Discrepancy of sequences and error estimates for the quasi-Monte Carlo method

Diskrepansen hos talföljder och feluppskattningar för kvasi-Monte Carlo metoden

Niklas Vesterinen

Faculty of Health, Science and Technology
Mathematics, Bachelor Degree Project
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Supervisor: Martin Lind
Examiner: Niclas Bernhoff
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Abstract

We present the notions of *uniform distribution* and *discrepancy* of sequences contained in the unit interval, as well as an important application of discrepancy in *numerical integration* by way of the *quasi-Monte Carlo* method. Some fundamental (and other interesting) results with regards to these notions are presented, along with some detalied and instructive examples and comparisons (some of which not often provided by the literature). We go on to analytical and numerical investigations of the asymptotic behaviour of the discrepancy (in particular for the *van der Corput*-sequence), and for the *general error estimates* of the *quasi-Monte Carlo* method. Using the discoveries from these investigations, we give a conditional proof of *the van der Corput theorem.* Furthermore, we illustrate that by using *low discrepancy sequences* (such as the *vdC*-sequence), a rather fast convergence rate of the *quasi-Monte Carlo* method may still be achieved, even for situations in which the famous theoretical result, *the Koksma inequality*, has been rendered unusable.

Sammanfattning

Vi presenterar begreppen *likformig distribution* och *diskrepans* hos talföljder på enhetsintervallet, såväl som en viktig tillämpning av diskrepans inom numerisk integration via *kvasi-Monte Carlo* metoden. Några fundamentala (och andra intressanta) resultat presenteras med avseende på dessa begrepp, tillsammans med några detaljerade och instruktiva exempel och jämförelser (varav några sällan presenterade i litteraturen). Vi går vidare med analytiska och numeriska undersökningar av det asymptotiska beteendet hos diskrepansen (särskilt för *van der Corput*-följden), såväl som för den *allmänna feluppskattningen* hos *kvasi-Monte Carlo* metoden. Utifrån upptäckterna från dessa undersökningar ger vi ett villkorligt bevis av *van der Corput's sats*, samt illustrerar att man genom att använda *lågdiskrepanstalföljder* (som *van der Corput*-följden) fortfarande kan uppnå tämligen snabb konvergenshastighet för *kvasi-Monte Carlo* metoden. Detta även för situationer där de kända teoretiska resultatet, *Koksma's olikhet*, är oandvändbart.

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Introduction

Quantitative investigations of the *regularity of distribution* of mathematical objects (arithmetic, geometric or analytic) form a central part of mathematics. Questions concerning the distribution of the primes or the zeroes of the Riemann zeta function drive a large part of modern number theory. In analysis, it is known that the asymptotic behaviour of the distribution of eigenvalues to certain differential operators can be precisely described (e.g. Weyl's law). In approximation theory and numerical analysis, the distribution of nodes or quadrature points fundamentally influence the quality of approximation (this will be discussed in detail in Chapter 3).

In this thesis, we study the distribution properties of countable point sets contained in the unit interval $I := [0, 1]$. Already this simple setting leads to many interesting results, questions and applications.

In Chapter 1, we present the notion of *uniform distribution* (or equidistribution) of an infinite sequence of points contained in I. This concept goes back to Weyl and appeared naturally in Diophantine approximation. Weyl also proved a characterization of uniform distribution in terms of integrals. This result provides the theoretical foundation for the *quasi-Monte Carlo method* which we study in Chapter 3, and give a detailed proof. We also prove that a certain simple sequence is uniformly distributed. Such calculations are quite instructive but rarely presented in the literature.

In Chapter 2, we present the notion of *discrepancy* of a finite sequence of numbers contained in I. This is a quantity that, in a sense, measures the deviation of the sequence from being uniformly distributed.

The main contribution of Chapter 2 concerns a certain *low discrepancy sequence*. A sequence is said to have low discrepancy if the asymptotic behaviour of the discrepancy of the first N terms behaves like $\log_2(N)/N$. The standard example of a low discrepancy sequence is the *van der Corput sequence* (abbreviated here as *vdC-sequence*). The standard calculation of the discrepancy of the *vdC-sequence* (referred to here as the *"vdC-theorem"*) is elementary but somewhat opaque [1]. Attempting to find an alternative proof, we investigate numerically the discrepancy of certain subsets of the *vdC-sequence* and discover a phenomenon that appears to have been overlooked (it was not mentioned in e.g. the survey paper [5]). We formulate this as Conjecture 2.1. Assuming this conjecture, we present a conditional proof of the *vdC-theorem* that is, in our opinion, both natural and elegant (but of course also <u>*conditional*</u> as long as Conjecture 2.1 remains unproven).

In Chapter 3, we consider an important application of discrepancy in numerical integration. The so-called *quasi-Monte Carlo* method (QMC method) uses low discrepancy sequences as quadrature points. The general error estimate of the QMC method is contained in a very elegant result widely known as *the Koksma inequality*. This result is often formulated and proved in a very concise way using Riemann-Stieltjes integration [1]. In this thesis however, we give a detailed proof of the inequality inspired by the discussion in [2].

If one uses the elements of the *vdC-sequence* as quadrature points in the QMC method, then for any function with finite *total variation*, the *convergence rate* of the quadrature error is of the order $\log_2(N)/N$. This is a direct consequence of *the Koksma inequality* and the *vdC-theorem*. However, the condition for the integrand to have finite total variation is rather strong. We demonstrate with numerical simulations that even for functions with infinite total variation, the QMC method may converge. Furthermore, the convergence rate can be very close to the target rate $\log_2(N)/N$. More specifically, in our example formulated as Conjecture 3.1, the rate of convergence is faster than $1/N^\alpha$ for any $\alpha < 1$ (but not $\alpha = 1$).

The arguments presented in this thesis are both analytical and numerical. We provide the MATLAB codes for our implementations in an appendix at the end of the thesis.

1 Uniform distribution of sequences

To begin with it should be noted that here, and throughout the rest of this thesis, every finite (or infinite) point set generated by a sequence $(x_n)_{n=1}^{N}$ and represented by the notation $\{(x_n)_{n=1}^{N}\} := \{x_1, x_2, \ldots, x_n\}$, is to be interpreted as an *ordered multi-set* in which the elements can have a multiplicity > 1. Furthermore, the notation $|\mathcal{A}|$ will be used to denote the *cardinality* of such a *ordered multi-set* $\mathcal{A}$, which will be referred to simply as a *point set*.

1.1 Definition

Definition 1.1. *Let $(x_n)_{n=1}^{\infty} := (x_1, x_2, \ldots)$ be a sequence of real numbers such that $x_n \in [0,1]$ for all n, with $\{(x_n)_{n=1}^{N}\} := \{x_1, x_2, \ldots, x_n\}$ being the point set consisting of the first N terms of $(x_n)_{n=1}^{\infty}$. Then we define $(x_n)_{n=1}^{\infty}$ as* ***uniformly distributed*** *(abbrivated* ***u.d.****)* ***in*** *$[0,1]$ if*

$$\lim_{N\to\infty} \frac{\left|\{(x_n)_{n=1}^{N}\} \cap [\alpha,\beta]\right|}{N} = \beta - \alpha \tag{1.1}$$

holds for all intervals $[\alpha,\beta] \subseteq [0,1]$.

Thus, a sequence of real numbers in the unit interval $I := [0,1]$ is u.d. (in I) if the proportion of terms of that sequence which lies inside an arbitrary subinterval of I, approaches the length of that subinterval as the number of terms increase. We could therefore say that a finite point set generated by such a sequence becomes more and more *evenly distributed* in I as the number of elements in that point set is increased.

One can easily generalize this definition from I to any subinterval of $\mathbb{R}$ and for any sequence of real numbers in $\mathbb{R}$ (not necessarily contained in I). In this thesis however we will only be concerned with sequences contained in I, why the given definition will suffice. Sequences satisfying (1.1) will be referred to simply as being u.d. without explicitly mentioning the interval I in which this property holds.

1.2 Integral criterion

Let $\chi_{[\alpha,\beta]}$ denote the characteristic function of the interval $[\alpha,\beta] \subseteq I$, i.e., let

$$\underset{[\alpha,\beta]}{\chi}(x) := \begin{cases} 1 & \text{for } x \in [\alpha,\beta] \\ 0 & \text{for } x \notin [\alpha,\beta]. \end{cases} \tag{1.2}$$

Then $\sum_{n=1}^{N} \underset{[\alpha,\beta]}{\chi}(x_n) = \left|\{(x_n)_{n=1}^{N}\} \cap [\alpha,\beta]\right|$ equals the number of elements in the point set $\{(x_n)_{n=1}^N\}$ that lies in $[\alpha, \beta]$. Furthermore, we have that

$$\int_0^1 \underset{[\alpha,\beta]}{\chi}(t)\,\mathrm{d}t = \int_\alpha^\beta \mathrm{d}t + \int \underset{[0,1]\setminus[\alpha,\beta]}{0 \cdot \mathrm{d}t} = \beta - \alpha.$$

Thus, using the characteristic function, (1.1) can be equivalently expressed as

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \underset{[\alpha,\beta]}{\chi}(x_n) = \int_0^1 \underset{[\alpha,\beta]}{\chi}(t)\,\mathrm{d}t \tag{1.3}$$

This observation, together with the progressively more and more *evenly distributed* elements of a point set consisting of the first N terms of a u.d. sequence, can lead one to think of the following plausible consequence of *uniform distribution.* Namely that a sequence which is u.d. could be used to approximate (or obtain) the value of an integral over I, by arithmetically averaging the values of the integrand over only some finite number of points of that sequence. Because the Riemann integral over I is equivalent to the mean value of the integrand over I, which is exactly what is being approximated by the arithmetic mean of function values over *evenly distributed* points in I.

This intuition is made rigorous in the following fundamental *uniform distribution criterion.*

Theorem 1.1 (An integral criterion for u.d.). *For any sequence of real numbers* $(x_n)_{n=1}^\infty$ *contained in* I *the following two conditions are equivalent.*

(a) $(x_n)_{n=1}^\infty$ *is u.d.*

(b) For every continuous function $f : I \to \mathbb{R}$ *and real-valued sequence* $(x_n)_{n=1}^\infty$ *contained in* I*, the following equality holds:*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(x_n) = \int_0^1 f(t)\mathrm{d}t \tag{1.4}$$

Proof: Since (1.3) is equivalent to (1.1), and (1.4) is equivalent to (1.3) if f is instead taken to belong to the function space of characteristic functions of all subintervals of I. Therefore (a) $\iff$ (b)$'$ if (b)$'$ denotes this alteration of (b) to the case of $f \in \{\chi_J : J \subset I\}$.

Furthermore, any arbitrary step function $f : I \to \mathbb{R}$ is just a finite linear combination of characteristic functions over non-overlapping unions of subintervals of I.

