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Michael Drmota Robert F. Tichy

Sequences, Discrepancies and Applications

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Dedicated to Professor Edmund Hlawka
on the occasion of his 80^{th} birthday

Preface

KRONECKER's approximation theorem says that the fractional parts of the multiples of an irrational lie dense in the unit interval. This result was the starting point of a long and fruitful development of the theory of uniformly distributed sequences. At the beginning of the 20^{th} century first refinements and generalizations of KRONECKER's theorem were established by various authors such as BOHL, SIERPINSKI, BERNSTEIN, HARDY and LITTLEWOOD, and WEYL who was the first establishing a systematic treatment of uniformly distributed sequences in his famous paper *'Über die Gleichverteilung von Zahlen mod. Eins'* [1953]. A historic survey on the theory of uniform distribution until 1916 is given by HLAWKA and BINDER [837] whereas the development of this subject after 1916 is contained in several monographs and survey articles. Some chapters of the classical books *'Aufgaben und Lehrsätze aus der Analysis'* by PÒLYA and SZEGÖ [1450] and *'Diophantische Approximationen'* by KOKSMA [941] are devoted to the early stage of the theory of uniform distribution. A detailed survey of the whole subject until 1960 was given by CIGLER and HELMBERG [369]. The first exhausting monograph *'Uniform Distribution of Sequences'* is due to KUIPERS and NIEDERREITER [983]. Some years later HLAWKA published his monograph [804, 815] on the theory of uniform distribution.

The beginning of the theory was the discovery that the fractional parts of the multiples of an irrational are not only dense in the unit interval but they are uniformly distributed. This means that the empirical distribution of the sequence is asymptotically equal to the uniform distribution. Therefore the main root of this theory is diophantine approximation and number theory, however there are strong connections to various fields of mathematics such as measure and probability theory, harmonic analysis, topological groups, summability theory, discrete mathematics, and numerical analysis. In the twenties and thirties several authors, for instance BEHNKE, VAN DER CORPUT, KOKSMA, and OSTROWSKI, established quantitative results concerned with the distribution behaviour of special sequences. As a quantitative measure of the distribution behaviour of a sequence VAN DER CORPUT considered the so-called discrepancy, i.e. the maximal deviation between the empirical distribution of the sequence and the uniform distribution. One problem is to find upper bounds for the discrepancy of special sequences. The main tool for proving such bounds is to apply analytic tools for estimating exponential sums. Another important problem is to prove general lower bounds for the discrepancy of sequences. This subject is called *Theory of Irregularities of Distribution* since it turns out that the distribution of a sequence cannot be too smooth. First significant results in this direction are due to VAN AARDENNE-EHRENFEST, ROTH, and SCHMIDT. There are two monographs on this subject, namely by SCHMIDT [1634] and more recently by BECK and CHEN [143].

In pioneering papers HLAWKA [782, 783] generalized the theory of uniform distribution to the setting of compact topological spaces and groups. These abstract aspects and connections to summability theory can be found in [983, chapters 3,4]. More recently the abstract theory of uniform distribution was further extended by several authors such as NIEDERREITER, LOSERT, and RINDLER. The special case of discrete spaces was extensively studied, mainly sequences of integers modulo m were considered. Distribution problems for integer sequences are surveyed by NARKIEWICZ [1260].

A very important application of uniformly distributed sequences is numerical integration since the approximation error can be estimated in terms of the discrepancy. Hence it is important to construct low-discrepancy sequences. Constructions of such sequences are due to HLAWKA and KOROBOV. A concise treatment of this so-called *Good Lattice Point Method* can be found in the monographs by KOROBOV [958] and by HUA and WANG [852]; see also HLAWKA, FIRNEIS, and ZINTERHOF [838]. More recently low-discrepancy and related sequences are used for several other applications: for simulation of random numbers, Quasi-Monte Carlo optimization, etc. In the meantime there exists a huge literature on various applications of Quasi-Monte Carlo methods to different kinds of problems; an excellent survey is NIEDERREITER's book [1336].

