AN IMPROVEMENT OF KOKSMA'S INEQUALITY AND CONVERGENCE RATES FOR THE QUASI-MONTE CARLO METHOD

MARTIN LIND

Abstract. When applying the quasi-Monte Carlo (QMC) method of numerical integration, Koksma’s inequality provides a basic estimate of the error in terms of the discrepancy of the used evaluation points and the total variation of the integrated function. We present an improvement of Koksma’s inequality that is also applicable for functions with infinite total variation. As a consequence, we derive error estimates for the QMC integration of functions of bounded $p$-variation.

1. Introduction

A natural way to numerically calculate the integral of a function $f : [0,1] \to \mathbb{R}$ is to take a sequence $x = \{x_n\}_{n=1}^{\infty} \subseteq [0,1]$ and use the approximation

\[ \int_{0}^{1} f(t)dt \approx \frac{1}{N} \sum_{n=1}^{N} f(x_n). \]

Introduce the error

\[ E_N(f; x) = \left| \frac{1}{N} \sum_{n=1}^{N} f(x_n) - \int_{0}^{1} f(t)dt \right|. \]

In the Monte Carlo method (MC), one takes $x$ in [1.1] to be a sequence of random numbers sampled uniformly from $[0,1]$. The expression inside the absolute value signs of [1.2] is then a random variable with expected value 0 and standard deviation of the order $1/\sqrt{N}$ as $N \to \infty$, see e.g. [1].

The quasi-Monte Carlo method (QMC) is based on instead taking a deterministic $x$ in [1.1] with "good spread" in $[0,1]$. This can lead to a better convergence rate of [1.2] than when taking random $x$. In fact, there exist deterministic $x \subseteq [0,1]$ such that the rate of decay of $E_N(f; x)$ is close to $1/N$ as $N \to \infty$ (see below).

Useful references for the theory and application of MC and QMC are e.g. [13, 7].

The aim of this note is to discuss error estimates for QMC on $[0,1]$. More specifically, we establish an improvement of the elegant Koksma’s inequality. Koksma’s inequality is the main general error estimate for QMC, we need some auxiliary notions in order to formulate it.
Let \( x = \{ x_n \}_{n=1}^\infty \subseteq [0, 1] \). The star discrepancy of the set \( \{ x_1, x_2, ..., x_N \} \) (i.e. set of the first \( N \) terms of \( x \)) is given by

\[
D_N^*(x) = \max_{0 \leq t \leq 1} \left| \frac{\sharp(\{ x_1, x_2, ..., x_N \} \cap [0, t])}{N} - t \right|
\]

(Here, \( \sharp(A) \) denotes the cardinality of the set \( A \).) In a sense, the quantity \( D_N^*(x) \) measures how much the distribution of the points of \( x \) deviates from the uniform distribution. One can show that for any \( x \) there holds \( D_N^*(x) \geq 1/(2N) \). On the other hand, there is a sequence \( x_C \subseteq [0, 1] \) (called the van der Corput sequence, see [1]) such that \( D_N^*(x_C) = O(\log(N)/N) \).

The total \( p \)-variation of a function \( f : [0, 1] \to \mathbb{R} \) is given by

\[
\text{Var}_p(f) = \sup \left( \sum_{j=1}^\infty |f(I_j)|^p \right)^{1/p}
\]

where the supremum is taken over all non-overlapping collections of intervals \( \{ I_j \}_{j=1}^\infty \) contained in \([0, 1]\) and \( f(I) = f(b) - f(a) \) if \( I = [a, b] \). If \( \text{Var}_p(f) < \infty \) we say that \( f \) has bounded \( p \)-variation (written \( f \in BV_p \)). Note that

\[
BV_1 \hookrightarrow BV_p \quad (1 < p < \infty).
\]

See [2] for a thorough discussion of bounded \( p \)-variation and applications.

