Upper Bounds in Discrepancy Theory

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Abstract Through the use of a few examples, we shall illustrate the use of probability theory, or otherwise, in the study of upper bound questions in the theory of irregularities of point distribution. Such uses may be Monte Carlo in nature but the most efficient ones appear to be quasi Monte Carlo in nature. Furthermore, we shall compare the relative merits of probabilistic and non-probabilistic techniques, as well as try to understand the actual role that the probability theory plays in some of these arguments.

1 Introduction

Discrepancy theory concerns the comparison of the discrete, namely an actual point count, with the continuous, namely the corresponding expectation. Since the former is always an integer while the latter can take a range of real values, such comparisons inevitably lead to discrepancies. Lower bound results in discrepancy theory support the notion that no point set can, in some sense, be too evenly distributed, while upper bound results give rise to point sets that are as evenly distributed as possible under such constraints.

Let us look at the problem from a practical viewpoint. Consider an integral

$$\int_{[0,1]^K} f(\mathbf{x})\,\mathrm{d}\mathbf{x},$$

where $f:[0,1]^K \to \mathbf{R}$ is a real valued function in K real variables. Of course, this integral simply represents the average value of the function f in $[0,1]^K$. If we are unable to evaluate this integral analytically, we may elect to select a large number of points $\mathbf{p}_1,\ldots,\mathbf{p}_N \in [0,1]^K$, and use the discrete average

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$$\frac{1}{N}\sum_{j=1}^{N} f(\mathbf{p}_j)$$

as an approximation, resulting in an error

$$\frac{1}{N}\sum_{j=1}^{N} f(\mathbf{p}_j) - \int_{[0,1]^K} f(\mathbf{x})\,\mathrm{d}\mathbf{x}.$$

Suppose next that $f = \chi_A$, the characteristic function of some measurable set $A \subseteq [0,1]^K$. Then the above error, without the normalization factor N^{-1}, becomes

$$\sum_{j=1}^{N} \chi_A(\mathbf{p}_j) - N\int_{[0,1]^K} \chi_A(\mathbf{x})\,\mathrm{d}\mathbf{x} = \#(\mathscr{P}\cap A) - N\mu(A),$$

the discrepancy of the set $\mathscr{P} = \{\mathbf{p}_1,\ldots,\mathbf{p}_N\}$ in A. Often we consider a collection $\mathscr{A}$ of such measurable sets $A \subseteq [0,1]^K$; an often considered example of $\mathscr{A}$ is the collection of all aligned rectangular boxes in $[0,1]^K$ which are anchored at the origin. Upper bound problems in discrepancy theory involve finding point sets that are good, in some sense, with respect to all the sets in $\mathscr{A}$.

Naturally, we try if possible to construct explicitly a good point set. However, when this is not possible, then the next best alternative is to show nevertheless that a good point set exists, by the use of probabilistic techniques. Thus, in upper bound arguments, we may use probability with great abandon, use probability with careful control, or not use probability at all. These correspond respectively to the three approaches, namely Monte Carlo, quasi Monte Carlo or deterministic.

There are a number of outcomes and questions associated with a probabilistic approach. First of all, we may end up with a very poor point distribution or a very good point distribution. It is almost certain that we lose explicitness. However, it is important to ask whether the probability is necessary, and if so, what it really does.

This brief survey is organized as follows. In Section 2, we discuss some basic ideas by considering a large discrepancy example. In Section 3, we take this example a little further and compare the merits of the three different approaches. We then discuss in Section 4 the classical problem, an example of small discrepancy. We continue with this example in Section 5 to give some insight into what the probability really does.

Notation. Throughout, $\mathscr{P}$ denotes a distribution of N points in $[0,1]^K$. For any measurable subset $B \subseteq [0,1]^K$, we let $Z[\mathscr{P};B] = \#(\mathscr{P}\cap B)$ denote the number of points of $\mathscr{P}$ that fall into B, with corresponding expected point count $N\mu(B)$. We then denote the discrepancy by $D[\mathscr{P};B] = Z[\mathscr{P};B] - N\mu(B)$.

Also, $\mathscr{Q}$ denotes a distribution of points in $[0,1)^k \times [0,\infty)$ with a density of one point per unit volume. For any measurable subset $B \subseteq [0,1)^k \times [0,\infty)$, we consider the corresponding discrepancy $E[\mathscr{Q};B] = \#(\mathscr{Q}\cap B) - \mu(B)$.

For any real valued function f and non-negative function g, we write $f = O(g)$ or $f \ll g$ to indicate that there exists a positive constant c such that $|f| < cg$. For any non-negative functions f and g, we write $f \gg g$ to indicate that there exists a positive constant c such that $f > cg$, and write $f \asymp g$ to denote that $f \ll g$ and $f \gg g$. The symbols $\ll$ and $\gg$ may be endowed with subscripts, and this means that the implicit constant c may depend on these subscripts.

Remark. The author has taken the liberty of omitting unnecessary details and concentrate mainly on the ideas, occasionally at the expense of accuracy. The reader will therefore find that some definitions and details in this survey will not stand up to closer scrutiny.

2 A Large Discrepancy Example

Let $\mathscr{A}$ denote the collection of all discs in the unit torus $[0,1]^2$ of diameter less than 1.

A special case of a result of Beck [3] states that for every distribution $\mathscr{P}$ of N points in $[0,1]^2$, we have the lower bound

$$\sup_{A\in\mathscr{A}} |D[\mathscr{P};A]| \gg N^{\frac{1}{4}}. \tag{1}$$

This lower bound is almost sharp, since for every natural number $N \geq 2$, there exists a distribution $\mathscr{P}$ of N points in $[0,1]^2$ such that

$$\sup_{A\in\mathscr{A}} |D[\mathscr{P};A]| \ll N^{\frac{1}{4}}(\log N)^{\frac{1}{2}}, \tag{2}$$

a special case of an earlier result of Beck [2]. We shall indicate some of the ideas behind this upper bound.

Let us assume, for simplicity, that $N = M^2$, where M is a natural number, and partition $[0,1]^2$ into $N = M^2$ little squares in the obvious and natural way to create the collection $\mathscr{S}$ of all the little squares S. We then place one point anywhere in each little square $S \in \mathscr{S}$, and let $\mathscr{P}$ denote the collection of all these points.