The present book attempts to summarize special developements and methods of the theory of uniform distribution since 1974 when KUIPERS' and NIEDERREITER's book [983] appeared. We emphasize on such topics which are not covered by some of the above mentioned monographs. Every section of this book consists of two parts, a self-contained one where main results and methods are established and a notes part where the corresponding literature is discussed. References of papers published before 1974 are only taken into account if they are necessary for the presentation and proofs of the results. For references of other papers we explicitely refer to the extensive bibliography in [983] and to a recent manuscript by HELMBERG [773].

In chapter 1 we discuss the classical theory of uniform distribution in the unit interval and in the k-dimensional unit cube. We present an improved version of the famous ERDÖS-TURÁN-KOKSMA inequality as well as BECK's proof of ROTH's lower bound for the discrepancy. Furthermore estimates for the discrepancy of special sequences are established, e.g. for the $(n\alpha)$-sequence, higher dimensional analogues, digital sequences, and exponential sequences. Here we also survey on BECK's recent metric result on the KRONECKER sequence as well as on special results on normal numbers. In a concluding section metric bounds for the discrepancy of sequences are proved.

In chapter 2 we shortly demonstrate BECK's Fourier-Transform approach for finding general lower bounds of the discrepancy. For a detailed presentation of this method we refer to BECK and CHEN [143]. However, a new method due to ALEXANDER is discussed in more details. Furthermore a quantitative treatment of the discrepancy with respect to summation methods is given. Continuous analogues are investigated as well as some new applications of BECK' method not contained in [143]. In a final section we study distribution problems in finite sets, in particular we present concepts of discrepancy for sequences in finite sets and some statistical results. This involves combinatorial methods and generating functions. The combinatorial discrepancy theory is not discussed exhaustively since there exists an excellent survey by BECK and SÓS [150] on this subject. Then we shortly deal with uniform distribution in integers and generalizations. For a detailed presentation of this topic we refer to NARKIEWICZ [1260]. However, we emphasize on recent results on the uniform distribution of linear recurring sequences.

The final chapter 3 is devoted to various applications of uniformly distributed sequences such as numerical integration and numerical solution of differential equations, random number generation, and Quasi-Monte Carlo methods. Furthermore we include as a very recent application some aspects of Mathematical Finance. During the last years all these applications have been a rapidly growing area of research. There were several important conferences on these topics, e.g. one in Lamprecht (Germany), subsequent ones in Fairbanks (Alaska, 1990), in Las Vegas (Nevada, 1994) and in Salzburg (Austria, 1996). NIEDERREITER's book [1336] is an extended version of his letures given at the Fairbanks conference. We try to focus on some application problems which we have selected following our own taste. We also include the explicit computation of the L^2-discrepancy which is the basic quantity for the average case analysis of numerical integration. For a detailed survey on average case analysis of numerical integration we refer to the monographs by NOVAK [1371] and by TRAUB, WASILKOWSKI and WOŹNIAKOWSKY [1872].

We are indebted to M. Blümlinger, M. Goldstern, P. Grabner, C. Heuberger, B. Klinger, A. Knappe, I. Radovic, T. Siegl, M. Skałba, J. Thuswaldner, G. Turnwald, M. Unterguggenberger, R. Winkler for helpful discussions and to Mrs. H. Panzenböck for typesetting. Especially we thank the Springer-Verlag for the kindness and support during the time we have written this volume. Finally we want to thank our wives for their patience and encouragement.

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Contents

Chapter 1

Discrepancy of Sequences

1.1 Basic Concepts

1.1.1 Basic Definitions

Let us consider the k-dimensional Euclidean space $\mathbf{R}^k$. We will identify two points $\mathbf{x}, \mathbf{y} \in \mathbf{R}^k$ if their difference $\mathbf{x} - \mathbf{y}$ is an integral lattice point $\in \mathbf{Z}^k$. Equivalently we can say that we consider the space $\mathbf{R}^k$ modulo 1 or we deal with the k-dimensional torus $\mathbf{T}^k = \mathbf{R}^k/\mathbf{Z}^k$.