Thus, for $f(x) := \sum_{i=0}^{m-1} c_i \underset{[d_i,d_{i+1}]}{\chi}(x_i)$ with $c_i \in \mathbb{R}$ and $0 = d_0 < d_1 < \ldots < d_m = 1$, we get due to the linearity of the sum and integral operators that

$$\begin{aligned}\lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N} f(x_n) &= \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\sum_{i=0}^{m-1} c_i \chi_{[d_i,d_{i+1}]}(x_n) = \lim_{N\to\infty}\frac{1}{N}\sum_{i=0}^{m-1} c_i \sum_{n=1}^{N}\chi_{[d_i,d_{i+1}]}(x_n)\\ &= \sum_{i=0}^{m-1} c_i\left(\lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\chi_{[d_i,d_{i+1}]}(x_n)\right) \overset{(1.3)}{=} \sum_{i=0}^{m-1} c_i \int_0^1 \chi_{[d_i,d_{i+1}]}(t)\,\mathrm{d}t\\ &= \int_0^1 \sum_{i=0}^{m-1} c_i\chi_{[d_i,d_{i+1}]}(t)\,\mathrm{d}t = \int_0^1 f(t)\mathrm{d}t\end{aligned}$$

Therefore, (a) $\Longrightarrow$ (b)$''$ if (b)$''$ denotes the alteration of (b) to any real-valued *step function* f defined on I.

To show that (b)$'' \Longrightarrow$ (b), assume that $f : I \to \mathbb{R}$ is continuous on I. Then the continuity of f implies that it is integrable on I. Thus, by the definition of the Darboux integral, given any fixed real number $\epsilon > 0$ there exists two step functions f_1 and f_2 for which $f_1(t) \leq f(t) \leq f_2(t)$ and $\int_0^1 \Big(f_2(t) - f_1(t)\Big)\mathrm{d}t \leq \epsilon$ holds for all $t \in I$. Using these inequalities, and letting $\varepsilon_N := \frac{1}{N}\sum_{n=1}^{N} f(x_n) - \int_0^1 f(t)\mathrm{d}t$, it follows that

$$\frac{1}{N}\sum_{n=1}^{N} f_1(x_n) - \int_0^1 f_1(t)\mathrm{d}t - \epsilon < \varepsilon_N < \frac{1}{N}\sum_{n=1}^{N} f_2(x_n) - \int_0^1 f_2(t)\mathrm{d}t + \epsilon,$$

which after taking the limit as $N \to \infty$ is reduced by (b)$''$ to

$$-\epsilon < \lim_{N\to\infty} \varepsilon_N < \epsilon.$$

Now, since ϵ can be chosen arbitrarily small, it follows from the *squeeze theorem* that $\lim_{N\to\infty} \varepsilon_N = 0$, so that (b)$'' \Longrightarrow$ (b) and hence that (a) $\Longrightarrow$ (b).

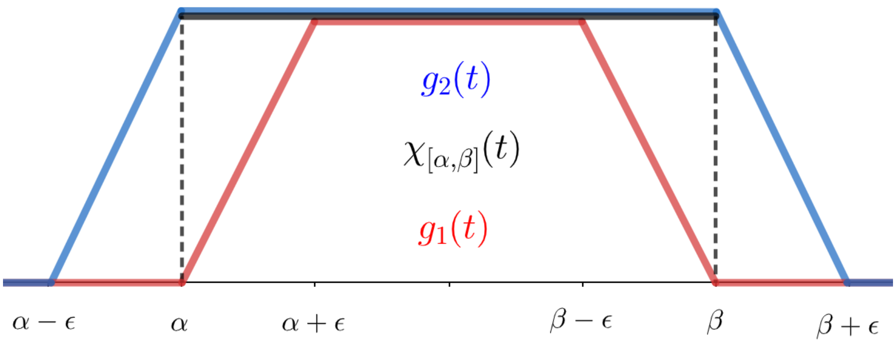
To show that (b) $\Longrightarrow$ (a), assume that (b) is true with $\alpha, \beta \in \mathbb{R}$ such that $0 \leq \alpha < \beta \leq 1$. Then for any fixed $\epsilon > 0$ there exists real numbers k, m_1, m_1', m_2 and m_2', all depending on ϵ, such that the two functions g_1 and g_2 defined by

$$g_1(t) := \begin{cases} 1 & \text{for } t \in [\alpha+\epsilon, \beta-\epsilon] \\ 0 & \text{for } t \in [0,\alpha] \cup [\beta, 1] \\ kt + m_1 & \text{for } t \in (\alpha, \alpha+\epsilon) \\ -kt + m_1' & \text{for } t \in (\beta-\epsilon, \beta) \end{cases} \qquad g_2(t) := \begin{cases} 1 & \text{for } t \in [\alpha, \beta] \\ 0 & \text{for } t \in [0,\alpha-\epsilon] \cup [\beta+\epsilon, 1] \\ kt + m_2 & \text{for } t \in (\alpha-\epsilon, \alpha) \\ -kt + m_2' & \text{for } t \in (\beta, \beta+\epsilon) \end{cases}$$

are continuous on I, and such that they satisfy $\int_0^1 \Big(g_2(t) - g_1(t)\Big)\mathrm{d}t \leq \epsilon$ for all $t \in I$.

It is also clear that $g_1(t) \leq \underset{[\alpha,\beta]}{\chi}(t) \leq g_2(t)$ holds for such values of k, m_1, m_1', m_2, m_2', and t, as shown in the Figure 1 below.

Figure 1:



Now, in a similar fashion as before, we can use these inequalities togehter with

$$\varepsilon_N := \frac{1}{N}\sum_{n=1}^{N} \underset{[\alpha,\beta]}{\chi}(x_n) - \int_0^1 \underset{[\alpha,\beta]}{\chi}(t)\,\mathrm{d}t = \frac{1}{N}\sum_{n=1}^{N} \underset{[\alpha,\beta]}{\chi}(x_n) - (\beta-\alpha),$$

to show that

$$\frac{1}{N}\sum_{n=1}^{N} g_1(x_n) - \int_0^1 g_1(t)\mathrm{d}t - \epsilon < \varepsilon_N < \frac{1}{N}\sum_{n=1}^{N} g_2(x_n) - \int_0^1 g_2(t)\mathrm{d}t + \epsilon$$

$$\implies \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N} g_1(x_n) - \int_0^1 g_1(t)\mathrm{d}t - \epsilon < \lim_{N\to\infty}\varepsilon_N < \lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N} g_2(x_n) - \int_0^1 g_2(t)\mathrm{d}t + \epsilon$$

$$\overset{(b)}{\implies} -\epsilon < \lim_{N\to\infty}\varepsilon_N < \epsilon \overset{\textit{squeeze theorem}}{\implies} \lim_{N\to\infty}\varepsilon_N = 0.$$

Hence $(x_n)_{n=1}^{\infty}$ satisfies (1.3) and therefore (b) $\implies$ (a) which completes the proof.

$\square$

1.3 Example

In this section, we provide an example of a sequence that is u.d.

Proposition 1.1. *Let* $(x_n)_{n=1}^{\infty} := \left(\frac{1}{2}, \frac{1}{3}, \frac{2}{3}, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, \frac{1}{5} \ldots\right)$, *then* $(x_n)_{n=1}^{\infty}$ *is u.d. in* I.

To prove this proposition we will use the following preliminary result.

Lemma 1.1. *If* $S_M := \{s_n = \frac{n}{M} : 1 \leq n \leq M-1\} = \{\frac{1}{M}, \frac{2}{M}, \ldots \frac{M-1}{M}\}$ *is a point-(multi)set for any positive integer* M, *and* $\alpha,\ \beta \in \mathbb{R}$ *such that* $0 \leq \alpha < \beta \leq 1$, *then*

$$\begin{aligned}\lim_{M\to\infty} \frac{\left|S_M \cap [\alpha,\beta]\right|}{M} &= \lim_{M\to\infty} \frac{\left|\{(s_n)_{n=1}^{M-1}\} \cap [\alpha,\beta]\right|}{M} \\ &= \lim_{M\to\infty} \left(\frac{1}{M-1} \sum_{n=1}^{M-1} \underset{[\alpha,\beta]}{\chi}(s_n)\right) = \beta - \alpha. \end{aligned} \tag{1.5}$$

Proof: Let $\Delta s = \Delta s(M) := s_{n+1} - s_n = \frac{n+1}{M} - \frac{n}{M} = \frac{1}{M}$ denote the constant difference between two consecutive elements in $S_M \subset I$. Since Δs is a strictly decreasing function of M, it follows that given large enough M one can find an element s_n arbitrarily close to any point in I. So that for any subinterval $[\alpha,\beta] \subseteq I$, the end points α and β can be enclosed by two, arbitraily close, consecutive elements in S_M.

To see this let $\epsilon > 0$ be any fixed but arbitrarily small real number. Then $\omega := \frac{1}{\epsilon}$ will be sufficiently large such that $M > \omega \implies \Delta s = \frac{1}{M} < \epsilon$. It is clear that under these conditions there exists natural numbers i_M and j_M, depending on M, such that $1 < i_M < j_M < M-1$ and for which that the following set of two-sided inequalities hold:

$$\begin{cases} s_{i_M} \leq \alpha < s_{i_M+1} = s_{i_M} + \Delta s < s_{i_M} + \epsilon \\ s_{j_M} \leq \beta < s_{j_M+1} = s_{j_M} + \Delta s < s_{j_M} + \epsilon \end{cases} \iff \begin{cases} \dfrac{i_M}{M} \leq \alpha < \dfrac{i_M+1}{M} < \dfrac{i_M}{M} + \epsilon \\ \dfrac{j_M}{M} \leq \beta < \dfrac{j_M+1}{M} < \dfrac{j_M}{M} + \epsilon \end{cases} \tag{1.6}$$

Because i_M and j_M represent the number of elements in S_M lying in the intervals $[0,\alpha]$ and $[0,\beta]$ respectively. It follows that $m_M := j_M - i_M$ is equal to the number of elements in S_M lying in the interval $[\alpha,\beta]$, so that

$$m_M = \sum_{n=1}^{M-1} \underset{[\alpha,\beta]}{\chi}(s_n) = \left|S_M \cap [\alpha,\beta]\right|.$$

Therefore, using (1.6), we can express the following bounds for the length of the interval $[\alpha, \beta]$:

$$\frac{m_M}{M} - \epsilon \leq \frac{m_M}{M} - \frac{1}{M} \leq \beta - \alpha \leq \frac{m_M}{M} + \frac{1}{M} \leq \frac{m_M}{M} + \epsilon.$$

Now, since $M > \omega \implies \dfrac{1}{M} < \epsilon$, it follows by the *squeeze theorem* that

$$\lim_{M\to\infty} \frac{m_M}{M} = \lim_{M\to\infty} \frac{m_M}{M-1} = \beta - \alpha. \tag{1.7}$$

Thus, (1.7) implies that (1.5) is true, which completes the proof of the lemma.