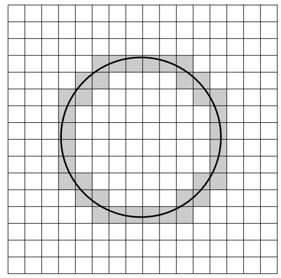
Now take any disc $A \in \mathscr{A}$, and try to bound the term $|D[\mathscr{P};A]|$ from above. Since discrepancy is additive with respect to disjoint unions, we have

$$D[\mathscr{P};A] = \sum_{S\in\mathscr{S}} D[\mathscr{P};S\cap A].$$

It is easy to see that for any little square $S \in \mathscr{S}$ such that $S \cap A = \emptyset$ or $S \subseteq A$, we have $D[\mathscr{P};S\cap A] = 0$. Hence

$$D[\mathscr{P};A] = \sum_{\substack{S\in\mathscr{S}\\ S\cap\partial A\neq\emptyset}} D[\mathscr{P};S\cap A],$$

where ∂A denotes the boundary of A.



It then follows easily that

$$|D[\mathscr{P};A]| \le \sum_{\substack{S\in\mathscr{S}\\ S\cap\partial A\neq\emptyset}} |D[\mathscr{P};S\cap A]| \ll M = N^{\frac{1}{2}},$$

rather weak in comparison to what we hope to obtain.

In order to improve on this rather trivial upper bound, we next adopt a quasi Monte Carlo approach.

For every little square $S \in \mathscr{S}$, let the point $\mathbf{p}_S$ be uniformly distributed within S, and independently from those points in the other little squares. In other words, we have a random point $\widetilde{\mathbf{p}}_S \in S$. Furthermore, we introduce the random variable

$$\xi_S = \begin{cases} 1, \text{ if } \widetilde{\mathbf{p}}_S \in A, \\ 0, \text{ if } \widetilde{\mathbf{p}}_S \notin A, \end{cases}$$

with discrepancy $\eta_S = \xi_S - \mathbf{E}\xi_S$. Clearly $\widetilde{\mathscr{P}} = \{\widetilde{\mathbf{p}}_S : S \in \mathscr{S}\}$ is a random point set, $\{\eta_S : S \in \mathscr{S}\}$ is a collection of independent random variables, and we have

$$D[\widetilde{\mathscr{P}};A] = \sum_{S\in\mathscr{S}} \eta_S = \sum_{\substack{S\in\mathscr{S}\\ S\cap\partial A\neq\emptyset}} \eta_S. \tag{3}$$

To obtain the desired result, we now simply invoke a large deviation type result in probability theory, for instance due to Hoeffding; see Pollard [19, Appendix B]. In summary, the probability theory enables us to obtain the squareroot of the trivial estimate, as is clear from the upper bound (2). Perhaps, we can think of the extra factor $(\log N)^{\frac{1}{2}}$ in (2) as the price of using probability.

In fact, for every distribution $\mathscr{P}$ of N points in $[0,1]^2$, the lower bound (1) follows from the stronger lower bound

$$\int_{\mathscr{A}} |D[\mathscr{P};A]|^2 \, \mathrm{d}A \gg N^{\frac{1}{2}},$$

also due to Beck [3]. We next proceed to show that this bound is best possible.

Let us choose $A \in \mathscr{A}$ and keep it fixed. It then follows from (3) that

$$|D[\widetilde{\mathscr{P}};A]|^2 = \sum_{\substack{S_1,S_2\in\mathscr{S}\\ S_1\cap\partial A\neq\emptyset\\ S_2\cap\partial A\neq\emptyset}} \eta_{S_1}\eta_{S_2}.$$

Taking expectation over all N random points, we obtain

$$\mathbf{E}\left(|D[\widetilde{\mathscr{P}};A]|^2\right) = \sum_{\substack{S_1,S_2\in\mathscr{S}\\ S_1\cap\partial A\neq\emptyset\\ S_2\cap\partial A\neq\emptyset}} \mathbf{E}(\eta_{S_1}\eta_{S_2}). \tag{4}$$

If $S_1 \neq S_2$, then η_{S_1} and η_{S_2} are independent, and so

$$\mathbf{E}(\eta_{S_1}\eta_{S_2}) = \mathbf{E}(\eta_{S_1})\mathbf{E}(\eta_{S_2}) = 0.$$

It follows that the only non-zero contributions to the sum in (4) come from those terms where $S_1 = S_2$, and so

$$\mathbf{E}\left(|D[\widetilde{\mathscr{P}};A]|^2\right) \leq \sum_{\substack{S\in\mathscr{S}\\ S\cap\partial A\neq\emptyset}} 1 \ll N^{\frac{1}{2}}.$$

We now integrate over all $A \in \mathscr{A}$ to obtain

$$\mathbf{E}\left(\int_{\mathscr{A}} |D[\widetilde{\mathscr{P}};A]|^2\,\mathrm{d}A\right) \ll N^{\frac{1}{2}},$$

and the desired result follows immediately.

3 Monte Carlo, Quasi Monte Carlo, or Not

Let $\mathscr{A}$ denote the collection of all discs in the unit torus $[0,1]^2$ of diameter equal to $\frac{1}{2}$. Consider a distribution $\mathscr{P}$ of $N = M^2$ points in $[0,1]^2$, with one point in each little square $S \in \mathscr{S}$. We now randomize these points, or otherwise, in one of the following ways: (i) The point in each S is uniformly distributed in $[0,1]^2$, and independently of other points. This is the Monte Carlo case. (ii) The point in each S is uniformly distributed in S, and independently of other points. This is the quasi Monte Carlo case. (iii) The point in each S is fixed in the centre of S, so that there is absolutely no probabilistic machinery. This is the deterministic case.

