The L^2 discrepancy of irrational lattices

Dmitriy Bilyk

Abstract It is well known that, when α has bounded partial quotients, the lattices $\left\{\left(k/N, \{k\alpha\}\right)\right\}_{k=0}^{N-1}$ have optimal extreme discrepancy. The situation with the L^2 discrepancy, however, is more delicate. In 1956 Davenport established that a *symmetrized* version of this lattice has L^2 discrepancy of the order $\sqrt{\log N}$, which is the lowest possible due to the celebrated result of Roth. However, it remained unclear whether this holds for the original lattices without any modifications. It turns out that the L^2 discrepancy of the lattice depends on much finer Diophantine properties of α, namely, the alternating sums of the partial quotients. In this paper we extend the prior work to arbitrary values of α and N. We heavily rely on Beck's study of the behavior of the sums $\sum\left(\{k\alpha\}-\frac{1}{2}\right)$.

1 Introduction

The present note is a sequel to the papers of the author with Temlyakov and Yu [7, 8] – we continue the study of the L^2 discrepancy of two-dimensional lattices of the form $\mathscr{L}_N(\alpha) := \left\{\left(k/N, \{k\alpha\}\right)\right\}_{k=0}^{N-1}$. Historically these lattices play a very important role in discrepancy theory. It has been known for a long time (cf., Lerch [12, 1904]) that, when α has bounded partial quotients of the continued fraction (α is badly approximable), the extreme discrepancy of these lattices satisfies the inequality

$$\left\|D_{\mathscr{L}_N(\alpha)}\right\|_\infty \le C_1(\alpha)\log N, \tag{1}$$

which is best possible in view of the famous result of Schmidt [16, 1972]. For $(x,y)\in[0,1)^2$, the discrepancy function is defined as

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Dmitriy Bilyk
School of Mathematics, University of Minnesota, Minneapolis, MN 55455 USA e-mail: dbilyk@math.umn.edu

$$D_{\mathscr{L}_N(\alpha)}(x,y) = \#\big(\mathscr{L}_N(\alpha)\cap[0,x)\times[0,y)\big) - Nxy. \tag{2}$$

Regarding the L^2 discrepancy, Davenport [10, 1956] has shown that the symmetrized lattice $\mathscr{L}_N^{sym}(\alpha) := \mathscr{L}_N(\alpha)\cup\mathscr{L}_N(-\alpha)$ consisting of $2N$ points satisfies the inequality

$$\big\|D_{\mathscr{L}_N^{sym}(\alpha)}\big\|_2 \le C_2(\alpha)\sqrt{\log(2N)}, \tag{3}$$

complementing the celebrated lower bound obtained by Roth [14, 1954] slightly earlier. Similar inequalities also hold for the rational approximations of irrational lattices (see [13, 7, 8]). Later Roth [15, 1979] established that random shifts of lattices also achieve the optimal order of the L^2 discrepancy.

Nevertheless, it still remained a mystery whether these modifications are indeed necessary and whether the original lattices have asymptotically minimal L^2 discrepancy. At least a couple of standard references in discrepancy theory erroneously stated without proof that $\big\|D_{\mathscr{L}_N(\alpha)}\big\|_2 \ge C''_\alpha \log N$.

The belief in this bound was partially justified by the fact that it holds for another classical low-discrepancy distribution – the Van der Corput set, while its modifications (symmetrizations, translations, digit shifts) have L^2 discrepancy of the order $\sqrt{\log N}$, i.e. in this case the modifications are really necessary.

However, in 1982 Sós and Zaremba [17] proved that if all the partial quotients of the (finite or infinite) continued fraction are equal, then $\big\|D_{\mathscr{L}_N(\alpha)}\big\|_2 \le C'_\alpha\sqrt{\log N}$. This result, in particular, applied to $\alpha = 1+\sqrt{2}$, the golden section $\alpha = \frac{1+\sqrt{5}}{2}$, the ratio of consecutive Fibonacci numbers $\alpha = \frac{F_n}{F_{n+1}}$. Unfortunately, the paper went largely unnoticed in the subject and the generalizations of this result only appeared recently. It turns out that the L^2 discrepancy estimates for lattices depend on much finer Diophantine properties than just boundedness of partial quotients.