Koksma’s inequality states that

\[
(1.3) \quad \mathcal{E}_N(f; x) \leq D_N^*(x) \text{Var}_1(f).
\]

In other words, the error of QMC is bounded by a product of two factors, the first measuring the "spread" of the sequence \( x \) and the second measuring the variation of the integrand \( f \). An immediate consequence of (1.3) is that we obtain the "almost optimal" error rate \( \mathcal{E}_N(f; x_C) = O(\log(N)/N) \) if \( f \in BV_1 \) and \( x_C \) is the previously mentioned van der Corput sequence.

A drawback of (1.3) is that it provides no error estimate in the case when \( f \not\in BV_1 \). For instance, we were originally interested in finding a general error estimates for \( f \in BV_p \) (\( p > 1 \)) (see Corollary 1.2 below). This led us to our main result (Theorem 1.1), which is a sharpening of (1.3) that is effective also when \( f \not\in BV_1 \). In fact, Theorem 1.1 provides an estimate of (1.2) for any function.

For this, we recall the notion of modulus of variation, first introduced in [3] (see also [2]). For any \( N \in \mathbb{N} \), we set

\[
\nu(f; N) = \sup \sum_{j=1}^N |f(I_j)|,
\]

where the supremum is taken over all non-overlapping collections of at most \( N \) sub-intervals of \([0, 1]\). An attractive feature of the modulus of variation is that it is finite for any bounded function. Of course, \( f \in BV_1 \) if and only if \( \nu(f; N) = O(1) \) as \( N \to \infty \) and the growth of \( \nu(f; N) \) then tells us how "badly" a function has unbounded 1-variation.

The next result is our main theorem.

**Theorem 1.1.** For any function \( f \) and \( N \in \mathbb{N} \) there holds

\[
(1.4) \quad \mathcal{E}_N(f; x) \leq 13D_N^*(x)\nu(f; N).
\]
The constant 13 in (1.3) is a consequence of our method of proof and certainly not optimal. However, the main point is that we can replace the total variation in (1.3) with a quantity that is finite for all functions. An immediate corollary of (1.4) is a Koksma-type inequality for $BV_p$ (which is not possible to derive from (1.3)).

**Corollary 1.2.** If $f \in BV_p$ $(1 \leq p < \infty)$, then

$$E_N(f; x) \leq 13N^{1-1/p}D_N^*(x)\operatorname{Var}_p(f).$$

In a sense the estimate (1.5) cannot be improved: there is a constant $c > 0$ such that for any $N$ we can find a sequence $x$ and a function $f$ with $\operatorname{Var}_p(f) = 1$ and

$$E_N(f; x) \geq cN^{1-1/p}D_N^*(x).$$

We shall also discuss error estimates for functions with some continuity properties. Our result here (Corollary 1.3) is known, see [5], but Theorem 1.1 allows us to derive it in a very simple way. Define the modulus of continuity of $f$ by

$$\omega(f; \delta) = \sup_{|x-y| \leq \delta} |f(x) - f(y)| \quad (0 \leq \delta \leq 1),$$

and let $\omega : [0, 1] \to [0, \infty)$ be a non-decreasing function with $\omega(0) = 0$, strictly concave and differentiable on $(0, 1)$. We denote by $H^\omega$ the class of functions such that

$$|f|_{H^\omega} = \sup_{0 < \delta \leq 1} \frac{\omega(f; \delta)}{\omega(\delta)} < \infty.$$

In particular, if $\omega(\delta) = \delta^\alpha$ $(0 < \alpha < 1)$, then $H^\omega$ is the space of $\alpha$-Hölder continuous functions.

**Corollary 1.3** (see e.g. [5], p. 146). If $f \in H^\omega$, then

$$E_N(f; x) \leq 13|f|_{H^\omega}N\omega\left(\frac{1}{N}\right)D_N^*(x).$$

Corollaries 1.2 and 1.3 follow from simple estimates of the quantity $\nu(f; N)$ (see Proposition 2.3 below).

## 2. Proofs

We first state a few results that we will use in the proof of Theorem 1.1.