We can take a different viewpoint, and let ν denote a probabilistic measure on $U = [0,1]^2$. Taking the origin as the reference point for ν, for every $S \in \mathscr{S}$, we let ν_S denote the translation of ν to the centre of S, and let $\widetilde{\mathbf{p}}_S$ denote the random point associated to ν_S. Repeating this for every $S \in \mathscr{S}$, we obtain a random point set $\widetilde{\mathscr{P}} = \{\widetilde{\mathbf{p}}_S : S \in \mathscr{S}\}$. Now write

$$D_\nu^2(N)=\int_U\ldots\int_U\left(\int_{\mathscr{A}}|D[\widetilde{\mathscr{P}};A]|^2\,\mathrm{d}A\right)\prod_{S\in\mathscr{S}}\mathrm{d}\nu_S.$$

We now choose ν in one of the following ways, corresponding to cases above: (i) We take ν to be the uniform measure supported by $[-\frac{1}{2},\frac{1}{2}]^2$. (ii) We take ν to be the uniform measure supported by $[-\frac{1}{2M},\frac{1}{2M}]^2$. (iii) We take ν to be the Dirac measure δ_0 concentrated at the origin.

Since $\mathscr{A}$ is the collection of all discs in the unit torus $[0,1]^2$ of diameter equal to $\frac{1}{2}$, each $A\in\mathscr{A}$ is a translate of any other, and so

$$\int_{\mathscr{A}}\mathrm{d}A \quad \text{is essentially} \quad \int_U \mathrm{d}\mathbf{x}$$

and this enables us to use Fourier transform techniques.

Let χ denote the characteristic function of the disc centred at the origin. Then one can show that

$$D_\nu^2(N)=N\sum_{\mathbf{0}\neq\mathbf{t}\in\mathbf{Z}^2}|\widehat{\chi}(\mathbf{t})|^2(1-|\widehat{\nu}(\mathbf{t})|^2)+N^2\sum_{\mathbf{0}\neq\mathbf{t}\in\mathbf{Z}^2}|\widehat{\chi}(M\mathbf{t})|^2|\widehat{\nu}(M\mathbf{t})|^2; \tag{5}$$

see Chen and Travaglini [10].

Consider first the Monte Carlo case, where the probabilistic measure ν is the uniform measure supported by $[-\frac{1}{2},\frac{1}{2}]^2$. Then the Fourier transform $\widehat{\nu}$ satisfies $\widehat{\nu}(\mathbf{0})=1$ and $\widehat{\nu}(\mathbf{t})=0$ whenever $\mathbf{0}\neq\mathbf{t}\in\mathbf{Z}^2$. In this case, the identity (5) becomes

$$D_\nu^2(N)=N\sum_{\mathbf{0}\neq\mathbf{t}\in\mathbf{Z}^2}|\widehat{\chi}(\mathbf{t})|^2\asymp N,$$

a very poor outcome.

Consider next the quasi Monte Carlo case, where the probabilistic measure ν is the uniform measure supported by $[-\frac{1}{2M},\frac{1}{2M}]^2$. Then

$$\widehat{\nu}(\mathbf{t})=N\,\frac{\sin(\pi M^{-1}t_1)}{\pi t_1}\,\frac{\sin(\pi M^{-1}t_2)}{\pi t_2},$$

so that $\widehat{\nu}(M\mathbf{t})=0$ whenever $\mathbf{0}\neq\mathbf{t}\in\mathbf{Z}^2$. In this case, the identity (5) becomes

$$D_\nu^2(N)=N\sum_{\mathbf{0}\neq\mathbf{t}\in\mathbf{Z}^2}|\widehat{\chi}(\mathbf{t})|^2(1-|\widehat{\nu}(\mathbf{t})|^2).$$

Consider finally the deterministic case, where the probabilistic measure ν is the Dirac measure concentrated at the origin. Then $\widehat{\nu}(\mathbf{t})=1$ identically. In this case, the identity (5) becomes

$$D_\nu^2(N)=N^2\sum_{\mathbf{0}\neq\mathbf{t}\in\mathbf{Z}^2}|\widehat{\chi}(M\mathbf{t})|^2.$$

Which of these two latter cases is superior?

To answer this question fully, it is necessary to consider all higher dimensional analogues of this question. Accordingly, in the K-dimensional unit torus $[0,1]^K$, where $K \geq 2$, we consider $N = M^K$ little cubes, where M is a natural number. All the definitions in dimension 2 are extended in the natural way to higher dimensions. In the quasi Monte Carlo case, the probabilistic measure ν is the uniform measure λ supported by $[-\frac{1}{2M}, \frac{1}{2M}]^K$, whereas in the deterministic case, the probabilistic measure ν is the Dirac measure δ_0 at the origin.

We now compare the quantities $D^2_{\delta_0}(M^K)$ and $D^2_{\lambda}(M^K)$, and have the following intriguing results due to Chen and Travaglini [10]:

∘ For dimension $K = 2$, $D^2_{\delta_0}(M^K) < D^2_{\lambda}(M^K)$ for all sufficiently large natural numbers M. Hence the deterministic model is superior.

∘ For all sufficiently large dimensions $K \not\equiv 1 \bmod 4$, $D^2_{\lambda}(M^K) < D^2_{\delta_0}(M^K)$ for all sufficiently large natural numbers M. Hence the quasi Monte Carlo model is superior.

∘ For all sufficiently large dimensions $K \equiv 1 \bmod 4$, $D^2_{\lambda}(M^K) < D^2_{\delta_0}(M^K)$ for infinitely many natural numbers M, and $D^2_{\delta_0}(M^K) < D^2_{\lambda}(M^K)$ for infinitely many natural numbers M. Hence neither model is superior.

We comment here that the last case is due to the unusual nature of lattices with respect to balls in these dimensions. A closer look at the Bessel functions that arise from the Fourier transforms of their characteristic functions will ultimately remove any intrigue.

4 The Classical Problem

The most studied example of small discrepancy concerns the classical problem of the subject.

Let $\mathscr{P}$ be distribution of N points in the unit cube $[0,1)^K$, where the dimension $K \geq 2$ is fixed. For every $\mathbf{x} = (x_1, \ldots, x_K) \in [0,1]^K$, we consider the rectangular box $B(\mathbf{x}) = [0,x_1) \times \ldots \times [0,x_K)$ anchored at the origin, with discrepancy

$$D[\mathscr{P};B(\mathbf{x})] = Z[\mathscr{P};B(\mathbf{x})] - Nx_1 \ldots x_k.$$

We are interested in the extreme discrepancy

$$\|D[\mathscr{P}]\|_\infty = \sup_{\mathbf{x}\in[0,1]^K} |D[\mathscr{P};B(\mathbf{x})]|,$$

as well as average discrepancies

$$\|D[\mathscr{P}]\|_W = \left(\int_{[0,1]^K} |D[\mathscr{P};B(\mathbf{x})]|^W \, \mathrm{d}\mathbf{x} \right)^{\frac{1}{W}},$$

where W is a positive real number.

