The L_2 Discrepancy of Two-Dimensional Lattices

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Dedicated to Konstantin Oskolkov, a dear friend and colleague, on the occasion of his 65th birthday.

Abstract Let α be an irrational number with bounded partial quotients of the continued fraction a_k. It is well known that *symmetrizations* of the irrational lattice $\{(\mu/N, \{\mu\alpha\})\}_{\mu=0}^{N-1}$ have optimal order of L_2 discrepancy, $\sqrt{\log N}$. The same is true for their rational approximations $\mathscr{L}_n(\alpha) = \{(\mu/q_n, \{\mu p_n/q_n\})\}_{\mu=0}^{q_n-1}$, where p_n/q_n is the nth convergent of α. However, the question whether and when the symmetrization is really necessary remained wide open.

We show that the L_2 discrepancy of the nonsymmetrized lattice $\mathscr{L}_n(\alpha)$ grows as

$$\|D(\mathscr{L}_n(\alpha), \mathbf{x})\|_2 \approx \max\left\{\log^{\frac{1}{2}} q_n, \left|\sum_{k=0}^{n}(-1)^k a_k\right|\right\},$$

in particular, characterizing the lattices for which the L_2 discrepancy is optimal.

1 Introduction

1.1 Discrepancy

The extent of equidistribution of a finite point set can be naturally measured using the discrepancy function. Let $\mathscr{P}_N$ be a set of N points in the unit cube $[0,1]^d$ in dimension d. The discrepancy function is then defined as

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$$D(\mathscr{P}_N, \mathbf{x}) := \#\{\mathscr{P}_N \cap [\mathbf{0}, \mathbf{x})\} - N \cdot |[\mathbf{0}, \mathbf{x})|, \tag{1}$$

where $\mathbf{x} = (x_1, \ldots, x_d)$, $[\mathbf{0}, \mathbf{x}) = \prod_{j=1}^{d} [0, x_j)$, and $|\cdot|$ denotes the Lebesgue measure. The L_p norm of the discrepancy function, usually referred to as the L_p discrepancy, is a benchmark that one uses to evaluate the quality of a particular set of N points. The fundamental problems of the discrepancy theory are to construct sets with small L_p discrepancy and to find optimal bounds.

The main principle of the theory of irregularities of distribution states the L_p discrepancy of a finite point set cannot be too small, that is, the quantity

$$D(N,d)_p := \inf_{\mathscr{P}_N} \|D(\mathscr{P}_N, \mathbf{x})\|_p$$

must necessarily go to infinity with N when $d \geq 2$. We refer the reader to [2,6,21,23] for detailed surveys. The famous lower bounds for $D(N,d)_p$ are:

Theorem 1 (Roth [26]). *In all dimensions $d \geq 2$, we have*

$$D(N,d)_2 \geq C(d)(\log N)^{\frac{d-1}{2}}, \tag{2}$$

where $C(d)$ is a positive constant that may depend on d.

This bound has been extended to L_p discrepancy ($1 < p < \infty$) by Schmidt [29], who has also obtained a lower estimate for the L_∞ (extremal) discrepancy:

Theorem 2 (Schmidt [28]). *In dimension $d = 2$,*

$$D(N,2)_\infty \geq C \log N, \tag{3}$$

where C is a positive absolute constant.

It is well known that both bounds are sharp in the order of magnitude. While Eq. (3) is harder to prove than Eq. (2) (in fact, higher-dimensional analogs of Eq. (3) are still very far from being understood; see [3]), its sharpness had been known long before Eq. (3) has been established, [10, 22]. The example which is relevant to our discussion is the irrational lattice:

$$\mathscr{A}_N(\alpha) := \left\{ \left(\frac{\mu}{N}, \{\mu\alpha\} \right) \right\}_{\mu=0}^{N-1}, \tag{4}$$

where α is an irrational number and $\{x\}$ is the fractional part of the number x. If the partial quotients of the continued fraction of α are bounded, then the L_∞ discrepancy of this set is of the order $\log N$ (see, e.g., [20, 23]). The idea of this example goes back to Lerch [22].

It is often more convenient and effective to work with rational approximations of such lattices. For an irrational number α with the continued fraction expansion

$$\alpha = [a_0; a_1, a_2, \dots] = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \dots}}}, \tag{5}$$

where $a_0 \in \mathbb{Z}$, $a_k \in \mathbb{N}$, $k \geq 1$, we denote by p_n/q_n the nth order convergents of α, that is, $p_n/q_n = [a_0; a_1, \dots, a_n]$.

We consider the sets

$$\mathscr{L}_n(\alpha) := \big\{ (\mu/q_n, \{\mu p_n/q_n\}) \big\}_{\mu=0}^{q_n-1}, \tag{6}$$

consisting of q_n points, which approximate $\mathscr{A}_{q_n}(\alpha)$. A particular example of such sets is the popular *Fibonacci lattice*. Let $\{b_n\}_{n=0}^{\infty}$ be the sequence of Fibonacci numbers:

$$b_0 = b_1 = 1, \quad b_n = b_{n-1} + b_{n-2}, \quad \text{for} \quad n \geq 2. \tag{7}$$

The b_n-point Fibonacci set $\mathscr{F}_n \subset [0,1]^2$ is then defined as

$$\mathscr{F}_n := \{ (\mu/b_n, \{\mu b_{n-1}/b_n\}) \}_{\mu=0}^{b_n-1}. \tag{8}$$

Obviously, for large n, the set $\mathscr{F}_n$ is close to the irrational lattice $\mathscr{A}_N(\alpha)$ with $N = b_n$ and $\alpha = \frac{\sqrt{5}-1}{2}$, that is, the reciprocal of the *golden section*. For this value of α, we have $a_0 = 1$, $a_k = 1$ for $k \geq 1$, and $p_n = b_{n-1}$, $q_n = b_n$. Therefore, $\mathscr{F}_n = \mathscr{L}_n\big((\sqrt{5}-1)/2\big)$. It is well known (see e.g., [24]) that

$$\|D(\mathscr{F}_n, \mathbf{x})\|_\infty \leq C \log b_n \leq C' n; \tag{9}$$

hence, Fibonacci sets also have optimal L_∞ discrepancy. Similar bounds hold for more general lattices $\mathscr{L}_n(\alpha)$ whenever the sequence $\{a_k\}$ of the partial quotients of α is bounded. These results can be derived either directly or as a perturbation of the corresponding results for the irrational lattice $\mathscr{A}_N(\alpha)$.