Obviously $\mathbf{T}^k$ can be identified with the unit cube $\mathbf{U}^k = [0,1)^k$. Formally this can be done by using the notion of fractional parts. The fractional part $\{x\}$ of a real number x is defined by $\{x\} = x - [x]$, where $[x]$ denotes the integral part of x, that is, the greatest integer $\leq x$. The fractional part $\{\mathbf{x}\}$ and the integral part $[\mathbf{x}]$ for $\mathbf{x} \in \mathbf{R}^k$ are defined componentwise.

Let $J = [a_1, b_1) \times \cdots \times [a_k, b_k) \subseteq \mathbf{R}^k$ be an interval (or a rectangle with sides parallel to the axes) in the k-dimensional space $\mathbf{R}^k$ with $0 < b_i - a_i \leq 1$, $i = 1, \ldots, k$. Then the reduction modulo 1, $I = J/\mathbf{Z}^k$ is called an interval (or a rectangle with sides parallel to the axes) of the torus $\mathbf{T}^k = \mathbf{R}^k/\mathbf{Z}^k$, e.g. $I = [0, \frac{1}{2}) \cup [\frac{2}{3}, 1) = [\frac{2}{3}, \frac{3}{2})/\mathbf{Z}$ is such an interval. The volume $\lambda_k(I)$ of an interval $I \subseteq \mathbf{R}^k/\mathbf{Z}^k$ is given by $\prod_{i=1}^{k}(b_i - a_i)$. (Of course, λ_k denotes the k-dimensional LEBESGUE measure.) For such an interval $I \subseteq \mathbf{R}^k/\mathbf{Z}^k$ and a sequence $(\mathbf{x}_n)_{n \geq 1}$, $\mathbf{x}_n \in \mathbf{R}^k$, let $A(I, N, \mathbf{x}_n)$ be the number of points $\mathbf{x}_n$, $1 \leq n \leq N$, for which $\{\mathbf{x}_n\} \in I$, i.e.

$$A(I, N, \mathbf{x}_n) = \sum_{n=1}^{N} \chi_I(\{\mathbf{x}_n\}), \tag{1.1}$$

where χ_I is the characteristic function of I.

Using these notations it is easy to define the notion of uniformly distributed sequences.

Definition 1.1 *A sequence* $(\mathbf{x}_n)_{n\geq 1}$ *of points in the k-dimensional space* $\mathbf{R}^k$ *is said to be* uniformly distributed modulo 1 *(for short u.d. mod 1) if for every interval* $I \subseteq \mathbf{R}^k/\mathbf{Z}^k$ *we have*

$$\lim_{N\to\infty} \frac{A(I,N,\mathbf{x}_n)}{N} = \lambda_k(I). \tag{1.2}$$

Furthermore $(\mathbf{x}_n)_{n\geq 1}$ *is called* well distributed modulo 1 *(for short w.d. mod 1) if for every interval* $I \subseteq \mathbf{R}^k/\mathbf{Z}^k$ *we have*

$$\lim_{N\to\infty} \frac{A(I,N,\mathbf{x}_{n+\nu})}{N} = \lambda_k(I) \tag{1.3}$$

uniformly for all $\nu \geq 0$.

Remark. Of course, well distribution is a stronger concept then uniform distribution. We postpone a systematic study of this notion to Section 2.2 ; some special w.d. sequences will be considered in Section 1.4.