The extreme discrepancy gives rise to the most famous open problem in the subject. First of all, an upper bound result of Halton [16] says that for every natural number $N \geq 2$, there exists a distribution $\mathscr{P}$ of N points in $[0,1]^K$ such that

$$\|D[\mathscr{P}]\|_\infty \ll_K (\log N)^{K-1}. \tag{6}$$

Also, it is well known that for every $K \geq 2$, there exists a real number $\eta(K) > 0$ such that for every distribution $\mathscr{P}$ of N points in $[0,1]^K$, we have the lower bound

$$\|D[\mathscr{P}]\|_\infty \gg_K (\log N)^{\frac{K-1}{2}+\eta(K)}. \tag{7}$$

In dimension $K = 2$, the inequality (7) holds with $\eta(2) = \frac{1}{2}$, and this goes back to the famous result of Schmidt [22]. The case $K \geq 3$ is the subject of very recent groundbreaking work of Bilyk, Lacey and Vagharshakyan [5]. However, the constant $\eta(K)$ is subject to the restriction $\eta(K) \leq \frac{1}{2}$, so there remains a huge gap between the lower bound (7) and the upper bound (6). This is known as the *Great Open Problem*. In particular, there has been no real improvement on the upper bound (6) for over 50 years.

On the other hand, the average discrepancies $\|D[\mathscr{P}]\|_W$ are completely resolved for every real number $W > 1$ in all dimensions $K \geq 2$. The amazing breakthrough result is due to Roth [20] and says that for every distribution $\mathscr{P}$ of N points in $[0,1]^K$, we have the lower bound

$$\|D[\mathscr{P}]\|_2 \gg_K (\log N)^{\frac{K-1}{2}}.$$

The generalization to the stronger lower bound

$$\|D[\mathscr{P}]\|_W \gg_{K,W} (\log N)^{\frac{K-1}{2}}$$

for all real numbers $W > 1$ is due to Schmidt [23], using an extension of Roth's technique. These lower bounds are complemented by the upper bound, established using quasi Monte Carlo techniques, that for every real number $W > 0$ and every natural number $N \geq 2$, there exists a distribution $\mathscr{P}$ of N points such that

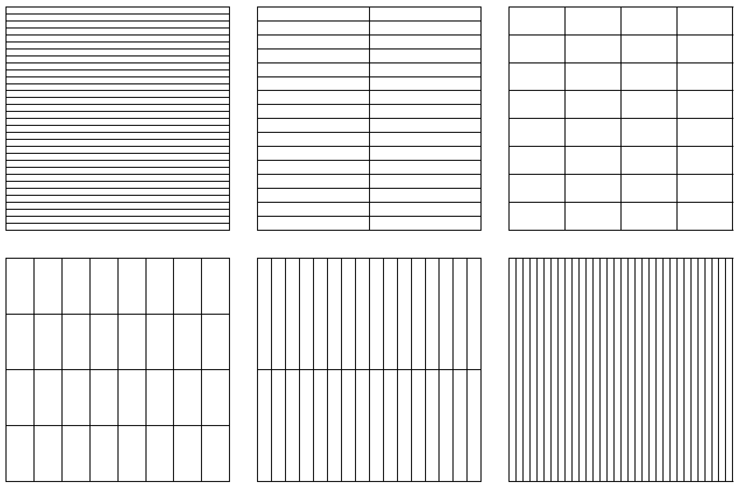
$$\|D[\mathscr{P}]\|_W \ll_{K,W} (\log N)^{\frac{K-1}{2}}. \tag{8}$$

The case $W = 2$ is due to Roth [21], the father of probabilistic techniques in the study of discrepancy theory. The general case is due to Chen [6].

4.1 Two Dimensions

We shall discuss some of the ideas behind the upper bounds (6) and (8) by first concentrating on the special case when the dimension $K = 2$.

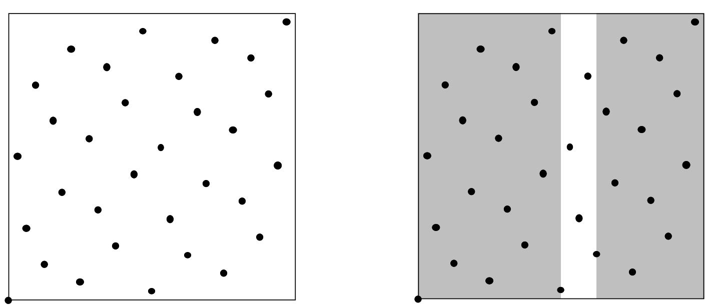
The van der Corput set $\mathscr{P}_h$ of 2^h points must satisfy the following requirement: Suppose that we partition $[0,1]^2$ in the natural way into 2^h congruent rectangles of size $2^{-h_1} \times 2^{-h_2}$, where $0 \leq h_1, h_2 \leq h$ and $h_1 + h_2 = h$. Whatever choice of h_1 and h_2 we make, any rectangle that arises from any such partition must contain precisely one point of $\mathscr{P}_h$. For instance, the van der Corput set $\mathscr{P}_5$ has 32 points, one in each rectangle below.



The 2^h points of $\mathscr{P}_h$ are best given in dyadic expansion. We have

$$\mathscr{P}_h = \{(0.a_1 \ldots a_h, 0.a_h \ldots a_1) : a_1, \ldots, a_h \in \{0,1\}\}. \tag{9}$$

Note that the digits of the second coordinates are in reverse order from the digits of the first coordinates. For instance, the 32 points of $\mathscr{P}_5$ are shown in the picture below on the left.



To describe the periodicity properties of the van der Corput set $\mathscr{P}_h$, we again look at $\mathscr{P}_5$. The picture above on the right shows that for those points with first coordinates in the dyadic interval $[4\times 2^{-3}, 5\times 2^{-3})$, the second coordinates have period 2^{-2}. Periodicity normally suggests the use of classical Fourier series.