Another standard example of a set with optimal L_∞ discrepancy is the *van der Corput set* $\mathscr{V}_n$ defined as the collection of 2^n points of the form

$$\big(0.x_1 x_2 \dots x_n, 0.x_n x_{n-1} \dots x_2 x_1\big), \; x_k = 0 \text{ or } 1, \tag{10}$$

where the coordinates are written in binary expansion. While this set is not directly related to our discussion, we shall sometimes compare the properties of $\mathscr{V}_n$ and the lattices $\mathscr{A}_N(\alpha)$ or $\mathscr{L}_n(\alpha)$. An interesting relation between the Fibonacci and van der Corput sequences is discussed in [15].

In contrast to the L_∞ case, the sharpness of the L_2 bound (2) is harder to demonstrate. Most constructions are obtained as modifications of the classical distributions with low L_∞ discrepancy. These modifications are often necessary—for instance, it is known that the L_2 discrepancy of the van der Corput set is not optimal: it is of the order $\log N$ rather than $\sqrt{\log N}$. The first example of a set with L_2 discrepancy of the order $\sqrt{\log N}$ has been constructed by Davenport [11] in 1956 by symmetrizing the irrational lattice $\mathscr{A}_N(\alpha)$:

$$\begin{aligned}\mathscr{A}'_{\mathscr{N}}(\alpha) &:= \{(\{\mu/N\},\{\mu\alpha\})\}_{\mu=-(N-1)}^{N-1} \\ &= \mathscr{A}_{\mathscr{N}}(\alpha) \cup \{(1-x,y) : (x,y) \in \mathscr{A}_{\mathscr{N}}(\alpha)\}.\end{aligned} \tag{11}$$

It has been shown by the authors of this chapter [5] that the same holds for the L_2 discrepancy of an analogous symmetrization $\mathscr{F}'_n$ of the Fibonacci set $\mathscr{F}_n$ (in this case, a naive perturbation argument does not work) and their method can be easily generalized to obtain the L_2 optimality of the symmetrizations of $\mathscr{L}_n(\alpha)$. Both in the case of $\mathscr{A}'_N(\alpha)$ and of $\mathscr{F}'_n$, the proofs used the Fourier series of the discrepancy function.

Davenport's work, however, has not addressed the question whether this symmetrization is really necessary; in other words, what is the L_2 discrepancy of the non-symmetrized lattices $\mathscr{A}_N(\alpha)$ or $\mathscr{L}_n(\alpha)$? In 1979, Sós and Zaremba [31] gave a partial answer to this question by proving that, when all the partial quotients of the (finite or infinite) continued fraction of α are equal, the set $\mathscr{A}_N(\alpha)$ has optimal L_2 discrepancy. In particular, their result covers the Fibonacci set $\mathscr{F}_n$ and the irrational lattice $\mathscr{A}_N((\sqrt{5}-1)/2)$ when all the partial quotients are equal to 1:

$$\|D(\mathscr{F}_n,\mathbf{x})\|_2 \asymp \|D\Big(\mathscr{A}_{b_n}\Big(\Big(\sqrt{5}-1\Big)/2,\mathbf{x}\Big)\|_2 \asymp \sqrt{\log b_n}. \tag{12}$$

It is also suggested in the same paper that perhaps the L_2 discrepancy is not optimal for some other values of α. This means that the L_2 discrepancy depends on much finer properties of α than simply the boundedness of its partial quotients.

In this chapter we continue this line of investigation. In Sect. 2, we give a Fourier-analytic proof of the fact that the nonsymmetrized Fibonacci lattice $\mathscr{F}_n$ has optimal order of magnitude of L_2 discrepancy. While this result is just a partial case of the aforementioned result of Sós and Zaremba, our proof, based on the computation of the Fourier coefficients, is much more direct and transparent. It also yields an exact formula for the L_2 discrepancy of $\mathscr{F}_n$, which opens the door to numerical experiments. In addition, this method easily generalizes and allows one to investigate other rational lattices $\mathscr{L}_n(\alpha)$.

In Sect. 3, we demonstrate how one can adapt the arguments used for the Fibonacci sets $\mathscr{F}_n$ to more general lattices. It is often the case that, when a low-discrepancy set fails to have the optimal L_2 discrepancy, the problem lies already in the Fourier coefficient of order zero: the integral $\int_{[0,1]^d} D(\mathscr{P}_N,\mathbf{x})d\mathbf{x}$; see, for example, [4, 17]. We show that this is indeed the case for the lattices $\mathscr{L}_n(\alpha)$, that is, the contribution of the other Fourier coefficients to the L_2 norm is of the order $\sqrt{\log N}$.