Note that (1.2) is equivalent to

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \chi_I(\{\mathbf{x}_n\}) = \int_{\mathbf{T}^k} \chi_I \, d\lambda_k \tag{1.4}$$

or for short

$$\lim_{N\to\infty} m_N(\chi_I) = m(\chi_I), \tag{1.5}$$

where

$$m_N(f) = \frac{1}{N} \sum_{n=1}^{N} f(\{\mathbf{x}_n\}) \tag{1.6}$$

and

$$m(f) = \int_{\mathbf{T}^k} f \, d\lambda_k \tag{1.7}$$

are positive linear functionals on the space of LEBESGUE integrable functions $f : \mathbf{T}^k \to \mathbf{R}$. Hence a sequence $(\mathbf{x}_n)_{n\geq 1}$ of points in $\mathbf{R}^k$ is u.d. mod 1 if and only if (1.5) holds for all characteristic functions χ_I of intervals $I \subseteq \mathbf{T}^k$. By linearity,

$$\lim_{N\to\infty} m_N(f) = m(f) \tag{1.8}$$

holds for all step functions f, too. Furthermore we have the following property.

Lemma 1.2 *Let* m_N $(N \in \mathbf{Z},\ N \geq 0)$ *and* m *be positive functionals on some space* $\mathcal{F}$ *of real-valued functions* $f : X \to \mathbf{R}$ $(X \neq \emptyset)$ *and let* $\mathcal{L} \subseteq \mathcal{F}$ *the subspace of these functions* f *satisfying (1.8). Suppose that* $f \in \mathcal{F}$ *has the property that for every* $\varepsilon > 0$ *there exist functions* $g_1, g_2 \in \mathcal{L}$ *with* $g_1 \leq f \leq g_2$ *and* $m(g_2) - m(g_1) < \varepsilon$. *Then* $f \in \mathcal{L}$, *too.*

Proof. By $m_N(g_1) \le m_N(f) \le m_N(g_2)$ and $m(g_1) \le m(f) \le m(g_2)$ we immediately get

$$\begin{aligned} m(g_1) &= \liminf_{N\to\infty} m_N(g_1) \le \liminf_{N\to\infty} m_N(f) \\ &\le \limsup_{N\to\infty} m_N(f) \le \limsup_{N\to\infty} m_N(g_2) \\ &= m(g_2) \end{aligned}$$

which implies

$$|m(f) - \liminf_{N\to\infty} m_N(f)| < \varepsilon$$

and

$$|m(f) - \limsup_{N\to\infty} m_N(f)| < \varepsilon$$

for every $\varepsilon > 0$. Thus $\lim_{N\to\infty} m_N(f) = m(f)$. □

This Lemma can be used to prove two criteria for sequences u.d. mod 1. Recall that the k-dimensional torus $\mathbf{T}^k$ can be identified with the cube $[0,1)^k \subseteq [0,1]^k$.

Theorem 1.3 (Criterion A) *A sequence $(\mathbf{x}_n)_{n\ge1}$ of points in the k-dimensional space $\mathbf{R}^k$ is u.d. mod 1 if and only if*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(\{\mathbf{x}_n\}) = \int_{[0,1]^k} f \, d\lambda_k \tag{1.9}$$

holds for all RIEMANN *integrable functions $f : [0,1]^k \to \mathbf{R}$.*

Theorem 1.4 (Criterion B) *A sequence $(\mathbf{x}_n)_{n\ge1}$ of points in the k-dimensional space $\mathbf{R}^k$ is u.d. mod 1 if and only if (1.9) holds for all continuous functions $f : [0,1]^k \to \mathbf{R}$.*

Proof. Let $\mathcal{L}$ be the space of all LEBESGUE integrable functions $f : [0,1]^k \to \mathbf{R}$ satisfying (1.9). Then $\mathcal{L}$ contains all stepfunctions. Now, if f is RIEMANN integrable then by definition for every $\varepsilon > 0$ there exist step functions g_1, g_2 with $g_1 \le f \le g_2$ and

$$\int_{[0,1]^k} (g_2 - g_1) \, d\lambda_k < \varepsilon. \tag{1.10}$$

Hence by Lemma 1.2 $f \in \mathcal{L}$. On the other hand all characteristic functions χ_I are RIEMANN integrable. This proves Criterion A.