$\square$

Proof of Proposition 1.1: Let $[\alpha, \beta]$ be a fixed but arbitrary subinterval of I. We shall prove that

$$\lim_{N\to\infty} \frac{\left|\left\{(x_n)_{n=1}^{N}\right\} \cap [\alpha, \beta]\right|}{N} = \beta - \alpha.$$

To this end, let $N \in \mathbb{N}$ also be fixed but arbitrary, and note that there exists a unique $M = M(N) \in \mathbb{N}$ such that

$$\bigcup_{j=2}^{M-1} S_j \subseteq \left\{(x_n)_{n=1}^{N}\right\} \subset \bigcup_{j=2}^{M} S_j.$$

Now, from the above inclusions and the finite point set $\left\{(x_n)_{n=1}^{N}\right\}$, two things immediately follow. Firstly,

$$\frac{(M-2)(M-1)}{2} \leq N < \frac{M(M-1)}{2}. \tag{1.8}$$

Secondly,

$$\sum_{j=2}^{M-1} |S_j \cap [\alpha, \beta]| \leq \left|\left\{(x_n)_{n=1}^{N}\right\} \cap [\alpha, \beta]\right| \leq \sum_{j=2}^{M} |S_j \cap [\alpha, \beta]|. \tag{1.9}$$

From Lemma 1.1 it follows that $\left|S_j \cap [\alpha, \beta]\right| = (j-1)(\beta - \alpha) + \mathcal{O}(1)$, which if inserted in (1.9) gives us

$$\sum_{j=2}^{M-1} \Big((j-1)(\beta-\alpha)+\mathcal{O}(1)\Big) \leq \left|\left\{(x_n)_{n=1}^{N}\right\} \cap [\alpha, \beta]\right| \leq \sum_{j=2}^{M} \Big((j-1)(\beta-\alpha)+\mathcal{O}(1)\Big).$$

By calculating the sums in the two-sided inequality above, we obtain

$$\frac{(M-2)(M-1)}{2}(\beta-\alpha)+\mathcal{O}(M) \leq \left|\left\{(x_n)_{n=1}^N\right\} \cap [\alpha,\beta]\right| \leq \frac{M(M-1)}{2}(\beta-\alpha)+\mathcal{O}(M),$$

or more concisely

$$\frac{M^2}{2}(\beta-\alpha)+\mathcal{O}(M) \leq \left|\left\{(x_n)_{n=1}^N\right\} \cap [\alpha,\beta]\right| \leq \frac{M^2}{2}(\beta-\alpha)+\mathcal{O}(M). \tag{1.10}$$

Furthermore, from (1.8) we obtain

$$N = \frac{M^2}{2} + \mathcal{O}(M) \iff M^2 = 2N + \mathcal{O}(M). \tag{1.11}$$

From which, together with $N = \mathcal{O}(M^2)$, it follows that

$$\begin{aligned}\frac{M^2}{2N} + \mathcal{O}\left(\frac{M}{N}\right) &= \frac{2N+\mathcal{O}(M)}{2N} + \mathcal{O}\left(\frac{M}{N}\right)\\ &= 1 + \frac{\mathcal{O}(M)}{N} + \mathcal{O}\left(\frac{M}{N}\right) = 1 + \mathcal{O}\left(\frac{M}{N}\right)\\ &= 1 + \mathcal{O}\left(\frac{1}{M}\right).\end{aligned}$$

Thus, dividing (1.10) by N and using (1.11), we get

$$(\beta-\alpha)+\mathcal{O}\left(\frac{1}{M}\right) \leq \frac{\left|\left\{(x_n)_{n=1}^N\right\} \cap [\alpha,\beta]\right|}{N} \leq (\beta-\alpha)+\mathcal{O}\left(\frac{1}{M}\right). \tag{1.12}$$

Since the previous inequalities hold for any N, this completes the proof. $\square$

2 Discrepancy of sequences

Thus far, the notion of *uniform distribution* (u.d.) of a sequence has been defined, a fundamental integral criterion for it has been established, and an example of a specific u.d. sequence has been given. We focused in the previous chapter on the *qualitative* property of *uniform distribution* of a sequence. In this chapter however, we shall study the distribution of sequences in a *quantiative* manner. We will demonstrate that not all u.d. sequences are equally "well" distributed, and in fact, we will see that there exists a family of sequences (the so-called *van der Corput sequences*) which have the best distribution behaviour among all u.d. sequences. To do this we will want to be able to distinguish between sequences of varying distribution behaviours. This will also be of great importance when considering their usefulness in numerical integration (to be explored in Section 3). For this purpose we shall now introduce the notion of *discrepancy.*

2.1 Definitions

Definition 2.1. *Let $(x_n)_{n=1}^{\infty}$ be a sequence of real numbers contained in I with $\{(x_n)_{n=1}^{N}\} := \{x_1, x_2, \ldots, x_N\}$ denoting the point set consisting of the first N terms of $(x_n)_{n=1}^{\infty}$.*[1] *Then we define the* ***discrepancy*** *of $\big\{(x_n)_{n=1}^{N}\big\}$ as the real number*

$$D_N = D_N\big(\big\{(x_n)_{n=1}^{N}\big\}\big) := \sup_{0\le\alpha<\beta\le 1}\left|\frac{\big|\big\{(x_n)_{n=1}^{N}\big\}\cap[\alpha,\beta]\big|}{N} - (\beta-\alpha)\right|. \qquad (2.1)$$

One can easily form alternative definitions of discrepancy by simply restricting the combinations of intervals $[\alpha, \beta] \subseteq I$ over which the supremum is taken. We will define one particularly useful such restriction of D_N for intervals of the type $[0, \alpha] \subseteq I$, call it the *star discrepancy*, and denote it by $D_N^{\star}$.

Definition 2.2. *Let $(x_n)_{n=1}^{\infty}$ be a sequence of real numbers contained in I with $\big\{(x_n)_{n=1}^{N}\big\} := \{x_1, x_2, \ldots, x_N\}$ denoting the point set consisting of the first N terms of $(x_n)_{n=1}^{\infty}$. Then we define the* ***star discrepancy*** *of $\big\{(x_n)_{n=1}^{N}\big\}$ as the real number*

$$D_N^{\star} = D_N^{\star}\big(\big\{(x_n)_{n=1}^{N}\big\}\big) := \sup_{0<\alpha\le 1}\left|\frac{\big|\big\{(x_n)_{n=1}^{N}\big\}\cap[0,\alpha]\big|}{N} - \alpha\right|. \qquad (2.2)$$

With Definition 1.1 of *uniform distribution* in mind, looking at the above definitions one can see that the supremum is taken over the absolute difference of two

[1] A reminder that all point sets are to be interpreted as *ordered multi-sets*, i.e., ordered sets in which elements can have a multiplicity > 1.

terms. One representing the actual fraction of the first N elements of a point set that lie in a given subinterval of I. The other representing the expected fraction of elements that would lie in it, if that point set were to be ideally u.d.
A *geometric interpretation of discrepancy* is thus that it represents the *maximum deviation* of a finite point set from an *ideal uniform distribution* in I.

Whether the sequence is infinite, or finite and containing at least N terms, the discrepancy is to be regarded with respect to the first N terms of the sequence.

As is shown in [3], these discrepancies are related by $D_N^\star \le D_N \le 2D_N^\star$. Therefore, since the two discrepancies have the same asymptotic behaviour, no loss in generality will occur by using the simpler *star discrepancy* in proving assertions about the discrepancy of sequences contained in I.

2.2 Discrepancy of u.d. sequences

While it follows immediately from definitions 2.1 and 2.2 that these discrepancies are bounded by $0 \le D_N^\star \le D_N \le 1$. We begin this section by showing that the discrepancy of finite point sets generated by u.d. sequences asymptotically tends to zero as the number of elements increase.

Theorem 2.1. *Let $(x_n)_{n=1}^{\infty}$ be a sequence of real numbers contained in I, and let $[\alpha, \beta] \subseteq I$ be a non-degenerate interval. Then the following conditions are equivalent.*

(a) $(x_n)_{n=1}^{\infty}$ *is u.d.*

(b) $\lim_{N\to\infty} D_N\left(\{(x_n)_{n=1}^N\}\right) = 0.$

***Proof**:* We begin by defining a counting function Δ_N representing the number of terms of the finite sequence $(x_n)_{n=1}^N$ which lie in the interval $[\alpha, \beta]$.

$$\Delta_N = \Delta_N\left(\{(x_n)_{n=1}^N\}, [\alpha, \beta]\right) := \left|\{(x)_{n=1}^N\} \cap [\alpha, \beta]\right|.$$

Using this notation the conditions (a) and (b) can be equivalently restated as

(a) $\lim_{N\to\infty} \left(\dfrac{\Delta_N}{N} - (\beta - \alpha)\right) = 0 \qquad \forall \alpha, \beta \in \mathbb{R} : 0 \le \alpha < \beta \le 1.$

(b) $\limsup_{\substack{0\le\alpha<\beta\le 1\\ N\to\infty}} \left|\dfrac{\Delta_N}{N} - (\beta - \alpha)\right| = 0.$

Clearly (b) $\implies$ (a) since $\limsup|*|=0 \implies \lim(*)=0$.

To prove that (a) $\implies$ (b) it suffices to show that if $(x_n)_{n=1}^{\infty}$ is u.d. then given any fixed interval $J := [\alpha, \beta] \subseteq I$, the difference $\dfrac{\Delta_N(J)}{N} - l(J)$, in which $l(J)$ denotes the length of J, can be made arbitrarily close to zero.

To this end we define a sequence of intervals $I_k := \left[\frac{k}{m}, \frac{k+1}{m}\right]$ with $m, k \in \mathbb{N}$ such that $m \geq 2$ is "suitably" chosen and $k = 0, 1, \ldots, m-1$. So that, for all k, $I_k \subseteq I$ and $l(I_k) = \frac{1}{m}$. Then by (a) there exists a large enough positive integer N_0, depending on m, such that for all possible values of k and for $N \geq N_0$, the following two-sided inequality holds:

$$\frac{1}{m}\left(1-\frac{1}{m}\right) \leq \frac{\Delta_N(I_k)}{N} \leq \frac{1}{m}\left(1+\frac{1}{m}\right). \tag{2.3}$$

Now, with J being given, choose m large enough such that $l(I_k) = \frac{1}{m} < l(J)$. Then there exists integers $k_1, k_2 \in \{0, 1, \ldots, m-1\}$ such that

$$\frac{k_1}{m} \leq \alpha < \frac{k_1+1}{m} \quad \text{and} \quad \frac{k_2}{m} \leq \beta < \frac{k_2+1}{m},$$

and intervals J_1, J_2 defined by

$$J_1 := \left[\frac{k_1+1}{m}, \frac{k_2}{m}\right] \quad \text{and} \quad J_2 := \left[\frac{k_1}{m}, \frac{k_2+1}{m}\right],$$

from which it is clear that

$$J_1 \subset J \subset J_2. \tag{2.4}$$

With J_1 and J_2 being finite unions of non-overlapping intervals I_k, it follows that

$$l(J_1) = \left|\bigcup_{k_1+1}^{k_2} I_k\right| \text{ and } l(J_2) = \left|\bigcup_{k_1}^{k_2+1} I_k\right| = l(J_1)+l(I_{k_1})+l(I_{k_2+1}) = l(J_1)+\frac{2}{m}. \tag{2.5}$$

From (2.4) and (2.5) it also follows that

$$l(J) - l(J_1) < \frac{2}{m} \text{ and } l(J_2) - l(J) < \frac{2}{m}. \tag{2.6}$$

Therefore, one can create lower and upper bounds for $\dfrac{\Delta_N(J)}{N} - l(J)$, depending only on the chosen value of m, as follows:

Using (2.4) in (2.3), we get

$$l(J_1)\left(1-\frac{1}{m}\right) \le \frac{\Delta_N(J_1)}{N} \le \frac{\Delta_N(J)}{N} \le \frac{\Delta_N(J_2)}{N} \le l(J_2)\left(1+\frac{1}{m}\right)$$

from which, using (2.6), we get

$$\left(l(J)-\frac{2}{m}\right)\left(1-\frac{1}{m}\right) \le \frac{\Delta_N(J)}{N} \le \left(l(J)+\frac{2}{m}\right)\left(1+\frac{1}{m}\right)$$

$$\iff l(J)-\frac{l(J)}{m}-\frac{2}{m}+\frac{2}{m^2} \le \frac{\Delta_N(J)}{N} \le l(J)+\frac{l(J)}{m}+\frac{2}{m}+\frac{2}{m^2}.$$

Furthermore, since $l(J) \le 1$, it follows that

$$\frac{2}{m^2}-\frac{3}{m} \le \frac{\Delta_N(J)}{N}-l(J) \le \frac{2}{m^2}+\frac{3}{m}.$$

Thus, the bounds for $\dfrac{\Delta_N(J)}{N}-l(J)$ can be made arbitrarily close to zero by choosing a large enough value m, which completes the proof. □

2.2.1 Convergence rates

With Theorem 2.1 established, one would naturally be interested in the convergence rate of the discrepancy for a given finite point set generated by a u.d. sequence. Let us therefore study the rate of convergence of the *star discrepancy* for finite point sets generated by the sequence $(x_n)_{n=1}^{\infty} = \{\frac{1}{2}, \frac{1}{3}, \frac{2}{3}, \frac{1}{4}, \ldots\}$, which was shown to be u.d. in Proposition 1.1.

