequality) *Let f be a function of bounded variation (in the sense of Hardy and Krause) on K and $\omega = (y_1, y_2, \dots)$ a sequence on K. The QMC integration error can be bounded by*

$$\left| \int_K f(\mathbf{x}) dH(\mathbf{x}) - \frac{1}{N} \sum_{n=1}^{N} f(y_n) \right| \leq V(f) D_{N,H}(\omega). \tag{5}$$

A proof of this central theorem can be found e.g. in [2] for the uniform distribution, and in [7] for general distributions H (using a slight specialization to variation in the measure sense).

In [4], Sobol looked at Quasi-Monte Carlo integration of singular functions with respect to the uniform distribution. He gave conditions for its convergence involving the function as well as the sequence used. In particular, his theorem reads:

Theorem 1.5 (Sobol, [4]) *Let $i' \subseteq \{1, \ldots, s\}$ and $\mathcal{K}_{i'}$ be the boundary of $[0,1]^s$ where all coordinates $x^{(i)} = 1$ for $i \notin i'$. Let furthermore $c < c_N$, where $c_N = \min_{1 \le \mu \le N}\left(x_\mu^{(1)}, \ldots, x_\mu^{(s)}\right)$, and $G_{i'}$ the part of $\mathcal{K}_{i'}$, where $x^{(i_1)}, \ldots, x^{(i_j)} \ge c$. If for every i' the integral*

$$\int_{\mathcal{K}_{i'}} x^{(i_1)} \cdots x^{(i_j)} \left| f^{(i')}(x^{(i')}) \right| dx^{(i')} \tag{6}$$

converges and

$$D_N^{i'}(x_1, x_2, \ldots) \int_{G_{i'}(c)} \left| f^{(i')}(x^{(i')}) \right| dx^{(i')} = o(1) \ , \tag{7}$$

then $\lim_{N\to\infty} \frac{1}{N} \sum_{\mu=1}^{N} f(x_\mu) = \int_{[0,1]^s} f(x)dx$.

In this paper we will generalize this result to weighted integration, which means integration with respect to arbitrary densities $h(x)$. We will also investigate several ways to construct the sequences needed for QMC integration w.r.t. arbitrary densities and propose ways to overcome some problems occurring in conventional methods.

2 The one-dimensional case

Let us first consider the one-dimensional case. The main theorem of this section generalizes and combines the Koksma inequality (1.4) in one dimension with Sobol's convergence theorem [4] for QMC integration of singular integrands. Instead of the uniform distribution, we will assume an arbitrary distribution $H(x)$ on $[a, b]$ and show convergence of the QMC integration. The multi-dimensional case will be treated in a similar manner in the next section, so we present the simpler one-dimensional case here to give a clear picture of the ideas.

Definition 2.1 *For a sequence $\omega = (y_1, y_2, \ldots)$ let $c_N = \min_{1 \le n \le N} y_n$ be the smallest value of the first N elements of the sequence.*

Theorem 2.2 *Let $a \le c \le c_N$. If a sequence $\{y_i\}_{i\in\mathbb{N}}$ and a differentiable function $f(x)$ on $[a, b]$ with a singularity only at the left boundary satisfy the condition*

$$D_{N,H}(\omega) \int_c^b |f'(x)|\, dx = o(1) \tag{8}$$

as well as $c_N \to a$ for $N \to \infty$, then the QMC estimator $\frac{1}{N}\sum_{n=1}^{N} f(y_n)$ converges to the value of the improper integral of $f(x)$ on $[a, b]$:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(y_n) = \int_a^b f(x) dH(x) \tag{9}$$

Remark 2.3 *For non-differentiable functions the condition is similar using the variation $V_{[c_N,b)}(f)$ instead of the integral of the derivative. The multidimensional case will be formulated in such a more general manner.*

PROOF. To prove (9) we will approximate $\int_c^b f(x)dH(x)$ with $\frac{1}{N}\sum_{n=1}^{N} f(y_n)$ and show that the remaining terms tend to zero. Without loss of generality we can assume the sequence to be sorted, and we define y_0 and y_{N+1} so that $c = y_0 \leq y_1 \leq \cdots \leq y_N \leq y_{N+1} = b$.