We introduce some notation. For $\alpha\in\mathbb{R}$ consider its continued fraction expansion

$$\alpha = [a_0; a_1, a_2, ...] = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + ...}}} \tag{4}$$

with the partial quotients $a_0\in\mathbb{Z}$, $a_k\in\mathbb{N}$, $k\ge 1$. This expansion is finite if α is rational, and infinite otherwise. We denote by p_n/q_n the n^{th} order convergents of α, i.e. $p_n/q_n = [a_0; a_1, ..., a_n]$. We say that $A\approx B$ if $A = \mathscr{O}(B)$ and vice versa.

In this note we prove the following theorem:

Theorem 1. *Assume that $\alpha = [a_0; a_1, a_2, ...]$ has bounded partial quotients and let p_n/q_n be its n^{th} order convergent. Then, for $q_{n-1} < N \le q_n$ we have*

$$\big\|D_{\mathscr{L}_N(\alpha)}\big\|_2 \approx \max\left\{\Big|\sum_{k=1}^{n}(-1)^k a_k\Big|, \sqrt{\log N}\right\}, \tag{5}$$

in particular,

$$\big\|D_{\mathscr{L}_N(\alpha)}\big\|_2 \approx \sqrt{\log N} \quad \text{if and only if} \quad \Big|\sum_{k=0}^{n}(-1)^k a_k\Big| \le C(\alpha)\sqrt{n}. \tag{6}$$

(If $\alpha = p_{n*}/q_{n*}$ is rational, we additionally assume that $N \le q_{n*}$.)

The classical recurrence relation $q_{n+1} = a_{n+1}q_n + q_{n-1}$ easily implies that q_n grows exponentially and thus whenever $q_{n-1} < N \le q_n$, we have $n \approx \log N$. Therefore, the first expression in the estimate above is at most of the order $\log N$.

We note that this theorem obviously includes the aforementioned result of Sós and Zaremba. In addition, a partial case of this theorem has been obtained by the author with Temlyakov and Yu [8] – this case deals with the situation when the rational $\alpha = p_n/q_n$ is the n^{th} convergent of a badly approximable number θ and the number of points $N = q_n$. This case, in particular, takes care of the famous Fibonacci lattice $\mathscr{F}_n = \left\{ (k/F_n, \{kF_{n-1}/F_n\}) \right\}_{k=0}^{F_n-1}$. Aicke Hinrichs (private communication) conjectures that the Fibonacci lattice has the lowest L^2 discrepancy among all lattices with F_n points. For more information on the Fibonacci lattice and its relation to discrepancy and numerical integration see [18, 19, 20, 7, 8].

We briefly mention some other values of α which yield a lattice with an optimal order of L^2 discrepancy. First of all, for any integer of the form $m = p^2+1$, we have $\sqrt{m} = [p;\overline{2p}]$. Hence it follows already from the Sós–Zaremba result that $\mathscr{L}_N(\sqrt{m})$ has L^2 discrepancy of order $\sqrt{N}$. Therefore, $\mathscr{L}_N(\sqrt{2})$ is optimal, while $\mathscr{L}_N(\sqrt{3})$ is not, since $\sqrt{3} = [1;\overline{1,2}]$ and the alternating sums grow linearly. We can also construct other examples. It is well known that quadratic irrationalities have periodic continued fraction expansions. Notice that if the length of the period is odd, then the alternating sums $\sum_{k=1}^{n}(-1)^k a_k$ stay bounded and the L^2 discrepancy is bounded by $\sqrt{\log N}$. We list the first few values of m (excluding $m = p^2+1$) such that the expansions of $\sqrt{m}$ have periods of odd length: 13, 29, 41, 53, 58, 61, 73, 74, 85, 89, 97. Notice that the periodicity implies an interesting dichotomy: for any quadratic irrational β, the L^2 discrepancy of $\mathscr{L}_N(\beta)$ is either of the order $\log N$ or $\sqrt{\log N}$. In general, it is not had to construct α so that $\mathscr{L}_N(\alpha)$ has any intermediate rate of the L^2 discrepancy.

We add a few words about the methods. Both the original paper of Davenport [10], and the work of Bilyk, Temlyakov, Yu [7, 8] used the Fourier series analysis of the discrepancy function. However, Davenport looked at discrepancy as a function of y and obtained estimates independent of x, while the author and collaborators considered the two-dimensional Fourier series, which for a rational lattice are supported on a very sparse set. In both cases, the main problem comes from the zero-order term of the Fourier expansion (the integral); indeed, both Davenport's symmetrization and Roth's translation are intended to handle this term. In this paper, we revert to Davenport's method.