Proposition 2.1. *If* $(x_n)_{n=1}^{\infty} := \{\frac{1}{2}, \frac{1}{3}, \frac{2}{3}, \frac{1}{4}, \ldots\}$, *then* $D_N^*\left(\{(x_n)_{n=1}^{N}\}\right) = \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$.

Proof: Using the results from Proposition 1.1, it follows that the M that solves (1.8) will be the integer part of the positive solution to $\frac{(M-1)(M-2)}{2} = N$, from which we get that

$$\frac{1}{2}+\sqrt{\frac{1}{4}+2N} \le M < \frac{3}{2}+\sqrt{\frac{1}{4}+2N} \implies M \ge C_1\sqrt{N} \quad \text{for some } C_1 > 0. \tag{2.7}$$

From (1.12) we have, by the definition of the 'big $\mathcal{O}$'-formalism, that there exist a constant $C_2 > 0$ such that

$$-\frac{C_2}{M} \le \frac{|\{(x_n)_{n=1}^{N}\} \cap [0,\alpha]|}{N} - \alpha \le \frac{C_2}{M},$$

holds for all $N \geq 1$ and $\alpha \in (0,1]$.

Hence

$$D_N^*\left(\{(x_n)_{n=1}^N\}\right) \overset{(2.2)}{:=} \sup_{0<\alpha\leq 1}\left|\frac{\left|\{(x)_{n=1}^N\} \cap [0,\alpha]\right|}{N} - \alpha\right| \leq \frac{C_2}{M},$$

and since $M \geq C_1\sqrt{N}$, it follows that

$$D_N^*\left(\{(x_n)_{n=1}^N\}\right) = \mathcal{O}\left(\tfrac{1}{\sqrt{N}}\right). \tag{2.8}$$

□

For the purpose of a later investigation we will now state, but not prove, a result often called the *triangle inequality for the discrepancy.* This result provides a sometimes very useful way to obtain an upper bound for the discrepancy of point sets that can be decomposed into smaller point sets for which the discrepancies have known, or easily calculated, useable upper bounds.

Proposition 2.2 (The triangle inequality for the discrepancy)**.** *Let $S \subset I$ be a finite point set with N elements that is decomposable into k subsets with the i:th subset S_i having N_i elements, such that $S = \bigcup_{i=1}^{k} S_i$ and $N = \sum_{i=1}^{k} N_i$. Then*

$$ND_N(S) \leq \sum_{i=1}^{k} N_i D_{N_i}(S_i) \quad \textit{and} \quad ND_N^\star(S) \leq \sum_{i=1}^{k} N_i D_{N_i}^\star(S_i) \tag{2.9}$$

Proof: For a proof the reader is referred to [1]. □

This result can be used to obtain the convergence rate (2.8) (shown above) in an alternative way. In Proposition 2.1, we have that $\left\{(x_n)_{n=1}^N\right\} = \bigcup_{j=2}^{M-1} S_j \cup S_R$ where $S_R \subset S_M$ can be thought of as a *remainder set.* A case in which $S_R = S_M$ would just be the same as $S_R = \varnothing$, i.e., $\left\{(x_n)_{n=1}^N\right\} = \bigcup_{j=2}^{M} S_j$. It follows therefore that the number of terms in S_R is bounded by $|S_R| \leq |S_M| - 1 = M - 2$. Furthermore, it is an immediate consequence of Lemma 1.1 that

$$\frac{\left|S_M \cap [0,\alpha]\right|}{M-1} - \alpha \leq \frac{C}{M-1} \quad \forall \alpha \in (0,1] \text{ and some } C > 0, \tag{2.10}$$

from which we get that

$$D^{\star}_{M-1}(S_M) = \mathcal{O}\left(\tfrac{1}{M-1}\right).$$

Using these results in the *triangle inequality* (2.9), together with the trivial bounds $0 \le D^{\star}_N \le D_N \le 1$ for the discrepancy of any point set, we get the following chain of inequalities:

$$\begin{aligned}
ND^{\star}_N\left(\{(x_n)_{n=1}^N\}\right) &\le \sum_{j=2}^{M-1}\Big((j-1)D^{\star}_{j-1}(S_j)\Big) + |S_R|D^{\star}_{|S_R|}(S_R) \\
&\le \sum_{j=2}^{M-1}\left((j-1)\frac{\overline{C}}{j-1}\right) + |S_R|\cdot 1 \le (\overline{C}+1)(M-2) \\
&\overset{(2.7)}{\le} (\overline{C}+1)\left(\sqrt{\frac{1}{4}+2N}-\frac{1}{2}\right), \quad (\overline{C}\in\mathbb{R}).
\end{aligned}$$

Which after division by N yields

$$\begin{aligned}
D^{\star}_N\left(\{(x_n)_{n=1}^N\}\right) &\le (\overline{C}+1)\left(\sqrt{\frac{1}{4N^2}+\frac{2}{N}}-\frac{1}{2N}\right) \\
&\le \frac{C}{\sqrt{N}},
\end{aligned}$$

from which we again obtain that $D^{\star}_N(\{(x_n)_{n=1}^N\}) = \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$.

2.3 The van der Corput sequence

We shall now introduce a u.d. sequence with particularly good distribution behavior and, as we shall se in Chapter 3, some ideal qualities for applications.
First discovered in 1935 by Dutch mathematician *J.G. van der Corput* (1890-1975), the so-called *van der Corput sequences* are, as mentioned in [1], likely still the lowest discrepancy sequences over I to be discovered.

Definition 2.3 (van der Corput sequences)**.** *Let $n \ge 1$ be an integer with base-b representation $n = \sum_{i=0}^{m-1} n_i b^i$, where $0 \le n_i < b$ is the i-th digit in this base-b expansion. Then the n-th term in the b-ary* ***van der Corput sequence*** *is given by $\omega(n) := \sum_{i=0}^{m-1} n_i b^{-(i+1)}$. So that the (infinite) b-ary* ***van der Corput sequence*** *$(x_n^{vdC})_{n=1}^{\infty}$ is generated by $x_n^{vdC} = \omega(n)$ for all $n \in \mathbb{Z} : n \ge 1$.*

In this thesis we will only be studying and applying the *binary van der Corput sequence*, which from now on will be referred to simply as the *vdC-sequence*.

We shall describe the *vdC-sequence* as being composed of building blocks $\mathcal{S}_j$, with the first four "*vdC-blocks*" indicated below.

$$\left\{\left(x_n^{vdC}\right)_{n=1}^{\infty}\right\} := \left\{x_n^{vdC} = \omega(n) : n \geq 1\right\} \tag{2.11}$$
$$= \left\{\underbrace{\frac{1}{2}}_{\mathcal{S}_1}, \underbrace{\frac{1}{4}, \frac{3}{4}}_{\mathcal{S}_2}, \underbrace{\frac{1}{8}, \frac{5}{8}, \frac{3}{8}, \frac{7}{8}}_{\mathcal{S}_3}, \underbrace{\frac{1}{16}, \frac{9}{16}, \frac{5}{16}, \frac{13}{16}, \frac{3}{16}, \frac{11}{16}, \frac{7}{16}, \frac{15}{16}}_{\mathcal{S}_4} \ldots\right\}.$$

In general, the M-th *vdC-block* consists of the elements $\mathcal{S}_M = \left\{\dfrac{2^i - 1}{2^M} : 1 \leq i \leq 2^M - 1\right\}$, but in the characteristic *vdC-order* as shown above for the first four *vdC-blocks*, and will be described in general below. In the finite case with N terms we get in general, (as we did previously with $(x_n)_{n=1}^{N}$ from Proposition 1.1 and 2.1) the inclusion of a *remainder block* $\mathcal{S}_R \subset \mathcal{S}_M$, bounded by $|\mathcal{S}_R| \leq |\mathcal{S}_M| - 1$, so that

$$\left\{\left(x_n^{vdC}\right)_{n=1}^{N}\right\} = \bigcup_{j=1}^{M-1} \mathcal{S}_j \cup \mathcal{S}_R.$$

There is a simple procedure for finding the correct ordering of the elements in each *vdC-block*, which does not require the use of $\omega(n)$ from Definition 2.3. Consider first that the M-th *vdC-block* $\mathcal{S}_M$ consists of 2^{M-1} elements, ranging from the 2^{M-1}-th to the $(2^M - 1)$-th term in the *vdC-sequence*. To find the correct ordering of these elements in $\mathcal{S}_M$, simply express the number $n \in \left\{2^{M-1}, 2^{M-1} + 1, \ldots, 2^M - 1\right\}$ representing the n-th term in the *vdC-sequence*, in binary form. Then rewriting it in reverse order as a binary decimal produces the n-th term in the *vdC-sequence*. This procedure is easily repeated for each term in each *vdC-block* as exemplified for $\mathcal{S}_4$ in Table 1.

n (base 10)	n (binary)	$n\left(\substack{\text{Reverse}\\\text{binary decimals}}\right)$	$\left(x_n^{vdC}\right)$(base 10)
8	1000	.0001	1/16
9	1001	.1001	9/16
10	1010	.0101	5/16
11	1011	.1101	13/16
12	1100	.0011	3/16
13	1101	.1011	11/16
14	1110	.0111	7/16
15	1111	.1111	15/16

Table 1: Procedure for finding the correct order of the elements in *vdC-block* $\mathcal{S}_4$.

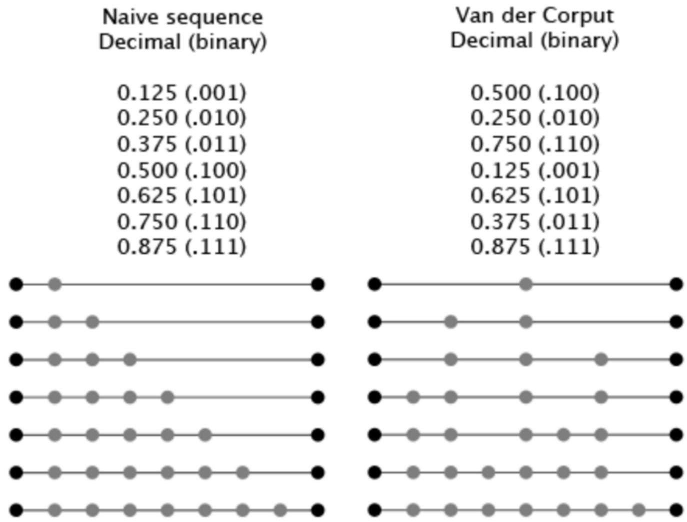
Some interesting properties of the *vdC-sequence* are now apparent. For starters, unlike the point sets generated by $(x_n)_{n=1}^N$ (from Proposition 1.1 and 2.1), no element in $\left\{\left(x_n^{vdC}\right)_{n=1}^N\right\} \subset I$ has a multiplicity higher than one (for any $N \in \mathbb{R}$). Also, if one chooses N such that $\mathcal{S}_R = \varnothing$, i.e., so that

$$\left\{\left(x_n^{vdC}\right)_{n=1}^N\right\} = \bigcup_{j=1}^{M} \mathcal{S}_j,$$

and rearranges the elements in an increasing order, then (from (2.11) above and Figure 2 below) it is clear that the elements in $\left\{\left(x_n^{vdC}\right)_{n=1}^N\right\}$ are *evenly distributed* with a distance of $\frac{1}{2^M}$ between any adjacent elements.