First, we establish an identity similar to Lemma 5.1 of [2]:

$$\frac{1}{N}\sum_{n=1}^{N} f(y_n) - \int_c^b f(x)dH(x) = H(c)\cdot f(b) - \int_c^b \Big(\frac{A_N([c,x),\omega)}{N} - H([c,x))\Big) df(x) \tag{10}$$

The above identity can be proved by inserting terms, applying integration by parts and using the fact that $H(x)$ is a distribution function on $[a,b]$.

$$\begin{aligned}
&\frac{1}{N}\sum_{n=1}^{N} f(y_n) - \int_c^b f(x)dH(x) \\
&\quad = \frac{1}{N}\sum_{n=1}^{N} f(y_n) - (1-H(c))\, f(b) + [H(x)-H(c)]\, f(x)|_c^b - \int_c^b f(x)dH(x) \\
&\quad = f(y_{N+1}) - \sum_{n=0}^{N} \frac{n}{N}\left(f(y_{n+1}) - f(y_n)\right) \\
&\qquad - f(b) + H(c)f(b) + \int_c^b [H(x)-H(c)]\, df(x) \\
&\quad = -\sum_{n=0}^{N} \int_{y_n}^{y_{n+1}} \frac{n}{N} df(x) + H(c)f(b) + \int_c^b [H(x)-H(c)]\, df(x) \\
&\quad = H(c)f(b) - \int_c^b \Big(\frac{A_N([c,x),\omega)}{N} - \cdot H([c,x))\Big) df(x)
\end{aligned}$$

Once this is established, the convergence is obvious:

$$\begin{aligned}
&\left|\frac{1}{N}\sum_{n=1}^{N} f(y_n) - \int_a^b f(x)dH(x)\right| \\
&\qquad\qquad \leq \left|\int_a^c f(x)dH(x)\right| + |H(c)|\,|f(b)| + D_{N,H}(\omega)\int_c^b |f'(x)|\, dx
\end{aligned}$$

According to the convergence of the improper integral on the whole interval, the first and second terms tend to zero as $c \to a$, and the condition of the theorem ensures that the third term is $o(1)$ and thus also tends to zero. □

Remark 2.4 *The minimal element c_N of the one-dimensional Halton-sequence in basis 2 (which coincides with the Faure and Sobol sequences) is larger than $1/2N$. In arbitrary bases p, the smallest element among the first N can be bounded from below by $1/p^{\lfloor \log_p N \rfloor + 1}$.*

The main drawback, from a practical point of view, of the preceding theorem is the lack of sequences with low H-discrepancy. In practical issues one has to generate these sequences by transformation from uniform low discrepancy sequences. For distributions, where explicit inverse distribution functions are available, the transformation of the uniform distributed sequence $(x_1, x_2, \dots)$ by an inversion method $y_i = H^{-1}(x_i)$ is obvious. This transformation preserves the discrepancy, i.e

$$D_N (x_1, x_2, \dots) = D_{N,H} (y_1, y_2, \dots) . \tag{11}$$

Unfortunately for most distributions the inverse distribution function is not given explicitly and direct numerical methods for the inversion are often inefficient.

In [8], Hlawka and Mück propose a systematic method for constructing H-distributed sequences, which just uses the distribution function but not its inverse. We focus on the case $K = [0, 1]$.

Definition 2.5 *Let $\omega = (x_1, x_2, \dots)$ be a sequence in $[0, 1)$ with discrepancy $D_N(\omega)$ with regard to the uniform distribution. The sequence $\tilde{\omega} = (\tilde{y}_1, \tilde{y}_2, \dots)$ is defined to be the sequence consisting of the points*

$$\tilde{y}_k = \frac{1}{N} \sum_{r=1}^{N} \lfloor 1 + x_k - H(x_r) \rfloor = \frac{1}{N} \sum_{r=1}^{N} \chi_{[0,x_k]} (H(x_r)) . \tag{12}$$

Lemma 2.6 *Let the sequence $\tilde{\omega}$ be defined by Eq. (12) and $M = sup_{x \in [0,1]} h(x)$. Then the H-discrepancy of $\tilde{\omega}$ can be bounded by the following inequality*

$$D_{N,H}(\tilde{\omega}) \leq (1 + M) D_N(\omega).$$

All points constructed by the Hlawka-Mück method are of the form i/N, $(i = 0, \dots, N)$, in particular, some elements $\tilde{y}_k$ of the transformed sequence $\tilde{\omega}$ might assume a value of 0. Since this is the singularity of $f(x)$, according to Theorem 2.2 these sequences are not directly suited for unbounded problems.