2 Preliminaries

Consider the 1-periodic *sawtooth* function $\psi(x) = \{x\} - \frac{1}{2}$. It will be crucial for us to understand the behavior of the sums

$$S_m(\alpha) = \sum_{k=0}^{m} \psi(k\alpha). \tag{7}$$

These objects have been extensively studied by Beck [2, 3, 4] (I would like to thank Nir Lev for pointing out these references to me). In particular, it turns out that the Cesaro mean of these sums

$$T_N(\alpha) := \frac{1}{N}\sum_{m=0}^{N-1} S_m(\alpha) = \sum_{m=0}^{N-1}\left(1-\frac{m}{N}\right)\psi(m\alpha) \tag{8}$$

satisfies the following (see Theorem 3.2 in [3])

$$T_N(\alpha) = \frac{1}{12}\sum_{k=1}^{n}(-1)^k a_k + \mathscr{O}(\max_{1\le i\le n} a_i), \tag{9}$$

where n is the smallest index such that $q_n \geq N$. It can also be shown (see [3]) that the second moment of these sums satisfy

$$V_N(\alpha) := \frac{1}{N}\sum_{m=0}^{N-1}\big(S_m(\alpha) - T_N(\alpha)\big)^2 \approx \sum_{m:\, q_m \le N} a_m^2. \tag{10}$$

In addition, the Central Limit Theorem holds for the sums $S_n(\alpha)$. The CLT takes the following form (see Theorem 4.1 in [3])

$$\frac{1}{N}\cdot \#\left\{0 \le m \le N-1 :\, \frac{S_m(\alpha) - T_N(\alpha)}{\sqrt{V_N(\alpha)}} \le \lambda\right\} \longrightarrow \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\lambda} e^{-t^2/2}dt \quad \text{as } N \to \infty \tag{11}$$

provided that $a_k^2/(\sum_{i=1}^k a_i^2) \to 0$ as $k \to \infty$.

This statement is applicable, in particular, when a_k's are bounded. In this case it follows from (10) that

$$V_N(\alpha) \le \max a_k^2 \cdot \#\{m :\, q_m \le N\} \le C_\alpha \log N \tag{12}$$

for some absolute constant $C_\alpha > 0$, since, as noted earlier, $q_{n-1} < N \le q_n$ implies $n \approx \log N$.

Now the CLT easily implies that

$$\left\| \frac{S_m(\alpha) - T_N(\alpha)}{\sqrt{V_N(\alpha)}} \right\|_{\ell^2(N)} = \mathscr{O}(1) \tag{13}$$

as $N \to \infty$, where $\|x\|_{\ell^2(N)} = \left(\frac{1}{N}\sum_{m=0}^{N-1}|x(m)|^2\right)^{1/2}$. Indeed, if x satisfies the CLT (11), then

$$\frac{1}{N}\sum_{m=0}^{N-1}|x(m)|^2 \leq \sum_{k\in\mathbb{Z}} \frac{\#\{m:\, 2^{k-1}<|x(m)|\leq 2^k\}}{N}\cdot 2^{2k}$$
$$\approx \sum_{k\in\mathbb{Z}} \frac{2^{2k}}{\sqrt{2\pi}}\int_{2^{k-1}}^{2^k} e^{-t^2/2}dt \leq \frac{4}{\sqrt{2\pi}}\int_0^\infty t^2\cdot e^{-t^2/2}dt$$

when N is large. Therefore,

$$T_N(\alpha) \leq \left(\frac{1}{N}\sum_{m=0}^{N-1} S_m^2(\alpha)\right)^{1/2} \leq K_\alpha\big(T_N(\alpha)+\sqrt{\log N}\big) \tag{14}$$

for some constant $K_\alpha > 0$. The first inequality is obvious by Cauchy–Schwartz, while the second one is a corollary of (13) and (12). This estimate will be crucial in the proof of Theorem 1.

In the end we would like to note that the mean values of $S_m(\alpha)$ arise naturally with respect to discrepancy. It is easy to check that

$$\int_{[0,1)^2} D_{\mathscr{L}_N(\alpha)}(x,y)\,dx\,dy = \sum_{m=0}^{N-1}\left(1-\frac{m}{N}\right)\big(1-\{m\alpha\}\big)-\frac{N}{4} = -T_N(\alpha)+\frac{1}{4}. \tag{15}$$

This, together with Roth's theorem, immediately implies the lower bound in (5) since $\|f\|_2 \geq |\int f|$. Estimate (14) for the quadratic mean of $S_m(\alpha)$ will arise in the proof of the upper bound.