However, perhaps the most interesting property is the actual ordering of the terms itself. It is not diffcult to construct a finite sequence for which the distance between adjacent elements in the corresponding point set is a constant. For example, consider the *"naive"* sequence that generates the point set $\left\{(x_n^{naive})_{n=1}^N\right\} := \left\{x_n = \frac{n}{N} : 1 \leq n < N\right\}$, which shares this property with $\left\{\left(x_n^{vdC}\right)_{n=1}^N\right\}$. If again N is chosen such that $\mathcal{S}_R = \varnothing$, then both point sets are equally *evenly distributed* in I. However their distribution behaviours are quite different as the number of elements is increased (now allowing for $\mathcal{S}_R \neq \varnothing$) as is illustrated in Figure 2 for $N \in \{1, 2, \ldots, 7\}$.

Figure 2: Comparing the *"naive"* sequence and *vdC-sequence* [6].



From this simple comparison it is apparent that subsets of $\left\{\left(x_n^{vdC}\right)_{n=1}^{N}\right\}$ will in general be better (more evenly) distributed in I than subsets of $\left\{\left(x_n^{naive}\right)_{n=1}^{N}\right\}$. This is one of the main properties which makes the *vdC-sequence* the superior of the two for certain applications (to be explored in Chapter 3).

Another one would be that if one needs to increase the number N and get a few more terms of the sequence. Then, in the case of the *vdC-sequence*, one can just add these to the N terms already calculated, whereas for the "naive" sequence one would have to start all over for each new N.

We continue with the main result in this chapter. This result was first proven by J.G. van der Corput himself, and we shall refer to it here as the *van der Corput theorem.*

Theorem 2.2 (The van der Corput theorem)**.** *The star discrepancy of the vdC-sequence satisfies*

$$D_N^{\star}\left(\left\{\left(x_n^{vdC}\right)_{n=1}^{N}\right\}\right) = \mathcal{O}\left(\frac{\log_2(N+1)}{N}\right). \tag{2.12}$$

A "standard proof" of the above theorem can be found in [1]. In our opinion however, the arguments presented there, although elementary, are not so transparent, which led us to try to find a new and more instructive proof. In this process we discovered a rather interesting property regarding the discrepancy of subsets of *vdC-blocks*, formulated as Conjecture 2.1 below. Assuming this conjecture, we shall give a conditional proof of Theorem 2.2.

Conjecture 2.1. *Let $\mathcal{S}_M(j) := \{s_n : 1 \le n \le j \le 2^{M-1}\}$ be the point set consisting of the first j elements of vdC-block $\mathcal{S}_M$ (in which the elements appear in the correct vdC-order). Then we have*

$$Y(M) := \max_{1\le j\le 2^{M-1}} jD_j^\star\big(\mathcal{S}_M(j)\big) = \frac{M}{3} + \epsilon_M, \tag{2.13}$$

where $\epsilon_M \to 0$ as $M \to \infty$.

We shall present a numerical justification of Conjecture 2.1. To this end we first introduce the following identity pertaining to the calculation of the *star discrepancy*. A result interesting in its own right.

Let $N \in \mathbb{N}$ be fixed and consider a finite point set $S = \{s_n : 1 \le n \le N\}$. Furhtermore, let $s_1^* \le s_2^* \le \ldots \le s_N^*$ be the elements of S rearranged in a non-decreasing order (note that $D_N^\star$ does not depend on the order of the elements). We then have the following identity for the *star discrepancy* of S,

$$D_N^\star(S) = \frac{1}{2N} + \max_{1\le n\le N}\left|s_n^* - \frac{2n-1}{2N}\right|. \tag{2.14}$$

We refer the reader to [1] for a proof.

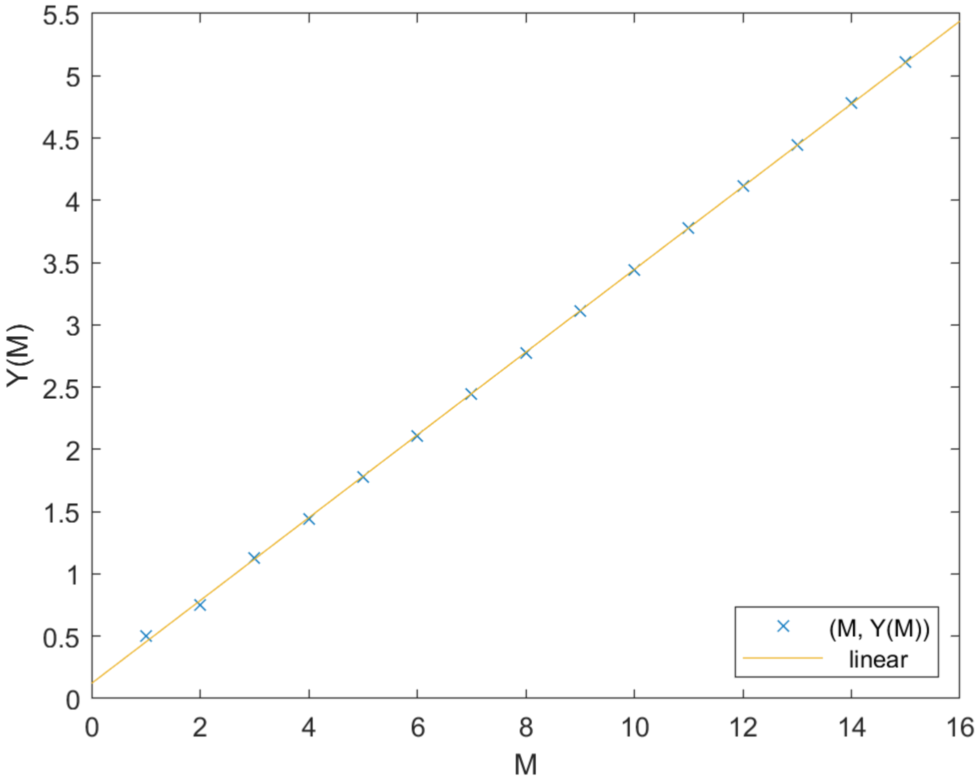
It follows directly from (2.14) that

$$Y(M) = \max_{1\le j\le 2^{M-1}}\left(\frac{1}{2} + j\max_{1\le n\le j}\left|s_n^* - \frac{2n-1}{2j}\right|\right) \tag{2.15}$$

where s_n^* $(1 \le n \le j)$ are the first j terms of the M-th *vdC-block*, but rearranged in increasing order.

We used (2.15) to write a program in the numerical computing software *MATLAB* that calculates $Y(M)$ for any M (see Appendix A for the code). The results are displayed in Figure 3 below, showing a plot of $Y(M)$ against M and the linear regression line of $(M, Y(M))$ (which was calculated using *MATLAB's basic fitting* tool).

Figure 3: Plot of $(M, (Y(M))$ including its linear regression line.



Clearly this result is very consistent with Conjecture 2.1.

Now, assuming the validity of Conjecture 2.1, we can give a conditional proof of Theorem 2.2.

Conditional proof of Theorem 2.2: Let us begin with the special case when $\mathcal{S}_R = \varnothing$, which will occur whenever the number of terms N is exactly equal to the sum of some number of M *complete vdC-blocks*. That is, when

$$N = \sum_{j=1}^{M} |\mathcal{S}_j| = \sum_{k=1}^{M} 2^{k-1} = 2^M - 1 \iff M = \log_2(N+1) \in \mathbb{Z}. \tag{2.16}$$

Thus, the corresponding *vdC-point set* $\left\{ \left(x_n^{vdC} \right)_{n=1}^{N} \right\} = \bigcup_{j=1}^{M} \mathcal{S}_j$ is composed of the union of the M *complete vdC-blocks*.

Now, the difference between any two adjacent terms in *vdC-block* $\mathcal{S}_M$ equals $\frac{2}{M}$ (a strictly decreasing function of M). Then by the exact same argument as was used to prove Lemma 1.1 from Chapter 1, it follows that the *vdC-block* $\mathcal{S}_M$ also satisfies (2.10), from which we get that

$$D^{\star}_{2^{M-1}}(\mathcal{S}_M) = \mathcal{O}\left(\tfrac{1}{2^{M-1}}\right).$$

Therefore, using this result in the *triangle inequality* (2.9) we get

$$ND^{\star}_N\left(\left\{\left(x^{vdC}_n\right)_{n=1}^N\right\}\right) \le \sum_{j=1}^{M} 2^{j-1} D^{\star}_{2^{j-1}}(\mathcal{S}_j) \le \sum_{j=1}^{M} 2^{j-1}\frac{C}{2^{j-1}} = CM \quad (C \in \mathbb{R}),$$

and after division by N we get

$$\begin{aligned} D^{\star}_N\left(\left\{\left(x^{vdC}_n\right)_{n=1}^N\right\}\right) &= \frac{CM}{N} \overset{(2.16)}{=} C\cdot\frac{\log_2(N+1)}{N} \\ &= \mathcal{O}\left(\frac{\log_2(N+1)}{N}\right). \end{aligned}$$

This proves the theorem for the special case when N is given by (2.16) (in which case $\mathcal{S}_R = \varnothing$).

In the general case however, we have $\left\{\left(x^{vdC}_n\right)_{n=1}^N\right\} = \bigcup_{j=1}^{M-1}\mathcal{S}_j \cup \mathcal{S}_R$, and are faced with the possibility of $\mathcal{S}_R \neq \varnothing$. So that a direct application of the *triangle inequality* (2.9) as above yields

$$\begin{aligned} ND^{\star}_N\left(\left\{\left(x^{vdC}_n\right)_{n=1}^N\right\}\right) &\le \sum_{j=1}^{M-1} 2^{j-1} D^{\star}_{2^{j-1}}(\mathcal{S}_j) + |\mathcal{S}_R| D^{\star}_{|\mathcal{S}_R|}(\mathcal{S}_R) \\ &\le C_1(M-1) + |\mathcal{S}_R| D^{\star}_{|\mathcal{S}_R|}(\mathcal{S}_R), \end{aligned} \tag{2.17}$$

where the problem remains to find a suitable upper bound for the term with the *remainder block*. The trivial bounds $0 \le D^{\star}_N \le D_N \le 1$ will no longer suffice because all we can say about $|\mathcal{S}_R|$ alone is that it satisfies $0 \le |\mathcal{S}_R| \le 2^M - 2$, an upper bound far greater then the upper bound $C_1(M-1)$ of the "main contributor" in (2.17).