Definition 2.7 *To overcome this problem, we define the sequence $\bar{\omega}$ for $i = 1, \dots, N$ as follows:*

$$\bar{y}_k = \begin{cases} \tilde{y}_k & \text{if } \tilde{y}_k \geq \frac{1}{N}, \\ \frac{1}{N} & \text{if } \tilde{y}_k = 0. \end{cases} \tag{13}$$

Theorem 2.8 *The H-discrepancy of $\bar{\omega}$ is bounded by*

$$D_{N,H}(\bar{\omega}) \leq (M+1)\left(D_N(\omega) + \frac{1}{N}\right).$$

PROOF. Let $(\bar{x}_1, \bar{x}_2, \dots)$ and $(\tilde{x}_1, \tilde{x}_2, \dots)$ be the sequences obtained by $\bar{x}_i = H(\bar{y}_i)$, resp. $\tilde{x}_i = H(\tilde{y}_i)$. By Eq. (11) it is sufficient to estimate the uniform discrepancy of $(\bar{x}_1, \bar{x}_2, \dots)$. For uniform discrepancies the following fact is well known (e.g. Niederreiter [3]): Let $(u_1, u_2, \dots)$ and $(v_1, v_2, \dots)$ be two sequences in $[0,1]$ with discrepancies D_1 and D_2, then $|D_1 - D_2| < \varepsilon$, whenever $\max_{1\leq i\leq N} |u_i - v_i| < \varepsilon$.

Now, the calculation

$$\begin{aligned} |x_k - \bar{x}_k| &\leq |x_k - \tilde{x}_k| + |\tilde{x}_k - \bar{x}_k| \\ &= \left|\int_{y_k}^{\tilde{y}_k} h(t)dt\right| + \left|\int_{\bar{y}_k}^{\tilde{y}_k} h(t)dt\right| \leq M\left(D_N(x_1, x_2, \dots) + \frac{1}{N}\right). \end{aligned}$$

completes the proof. □

Remark 2.9 *The discrepancy of uniform low discrepancy sequences is typically of the order $\mathcal{O}(\frac{\log N}{N})$ (resp. $\mathcal{O}(\frac{1}{N})$ for nets). Therefore the additional factor $(1/N)$ one inherits though the shift (13) does not affect the asymptotic behavior of the integration error.*

Remark 2.10 *Another method to avoid the inversion can be obtained by a suitable integral transformation. With the help of such a transformation, in Monte Carlo algorithms often referred to as importance sampling, it might even be possible to avoid some singularities.*

3 Multivariate singular integration

We will now look at arbitrary-dimensional integrals

$$\int_{[\mathbf{a},\mathbf{b}]} f(\mathbf{x})dH(\mathbf{x}), \tag{14}$$

where the integration domain is taken as a compact subinterval $[\mathbf{a}, \mathbf{b}]$ of $\mathbb{R}^s$.

Remark 3.1 *This is no restriction: If any of the dimensions is unbounded, we can first carry out the calculation on compact intervals and then take the limits to infinity as indicated in Section 1.*

The notations and operators used in the sequel are defined in Section 1. In addition we need the summation symbol $\sum^*$:

Definition 3.2 *Given an expression F depending on variables $x^{(r)}, \dots, x^{(s)}$ and a partition of $N_{r,s} = \{r, r+1, \dots, s\}$ into two subsets $L = \{x^{(l_1)}, \dots, x^{(l_p)}\}$ and $N_{r,s} \setminus L = \{x^{(l_{p+1})}, \dots, x^{(l_{s-r})}\}$, we use the notation*

$$F(L) = F\left(x^{(l_1)}, \dots, x^{(l_p)}; x^{(l_{p+1})}, \dots, x^{(l_{s-r})}\right).$$