We also observe that the main term [the integral of the discrepancy function of $\mathscr{L}_n(\alpha)$] is closely related to the Dedekind sums, an object often arising in number theory and geometry. In particular, it allows us to show that the behavior of the integral of the discrepancy function is controlled by the growth of the alternating sums of the partial quotients of α: $\sum_{k=0}^{n}(-1)^k a_k$, which, in particular, reveals the nature of the condition that all a_k's are the same in the result of Sós and Zaremba [31]. To be more precise, we prove the following theorem:

Theorem 3. *Let $\alpha = [a_0; a_1, a_2, \ldots]$ be an irrational number with bounded partial quotients. Denote the nth convergents of α by p_n/q_n and consider the lattice $\mathscr{L}_n(\alpha)$ as defined in Eq.* (6)*. Then its L_2 discrepancy satisfies*

$$\|D(\mathscr{L}_n(\alpha), \mathbf{x})\|_2 \approx \max\left\{\sqrt{\log q_n}, \left|\sum_{k=0}^{n}(-1)^k a_k\right|\right\}. \tag{13}$$

By $A \approx B$, we mean that "A is of the same order as B", that is, $A = \mathscr{O}(B)$ and $B = \mathscr{O}(A)$, as n (or N) tends to infinity (the implicit constants are independent of n or N, but may depend on the number α). Therefore, when the alternating sum of a_k's does not grow too fast, the lattices $\mathscr{L}_n(\alpha)$ have optimal order of L_2 discrepancy even *without the symmetrization*. Since $\log q_n \approx n$, this happens precisely when

$$\left|\sum_{k=0}^{n}(-1)^k a_k\right| \ll \sqrt{n}, \tag{14}$$

where $A \ll B$ means $A = \mathscr{O}(B)$. We thus characterize all the lattices $\mathscr{L}_n(\alpha)$ for which the L_2 discrepancy is minimal in the sense of order. In Sect. 4, we make some further remarks concerning the behavior of the L_2 discrepancy for certain specific values of α.

To finish the introduction, we would like to mention that constructions of sets with optimal L_2 or L_p discrepancies are an important problem in discrepancy theory and quasi-Monte Carlo methods. Following the result of Davenport [11] in dimension $d = 2$, Roth [27] constructed sets with optimal L_2 discrepancy in all dimensions. Chen [7] and Frolov [14] have constructed sets with minimal order of L_p discrepancy for $1 < p < \infty$. It is interesting to point out that in dimensions $d \geq 3$, all the known constructions until recently were probabilistic. The first deterministic examples were provided in the last decade by Chen and Skriganov [8, 9, 30].

Cubature formulas based on Fibonacci lattice have been thoroughly studied in approximation theory [34, 35]. Rational lattices $\mathscr{L}_n(\alpha)$ are obviously more practical than the irrational lattices $\mathscr{A}_N(\alpha)$; besides, cubature formulas built on $\mathscr{L}_n(\alpha)$ perform better in spaces with mixed smoothness of order $r > 2$; see [5, 18, 36].

2 The L_2 Discrepancy of the Fibonacci Set

In this section, we prove the L_2 bound for the discrepancy of the Fibonacci set, particularly giving a new proof of the result of Sós and Zaremba [31]. Recall that the discrepancy function of the Fibonacci set is

$$D(\mathscr{F}_n,\mathbf{x}) := \#\{\mathscr{F}_n \cap [\mathbf{0},\mathbf{x})\} - b_n x_1 x_2 = \sum_{\mathbf{p}=(p_1,p_2)\in\mathscr{F}_n} \chi_{[p_1,1)\times[p_2,1)}(\mathbf{x}) - b_n x_1 x_2,$$

where $\mathbf{x} = (x_1,x_2) \in [0,1]^2$. We compute the Fourier coefficients of the $D(\mathscr{F}_n,\mathbf{x})$:

$$\begin{aligned}\widehat{D}(\mathscr{F}_n,\mathbf{k}) = &\sum_{\mathbf{p}\in\mathscr{F}_n} \int_{p_1}^1 e^{-2\pi i k_1 x_1} dx_1 \int_{p_2}^1 e^{-2\pi i k_2 x_2} dx_2 \\ &- b_n \int_0^1 x_1 e^{-2\pi i k_1 x_1} dx_1 \int_0^1 x_2 e^{-2\pi i k_2 x_2} dx_2.\end{aligned} \tag{15}$$

Note that

$$\sum_{\mu=1}^{b_n} e^{-2\pi i l \mu / b_n} = \begin{cases} b_n, & l \equiv 0 \pmod{b_n}, \\ 0, & l \not\equiv 0 \pmod{b_n}. \end{cases} \tag{16}$$

Let $L(n) := \{\mathbf{k} = (k_1,k_2) \in \mathbf{Z}^2 : k_1 + b_{n-1}k_2 \equiv 0 \pmod{b_n}\}$, then

$$\sum_{\mu=1}^{b_n} e^{-2\pi i (k_1 + b_{n-1}k_2)\mu / b_n} = \begin{cases} b_n, & (k_1,k_2) \in L(n), \\ 0, & (k_1,k_2) \notin L(n). \end{cases} \tag{17}$$

We consider different cases.

Case 1. $\mathbf{k} = (0,0)$. (*The integral of* $D(\mathscr{F}_n,\mathbf{x})$). Standard heuristics in discrepancy theory state that this case usually presents the most important complications in obtaining favorable L_2 estimates. In fact, in the case of the van der Corput set, this term is solely responsible for the L_2 discrepancy being too large; see [4, 17]. Davenport's symmetrization was created precisely to eliminate this term in the Fourier series of the discrepancy function. One can compute this term precisely in the case of the Fibonacci lattice:

Lemma 1.

$$\widehat{D}(\mathscr{F}_n,\mathbf{0}) = \begin{cases} \dfrac{3}{4}, & \textit{for } n \textit{ even}, \\ \dfrac{b_{n-1}}{6b_n} + \dfrac{7}{12}, & \textit{for } n \textit{ odd}. \end{cases} \tag{18}$$

Proof. From Eq. (15), we obtain

$$\begin{aligned}\widehat{D}(\mathscr{F}_n,\mathbf{0}) &= \sum_{\mu=0}^{b_n-1} \left(1 - \frac{\mu}{b_n}\right)\left(1 - \left\{\frac{\mu b_{n-1}}{b_n}\right\}\right) - \frac{b_n}{4} \\ &= \sum_{\mu=1}^{b_n-1} \mu/b_n \cdot \{\mu b_{n-1}/b_n\} - \frac{b_n}{4} + 1,\end{aligned} \tag{19}$$

where we have used the fact that $\sum_{\mu=0}^{b_n-1} \mu/b_n = \sum_{\mu=0}^{b_n-1} \{\mu b_{n-1}/b_n\} = \frac{b_n-1}{2}$.