In the case considered in [8] when $\alpha = p/q$ is rational and $N = q$, the integral above equals $\mathscr{D}(p,q)+\frac{1}{2}$, where

$$\mathscr{D}(p,q) = \sum_{k=0}^{q-1}\frac{k}{q}\cdot\psi\left(k\frac{p}{q}\right) \tag{16}$$

is the *Dedekind sum*. The fact that its behavior is controlled by the alternating sums of partial quotients of p/q has been known independently of Beck's work (e.g. [1, 11]) and has been used in the present setting in [8].

3 The proof of Theorem 1 (upper bound)

We follow Davenport's approach. For a moment, let us fix $x\in[0,1)$ and set $U = U(x) = \lceil Nx-1\rceil$. It is well known (see [10, 15]) that the discrepancy function may be approximated as $D_{\mathscr{L}_N(\alpha)}(x,y) = M_U(y)+\mathscr{O}(1)$, where

$$M_U(y) = \sum_{k=0}^{U}\big(\psi(k\alpha-y)-\psi(k\alpha)\big) = \frac{1}{2\pi i}\sum_{m\neq 0}\frac{1}{m}\left(\sum_{k=0}^{U} e^{2\pi imk\alpha}\right)\big(1-e^{-2\pi imy}\big), \tag{17}$$

where the equality is understood in the L^2 sense. We have used the Fourier expansion $\psi(x) \sim -\sum_{m\neq 0} \frac{e^{2\pi imy}}{2\pi im}$. Using Parseval's identity one obtains:

$$\left\|M_U\right\|^2_{L^2(dy)} \leq |\widehat{M_U}(0)|^2 + C\sum_{m=1}^{\infty} \frac{1}{m^2}\left|\sum_{k=0}^{U} e^{2\pi imk\alpha}\right|^2. \tag{18}$$

The sum above is bounded by a constant multiple of $\log U \leq \log N$ (see [10, 9] for details – this estimate was the heart of Davenport's proof). The zero-order Fourier coefficient (the constant term) is

$$\widehat{M_U}(0) = \frac{1}{2\pi i}\sum_{m\neq 0} \frac{1}{m}\left(\sum_{k=0}^{U} e^{2\pi imk\alpha}\right) = -\sum_{k=0}^{U} \psi(k\alpha) = -S_U(\alpha). \tag{19}$$

We thus arrive to

$$\left\|M_U\right\|^2_{L^2(dy)} \leq S_U^2(\alpha) + C'_\alpha \log N. \tag{20}$$

We now integrate estimate (20) over $x \in [0,1)$. Notice that as x runs over $[0,1)$, the discrete parameter $U = U(x)$ changes between 0 and $N-1$, hence the first term results in

$$\frac{1}{N}\sum_{U=0}^{N-1} S_U^2(\alpha) \leq C''_\alpha (T_N^2(\alpha) + \log N) \tag{21}$$

according to (14). Putting together these estimates and (9) we find that

$$\left\|M_{U(x)}(y)\right\|^2_{L^2(dx\,dy)} \leq K_1(\alpha)\log N + K_2(\alpha)\left|\sum_{k:\, q_k\leq N} (-1)^k a_k\right|^2, \tag{22}$$

for some constants $K_1(\alpha)$ and $K_2(\alpha)$, which yields the upper bound in (5) and finishes the proof of Theorem 1. □

We would like to make a concluding remark. It seems to be a recurrent feature that whenever a well-distributed set fails to meet the optimal L^2 discrepancy bounds, the problem is always already in the constant term, i.e. the integral of the discrepancy function [10, 15, 6, 5, 8]. We conjecture that this should be true in general, in other words the following statement should hold: *there exist constans C_1, C_2, $C_3 > 0$ such that whenever $\mathscr{P}_N \subset [0,1)^2$, $\#\mathscr{P}_N = N$ satisfies $\left\|D_{\mathscr{P}_N}\right\|_\infty \leq C_1 \log N$ and $\left\|D_{\mathscr{P}_N}\right\|_2 \geq C_2 \log N$, it should also satisfy*

$$\left|\int_{[0,1)^2} D_{\mathscr{P}_N}(x,y)\,dx\,dy\right| \geq C_3 \log N. \tag{23}$$

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