The summation operator $\sum^*$ is defined as the sum over all elements of the set $\mathcal{P}_p = \{L \subseteq N_{r,s} : card(L) = p\}$, i.e.

$$\sum_{r,\dots,s;p}^{*} F = \sum_{L \in \mathcal{P}_p} F(L).$$

The integration by parts formula used in the proof of the previous section for differentiable one-dimensional functions can be generalized to arbitrary s-dimensional functions. It is commonly referred to as Abel's summation formula:

Lemma 3.3 (Abel's summation formula, e.g. [2]) *Let $\left(\eta_0^{(j)}, \eta_1^{(j)}, ..., \eta_{m_j}^{(j)}\right)$ and $\left(\xi_0^{(j)}, \xi_1^{(j)}, \dots, \xi_{m_j}^{(j)}\right)$ with $j = 1, \dots, s$ be two partitions of the interval $[\mathbf{a}, \mathbf{b}]$, and $f(\mathbf{x})$ and $g(\mathbf{x})$ two functions on $[\mathbf{a}, \mathbf{b}]$. Then*

$$\begin{aligned} &\sum_{i_1=0}^{m_1-1} \cdots \sum_{i_s=0}^{m_s-1} f\left(\xi_{i_1+1}^{(1)}, \dots, \xi_{i_s+1}^{(s)}\right) \Delta_{1,\dots,s} g\left(\eta_{i_1}^{(1)}, \dots, \eta_{i_s}^{(s)}\right) \\ &\quad = \sum_{p=0}^{s} (-1)^p \sum_{1,\dots,s;p}^{*} \Delta_{p+1,\dots,s}^{*} \sum_{i_1=0}^{m_1-1} \cdots \sum_{i_p=0}^{m_p-1} g\left(\eta_{i_1}^{(1)}, \dots, \eta_{i_p}^{(p)}, x^{(p+1)}, \dots, x^{(s)}\right) \\ &\qquad\qquad \times \Delta_{1,\dots,p} f\left(\xi_{i_1}^{(1)}, \dots, \xi_{i_p}^{(p)}, x^{(p+1)}, \dots, x^{(s)}\right). \end{aligned} \tag{15}$$

For a proof of this important equation we refer to the monograph [2] of Kuipers and Niederreiter.

Using this summation formula, we can now prove the convergence of the s-dimensional Quasi-Monte Carlo estimator to the value of the improper integral (14), even though the integrand can be singular on the whole left boundary of the integration area. Conventional methods usually apply the Koksma-Hlawka inequality (5). Here this inequality does not give an upper bound for the integration error, because the singularity causes the function to be of unbounded variation on $[\mathbf{a}, \mathbf{b}]$. We only require the function to be of bounded variation on every compact subinterval of $(\mathbf{a}, \mathbf{b}]$. The proof will follow the lines of the proof of the Koksma-Hlawka inequality given in [2], so for some parts of the proof we just refer to that book.

Theorem 3.4 (Convergence of the multidimensional QMC estimator) *Let $f(\mathbf{x})$ be a function on $[\mathbf{a},\mathbf{b}]$ with singularities only at the left boundary of the definition interval (i.e. $f(\mathbf{x}) \to \pm\infty$ only if $x^{(j)} \to a_j$ for at least one j), and let furthermore $c_{N,j} = \min_{1\le n\le N} y_n^{(j)}$ and $a_j < c_j \le c_{N,j}$. If the improper integral (14) exists in the sense of Section 1, and if*

$$D_{N,H}(\omega) \cdot V_{[\mathbf{c},\mathbf{b}]}(f) = o(1), \tag{16}$$

then the QMC estimator converges to the value of the improper integral:

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{y}_n) = \int_{[\mathbf{a},\mathbf{b}]} f(\mathbf{x}) dH(\mathbf{x}) \ . \tag{17}$$

PROOF. Like in the one-dimensional case we estimate the integration error on the interval $[\mathbf{c},\mathbf{b}]$, where the function $f(\mathbf{x})$ is regular for any choice of $\mathbf{c}$, and show that the remaining terms vanish as $\mathbf{c} \to \mathbf{a}$. Again similar to the proof of Theorem 2.2 we use a function

$$g(\mathbf{x}) = \frac{1}{N} A([\mathbf{c},\mathbf{x}), \omega) - H([\mathbf{c},\mathbf{x})) \tag{18}$$

for a given sequence $\omega = (y_n^{(j)})$, $1 \le n \le N$, $1 \le j \le s$. One has to notice that this function is merely the function used in the definition of the discrepancy, so that $\sup_{\mathbf{x}\in[\mathbf{c},\mathbf{b}]} |g(\mathbf{x})| \le D_{N,H}(\omega)$.