We shall now connect $\widehat{D}(\mathscr{F}_n,\mathbf{0})$ to a well-known object in number theory—the Dedekind sum. The (inhomogeneous) Dedekind sum is defined as

$$\mathscr{D}(p,q) = \sum_{\mu=1}^{q-1} \rho\left(\frac{\mu}{q}\right)\rho\left(\frac{p\mu}{q}\right), \tag{20}$$

where $\rho(x) = \frac{1}{2} - \{x\}$ is the sawtooth function and p, q are positive integers. These sums have already appeared in the context of discrepancy, uniform distribution, and Fibonacci numbers, for example, [25, 37, 38]. We have the following relation:

$$\begin{aligned} \mathscr{D}(b_{n-1},b_n) &= \sum_{\mu=1}^{b_n-1}\left(\frac{1}{2}-\frac{\mu}{b_n}\right)\left(\frac{1}{2}-\left\{\frac{\mu b_{n-1}}{b_n}\right\}\right) \\ &= \sum_{\mu=1}^{b_n-1} \mu/b_n \cdot \{\mu b_{n-1}/b_n\} - \frac{b_n}{4} + \frac{1}{4}. \end{aligned} \tag{21}$$

We thus see from Eqs. (19) and (21) that

$$\widehat{D}(\mathscr{F}_n,\mathbf{0}) = \mathscr{D}(b_{n-1},b_n) + \frac{3}{4}. \tag{22}$$

The Dedekind sum $\mathscr{D}(p,q)$ can be computed in terms of the continued fraction expansion of p/q. The following formula holds [1, 16]:

Proposition 1. *Let n be the length of the continued fraction expansion of p/q and let p_k/q_k denote the kth convergents of p/q, $k \le n$, and a_0, a_1, …, a_n be the partial quotients. Then*

$$\mathscr{D}(p,q) = \begin{cases} \dfrac{1}{12}\left(\dfrac{p_n - q_{n-1}}{q_n} - \displaystyle\sum_{k=0}^{n}(-1)^k a_k\right), & \textit{for } n \textit{ even}, \\[2ex] \dfrac{1}{12}\left(\dfrac{p_n + q_{n-1}}{q_n} - \displaystyle\sum_{k=0}^{n}(-1)^k a_k\right) - \dfrac{1}{4}, & \textit{for } n \textit{ odd}. \end{cases} \tag{23}$$

In our case, $p = b_{n-1}$ and $q = b_n$, $p_n = q_{n-1} = b_{n-1}$, $q_n = b_n$, $a_0 = 0$, and $a_1 = a_2 = \cdots = a_n = 1$, which yields the result of Lemma 1. □

Case 2. $k_1 \neq 0$, $k_2 \neq 0$. In this case, Eq. (15) becomes

$$\widehat{D}(\mathscr{F}_n,\mathbf{k}) = \frac{-1}{4\pi^2 k_1 k_2}\sum_{\mathbf{p}\in\mathscr{F}_n}(1-e^{-2\pi i k_1 p_1})(1-e^{-2\pi i k_2 p_2}) + \frac{b_n}{4\pi^2 k_1 k_2}, \tag{24}$$

which together with Eqs. (16) and (17) leads to the following lemmas:

Lemma 2. *If* $k_1 \neq 0$, $k_2 \neq 0$, *then*

$$\widehat{D}(\mathscr{F}_n, \mathbf{k}) = \frac{b_n}{4\pi^2 k_1 k_2} \tag{25}$$

provided that at least one of k_1 *and* k_2 *is* 0 *modulo* b_n.

Lemma 3. *Assume* $k_1 \not\equiv 0 \pmod{b_n}$ *and* $k_2 \not\equiv 0 \pmod{b_n}$, *then*

$$\widehat{D}(\mathscr{F}_n, \mathbf{k}) = \begin{cases} \dfrac{-b_n}{4\pi^2 k_1 k_2}, & k_1 + k_2 b_{n-1} \equiv 0, \ \text{i.e. } \mathbf{k} \in L(n) \\ 0, & k_1 + k_2 b_{n-1} \not\equiv 0, \ \text{i.e. } \mathbf{k} \notin L(n), \end{cases} \tag{26}$$

where all congruences are taken modulo b_n.

Case 3. $k_1 = 0, k_2 \neq 0$. We have the following lemma:

Lemma 4. *If* $k_1 = 0, k_2 \neq 0$,

$$\widehat{D}(\mathscr{F}_n, \mathbf{k}) = \begin{cases} \dfrac{b_n}{4\pi i k_2}, & k_2 \equiv 0 \pmod{b_n}, \\ -\dfrac{1}{4\pi i k_2} \cdot \dfrac{e^{-2\pi i k_2 b_{n-1}/b_n} + 1}{e^{-2\pi i k_2 b_{n-1}/b_n} - 1}, & k_2 \not\equiv 0 \pmod{b_n}. \end{cases} \tag{27}$$

Proof. From Eq. (15), we obtain

$$\widehat{D}(\mathscr{F}_n, \mathbf{k}) = \frac{-1}{2\pi i k_2} \sum_{\mathbf{p} \in \mathscr{F}_n} (1 - p_1)(1 - e^{-2\pi i k_2 p_2}) + \frac{b_n}{4\pi i k_2}.$$

The case $k_2 \equiv 0$ is trivial. When $k_2 \not\equiv 0$, one is faced with the sum $\sum_{\mu=0}^{b_n-1} \frac{\mu}{b_n} e^{-\frac{2\pi i k_2 \mu b_{n-1}}{b_n}}$, which can be computed by considering the function $f(x) = \sum_{\mu=0}^{b_n-1} e^{\frac{2\pi i \mu x}{b_n}} = \frac{e^{2\pi i x} - 1}{e^{\frac{2\pi i x}{b_n}} - 1}$ and observing that the aforementioned sum equals $f'(-k_2 b_{n-1})/2\pi i$.