Let us choose a real number $x_1 \in [0,1)$ and keep it fixed. For simplicity, let us assume that x_1 is an integer multiple of 2^{-h}, so that $x_1 = 0.a_1 \ldots a_h$ for some digits $a_1, \ldots, a_h \in \{0,1\}$. Then

$$[0,x_1) = \bigcup_{\substack{i=1\\a_i=1}}^{h} [0.a_1 \ldots a_{i-1}, 0.a_1 \ldots a_i).$$

Consider now a rectangle of the form $B(x_1,x_2) = [0,x_1) \times [0,x_2)$. Then one can show without too much difficulty that

$$\begin{aligned} D[\mathscr{P}_h; B(x_1,x_2)] &= \sum_{\substack{i=1\\a_i=1}}^{h} D[\mathscr{P}_h; [0.a_1 \ldots a_{i-1}, 0.a_1 \ldots a_i) \times [0,x_2)] \\ &= \sum_{\substack{i=1\\a_i=1}}^{h} \left(\alpha_i - \psi\left(\frac{x_2+\beta_i}{2^{i-h}} \right) \right), \end{aligned} \tag{10}$$

where $\psi(z) = z - [z] - \frac{1}{2}$ is the sawtooth function and the numbers α_i and β_i are constants. Note that the summand is periodic in the variable x_2 with period 2^{i-h}.

Since the summands are bounded, the inequality $|D[\mathscr{P}_h; B(x_1,x_2)]| \ll h$ follows immediately, and we can go on to show that $\|D[\mathscr{P}_h]\|_\infty \ll h$. This is essentially inequality (6) in the case $K=2$ and $N=2^h$. A little elaboration of the argument will lead to the inequality (6) in the case $K=2$ for all $N \geq 2$.

Next, let us investigate $\|D[\mathscr{P}_h]\|_2$. Squaring the expression (10) and expanding, we see clearly that $|D[\mathscr{P}_h; B(x_1,x_2)]|^2$ contains a term of the form

$$\sum_{\substack{i,j=1\\a_i=a_j=1}}^{h} \alpha_i \alpha_j.$$

This ultimately leads to the estimate

$$\int_{[0,1]^2} |D[\mathscr{P}_h; B(\mathbf{x})]|^2 \, \mathrm{d}\mathbf{x} = 2^{-6}h^2 + O(h),$$

as first observed by Halton and Zaremba [17]. Thus the van der Corput point sets $\mathscr{P}_h$ will not lead to the estimate (8) in the special case $K = W = 2$.

The periodicity in the x_2-direction suggests a quasi Monte Carlo approach. In Roth [21], we consider translating the set $\mathscr{P}_h$ in the x_2-direction modulo 1 by a quantity t to obtain the translated set $\mathscr{P}_h(t)$. Now keep x_2 as well as x_1 fixed. Then one can show without too much difficulty that

$$D[\mathscr{P}_h(t);B(x_1,x_2)] = \sum_{\substack{i=1\\a_i=1}}^{h} \left(\psi\left(\frac{z_i+t}{2^{i-h}}\right) - \psi\left(\frac{w_i+t}{2^{i-h}}\right)\right), \tag{11}$$

where the numbers z_i and w_i are constants. This is a sum of quasi-orthogonal functions in the probabilistic variable t, and one can show that

$$\int_0^1 |D[\mathscr{P}_h(t);B(x_1,x_2)]|^2 \,\mathrm{d}t \ll h. \tag{12}$$

Integrating trivially over $\mathbf{x} = (x_1,x_2) \in [0,1]^2$, we finally conclude that there exists $t^* \in [0,1]$ such that

$$\int_{[0,1]^2} |D[\mathscr{P}_h(t^*);B(x_1,x_2)]|^2 \,\mathrm{d}\mathbf{x} \ll h.$$

Note that the probabilistic technique eschews the effect of the constants α_i in the expression (10). This leads us to wonder whether we can superimpose another van der Corput like point set on the set $\mathscr{P}_h$ in order to remove the constants α_i. If this is possible, then it will give rise to a non-probabilistic approach and an explicit point set. Consider the point set

$$\mathscr{P}_h^* = \{(p_1, 1-p_2) : (p_1,p_2) \in \mathscr{P}_h\},$$

obtained from $\mathscr{P}_h$ by a reflection across the horizontal line $x_2 = \frac{1}{2}$. Then one can show without too much difficulty that

$$D[\mathscr{P}_h^*;B(x_1,x_2)] = \sum_{\substack{i=1\\a_i=1}}^{h} \left(-\alpha_i - \psi\left(\frac{x_2+\gamma_i}{2^{i-h}}\right)\right),$$

where the numbers γ_i are constants. Combining this with (11), we conclude that

$$D[\mathscr{P}_h \cup \mathscr{P}_h^*;B(x_1,x_2)] = -\sum_{\substack{i=1\\a_i=1}}^{h} \left(\psi\left(\frac{x_2+\beta_i}{2^{i-h}}\right) + \psi\left(\frac{x_2+\gamma_i}{2^{i-h}}\right)\right).$$

This is a sum of quasi-orthogonal functions in the variable x_2, and one can show that for the set $\mathscr{P}_h \cup \mathscr{P}_h^*$ of 2^{h+1} points in $[0,1]^2$,

$$\int_{[0,1]} |D[\mathscr{P}_h \cup \mathscr{P}_h^*;B(x_1,x_2)]|^2 \,\mathrm{d}x_2 \ll h.$$

This argument is an example of a reflection principle introduced by Davenport [12].

To summarize, if (10) were a sum of quasi-orthogonal functions with respect to the variable x_2, then we would be able to derive the inequality

$$\int_{[0,1]} |D[\mathscr{P}_h; B(x_1,x_2)]|^2 \, \mathrm{d}x_2 \ll h. \tag{13}$$

However, there is no quasi-orthogonality. By introducing the probabilistic variable t, we are able to replace the expression (10) with the expression (11) which is a sum of quasi-orthogonal functions in the probabilistic variable t, and this leads to the inequality (12) which has the same strength as the inequality (13). In other words, the probability leads to crucial quasi-orthogonality. On the other hand, some crucial quasi-orthogonality can also be brought in by the Davenport reflection principle.

Remark. The Davenport reflection principle is only valid in dimension $K = 2$. The absence of such a principle in higher dimensions contributes greatly to the difficulty of finding explicit point sets that satisfy the inequality (8), a problem eventually solved by Chen and Skriganov [9] for the case $W = 2$ and later by Skriganov [25] for all positive real numbers W.