Using a double partition $c_j = \xi_0^{(j)} = \eta_0^{(j)} \le \xi_1^{(j)} < \eta_1^{(j)} \le \cdots < \eta_{m_j}^{(j)} = \xi_{m_j+1}^{(j)} = b_j$ $(j = 1, \ldots, s)$ of the interval $[\mathbf{c},\mathbf{b}]$ with the additional condition that the $\xi_1^{(1)}, \ldots, \xi_{m_j}^{(j)}$ contain at least our sequence ω, we now apply Lemma 3.3 to the function $g(\mathbf{x})$. As argued in [2], the left hand side of Eq. (15),

$$\sum_{i_1=0}^{m_1-1} \cdots \sum_{i_s=0}^{m_s-1} f\left(\xi_{i_1+1}^{(1)}, \ldots, \xi_{i_s+1}^{(s)}\right) \Delta_{1,\ldots s} g\left(\eta_{i_1}^{(1)}, \ldots \eta_{i_s}^{(s)}\right),$$

can be simplified to

$$\text{LHS} = \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{y}_n) - \sum_{i_1=0}^{m_1-1} \cdots \sum_{i_s=0}^{m_s-1} f\left(\xi_{i_1+1}^{(1)}, \ldots, \xi_{i_s+1}^{(s)}\right) \Delta_{1,\ldots s} H\left(\bigotimes_{l=1}^{s} \left[c_l, \eta_{i_l}^{(l)}\right)\right), \tag{19}$$

where $\otimes$ denotes the Cartesian product.

For the right hand side we notice that $g(\mathbf{x}) = 0$ if any of the $x^{(j)} = c_j$. Also, $g(\mathbf{b}) = 1 - H([\mathbf{c},\mathbf{b}))$, so that the summand of $p = 0$ can be simplified as

$$\Delta^*_{1,\ldots,s} g\left(x^{(1)}, \ldots x^{(s)}\right) f\left(x^{(1)}, \ldots, x^{(s)}\right) = g(\mathbf{b}) f(\mathbf{b}). \tag{20}$$

Similarly, for $1 \leq p \leq s$, only terms with $x^{(p+1)} = b_{p+1}, \ldots, x^{(s)} = b_s$ contribute (if any $x^{(p+j)} = c_{p+j}$, the function value of $g(\mathbf{x})$ vanishes):

$$\begin{aligned}|\mathrm{RHS}| \leq |g(\mathbf{b})f(\mathbf{b})| + \sum_{p=1}^{s} |(-1)^p| \sum_{1,\ldots,s;p}^{*} \sum_{i_1=0}^{m_1} \cdots \sum_{i_s=0}^{m_s} \left| g\left(\eta_{i_1}^{(1)}, \ldots, \eta_{i_p}^{(p)}\right)\right| \\ \times \left|\Delta_{1,\ldots,p} f\left(\xi_{i_1}^{(1)}, \ldots, \xi_{i_p}^{(p)}, b_{p+1}, \ldots, b_s\right)\right| \\ \leq |g(\mathbf{b})f(\mathbf{b})| + \sum_{p=1}^{s} \sum_{1,\ldots,s;p}^{*} D_{N,H}(\omega_{p+1,\ldots,s}) V^{(p)}(f(x^{(1)}, \ldots, x^{(p-1)}, b_{p+1}, \ldots, b_s).\end{aligned} \tag{21}$$

with $\omega_{p+1,\ldots,s}$ denoting the projection of the sequence ω on the upper boundary of $[\mathbf{a}, \mathbf{b}]$ so that the components $i_{p+1}, \ldots, i_s$ are set to $b^{(i_{p+1})}, \ldots, b^{(i_s)}$, and the discrepancy is computed on the face of $[\mathbf{a}, \mathbf{b}]$, in which $\omega_{p+1,\ldots,s}$ is contained.