Case 4. $k_1 \neq 0$, $k_2 = 0$. This case is the same as the previous case due to the well-known relation $b_n^2 - b_{n+1} b_{n-1} = (-1)^n$, which implies that

$$\mathscr{F}_n = \left\{ \left(\frac{\mu}{b_n}, \left\{ \frac{\mu b_{n-1}}{b_n} \right\} \right) \right\}_{\mu=0}^{b_n-1} = \left\{ \left(\left\{ \frac{(-1)^{n-1} r b_{n-1}}{b_n} \right\}, \frac{r}{b_n} \right) \right\}_{r=0}^{b_n-1}.$$

In other words, the Fibonacci set possesses some inner symmetry: if n is odd, it is simply symmetric with respect to the diagonal $x = y$; if n is even, the symmetry involves an additional reflection about the axis $x = \frac{1}{2}$.

Lemma 5. *If* $k_1 \neq 0, k_2 = 0$,

$$\widehat{D}(\mathscr{F}_n, \mathbf{k}) = \begin{cases} \dfrac{b_n}{4\pi i k_1}, & k_1 \equiv 0 \pmod{b_n}, \\ -\dfrac{1}{4\pi i k_1} \cdot \dfrac{e^{(-1)^n 2\pi i k_1 b_{n-1}/b_n} + 1}{e^{(-1)^n 2\pi i k_1 b_{n-1}/b_n} - 1}, & k_1 \not\equiv 0 \pmod{b_n}. \end{cases}$$

Theorem 4. *For the Fibonacci set* $\mathscr{F}_n \subset [0,1]^2$*, we have*

$$\|D(\mathscr{F}_n, \mathbf{x})\|_2 \ll \sqrt{\log b_n}. \tag{28}$$

We first derive a formula providing the exact value of $\|D(\mathscr{F}_n, \mathbf{x})\|_2$. We start with the contribution of Lemma 3. In this case, $\widehat{D}(\mathscr{F}_n, \mathbf{k}) = -\frac{b_n}{4\pi^2 k_1 k_2}$. We make use of the well-known identity (see e.g., [32], p. 165, ex. 15):

$$\sum_{n \in \mathbb{Z}} \frac{1}{(n+x)^2} = \frac{\pi^2}{\sin^2(\pi x)}. \tag{29}$$

For $\mathbf{k} \in L(n)$, $k_i \not\equiv 0 \pmod{b_n}$, denote $k_1 + k_2 b_{n-1} = l b_n$, for $l \in \mathbb{Z}$ and $k_2 = m b_n + r$, where $m \in \mathbb{Z}$ and $r = 1, \ldots, b_n - 1$. Lemma 3 implies

$$\begin{aligned} \sum_{\mathbf{k} \in L(n), k_i \neq 0} \left| \widehat{D}(\mathscr{F}_n, \mathbf{k}) \right|^2 &= \frac{b_n^2}{16\pi^4} \sum_{k_2 \neq 0 \bmod b_n} \frac{1}{k_2^2} \sum_{l \in \mathbb{Z}} \frac{1}{b_n^2} \cdot \frac{1}{\left(l - \frac{b_{n-1} k_2}{b_n}\right)^2} \\ &= \frac{1}{16\pi^2} \sum_{r=1}^{b_n - 1} \frac{1}{\sin^2\left(\frac{\pi b_{n-1} r}{b_n}\right)} \sum_{m \in \mathbb{Z}} \frac{1}{b_n^2} \cdot \frac{1}{\left(m + \frac{r}{b_n}\right)^2} \\ &= \frac{1}{16 b_n^2} \sum_{r=1}^{b_n - 1} \frac{1}{\sin^2\left(\frac{\pi b_{n-1} r}{b_n}\right) \cdot \sin^2\left(\frac{\pi r}{b_n}\right)}. \end{aligned} \tag{30}$$

In the setting of Lemma 2 ($k_1, k_2 \neq 0$ and at least one of them is zero modulo b_n), inclusion-exclusion principle and the identity $\sum_{l \in \mathbb{N}} \frac{1}{l^2} = \frac{\pi^2}{6}$ yield

$$\begin{aligned} \sum_{\mathbf{k} \sim \text{Lemma 2}} \left| \widehat{D}(\mathscr{F}_n, \mathbf{k}) \right|^2 &= 4 \cdot \frac{b_n^2}{16\pi^4} \cdot \left(2 \cdot \sum_{l,k \in \mathbb{N}} \frac{1}{l^2 b_n^2 \cdot k^2} - \sum_{l_1, l_2 \in \mathbb{N}} \frac{1}{b_n^4 l_1^2 l_2^2} \right) \\ &= \frac{b_n^2}{4\pi^4} \cdot \left(\frac{2\pi^4}{36 b_n^2} - \frac{\pi^4}{36 b_n^4} \right) = \frac{1}{72} \left(1 - \frac{1}{2 b_n^2} \right), \end{aligned} \tag{31}$$

where multiplication by 4 accounts for all possible choices of signs. We now turn to the first contribution of Lemma 4: $k_1 = 0$, $k_2 \not\equiv 0 \pmod{b_n}$:

$$\left|\widehat{D}(\mathscr{F}_n,\mathbf{k})\right|^2 = \frac{1}{16\pi^2k_2^2}\cdot\frac{e^{-2\pi i k_2 b_{n-1}/b_n}+1}{e^{-2\pi i k_2 b_{n-1}/b_n}-1}\cdot\frac{e^{2\pi i k_2 b_{n-1}/b_n}+1}{e^{2\pi i k_2 b_{n-1}/b_n}-1}$$
$$= \frac{1}{16\pi^2k_2^2}\cdot\frac{1+\cos\left(\frac{2\pi k_2 b_{n-1}}{b_n}\right)}{1-\cos\left(2\pi\frac{k_2 b_{n-1}}{b_n}\right)} = \frac{1}{16\pi^2k_2^2}\cdot\frac{\cos^2\left(\frac{\pi k_2 b_{n-1}}{b_n}\right)}{\sin^2\left(\frac{\pi k_2 b_{n-1}}{b_n}\right)}. \quad (32)$$