**Lemma 2.1.** Let $M \in \mathbb{N}$ and $s_M$ be the continuous first-order spline interpolating $f$ at the knots $0 = x_0 < x_1 < \ldots < x_M = 1$. Then

$$\operatorname{Var}_1(s_M) \leq \nu(f; M).$$

**Proof.** Let $\{x_{n_k}\}$ be the subset of $\{x_n\}$ consisting of points of local extremum of $s_M$. It is easy to see that

$$\operatorname{Var}_1(s_M) = \sum_k |s_M(x_{n_{k+1}}) - s_M(x_{n_k})| = \sum_k |f(x_{i_{k+1}}) - f(x_{i_k})| \leq \nu(f; M),$$

where the last inequality holds since the sum extends over at most $M$ terms. \qed

**Lemma 2.2.** Let $f$ be a measurable function and $J \subseteq [0, 1]$ an interval. Then there exists $x_0 \in J$ such that

$$\int_J |f(t)| dt \leq 2|J||f(x_0)|.$$
Proof. Clearly we cannot have \(|f(x)| < (2|J|)^{-1} \int_J |f(t)| dt\) for all \(x \in J\), since then it would follow
\[
\int_J |f(x)| dx < \frac{1}{2} \int_J |f(t)| dt,
\]
which is of course a contradiction.

We now prove Theorem 1.1.

Proof of Theorem 1.1. Without loss of generality, we may assume that
\[x_1 < x_2 < ... < x_N.\]

Set \(x_0 = 0\) and \(x_{N+1} = 1\) and let \(s_N\) be the continuous first-order spline interpolating \(f\) at the knots \(x_0, x_1, ..., x_N, x_{N+1}\). Then
\[
\frac{1}{N} \sum_{n=1}^{N} f(x_n) - \int_0^1 f(t) dt = \frac{1}{N} \sum_{n=1}^{N} s_N(x_n) - \int_0^1 s_N(t) dt + \int_0^1 [s_N(t) - f(t)] dt
\]
Hence,
\[
\mathcal{E}_N(f; x) \leq \mathcal{E}_N(s_N, x) + \|f - s_N\|_{L^1(0,1)}
\]
By (1.3) and Lemma 2.2, we have
(2.1)
\[
\mathcal{E}_N(f; x) \leq D_N^*(x) \nu(f; N) + \|f - s_N\|_{L^1(0,1)}
\]
We shall estimate \(\|f - s_N\|_{L^1(0,1)}\). We have
\[
\|f - s_N\|_{L^1(0,1)} = \sum_{n=0}^{N} \int_{x_n}^{x_{n+1}} |f(t) - s_N(t)| dt
\]
By Lemma 2.2 there are \(y_n \in (x_n, x_{n+1})\) for \(n = 0, 1, ..., N\) such that
\[
\int_{x_n}^{x_{n+1}} |f(t) - s_N(t)| dt \leq 2(x_{n+1} - x_n) |f(y_n) - s_N(y_n)|.
\]
Thus,
(2.2)
\[
\|f - s_N\|_{L^1(0,1)} \leq 2\delta_N(x) \sum_{n=0}^{N} |f(y_n) - s_N(y_n)|,
\]
where \(\delta_N(x) = \max_{0 \leq n \leq N} (x_{n+1} - x_n)\). We shall first prove that
(2.3)
\[
\delta_N(x) \leq 4D_N^*(x).
\]
Indeed, the discrepancy of \(x\) is defined as
\[
D_N(x) = \sup_{J \subset [0,1]} \left| \frac{|J \cap \{x_1, x_2, ..., x_N\}|}{N} - |J| \right|.
\]
It is well-known (see [5], p. 91) that
\[
D_N(x) \geq \frac{1}{N} \quad \text{and} \quad D_N(x) \leq 2D_N^*(x).
\]
Note that if \(J_n = [x_n, x_{n+1})\) (\(0 \leq n \leq N\)) we have
\[
J_n \cap \{x_0, x_1, ..., x_{N+1}\} = \{x_n\}.
\]
Thus, for \(1 \leq n \leq N\) we have
\[
|J_n| = \left| \frac{1}{N} \sum_{j=0}^{N} \chi_{\{x_0, x_1, \ldots, x_N, x_{N+1}\}}(x) \right| - \frac{1}{N} |J_n| \\
\leq \frac{1}{N} + \left| \frac{1}{N} \sum_{j=1}^{N} \chi_{\{x_1, \ldots, x_N\}}(x) \right| - |J_n| \\
\leq \frac{1}{N} + D_N(x) \leq 2D_N(x) \\
\leq 4D_N^*(x).
\]
A similar inequality holds for \(J_0 = [x_0, x_1]\). This proves (2.3). Hence, by (2.2), we have
\[
\|f - s_N\|_{L^1(0,1)} \leq 4D_N^*(x) \sum_{n=0}^{N} |f(y_n) - s_N(y_n)|.
\]
Furthermore,
\[
|f(y_n) - s_N(y_n)| \leq |f(y_n) - f(x_n)| + |f(x_n) - s_N(y_n)| \\
= |f(y_n) - f(x_n)| + |s_N(x_n) - s_N(y_n)|
\]
and it follows that
\[
\sum_{n=0}^{N} |f(y_n) - s_N(y_n)| \leq \sum_{n=0}^{N} |f(y_n) - f(x_n)| + \sum_{n=0}^{N} |s_N(x_n) - s_N(y_n)| \\
\leq \nu(f; N+1) + \text{Var}_1(s_N) \\
\leq \nu(f; N+1) + \nu(f; N) \\
\leq 3\nu(f; N).
\]
Consequently,
\[
\|f - s_N\|_{L^1(0,1)} \leq 12D_N^*(x)\nu(f; N).
\]
and by (2.1) we obtain
\[
\mathcal{E}_N(f; x) \leq 13D_N^*(x)\nu(f; N).
\]