However, it follows from Conjecture 2.1 that

$$|\mathcal{S}_R| D^{\star}_{|\mathcal{S}_R|}(\mathcal{S}_R) \le \max_{1\le j\le 2^M-1} jD^{\star}_j\big(\mathcal{S}_M(j)\big) =: Y(M) = \frac{M}{3} + \epsilon_M.$$

For our purposes this is a very nice upper bound indeed, since when inserted into (2.17) we get

$$
\begin{aligned}
ND_N^\star\left(\left\{\left(x_n^{vdC}\right)_{n=1}^N\right\}\right) &\le C_1(M-1) + |\mathcal{S}_R| D^\star_{|\mathcal{S}_R|}(\mathcal{S}_R) \\
&\le C_1(M-1) + \frac{M}{3} + \epsilon_M = \left(C_1 + \frac{1}{3}\right) M + \epsilon_M - C_1 \\
&\le CM \quad \text{(for some } C > 0). \qquad (2.18)
\end{aligned}
$$

Now, in the general case we get the following relation between the total number of elements N and the number M of the final *vdC-block* (in which the last element x_N^{vdC} lies).

$$
\begin{aligned}
\sum_{j=1}^{M-1} |\mathcal{S}_j| \le N < \sum_{j=1}^{M} |\mathcal{S}_j| &\iff 2^{M-1} - 1 \le N < 2^M - 1 \\
&\iff 2^{M-1} \le N + 1 < 2^M \\
&\iff M - 1 \le \log_2(N+1) < M \\
&\implies \log_2(N+1) < M \le \log_2(N+1) + 1 \qquad (2.19)
\end{aligned}
$$

Finally, dividing (2.18) by N and using (2.19) we get

$$
D_N^\star\left(\left\{\left(x_n^{vdC}\right)_{n=1}^N\right\}\right) \le \frac{CM}{N} \le C \cdot \frac{\log_2(N+1)+1}{N} = \mathcal{O}\left(\frac{\log_2(N+1)}{N}\right)
$$

which completes the conditional proof of Theorem 2.2. □

Remark 2.3. We have previously alluded to the fact that the *vdC-sequence*, in a sense, has the smallest discrepancy of all sequences contained in I. Indeed, there is a celebrated result of Schmidt (see [1]) which states that given *any* infinite sequence $(x_n)_{n=1}^\infty$, there is a constant $c > 0$ and a set of natural numbers $N_1 < N_2 < N_3 < \ldots$ such that

$$
D_{N_j}^\star\left(\left\{(x_n)_{n=1}^{N_j}\right\}\right) \ge c \cdot \frac{\log_2(N_j)}{N_j} \quad (j = 1, 2, \ldots).
$$

In other words, we cannot expect $D_N^\star$ to converge to 0 any faster than $\dfrac{\log_2(N)}{N}$, and this rate is attained for the *vdC-sequence*.

3 Numerical integration & error estimates

In this chapter we will demonstrate how one can put the results from the previous two chapters to use in numerical integration. More precisely, why and how *low discrepancy sequences*, in particular the *vdC-sequence* from Section 2.3, can be used to approximate integrals over I for a suitable class of functions.
This will be done using the *quasi-Monte Carlo method* (abbrivated *QMC method*) which will be introduced first. Thereafter we will show an important theoretical result: the *Koksma inequality*, which gives an upper bound to the error in our integral approximation. Then, after an illustrative example, we will conclude this chapter (and thesis) with the presentation of our main result. Namely, how usable upper bounds for the approximation error can be achieved even for situations when the *Koksma inequality* does not yield a usable result, given that a sequence with low enough discrepancy is used in the approximation.

3.1 The numerical algorithm & error function

Let $f : I \to \mathbb{R}$ be a Riemann integrable function on I. Say that we want to know the value of $\mathcal{I} := \int_0^1 f(t)\mathrm{d}t$, and that we will approximate this integral with the numerical algorithm $Q_N := \frac{1}{N}\sum_{n=1}^{N} f(x_n)$, consisting of the average of f evaluated over a set of points $x_n \in \mathcal{P}_N := \{(x_n)_{n=1}^N\} \subset I$. I.e., that we will use the approximation

$$\mathcal{I} := \int_0^1 f(t)\mathrm{d}t \approx Q_N := \frac{1}{N}\sum_{n=1}^{N} f(x_n) \quad (x_n \in \mathcal{P}_N). \tag{3.1}$$

Naturally, we will be interested in the error in this approximation.

Definition 3.1 (The error function)**.** *Let $f : I \to \mathbb{R}$ be a given Riemann integrable function on I. Then for any point set $\mathcal{P}_N$, and corresponding numerical algorithm Q_N, we define the* ***error function*** *ε_N as*

$$\begin{aligned}\varepsilon_N = \varepsilon(f, \mathcal{P}_N) &:= \left|\int_0^1 f(x)\mathrm{d}x - \frac{1}{N}\sum_{n=1}^{N} f(x_n)\right| \quad (x_n \in \mathcal{P}_N) \\ &= \left|\mathcal{I} - Q_N\right|.\end{aligned} \tag{3.2}$$

The magnitude of ε_N will of course depend on both the point set $\mathcal{P}_N$ and the function f. Since f is to be given, we are left with the problem of choosing $\mathcal{P}_N$ so as to make $\varepsilon_N \geq 0$ as small as desired. We would therefore like to be able to assess the quality of some given $\mathcal{P}_N$, as well as being able to find a $\mathcal{P}_N$ of particularly high quality. Next we will present two ways to deal with this problem.

3.1.1 The Monte Carlo (MC) method

Let $X_1, X_2, ..., X_N$ be finite sequence of independent random variables that are uniformly distributed on I.[2] The idea of the MC method is to take each point $x_n \in \mathcal{P}_N$ to be a sample from X_n for $n = 1, 2, \ldots, N$. Then the approximation Q_N is simply an observation of the random variable $\mathcal{R}_N := \dfrac{1}{N}\displaystyle\sum_{n=1}^{N} f(X_n)$.

Standard calculations for the expectation and variance then show that

$$E(\mathcal{R}_N) = \mathcal{I} \quad \text{and} \quad V(\mathcal{R}_N) = \frac{\sigma^2}{N},$$

where $\sigma^2 = V(f(X_n))$ (which is finite if f is continuous).

By the *law of large numbers*, we get that $\mathcal{R}_N \to \mathcal{I}$ in probability. Furthermore, by the *central limit theorem*, we also have that

$$\lim_{N\to\infty} P\left(|\mathcal{I} - \mathcal{R}_N| \geq \frac{\alpha\sigma}{\sqrt{N}}\right) = 1 - \Phi(\alpha),$$

where $\Phi(t)$ is the distribution function of the standard gaussian. Hence, for any $\epsilon > 0$ there is a $C > 0$ and an $M \in \mathbb{N}$ such that for all $N \geq M$ we have

$$P\left(|\mathcal{I} - \mathcal{R}_N| \geq \frac{C\sigma}{\sqrt{N}}\right) < \epsilon.$$

In other words, for any $\epsilon > 0$, there is an $M \in \mathbb{N}$ such that for $N \geq M$ we have

$$\varepsilon_N = |\mathcal{I} - \mathcal{R}_N| = \mathcal{O}\left(\frac{1}{\sqrt{N}}\right) \quad \text{with probability} > 1 - \epsilon. \tag{3.3}$$

This is a sort of *probabilistic convergence rate* of the *MC* method.

One immediate drawback of the MC method is that any convergence statement about ε_N is probabilistic (as above), thus adding an inherent uncertainty to the value of ε_N. Another drawback is that when the points of $\mathcal{P}_N$ are sampled randomly, they are not necessarily very evenly spread out in I (see Figure 4 on page 26). As a means counter these drawbacks, we now introduce the so-called *quasi-Monte Carlo method*.

[2] In this context, "uniformly distributed" refers to the probabilistic concept, not u.d. as defined in Chapter 1.

3.1.2 The quasi-Monte Carlo (QMC) method

The idea of the *QMC method* is that each $x_n \in \mathcal{P}_N$ is chosen deterministically, using the first N terms of a *low discrepancy sequence*. Then the problem of assessing the quality of a given $\mathcal{P}_N$, or finding a $\mathcal{P}_N$ with particularly high quality, are dealt with through the use of discrepancy, and the readily available sequences of particularly low discrepancy (such as the *vdC-sequence*).

Intuitively one can expect an *evenly distributed* $\mathcal{P}_N$ is neccessary for Q_N to be a good approximation for $\mathcal{I}$, with higher number of elements N yielding better approximations. It is also intuitive that the more *"varying"* the function f, the higher the requirement on $\mathcal{P}_N$ in terms of its (*even*)distribution and cardinality.

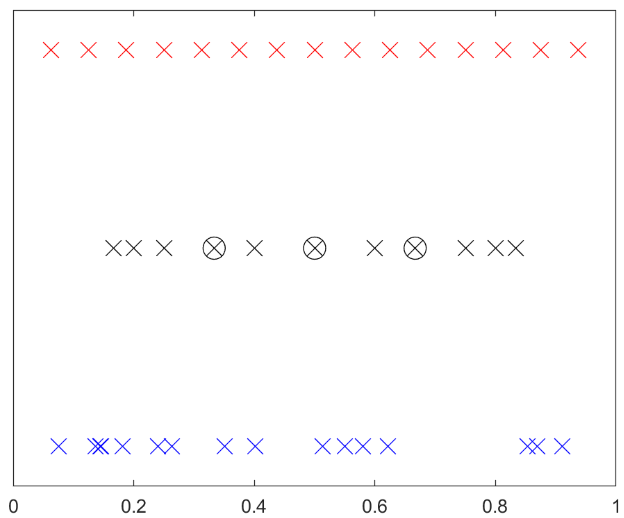
In Section 3.3, we shall investigate the convergence and convergence rates for ε_N using the *QMC method*. This investigation will lead to what we consider to be our main result of this thesis. Before venturing any deeper into that inquiry however, we begin by observing the following convergence result highlighting our intuition.

Proposition 3.1. *If* $(x_n)_{n=1}^{\infty}$ *u.d. and* $f \in C[0,1]$ *then* $\lim_{N\to\infty} \varepsilon_N = 0$.

Proof: This result follows immediately from the *integral criterion for u.d.* presented here as Theorem 1.1. □

The distribution comparison in Figure 4 (below) highlights the advantage of the *QMC method* over the MC method, and the advantage of the *vdC-sequence* over other u.d. sequences, for application in numerical integration over I (see also Figure 2 on page 18).

Figure 4: Distribution comparison



In Figure 4 we can see the difference in the distribution of the first fifteen terms of the *vdC-sequence* (top, red), the sequence $\left(\frac{1}{2}, \frac{1}{3}, \frac{2}{3}, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, \frac{1}{5} \ldots\right)$ from Proposition 1.1, page 7, and Proposition 2.1, page 13 (middle, black). And fifteen samples of a uniformly distributed random variable (bottom, blue). Each cross represent a term in the sequence (or sample) with a circle around a cross denoting a multiplicity greater then one.

3.2 Error bounds: The Koksma inequality

In this section we will present one of the most significant results in this thesis. A truly quite beautiful inequality, due to (another) Dutch mathematician *Jurjen Ferdinand Koksma* (1904-1964), which gives an upper bound to the *error function* ε_N when using the *QMC method*. What makes this result so elegant is that ε_N is bounded by the product of two terms. One that quanitifies how *"nice"* the integrand f is, and another which quantifies how *"well" distributed* $\mathcal{P}_N$ (used in the *QMC-algorithm* Q_N) is. Before we introduce the next theorem, we first define the *total variation* of a certain class of functions.