Writing $k_2 = lb_n + r$, $l \in \mathbb{Z}$, $r = 1,\dots,b_n - 1$ and using Eq. (29), we obtain

$$\sum_{k_2\neq 0}\left|\widehat{D}(\mathscr{F}_n,(0,k_2))\right|^2 = \frac{1}{16\pi^2}\sum_{l\in\mathbb{Z}}\sum_{r=1}^{b_n-1}\frac{1}{b_n^2\cdot\left(l+\frac{r}{b_n}\right)^2}\cdot\frac{\cos^2(\pi k_2 b_{n-1}/b_n)}{\sin^2(\pi k_2 b_{n-1}/b_n)}$$
$$= \frac{1}{16b_n^2}\sum_{r=1}^{b_n-1}\frac{\cos^2\left(\frac{\pi r b_{n-1}}{b_n}\right)}{\sin^2\left(\frac{\pi r}{b_n}\right)\cdot\sin^2\left(\frac{\pi r b_{n-1}}{b_n}\right)}. \quad (33)$$

Finally, the second contribution of Lemma 4 ($k_2 \neq 0$, $k_2 \equiv 0 \pmod{b_n}$) is

$$\sum_{k_2\equiv 0, k_2\neq 0}\left|\widehat{D}(\mathscr{F}_n,(0,k_2))\right|^2 = \frac{b_n^2}{16\pi^2}\sum_{l\in\mathbb{Z}\setminus\{0\}}\frac{1}{b_n^2 l^2} = \frac{1}{48}. \quad (34)$$

Obviously, when $k_2 = 0$, the contributions are identical to Eqs. (33) and (34).

We are now ready to prove the main theorem and to derive the exact formula for $\|D(\mathscr{F}_n,\mathbf{x})\|_2^2$.

Proof of Theorem 4: Both $\widehat{D}(\mathscr{F}_n,\mathbf{0})$ and the contributions described in Eqs. (31) and (34) are bounded by an absolute constant. By comparing Eq. (33) to Eq. (30), we see that all the other contributions to the L_2 norm are dominated by the contribution of the terms corresponding to Lemma 3, that is, $\mathbf{k} \in L(n)$. However, dealing with these terms is a standard issue, which relies on the properties of $L(n)$. See, for example, Sect. 3 (Lemma 7) or [5, 34] for details. □

Putting together Eqs. (30), (31), (33), and (34), and the value of $\widehat{D}(\mathscr{F}_n,\mathbf{0})$ (Lemma 1), we obtain

Theorem 5. *For $n \geq 2$, we have*

$$\|D(\mathscr{F}_n,\mathbf{x})\|_2^2 = \frac{1}{16b_n^2}\sum_{r=1}^{b_n-1}\frac{1+2\cos^2\left(\frac{\pi r b_{n-1}}{b_n}\right)}{\sin^2\left(\frac{\pi r}{b_n}\right)\cdot\sin^2\left(\frac{\pi r b_{n-1}}{b_n}\right)} + \frac{89}{144} - \frac{1}{144b_n^2} \quad (35)$$

when n is even and

$$\|D(\mathscr{F}_n,\mathbf{x})\|_2^2 = \frac{1}{16b_n^2}\sum_{r=1}^{b_n-1}\frac{1+2\cos^2\left(\frac{\pi r b_{n-1}}{b_n}\right)}{\sin^2\left(\frac{\pi r}{b_n}\right)\cdot\sin^2\left(\frac{\pi r b_{n-1}}{b_n}\right)} + \frac{1}{18} - \frac{1}{144b_n^2} + \left(\frac{b_{n-1}}{6b_n} + \frac{7}{12}\right)^2$$

when n is odd.

Numerical experiments indicate that the main term in the formulae above

$$S_n = \frac{1}{16b_n^2}\sum_{r=1}^{b_n-1}\frac{1+2\cos^2\left(\frac{\pi r b_{n-1}}{b_n}\right)}{\sin^2\left(\frac{\pi b_{n-1}}{b_n}\right)\cdot\sin^2\left(\frac{\pi r b_{n-1}}{b_n}\right)} \approx 0.0224\cdot n, \tag{36}$$

which is worse than $S_n' = \frac{1}{8b_n^2}\sum_{r=1}^{b_n-1}\frac{1}{\sin^2\left(\frac{\pi b_{n-1} r}{b_n}\right)\cdot\sin^2\left(\frac{\pi r}{b_n}\right)} \approx 0.0149\cdot n$, the corresponding leading term of the analogous formula for the *symmetrized* Fibonacci set [5]. In fact, it is easy to see that $S_n = \frac{3}{2}S_n' + \mathscr{E}_n$, where the error term $\mathscr{E}_n$ converges to a finite limit as $n\to\infty$. Hence, the L_2 discrepancy of the Fibonacci set exceeds the L_2 discrepancy of its symmetrized version by about 50 % for large n.

One can show directly that the term S_n is of the order $\log b_n \approx n$, which would give a different proof of Theorem 4. A number-theoretic argument to that effect has been pointed out to us by Konstantin Oskolkov.