Since every continuous function f is RIEMANN integrable (1.9) surely holds for continuous functions. Conversely it is easy to see that for every characteristic function χ_I and every $\varepsilon > 0$ there exist continuous functions g_1, g_2 with $g_1 \le \chi_I \le g_2$ and (1.10). Thus a second application of Lemma 1.2 proves Criterion B. □

Remark 1. It should be noted that Criterion B is a proper version to generalize the definition of u.d. sequences to compact topological spaces whereas the first definition has no direct analogue at a first glance.

Remark 2. There is no sequence satisfying (1.9) for all LEBESGUE integrable functions.

Remark 3. Property (1.9) is also the starting point to apply u.d. sequences for numerical integration.

1.1.2 Discrepancies

In order to quantify the convergence in (1.2) the discrepancy D_N of a sequence $(\mathbf{x}_n)_{n\geq 1}$ has been introduced.

Definition 1.5 *Let $\mathbf{x}_1, \ldots, \mathbf{x}_N$ be a finite sequence of points in the k-dimensional space $\mathbf{R}^k$. Then the number*

$$D_N = D_N(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sup_{I\subseteq \mathbf{T}^k} \left| \frac{A(I, N, \mathbf{x}_n)}{N} - \lambda_k(I) \right| \tag{1.11}$$

is called the discrepancy of the given sequence. For an infinite sequence $(\mathbf{x}_n)_{n\geq 1}$ $D_N(\mathbf{x}_n)$ should denote the discrepancy of $(\mathbf{x}_n)_{n=1}^N$ and is called discrepancy, too.

The essential point of the concept of discrepancy is that the notion of uniform distribution can be covered by it; i.e. the convergence in (1.2) is uniform with respect to all intervals $I \subseteq \mathbf{T}^k$.

Theorem 1.6 *A sequence $(\mathbf{x}_n)_{n\geq 1}$ is u.d. mod 1 if and only if*

$$\lim_{N\to\infty} D_N(\mathbf{x}_n) = 0. \tag{1.12}$$

Proof. (1.12) immediately implies (1.2) for all intervals $I \subseteq \mathbf{T}^k$. So we only have to show that every u.d. sequence satisfies (1.12). For this reason let M be an arbitrary positive integer and set

$$I_{m_1,\ldots,m_k} = \left[\frac{m_1}{M}, \frac{m_1+1}{M}\right) \times \cdots \times \left[\frac{m_k}{M}, \frac{m_k+1}{M}\right)$$

for $0 \leq m_i < M$, $i = 1, \ldots, k$. By (1.2) there exists a positive integer N_0 such that

$$\frac{1}{M^k}\left(1 - \frac{1}{M}\right) \leq \frac{A(I_{m_1,\ldots,m_k}, N, \mathbf{x}_n)}{N} \leq \frac{1}{M^k}\left(1 + \frac{1}{M}\right) \tag{1.13}$$

for $N \geq N_0$ and for all cubes $I_{m_1,\ldots,m_k}$. Now consider an arbitrary interval $I \subseteq \mathbf{T}^k$. Clearly there exist intervals $\underline{I}, \overline{I}$, finite unions of cubes $I_{m_1,\ldots,m_k}$, such that $\underline{I} \subseteq I \subseteq \overline{I}$ and

$$\lambda_k(\overline{I}) - \lambda_k(\underline{I}) \leq 1 - \left(1 - \frac{2}{M}\right)^k = \frac{2k}{M} + \mathcal{O}\left(\frac{2}{M^2}\right). \tag{1.14}$$

From (1.13) we get

$$\begin{aligned} \lambda_k(\underline{I})\left(1 - \frac{1}{M}\right) &\leq \frac{A(\underline{I}, N, \mathbf{x}_n)}{N} \leq \frac{A(I, N, \mathbf{x}_n)}{N} \\ &\leq \frac{A(\overline{I}, N, \mathbf{x}_n)}{N} \leq \lambda_k(\overline{I})\left(1 + \frac{1}{M}\right) \end{aligned} \tag{1.15}$$