4.2 Higher Dimensions

Many new ideas in the study of upper bounds only come in when we consider the problem in higher dimensions.

Our first task is to generalize the van der Corput sets. To do this, we first rescale the second coordinate of every point in the van der Corput set $\mathscr{P}_h$ given by (9) by a factor 2^h to obtain the set

$$\mathscr{Q}_h = \{(0.a_1 \ldots a_h, a_h \ldots a_1) : a_1, \ldots, a_h \in \{0,1\}\}.$$

Clearly $0 \le a_h \ldots a_1 < 2^h$, and so $\mathscr{Q}_h \subseteq [0,1) \times [0,2^h)$. We next extend $\mathscr{Q}_h$ to an infinite set as follows. Every non-negative integer n can be written in the form

$$n = \sum_{i=1}^{\infty} 2^{i-1} a_i = \ldots a_3 a_2 a_1, \quad a_i \in \{0,1\}.$$

Writing the digits in reverse order and placing them behind the decimal point, we then arrive at the expression

$$x_2(n) = \sum_{i=1}^{\infty} 2^{-i} a_i = 0.a_1 a_2 a_3 \ldots.$$

We now consider the set

$$\mathscr{Q} = \{(x_2(n), n) : n = 0,1,2,\ldots\} \subseteq [0,1) \times [0,\infty).$$

Clearly $\mathscr{Q}_h \subseteq \mathscr{Q}$. It is not difficult to show that every rectangle of the form

$$[\ell 2^{-s}, (\ell+1)2^{-s}) \times [m2^s, (m+1)2^s)$$

in $[0,1)\times[0,\infty)$, where ℓ and m are integers, has unit area and contains precisely one point of $\mathscr{Q}$.

Next we consider van der Corput sets in higher dimensions. We follow the ideas of Halton [16]. Let p be a prime number. Similar to our earlier considerations, every non-negative integer n can be written in the form

$$n=\sum_{i=1}^{\infty}p^{i-1}a_i=\ldots a_3a_2a_1,\quad a_i\in\{0,1,\ldots,p-1\}.$$

Writing the digits in reverse order and placing them behind the decimal point, we then arrive at the expression

$$x_p(n)=\sum_{i=1}^{\infty}p^{-i}a_i=0.a_1a_2a_3\ldots.$$

Now let $p_1,\ldots,p_k$ be prime numbers, and consider the set

$$\mathscr{Q}=\{(x_{p_1}(n),\ldots,x_{p_k}(n),n):n=0,1,2,\ldots\}\subseteq[0,1)^k\times[0,\infty).$$

It can then be shown, using the Chinese remainder theorem, that every rectangular box of the form

$$\begin{aligned}&[\ell_1p_1^{-s_1},(\ell_1+1)p_1^{-s_1})\times\ldots\times[\ell_kp_k^{-s_k},(\ell_k+1)p_k^{-s_k})\\&\quad\times[mp_1^{s_1}\ldots p_k^{s_k},(m+1)p_1^{s_1}\ldots p_k^{s_k})\end{aligned}\tag{14}$$

in $[0,1)^k\times[0,\infty)$, where $\ell_1,\ldots,\ell_k$ and m are integers, has unit volume and contains precisely one point of $\mathscr{Q}$, provided that $p_1,\ldots,p_k$ are distinct.

The inequality (8) for $W=2$ can now be established by quasi Monte Carlo techniques if we consider translations

$$\mathscr{Q}(t)=\{(x_{p_1}(n),\ldots,x_{p_k}(n),n+t):n=0,1,2,\ldots\}$$

of the set $\mathscr{Q}$ using a probabilistic parameter t. We omit the rather messy details.

Remark. Strictly speaking, before we consider the translation by t, we should extend the set $\mathscr{Q}$ further to one in $[0,1)^k\times(-\infty,\infty)$ in a suitable way.

4.3 Good Distributions

The important condition above is that the primes $p_1,\ldots,p_k$ are distinct. We now ask the more general question of whether there exist primes $p_1,\ldots,p_k$, not necessarily distinct, and a point set $\mathscr{Q}\subseteq[0,1)^k\times[0,\infty)$ such that every rectangular box of the form (14), of unit volume and where $\ell_1,\ldots,\ell_k$ and m are integers, contains precisely one point of $\mathscr{Q}$. For any such instance, we shall say that $\mathscr{Q}$ is good with respect to the primes $p_1,\ldots,p_k$.

Halton's argument shows that good sets $\mathscr{Q}$ exist with respect to distinct primes $p_1,\ldots,p_k$. A construction of Faure [15] shows that good sets $\mathscr{Q}$ exist with respect to primes $p_1,\ldots,p_k$, provided that $p_1=\ldots=p_k\geq k$. No other good sets $\mathscr{Q}$ are currently known.

The good sets constructed by Halton have good periodicity properties, and thus permit a quasi Monte Carlo technique using a translation parameter t. However, the good sets constructed by Faure do not have such periodicity properties, and so do not permit a similar quasi Monte Carlo technique. The challenge now is to find a quasi Monte Carlo technique that works in both instances as well as for any other good point sets that may arise. The answer lies in digit shifts introduced by Chen [7].

Let us first restrict ourselves to two dimensions, and consider a good set

$$\mathscr{Q}=\{(x_p(n),n):n=0,1,2,\ldots\}\subseteq[0,1)\times[0,\infty);$$

note that here $x_p(n)$ may not be obtained from n by the digit-reversing process we have described earlier for Halton sets. The number of digits that we shift depends on the natural number $N\geq 2$, the cardinality of the finite point set $\mathscr{P}$ we wish to find. Normally, we choose a non-negative integer h determined uniquely by the inequalities $2^{h-1}<N\leq 2^h$, so that $h\asymp\log N$. Suppose that

$$x_p(n)=\sum_{i=1}^{\infty}p^{-i}a_i=0.a_1a_2a_3\ldots.$$

For every $\mathbf{b}=(b_1,\ldots,b_h)$, where $b_1,\ldots,b_h\in\{0,1,\ldots,p-1\}$, let

$$x_p^{\mathbf{b}}(n)=0.a_1a_2a_3\ldots\oplus 0.b_1\ldots b_h000\ldots,$$

where $\oplus$ denotes digit-wise addition modulo p, and write

$$\mathscr{Q}^{\mathbf{b}}=\{(x_p^{\mathbf{b}}(n),n):n=0,1,2,\ldots\}.$$

Analogous to (12), we can show that

$$\frac{1}{p^h}\sum_{\mathbf{b}\in\{0,1,\ldots,p-1\}^h}|E[\mathscr{Q}^{\mathbf{b}};B(x,y)]|^2\ll_p h.$$