It is worth pointing out that the best currently known value of the constant $\lim_n \frac{\|D(\mathscr{P}_N,\mathbf{x}\|_2}{\sqrt{\log N}}$ is about 0.17907 [12]. The results of our numerical experiments (see also [5]) suggest that perhaps for the symmetrized Fibonacci lattice, this value may be slightly better, ≈ 0.176006, while for $\mathscr{F}_n$, it is about 0.264009. The largest known constant in the lower bound (2) in dimension $d=2$ is approximately 0.038925 [19].

3 General Lattices

It is fairly straightforward to extend the argument of the previous section to general lattices $\mathscr{L}_n(\alpha)$. Denote

$$L_\alpha(n) := \{\mathbf{k} : k_1 + p_n k_2 \equiv 0 \pmod{q_n}\}. \tag{37}$$

Repeating all the computations almost line by line, we obtain

Lemma 6. *When $k_1 \neq 0$, $k_2 \neq 0$, we have*

$$\widehat{D}(\mathscr{L}_n(\alpha),\mathbf{k}) = \begin{cases} \dfrac{q_n}{4\pi^2 k_1 k_2}, & k_1 \equiv 0 \text{ or } k_2 \equiv 0,\\ \dfrac{-q_n}{4\pi^2 k_1 k_2}, & k_1, k_2 \not\equiv 0,\ \mathbf{k}\in L_\alpha(n),\\ 0, & k_1,k_2\not\equiv 0,\ \mathbf{k}\notin L_\alpha(n). \end{cases} \tag{38}$$

If $k_1 = 0, k_2 \neq 0$,

$$\widehat{D}(\mathscr{L}_n(\alpha),(0,k_2)) = \begin{cases} \dfrac{q_n}{4\pi i k_2}, & k_2 \equiv 0,\\ -\dfrac{1}{4\pi i k_2}\cdot\dfrac{e^{-2\pi i k_2 p_n/q_n}+1}{e^{-2\pi i k_2 p_n/q_n}-1}, & k_2\not\equiv 0. \end{cases} \tag{39}$$

If $k_1 \neq 0, k_2 = 0$,

$$\widehat{D}(\mathscr{L}_n(\alpha),(k_1,0)) = \begin{cases} \dfrac{q_n}{4\pi i k_1}, & k_1 \equiv 0, \\ -\dfrac{1}{4\pi i k_1} \cdot \dfrac{e^{(-1)^n 2\pi i k_1 q_{n-1}/q_n}+1}{e^{(-1)^n 2\pi i k_1 q_{n-1}/q_n}-1}, & k_1 \not\equiv 0. \end{cases} \tag{40}$$

Moreover, we have

$$|\widehat{D}(\mathscr{L}_n(\alpha),\mathbf{0})| = \left|\mathscr{D}(p_n,q_n)+\frac{3}{4}\right| \leq \mathscr{O}(1)+\frac{1}{12}\left|\sum_{k=0}^{n}(-1)^k a_k\right|, \tag{41}$$

where $\mathscr{D}(p,q)$ *is the Dedekind sum defined in Eq.* (20) *and the implicit constant in* $\mathscr{O}(1)$ *depends only on* α. *All the congruences above are modulo* q_n.

To pass from the case $k_2 = 0$ to $k_1 = 0$, we used the identity $p_n q_{n-1} - p_{n-1} q_n = (-1)^{n-1}$, which implies that $\mathscr{L}_n(\alpha) = \left\{(\{(-1)^{n-1} q_{n-1} r/q_n\}, r/q_n\right\}_{r=0}^{q_n-1}$. The exact formula for the L_2 discrepancy can also be derived.

Theorem 6. *We have the following relation:*

$$\|D(\mathscr{L}_n(\alpha),\mathbf{x})\|_2^2 = \frac{1}{16q_n^2}\sum_{r=1}^{q_n-1}\frac{1+2\cos^2(\pi r p_n/q_n)}{\sin^2(\pi r/q_n)\cdot\sin^2(\pi r p_n/q_n)} + \left(\mathscr{D}(p_n,q_n)+\frac{3}{4}\right)^2 + \frac{1}{18} - \frac{1}{144q_n^2}. \tag{42}$$

We are now ready to estimate the size of L_2 discrepancy of $\mathscr{L}_n(\alpha)$.

Proof of Theorem 3. Obviously, the zero-order Fourier coefficient (41) grows exactly as the alternating sum of a_k's. We shall show that the contribution of the other terms is of the order $\sqrt{\log q_n}$. One can easily see from Lemma 6 and Eq. (42) that this contribution is dominated by the input of the coefficients corresponding to $\mathbf{k} \in L_\alpha(n)$. Define the hyperbolic cross $\Gamma(M) = \{(k_1,k_2) \in \mathbb{Z}^2 : |k_1 k_2| \leq M;\ |k_1|,|k_2| \leq M\}$. We have the following lemma concerning the structure of the set $L_\alpha(n)$:

Lemma 7. *There exists* $\gamma > 0$ *depending only on* α, *such that for* $n > 2$,

$$\Gamma(\gamma q_n) \cap L_\alpha(n) = \mathbf{0}. \tag{43}$$

A version of this lemma restricted to $p_n = b_{n-1}$, $q_n = b_n$ is known and has been used repeatedly to obtain discrepancy estimates and errors of cubature formulas for the Fibonacci set [5, 33, 34]. Here, we prove the lemma in full generality:

Proof. Let $k_1 + p_n k_2 = l q_n$, $l \in \mathbb{Z}$. It suffices to assume $0 < |k_1|, |k_2| < q_n$. We have $k_1 k_2 = q_n k_2^2 \left(\frac{l}{k_2} - \frac{p_n}{q_n}\right)$. Denote $\Delta = \frac{l}{k_2} - \frac{p_n}{q_n}$. Since $|k_2| < q_n$ and the convergent p_n/q_n is the best approximation to α, we have $|\alpha - l/k_2| > |\alpha - p_n/q_n|$. Choose $\nu \in \mathbb{N}$ to be the smallest index such that $q_\nu > |k_2|$ and l/k_2 and p_ν/q_ν lie on the same side from α. Then $\nu \le n$, $q_{\nu-2} \le |k_2| < q_\nu$, and $|\alpha - l/k_2| > |\alpha - p_\nu/q_\nu|$. Moreover, the relation $q_\nu = a_\nu q_{\nu-1} + q_{\nu-2}$ implies that $q_\nu \le (A+1)^2 q_{\nu-2}$, where $A = \max a_k$: incidentally, here we use the fact that α has bounded partial quotients. We have $|\Delta| \ge \left|\frac{l}{k_2} - \frac{p_\nu}{q_\nu}\right|$ (if p_n/q_n is on the other side of α it is obvious; otherwise, it is closer to α since $n \ge \nu$). Therefore, since p_ν/q_ν is irreducible and $\frac{l}{k_2} \ne \frac{p_\nu}{q_\nu}$,

$$|\Delta| \ge \left|\frac{l}{k_2} - \frac{p_\nu}{q_\nu}\right| \ge \frac{1}{|k_2| q_\nu} \ge \frac{1}{(A+1)^2} \frac{1}{|k_2| q_{\nu-2}} \ge \frac{\gamma}{k_2^2}. \tag{44}$$

Hence, $|k_1 k_2| \ge \gamma q_n$ with $\gamma = 1/(A+1)^2$. □

Denoting $Z_l := \big(\Gamma(2^{l+1}\gamma b_n) \setminus \Gamma(2^l \gamma b_n)\big) \cap L_\alpha(n)$, it is now easy to deduce from Eq. (43) that $\#Z_l \ll 2^l (l+1) \log q_n$. Then one obtains using Eq. (38)

$$\sum_{\mathbf{k} \in L_\alpha(n)} |\widehat{D}(\mathscr{L}_n(\alpha), \mathbf{k})|^2 \ll \sum_{l=0}^{\infty} \sum_{\mathbf{k} \in Z_l} \frac{1}{(2^l)^2} \ll \log q_n. \tag{45}$$

Together with Roth's lower estimate (2), this finishes the proof of Theorem 3. □

4 Further Remarks

It is interesting to discuss how the L_2 discrepancy of various specific lattices $\mathscr{L}_n(\alpha)$ behaves depending on the value of α. We list only a few observations here; a more comprehensive study of the number-theoretic aspects of this question will be conducted in the subsequent work of the authors.

It is evident from Theorem 3 that, while some lattices $\mathscr{L}_n(\alpha)$ have optimal L_2 discrepancy, others do not. Set, for example, $a_{2j} = 2$ and $a_{2j+1} = 1$, in this case, the alternating sums grow as $n \approx \log q_n$. At the same time, it follows from the arguments in [5] that symmetrizations of these lattices always have asymptotically minimal L_2 discrepancy. We make some peculiar remarks:

- It is not hard to construct numbers α such that the corresponding lattices $\mathscr{L}_n(\alpha)$ would have any prescribed rate of growth of L_2 discrepancy between $\sqrt{\log N}$ and $\log N$—one just needs to build a sequence $\{a_k\}$ for which the alternating sums behave appropriately. We are not aware of any prior results of this flavor.
- However, if $\alpha = k + l\sqrt{m}$ is a quadratic irrationality, there is a certain dichotomy: the L_2 discrepancy of $\mathscr{L}_n(\alpha)$ grows either as $\sqrt{\log N}$ or as $\log N$, intermediate rates are not possible. Indeed, it is well known that the continued fractions of quadratic irrationalities are periodic. Hence, the alternating sums of a_k are either bounded by a constant (e.g., if the length of the period is odd) or grow as n (when the period is even and the alternating sum within one cycle is nonzero).

- In particular, $\mathscr{L}_n(\sqrt{2})$ has optimal L_2 discrepancy since $\sqrt{2} = [1;\overline{2}]$, while the L_2 discrepancy of $\mathscr{L}_n(\sqrt{3})$ is of the order n. In general, it would be interesting to understand which square roots $\alpha = \sqrt{m}$ have odd periods of continued fractions. One common example is $m = p^2 + 1$. In this case, $\sqrt{m} = [p;\overline{2p}]$, so this example was essentially covered by the Sós and Zaremba [31] result.
- We list those values of m between 1 and 250 (other than $m = p^2 + 1$) for which the period of $\sqrt{m}$ is odd: 13, 29, 41, 53, 58, 61, 73, 74, 85, 89, 97, 106, 109, 113, 125, 130, 137, 149, 157, 173, 181, 185, 193, 202, 218, 229, 241, and 250. For these values of m, $\mathscr{L}_n(\sqrt{m})$ has optimal L_2 discrepancy.
- It is known that for any $P \in \mathbb{N}$, there exists $m \in \mathbb{N}$ such that the length of the period of the continued fraction of $\sqrt{m}$ is P [13].
- We do not know any values of m such that the length of the period of $\sqrt{m}$ is even, but the L_2 discrepancy of $\mathscr{L}_n(\sqrt{m})$ is of the order $\sqrt{n}$ (i.e., the alternating sum of a_k over one period is zero). In the following examples, for instance, the alternating sum of the partial quotients grows as n: $m = p^2 + 2$, $(p+1)^2 - 1$, or $p^2 + p$ ($\sqrt{p^2+2} = [p;\overline{p,2p}]$, $\sqrt{(p+1)^2-1} = [p;\overline{1,p-1,1,2p}]$, and $\sqrt{p^2+p} = [p;\overline{2,2p}]$). For such m, the $\mathscr{L}_n(\sqrt{m})$ is of the order $\log N$.

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