Since the second term in Eq. (19) is nothing else but a Riemann-Stieltjes sum to the integral $\int_{[\mathbf{c},\mathbf{b}]} f(\mathbf{x}) dH(\mathbf{x})$, and the rest is independent of the double partition, we let the mesh size of the double partition tend to zero

$$\max_{1 \leq j \leq s} \max_{0 \leq i \leq m_j} (\eta_{i+1}^{(j)} - \eta_i^{(j)}) \to 0$$

to obtain the multidimensional version of Eq. (10):

$$\left| \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{y}_n) - \int_{[\mathbf{c},\mathbf{b}]} f(\mathbf{x}) dH(\mathbf{x}) \right| \leq |(1 - H([\mathbf{c}, \mathbf{b}))) f(\mathbf{b})| + |D_{N,H}(\omega)| \cdot \left| V_{[\mathbf{c},\mathbf{b}]}(f) \right| \tag{22}$$

The existence of the improper integral in the sense of Section 1 guarantees that

$$I_{\mathrm{rest}} := \left| \int_{[\mathbf{a},\mathbf{b}]} f(\mathbf{x}) dH(\mathbf{x}) - \int_{[\mathbf{c},\mathbf{b}]} f(\mathbf{x}) dH(\mathbf{x}) \right|$$

tends to zero as we let $\mathbf{c} \to \mathbf{a}$. Thus, we have

$$\begin{aligned}\left| \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{y}_n) - \int_{[\mathbf{a},\mathbf{b}]} f(\mathbf{x}) dH(\mathbf{x}) \right| \leq \left| \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{y}_n) - \int_{[\mathbf{c},\mathbf{b}]} f(\mathbf{x}) dH(\mathbf{x}) \right| + I_{\mathrm{rest}} \\ \leq |[1 - H([\mathbf{c}, \mathbf{b}))] f(\mathbf{b})| + D_{N,H}(\omega) \cdot V_{[\mathbf{c},\mathbf{b}]}(f) + I_{\mathrm{rest}} \,.\end{aligned} \tag{23}$$

For $N \to \infty$ and so $\mathbf{c} \to \mathbf{a}$, the first and third terms obviously tend to zero, while the conditions of the theorem guarantee this also for the second term. Thus the proof is finished. □

As in the one-dimensional case, one faces the problem of generating H-distributed sequences. Multidimensional versions for inversion methods are well known (e.g. Devroye [9]). Under weak, Lipschitz type conditions, Hlawka and Mück [10] showed the following bound for the H-discrepancy of sequences $\tilde{\omega}$ generated by multidimensional inversion methods:

$$D_{N,H}(\tilde{\omega}) \leq c\,(D_N(\omega))^{1/s}\,, \tag{24}$$

where ω denotes the original uniformly distributed sequence. Furthermore in [10] a multidimensional approach similar to Eq. (12) is given.

We again focus on distributions on $[0,1]^s$ and specialize our analysis to distributions with independent marginals, i.e. $H(\mathbf{x}) = \prod_{i=1}^{s} H_i(x^{(i)})$.

In this case one can transform each dimension separately by one-dimensional inversion methods and improve the bound (24) similar to the one-dimensional case to

$$D_{N,H}(\tilde{\omega}) = D_N(\omega). \tag{25}$$

Hlawka [11] suggested to apply the construction (12) to every dimension individually to avoid an inversion of $H_1, \ldots, H_s$ and gave a bound on the H-discrepancy of sequences $\bar{\omega}$ generated by this procedure:

$$D_{N,H}(\bar{\omega}) \leq (1 + 3sM) D_N(\omega),$$

where $M = \sup h(\mathbf{x})$.

Similar to one dimension, Hlawka's method might lead to sequences, which are not suited for unbounded integrands. Our final theorem shows a modification, which leads to QMC estimators for a wide range of functions. Before we can state it, we need to recall a lemma, which will be essential for the proof.