In higher dimensions, we consider a good set

$$\mathscr{Q}=\{(x_{p_1}(n),\ldots,x_{p_k}(n),n):n=0,1,2,\ldots\}\subseteq[0,1)^k\times[0,\infty),$$

and choose h as above. For every $j=1,\ldots,k$ and $\mathbf{b}_j\in\{0,1,\ldots,p_j-1\}^h$, we define $x_{p_j}^{\mathbf{b}_j}(n)$ in terms of $x_{p_j}(n)$ as before for every $n=0,1,2,\ldots$, and write

$$\mathscr{Q}^{\mathbf{b}_1,\ldots,\mathbf{b}_k}=\{(x_{p_1}^{\mathbf{b}_1}(n),\ldots,x_{p_k}^{\mathbf{b}_k}(n),n):n=0,1,2,\ldots\}.$$

We can then show that

$$\frac{1}{(p_1 \dots p_k)^h} \sum_{\substack{j=1,\dots,k \\ \mathbf{b}_j \in \{0,1,\dots,p_j-1\}^h}} |E[\mathscr{Q}^{\mathbf{b}_1,\dots,\mathbf{b}_k};B(x_1,\dots,x_k,y)]|^2 \ll_{p_1,\dots,p_k} h^k.$$

We emphasize that this quasi Monte Carlo approach is independent of choice of $p_1,\dots,p_k$, so long as $\mathscr{Q}$ is good with respect to the primes $p_1,\dots,p_k$.

5 Fourier–Walsh Analysis

Much greater insight on the role of probability theory has been gained recently through the study of the classical problem via Fourier–Walsh analysis.

The van der Corput set (9) of 2^h points, together with coordinate-wise and digit-wise addition modulo 2, forms a group which is isomorphic to $\mathbf{Z}_2^h$. The characters of these groups are the classical Walsh functions with values ± 1. To study the discrepancy of these sets, it is therefore natural to appeal to Fourier–Walsh analysis, in particular Fourier–Walsh series.

The more general van der Corput set

$$\mathscr{P}_h = \{(0.a_1 \dots a_h, 0.a_h \dots a_1) : 0 \le a_1,\dots,a_k < p\}$$

of p^h points, together with coordinate-wise and digit-wise addition modulo p, forms a group which is isomorphic to $\mathbf{Z}_p^h$. The characters of these groups are the base p Walsh functions, or Chrestenson–Levy functions, with values p-th roots of unity. To study the discrepancy of these sets, it is therefore natural to appeal to base p Fourier–Walsh analysis, in particular base p Fourier–Walsh series.

Suppose that a point set $\mathscr{P}$ possesses the structure of vector spaces over $\mathbf{Z}_p$. The work of Skriganov [24] shows that $\mathscr{P}$ is a good point distribution with respect to the norm $\|D[\mathscr{P}]\|_\infty$ provided that the corresponding vector spaces have large weights relative to a special metric. Furthermore, the work of Chen and Skriganov [9] shows that $\mathscr{P}$ is a good point distribution with respect to the norm $\|D[\mathscr{P}]\|_2$ provided that the corresponding vector spaces have large weights simultaneously relative to two special metrics, a Hamming metric and a non-Hamming metric arising from coding theory. Indeed, these large weights are guaranteed by taking $p \ge 2K^2$ if we consider the classical problem in $[0,1]^K$. This is sufficient for dispensing with the quasi Monte Carlo approach.

Suppose now that a distribution $\mathscr{P}$ possesses the structure of vector spaces over $\mathbf{Z}_p$, and suppose that $\mathscr{P}$ contains $N = p^h$ points. Then it can be shown that a good approximation of the discrepancy function $D[\mathscr{P};B(\mathbf{x})]$ given by

$$F[\mathscr{P};B(\mathbf{x})] = N \sum_{\mathbf{l} \in \mathscr{L}} \phi_{\mathbf{l}}(\mathbf{x}),$$

where $\mathscr{L}$ is a finite set depending on $\mathscr{P}$ and $\phi_{\mathbf{l}}(\mathbf{x})$ is a product of certain coefficients of the Fourier–Walsh series of the characteristic functions $\chi_{[0,x_i)}$ of the intervals forming the rectangular box $B(\mathbf{x})$.

If $p \geq 2K^2$, then the functions $\phi_{\mathbf{l}}(\mathbf{x})$ are orthogonal, and so

$$\int_{[0,1]^K} |F[\mathscr{P};B(\mathbf{x})]|^2 \,\mathrm{d}\mathbf{x} = N^2 \sum_{\mathbf{l}\in\mathscr{L}} \int_{[0,1]^K} |\phi_{\mathbf{l}}(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x}.$$

On ther other hand, if $p < 2K^2$, so that we do not know whether the functions $\phi_{\mathbf{l}}(\mathbf{x})$ are orthogonal, then we consider a suitable group $\mathscr{T}$ of digit shifts $\mathbf{t}$, so that

$$F[\mathscr{P}\oplus\mathbf{t};B(\mathbf{x})] = N \sum_{\mathbf{l}\in\mathscr{L}} \overline{W_{\mathbf{l}}(\mathbf{t})}\phi_{\mathbf{l}}(\mathbf{x}),$$

where $W_{\mathbf{l}}(\mathbf{t})$ are K-dimensional base p Walsh functions. This quasi Monte Carlo argument then leads to

$$\sum_{\mathbf{t}\in\mathscr{T}} |F[\mathscr{P}\oplus\mathbf{t};B(\mathbf{x})]|^2 = N^2 \sum_{\mathbf{l}',\mathbf{l}''\in\mathscr{L}} \left(\sum_{\mathbf{t}\in\mathscr{T}} \overline{W_{\mathbf{l}'}(\mathbf{t})} W_{\mathbf{l}''}(\mathbf{t}) \right) \phi_{\mathbf{l}'}(\mathbf{x})\overline{\phi_{\mathbf{l}''}(\mathbf{x})}.$$