The next result proves the corollaries 1.2 and 1.3

**Proposition 2.3.** Let \(N \in \mathbb{N}\), then we have
\[
\nu(f; N) \leq N^{1-1/p} \text{Var}_p(f) \quad (1 \leq p < \infty),
\]
and
\[
\nu(f; N) \leq |f|_{H^{-N, \omega}} \left( \frac{1}{N} \right).
\]

**Proof.** The inequality (2.4) follows immediately from Hölder’s inequality. For (2.5), take \(N\) intervals \(\{I_j\}_{j=1}^{N}\), then clearly
\[
\sum_{j=1}^{N} |f(I_j)| \leq |f|_{H^{-N, \omega}} \sum_{j=1}^{N} \omega(|I_j|).
\]
Define

\[ M_\omega(N) = \max \left( \sum_{j=1}^{N} \omega(t_j) \right) \text{ subject to } \sum_{j=1}^{N} t_j = 1, \ t_j > 0. \]

Since \( \sum_{j=1}^{N} |I_j| \leq 1 \) and \( \omega \) is non-decreasing, we clearly have

\[ \nu(f; N) \leq |f|_{H^\omega} M_\omega(N). \]

To calculate \( M_\omega(N) \), we use Lagrange multipliers. The critical point \( (t_1, t_2, ..., t_N, \lambda) \) of the Lagrangian function solves

\[ \omega'(t_j) - \lambda = 0 \quad (1 \leq j \leq N) \quad \text{and} \quad \sum_{j=1}^{N} t_j - 1 = 0. \]

By the strict concavity of \( \omega \), the above system has the unique solution \( t_1 = t_2 = ... = t_N \). Hence, the maximum (2.6) is

\[ M_\omega(N) = N\omega \left( \frac{1}{N} \right). \]

\[ \square \]

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DEPARTMENT OF MATHEMATICS, KARLSTAD UNIVERSITY, UNIVERSITETSGATAN 2, 651 88 KARLSTAD, SWEDEN

E-mail address: martin.lind@kau.se