Lemma 3.5 (e.g. [8]) *Let $\Omega_1 = (u_1, \ldots, u_N)$ and $\Omega_2 = (v_1, \ldots, v_N)$ be two sequences in $[0,1]^s$. If the condition*

$$|u_i^{(j)} - v_i^{(j)}| \leq \varepsilon_j,$$

holds for all $1 \leq j \leq s$ and all $1 \leq i \leq N$, we get the following bound on the difference of the discrepancies

$$|D_N(\Omega_1) - D_N(\Omega_2)| \leq \prod_{j=1}^{s} (1 + 2\varepsilon_j) - 1. \tag{26}$$

Theorem 3.6 *Let H be a s-dimensional distribution with independent marginal distributions $H_1, \ldots, H_s$ and $M = \sup h(\mathbf{x}) < \infty$. Let furthermore $\omega = (x_1, x_2, \ldots)$ be a sequence with (uniform) discrepancy $D_N(\omega)$ and define the sequence $\tilde{\omega} = (\tilde{y}_1, \tilde{y}_2, \ldots)$ by*

$$\tilde{y}_i^{(j)} = \frac{1}{N} \sum_{n=1}^{N} \lfloor 1 + x_i^{(j)} - H_i(x_n^{(j)}) \rfloor,$$

for $j = 1, \dots, s$ and $n = 1, \dots, N$. Then the sequence $\bar{\omega}$

$$\bar{y}_k^{(j)} = \begin{cases} \tilde{y}_k^{(j)} & \text{if } \tilde{y}_k^{(j)} \geq \frac{1}{N}, \\ \frac{1}{N} & \text{if } \tilde{y}_k^{(j)} = 0 \end{cases} \tag{27}$$

has the following two properties:

$$D_{N,H}(\bar{\omega}) \leq (1 + 4M)^s D_N(\omega)$$

$$\min_{1 \leq j \leq s, 1 \leq i \leq N} \tilde{y}_i^{(j)} \geq \frac{1}{N}$$

PROOF. Let $\bar{x}_i^{(j)} = H_i^{-1}(\bar{y}_i^{(j)})$. Similar to Theorem 2.8 we get the inequality

$$|x_i^{(j)} - \bar{x}_i^{(j)}| \leq M \left(D_N(\omega) + \frac{1}{N} \right).$$

Using Lemma 3.5 we obtain

$$D_N(\bar{x}_1, \bar{x}_2, \dots) \leq D_N(\omega) - 1 + \left(1 + M \left(D_N(\omega) + \frac{1}{N} \right) \right)^s.$$

By Eq. (25) and the inequality $\frac{1}{N} \leq D_N(\omega) \leq 1$ it follows that

$$D_{N,H}(\bar{\omega}) \leq D_N(\omega) - 1 + \left(1 + M \left(D_N(\omega) + \frac{1}{N} \right) \right)^s \leq (1 + 4M)^s D_N(\omega). \qquad \square$$

4 Conclusion

In this article we successfully showed that Quasi-Monte Carlo methods can also be applied to improper s-dimensional integrals, where the integrand function $f(\mathbf{x})$ becomes singular at the integration boundary, assuming the function and the low-discrepancy sequence in use display certain properties as listed in Theorem 3.4. While similar conditions have long been known [4] for integration with respect to the uniform distribution (i.e. using uniformly distributed low-discrepancy sequences), we were able to generalize these results to integration with respect to arbitrary multidimensional densities, often called weighted integration.

In [8] and [11] Hlawka and Mück proposed a scheme to transform a uniformly distributed low-discrepancy to a low-discrepancy sequence with given density. However, the new sequence does not in general fulfill the conditions set forth in our convergence theorems and so cannot be used for the QMC integration of singular integrands. We were able to give a slight modification of the transformed sequence so that it does not loose its low discrepancy, but can be used for QMC weighted integration of singular integrands as our convergence theorems show.

We looked at one-dimensional densities and multidimensional densities which can be factored. Arbitrary multidimensional densities lead to the problem that even the inversion method does in general not preserve the discrepancy of a low-discrepancy sequence. Therefore the creation of low-H-discrepancy sequences still poses an open problem, in particular sequences suited for singular integrands.

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