Using the orthogonality property

$$\sum_{\mathbf{t}\in\mathscr{T}} \overline{W_{\mathbf{l}'}(\mathbf{t})} W_{\mathbf{l}''}(\mathbf{t}) = \begin{cases} \#\mathscr{T}, & \text{if } \mathbf{l}'=\mathbf{l}'', \\ 0, & \text{otherwise,} \end{cases}$$

we conclude immediately that

$$\frac{1}{\#\mathscr{T}} \sum_{\mathbf{t}\in\mathscr{T}} |F[\mathscr{P}\oplus\mathbf{t};B(\mathbf{x})]|^2 = N^2 \sum_{\mathbf{l}\in\mathscr{L}} |\phi_{\mathbf{l}}(\mathbf{x})|^2.$$

Integrating with respect to $\mathbf{x}$ trivially over $[0,1]^K$, we conclude that

$$\frac{1}{\#\mathscr{T}} \sum_{\mathbf{t}\in\mathscr{T}} \int_{[0,1]^K} |F[\mathscr{P}\oplus\mathbf{t};B(\mathbf{x})]|^2 \,\mathrm{d}\mathbf{x} = N^2 \sum_{\mathbf{l}\in\mathscr{L}} \int_{[0,1]^K} |\phi_{\mathbf{l}}(\mathbf{x})|^2 \,\mathrm{d}\mathbf{x}.$$

Hence the quasi Monte Carlo methods gives rise to orthogonality via the back door.

6 Further Reading

The oldest monograph on discrepancy theory is due to Beck and Chen [4], and covers the subject from its infancy up to the mid-1980s, with fairly detailed proofs, but is naturally very out of date. A more recent attempt is the beautifully written monograph of Matoušek [18].

The comprehensive volume by Drmota and Tichy [14] contains many results and a very long list of precisely 2000 references, whereas the recent volume by Dick and Pillichshammer [13] concentrates on quasi Monte Carlo methods in both discrepancy theory and numerical integration.

The survey by Alexander, Beck and Chen [1] covers the majority of the main results in discrepancy theory up to the turn of the century, and provides references for the major developments. Shorter surveys, on selected aspects of the subject, are given by Chen [8] and by Chen and Travaglini [11].

References

1. Alexander, J.R., Beck, J., Chen, W.W.L.: Geometric discrepancy theory and uniform distribution. In: Goodman, J.E., O'Rourke, J. (eds.) Handbook of Discrete and Computational Geometry (2nd edition), pp. 279–304. CRC Press (2004)
2. Beck, J.: Balanced two-colourings of finite sets in the square I. Combinatorica **1**, 327–335 (1981)
3. Beck, J.: Irregularities of distribution I. Acta Math. **159**, 1–49 (1987)
4. Beck, J., Chen, W.W.L.: Irregularities of Distribution. Cambridge Tracts in Mathematics **89**, Cambridge University Press (1987)
5. Bilyk, D., Lacey, M.T., Vagharshakyan, A.: On the small ball inequality in all dimensions. J. Funct. Anal. **254**, 2470–2502 (2008)
6. Chen, W.W.L.: On irregularities of distribution. Mathematika **27**, 153–170 (1980)
7. Chen, W.W.L.: On irregularities of distribution II. Quart. J. Math. Oxford **34**, 257–279 (1983)
8. Chen, W.W.L.: Fourier techniques in the theory of irregularities of point distribution. In: Brandolini, L., Colzani, L., Iosevich, A., Travaglini, G. (eds.) Fourier Analysis and Convexity, pp. 59–82. Birkhäuser Verlag (2004)
9. Chen, W.W.L., Skriganov, M.M.: Explicit constructions in the classical mean squares problem in irregularities of point distribution. J. reine angew. Math. **545**, 67–95 (2002)
10. Chen, W.W.L., Travaglini, G.: Deterministic and probabilistic discrepancies. Ark. Mat. **47**, 273–293 (2009)
11. Chen, W.W.L., Travaglini, G.: Some of Roth's ideas in discrepancy theory. In: Chen, W.W.L., Gowers, W.T., Halberstam, H., Schmidt, W.M., Vaughan, R.C. (eds.) Analytic Number Theory: Essays in Honour of Klaus Roth, pp. 150–163. Cambridge University Press (2009)
12. Davenport, H.: Note on irregularities of distribution. Mathematika **3**, 131–135 (1956)
13. Dick, J., Pillichshammer, F.: Digital Nets and Sequences. Cambridge University Press (2010)
14. Drmota, M., Tichy, R.F.: Sequences, Discrepancies and Applications. Lecture Notes in Mathematics **1651**, Springer Verlag (1997)
15. Faure, H.: Discrépance de suites associées à un système de numération (en dimension s). Acta Arith. **41**, 337–351 (1982)
16. Halton, J.H.: On the efficiency of certain quasirandom sequences of points in evaluating multidimensional integrals. Num. Math. **2**, 84–90 (1960)
17. Halton, J.H., Zaremba, S.K.: The extreme and L^2 discrepancies of some plane sets. Monatsh. Math. **73**, 316–328 (1969)
18. Matoušek, J.: Geometric Discrepancy. Algorithms and Combinatorics **18**, Springer Verlag (1999, 2010)
19. Pollard, D.: Convergence of Stochastic Processes. Springer Verlag (1984)
20. Roth, K.F.: On irregularities of distribution. Mathematika **1**, 73–79 (1954)
21. Roth, K.F.: On irregularities of distribution IV. Acta Arith. **37**, 67–75 (1980)
22. Schmidt, W.M.: Irregularities of distribution VII. Acta Arith. **21**, 45–50 (1972)

23. Schmidt, W.M.: Irregularities of distribution X. In: Zassenhaus, H. (ed.) Number Theory and Algebra, pp. 311–329. Academic Press (1977)
24. Skriganov, M.M.: Coding theory and uniform distributions. Algebra i Analiz **13** (2), 191–239 (2001). English translation: St. Petersburg Math. J. **13**, 301–337 (2002)
25. Skriganov, M.M.: Harmonic analysis on totally disconnected groups and irregularities of point distributions. J. reine angew. Math. **600**, 25–49 (2006)