Definition 3.2. *Let $f : I \to \mathbb{R}$ be differentiable on I, such that $f' : (0, 1) \to \mathbb{R}$ is Riemann-integrable on I. Then the* ***total variation*** *of f, denoted by $TV(f)$, is defined as* $TV(f) := \displaystyle\int_0^1 |f'(t)|\mathrm{d}t.$

Theorem 3.1 (The Koksma inequality)**.** *Let $f : I \to \mathbb{R}$ be differentiable on I, such that $f' : (0,1) \to \mathbb{R}$ is Riemann-integrable on I. Let $Q_N := \frac{1}{N}\sum_{n=1}^{N} f(x_n)$ using $\mathcal{P}_N := \{(x_n)_{n=1}^N\}$ as quadrature points, with $(x_n)_{n=1}^N$ being any finite sequence of real numbers in I. Then the approximation error ε_N given by Definition 3.1 has the following upper bound:*

$$\varepsilon_N \leq \int_0^1 |f'(x)|\mathrm{d}x \cdot D_N^\star\big(\mathcal{P}_N\big) = TV(f) \cdot D_N^\star\big(\mathcal{P}_N\big) \tag{3.4}$$

Our proof of Theorem 3.1 will be an extended, more detailed, and (in our opinion) more instructive presentation of the arguments given for a similar result in [2].

Proof: Using the fact that

$$f(1) - \int_x^1 f'(y)\mathrm{d}y = f(1) - \big(f(1) - f(x)\big) = f(x)$$

we can subsitute $f(x)$ in (3.2) for $f(1) - \int_x^1 f'(y)\mathrm{d}y$ and thus obtain

$$\begin{aligned}
\varepsilon_N &= \left|\int_0^1 \left(f(1) - \int_x^1 f'(y)\mathrm{d}y\right)\mathrm{d}x - \frac{1}{N}\sum_{n=1}^{N}\int_0^1 \left(f(1) - \int_{x_n}^1 f'(y)\mathrm{d}y\right)\mathrm{d}x\right| \\
&= \left|\int_0^1 f(1)\mathrm{d}y - \int_0^1\int_x^1 f'(y)\mathrm{d}y\mathrm{d}x - \frac{1}{N}\sum_{n=1}^{N} f(1) + \frac{1}{N}\sum_{n=1}^{N}\int_{x_n}^1 f'(y)\mathrm{d}y\right| \\
&= \left|\frac{1}{N}\sum_{n=1}^{N}\int_{x_n}^1 f'(y)\mathrm{d}y - \int_0^1\int_x^1 f'(y)\mathrm{d}y\mathrm{d}x\right|
\end{aligned} \tag{3.5}$$

due to the integral and sum of $f(1)$ canceling each other in the last step.

Now, using the characteristic function and linearity of the sum and integral operators, the first term in (3.5) can be rewritten in the following manner.

$$\frac{1}{N}\sum_{n=1}^{N}\int_{x_n}^1 f'(y)\mathrm{d}y = \frac{1}{N}\sum_{n=1}^{N}\int_0^1 \underset{[x_n,1]}{\chi}(y)\, f'(y)\mathrm{d}y = \int_0^1 \frac{1}{N}\sum_{n=1}^{N} \underset{[x_n,1]}{\chi}(y)\, f'(y)\mathrm{d}y \tag{3.6}$$

Furthermore, the second term in (3.5) can be interpreted as an iteration of the double integral $\iint\limits_{\mathcal{D}} f'(y)\mathrm{d}A$, over the domain $\mathcal{D} := \{(x, y) \in \mathbb{R} : 0 \leq x \leq y \leq 1\}$. Which of course can be re-iterated as

$$\int_0^1\int_0^y f'(y)\mathrm{d}x\mathrm{d}y = \int_0^1 yf'(y)\mathrm{d}y. \tag{3.7}$$

Therefore, by substituting the first and second terms of (3.5) with (3.6) and (3.7) respectively, we obtain

$$\begin{aligned}
\varepsilon_N &= \left| \frac{1}{N} \sum_{n=1}^{N} \int_{x_n}^{1} f'(y) \mathrm{d}y - \int_0^1 \int_x^1 f'(y) \mathrm{d}y \mathrm{d}x \right| \\
&= \left| \int_0^1 f'(y) \left(\frac{1}{N} \sum_{n=1}^{N} \underset{[x_n,1]}{\chi}(y) - y \right) \mathrm{d}y \right|. \qquad (3.8)
\end{aligned}$$

Now, with $\mathcal{D}$ giving the relationship between x and y, it is easily verified from the definition of the characteristic function (1.2) that $\underset{[x_n,1]}{\chi}(y) = \underset{[0,y]}{\chi}(x_n)$.

Thus, the second factor in (3.8) can be equivalently expressed as

$$\begin{aligned}
\frac{1}{N} \sum_{n=1}^{N} \underset{[x_n,1]}{\chi}(y) - y &= \frac{1}{N} \sum_{n=1}^{N} \underset{[0,y]}{\chi}(x_n) - y = \frac{\left| \mathcal{P}_N \cap [0,y] \right|}{N} - y \\
&= \frac{\Delta_N \big(\mathcal{P}_N, [0,y] \big)}{N} - y = \frac{\Delta_N(y)}{N} - y \qquad (3.9)
\end{aligned}$$

Where $\Delta_N(y)$ is the previously defined "counting function" from Theorem 2.1.

Clearly (3.9) is the same expression that appears in Definition 2.2 of the *star discrepancy* of the finite point set $\mathcal{P}_N$.

With this in mind, we can substitute (3.9) in (3.8) to obtain

$$\begin{aligned}
\varepsilon_N &= \left| \int_0^1 f'(y) \left(\frac{1}{N} \sum_{n=1}^{N} \underset{[x_n,1]}{\chi}(y) - y \right) \mathrm{d}y \right| = \left| \int_0^1 f'(y) \left(\frac{\Delta_N(y)}{N} - y \right) \mathrm{d}y \right| \\
&\leq \int_0^1 \left| f'(y) \right| \left| \frac{\Delta_N(y)}{N} - y \right| \mathrm{d}y \leq \int_0^1 \left| f'(y) \right| \sup_{0<y\leq 1} \left(\left| \frac{\Delta_N(y)}{N} - y \right| \right) \mathrm{d}y \\
&= TV(f) \cdot D_N^{\star} \left(\mathcal{P}_N \right),
\end{aligned}$$

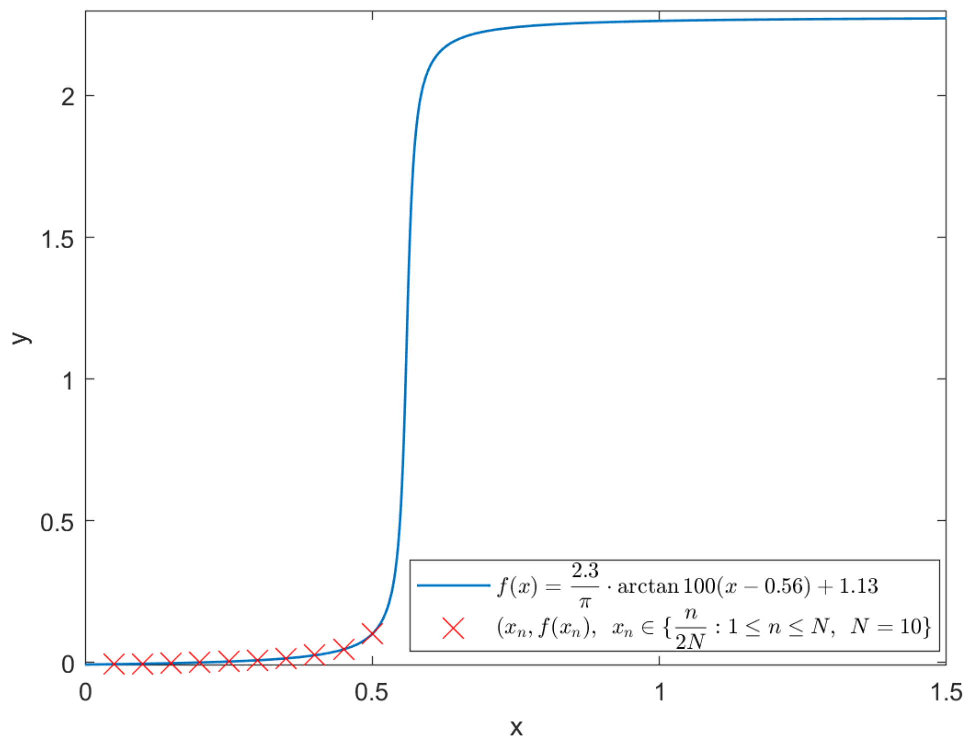
which completes the proof. □

3.2.1 Low-varying function, high discrepancy sequence

Next we will present an example which, although somewhat artifical, nonetheless illustrates the importance that a *low discrepancy sequence* is used in the *QMC-algorithm.* For as we shall see, even if $TV(f)$ is very small (i.e., f is *"very nice"* as is desired in the *Koksma inequality*), ε_N can still be very large if $\mathcal{P}_N$ has high discrepancy.

So then, for the sake of a simple illustration.
Let f be the function given by $f(x) := \frac{2.3}{\pi} \arctan 100(x - 0.56) + 1.13$, and let $\mathcal{P}_N := \{x_n = \frac{n}{2N} : 1 \leq n \leq N, \;\; N = 10\} \subset [0, \frac{1}{2}]$ (see Figure 5).

Figure 5: Low-varying function and high discrepancy sequence



Suppose we want to approximate $\mathcal{I} := \displaystyle\int_0^1 f(x)\mathrm{d}x$ using $Q_N := \displaystyle\frac{1}{N}\sum_{n=1}^{N} f(x_n)$ with $x_n \in \mathcal{P}_N$. Since f is a strictly increasing function, we get that $|f'(x)| = f'(x) > 0$, from which it follows that

$$TV(f) := \int_0^1 |f'(x)| \, \mathrm{d}x = \int_0^1 f'(x)\mathrm{d}x = f(1) - f(0).$$

Furthermore, since the elements of $\mathcal{P}_N$ are evenly distributed in $\left[0, \frac{1}{2}\right]$, with the constant difference $\frac{1}{2N}$ between consecutive elements. It is obvious that $\displaystyle\frac{\Delta_N(\alpha)}{N}$ is an increasing function of α on the interval $\left[0, \frac{1}{2}\right]$, as more and more of the elements of $\mathcal{P}_N$ will lie inside the interval $[0, \alpha]$. It follows that $\dfrac{\Delta_N(\alpha)}{N} - \alpha$ is strictly increasing for $\alpha \in \left\{\frac{n}{20} : 1 \leq n \leq 10\right\}$, and strictly decreasing for $\alpha \in \left[\frac{1}{2}, 1\right]$. Thus, since an absolute maximum of $\frac{1}{2}$ is attained at $\alpha = \frac{1}{2}$, we can conclude that

$$D_N^\star(\mathcal{P}_N) = \frac{1}{2}.$$

Now, numerical calculations (using MATLAB) gives us that

$$\mathcal{I} \approx 1, \qquad Q_N \approx 0, \qquad TV(f) \approx 2.27.$$

From which we get, together with the *Koksma inequality* (3.4) that

$$\varepsilon_N \leq 2.27 \cdot \frac{1}{2} \approx 1.14 \qquad \text{and} \qquad \varepsilon_N = |\mathcal{I} - Q_N| \approx 1 = \mathcal{I}.$$

We see that the *Koksma inequality* (3.4), despite the high discrepancy of $\mathcal{P}_N$, still yielded a reasonable upper bound to ε_N. However the discrepancy of $\mathcal{P}_N$ was high enough for this approximation to produce an error large enough to be roughly the size of the value of the integral being approximated for, i.e., not a very good approximation.

3.3 On the assumptions underlying the Koksma inequality

We have seen that the *Koksma inequality* provides an estimate on the size of the error ε_N whenever $TV(f) < \infty$. In particular, if $\mathcal{P}_N$ consists of the first N terms of the *vdC-sequence*, then

$$\varepsilon_N(f, \mathcal{P}_N) = \mathcal{O}\left(\frac{\log_2(N+1)}{N}\right) \tag{3.10}$$

for any f such that $TV(f) < \infty$.

However, the condition of finite total variation is quite strong, and in this section we shall demonstrate that $TV(f) < \infty$ is not a necessary condition in order to have $\epsilon_N \to 0$. In fact, we shall demonstrate the following conjecture.

Conjecture 3.1. *Let $\mathcal{F}(x) := x \sin\left(\frac{1}{x}\right)$ for $x \in (0, 1]$ with $\mathcal{F}(0) = 0$, then the following statements are true:*

1. *$TV(\mathcal{F}) = \infty$,*
2. *If $\mathcal{P}_N$ consists of the first N terms of the vdC-sequence, then*

$$\varepsilon_N(\mathcal{F}, \mathcal{P}_N) = \mathcal{O}\left(\frac{1}{N^\alpha}\right) \tag{3.11}$$

for any $\alpha < 1$ (note the strict inequality).

In other words: ε_N **may converge to zero even if the integrand has infinite total variation. Moreover, the convergence rate can be very close to the rate (3.10), obtained for functions with finite total variation!**

We shall verify Conjecture 3.1 as follows.

We begin by proving that $\mathcal{F}'$ is not integrable (thus proving the first statement).

Proof of statement 1: We have $\mathcal{F}'(x) = \sin\left(\frac{1}{x}\right) - \frac{1}{x}\cos\left(\frac{1}{x}\right)$ for $x \in (0,1)$. Thus,

$$TV(\mathcal{F}) = \int_0^1 \left|\sin\left(\frac{1}{x}\right) - \frac{1}{x}\cos\left(\frac{1}{x}\right)\right| \mathrm{d}x = \int_1^\infty \left|\frac{\sin u}{u^2} - \frac{\cos u}{u}\right| \mathrm{d}u,$$

where the last equality follows simply from the change of variable $u = x^{-1}$.
By the (ordinare) triangle inequality we get

$$\begin{aligned} TV(\mathcal{F}) &= \int_1^\infty \left|\frac{\sin u}{u^2} - \frac{\cos u}{u}\right| \mathrm{d}u = \int_1^\infty \left|\frac{\cos u}{u} - \frac{\sin u}{u^2}\right| du \\ &\geq \int_1^\infty \frac{|\cos u|}{u} \mathrm{d}u - \int_1^\infty \frac{|\sin u|}{u^2} \mathrm{d}u = I_1 - I_2. \end{aligned}$$

Thus it is sufficient to prove that $I_1 = \infty$ and $I_2 < \infty$.

Firstly, since $|\sin(u)| \leq 1$ for all $u \in \mathbb{R}$ we get

$$I_2 < \int_1^\infty \frac{1}{u^2} \mathrm{d}u = \left[\frac{-1}{u}\right]_1^\infty = 1 < \infty.$$

Secondly, let $\mathcal{D} := \{u \in \mathbb{R} : |\cos u| > \frac{1}{2}, u \geq 1\} = \bigcup_{n=0}^{\infty} J_n$, with $J_n := \left[\frac{2\pi}{3} + n\pi, \frac{4\pi}{3} + n\pi\right]$ so that $l(J_n) = \frac{2\pi}{3}$ for all $n \in \mathbb{N}$.

Note that $I_1 > \displaystyle\int_{\mathcal{D}} \left|\frac{\cos u}{u}\right| \mathrm{d}u$.

Now, using the lower bound of $\frac{1}{2}$ for $|\cos u|$ for all $u \in \mathcal{D}$, and that $\frac{1}{u}$ is *strictly decreasing* in $\mathcal{D}$, we get

$$\begin{aligned}
I_1 &> \int_{\mathcal{D}} \left|\frac{\cos u}{u}\right| \mathrm{d}u > \frac{1}{2}\int_{\mathcal{D}} \frac{1}{u}\mathrm{d}u = \frac{1}{2}\sum_{n=0}^{\infty}\int_{J_n} \frac{1}{u}\mathrm{d}u \\
&> \frac{1}{2}\sum_{n=0}^{\infty}\left(\frac{1}{\frac{4\pi}{3}+n\pi}\cdot\frac{2\pi}{3}\right) = \frac{1}{4}\sum_{n=0}^{\infty}\frac{1}{1+n} > \frac{1}{4}\sum_{n=1}^{\infty}\frac{1}{2n} \\
&= \frac{1}{8}\sum_{n=1}^{\infty}\frac{1}{n} = \infty \quad \text{(divergent harmonic series).}
\end{aligned}$$

Which concludes the proof of statement 1.

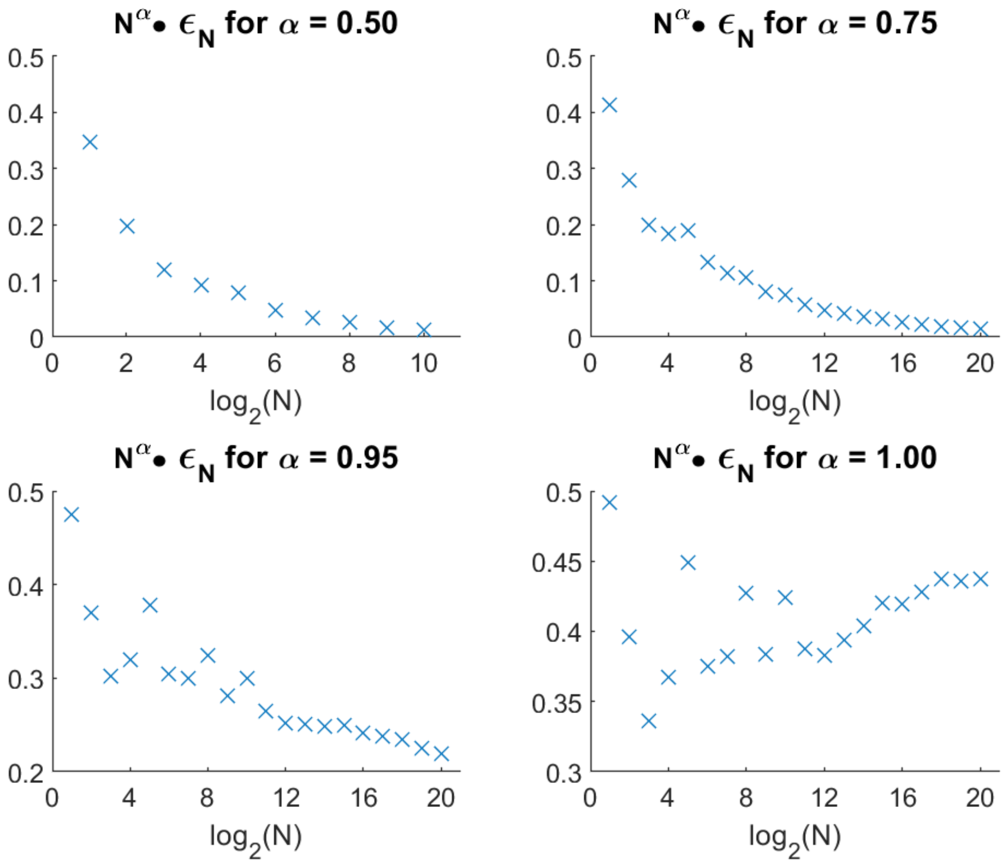
$\square$

Verification of statement 2: We verify the second statement with simulations for which we outline the argument below:

1. Use MATLAB to numerically calculate $\mathcal{I} = \displaystyle\int_0^1 x \sin\left(\frac{1}{x}\right) dx$ with high precision.
2. Use the MATLAB routine to generate the first N terms of the vdC-sequence, and then form the *QMC-algorithm* Q_N.
3. Calculate $\varepsilon_N = |\mathcal{I} - Q_N|$.
4. Perform steps 2 and 3 for $N = 1, 2, 4, 8, ...$ and plot $N^\alpha \cdot \varepsilon_N$ against $\log_2 N$ for a fixed $\alpha \leq 1$ (we use a logarithmic scale for the sake of clarity).

The results of our simulations are presented in Figure 6 below for different values of α (see Appendix A for the code).

Figure 6: Plots of $N^\alpha \cdot \varepsilon_N$ against $\log_2(N)$ for different fixed values of $\alpha \leq 1$.



These results clearly demonstrate the convergence rate (3.11) (repeated below)

$$\varepsilon_N(\mathcal{F}, \mathcal{P}_N) = \mathcal{O}\left(\frac{1}{N^\alpha}\right),$$

for a fixed $\alpha \leq 0.95$, with a clear divergence for $\alpha = 1$.

We decided against using higher values then $\alpha = 0.95$ due to the high computational demands of performing steps 2 and 3 for the much higher values of N necessary to illustrate (3.11) for $0.95 < \alpha < 1$. As we deemed the values of α displayed in Figure 6 to be sufficiently satisfactory for the verification of the second statement of Conjecture 3.1.

4 Conclusions

The main contributions of this thesis concerns the discrepancy of the *vdC-sequence*, and the convergence rates of the *QMC method* provided by the *Koksma inequality*.

We presented Conjecture 2.1 concerning the maximum discrepancy of subsets of *vdC-blocks*. Assuming this conjecture, we gave a conditional proof of Theorem 2.2, the *van der Corput theorem* (i.e., calculation of the order of the discrepancy of *vdC-point sets*).

Concerning the convergence rates of the *QMC method*, we have illustrated in Conjecture 3.1 that the general error estimate provided by the *Koksma inequality* may be too pessimistic. If one uses quadrature points with low discrepancy, one can obtain convergence (even fast convergence) even if the integrand has infinite total variation.

A MATLAB code

Script A (used in Conjecture 2.1):

```
vdc=vdcorput(100000,2);%vdC-sequence(number of elements, base)
M_tot=15;
H=0;
for M=1:M_tot
 N=2^(M-1);
  S_M=vdc(2.^(M-1)+1:2.^M);
  for j=1:N
      S_Mj=sort(S_M(1:j));%1st j elements in S_M in non-decreasing order.
      y=(2.*sort(1:j)-1)./(2*j);%2nd term in proposition (2.13).
      z=0.5+j.*max(abs(S_Mj'-y));
      H(1,j)=max(z);
  end
  Y(1,M)=max(H)%Y(M) to be plotted against M
end
```

Script B (used in Conjecture 3.1):

```
syms x;
f=@(x)x.*sin(1./x);
I=integral(@(x)x.*sin(1./x),0,1);
vdc=vdcorput(2000,2); %vdC-sequence(Number of elements, base)
alfa=0.5;
for i=1:10
    y=i;
    N=2.^y;
    Q=0;
    Y(1,i)=0;
    for x=2:N+1
        Q=Q+1./N.*f(vdc(x))
    end
epsilon=abs(I-Q);
Y(1,i)=N.^(alfa).*epsilon
end
```

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