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BENFORD'S LAW FOR THE $3x + 1$ FUNCTION

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Abstract

Benford's law (to base B) for an infinite sequence $\{x_k : k \geqslant 1\}$ of positive quantities x_k is the assertion that $\{\log_B x_k : k \geqslant 1\}$ is uniformly distributed (mod 1). The $3x+1$ function $T(n)$ is given by $T(n) = (3n+1)/2$ if n is odd, and $T(n) = n/2$ if n is even. This paper studies the initial iterates $x_k = T^{(k)}(x_0)$ for $1 \leqslant k \leqslant N$ of the $3x+1$ function, where N is fixed. It shows that for most initial values x_0, such sequences approximately satisfy Benford's law, in the sense that the discrepancy of the finite sequence $\{\log_B x_k : 1 \leqslant k \leqslant N\}$ is small.

1. *Introduction*

The $3x + 1$ problem concerns the behavior under iteration of the map $T : \mathbb{Z} \to \mathbb{Z}$ given by $T(n) = n/2$ or $T(n) = (3n + 1)/2$ according to whether n is even or odd. That is, $T(2m) = m$ and $T(2m + 1) = 3m + 2$. The notorious $3x + 1$ conjecture asserts that when started from any positive integer n, some iterate $T^{(k)}(n) = 1$; it remains unsolved. Surveys of work on this problem have been carried out by Lagarias [**14**] and Wirsching [**25**].

It is well known that the initial iterates of this map exhibit a 'random' character. This holds in the sense that the initial iterates of a randomly selected integer appear to be even or odd with equal probability. Such a result can be rigorously justified if one takes the interval $1 \leqslant n \leqslant X = 2^k$ and considers only the first $k = \log_2 X$ iterations (see [**14**, Theorem A]). This leads to the rapid decay of most trajectories of the iteration under T, at an exponential rate, with an expected decrease by a multiplicative factor $\sqrt{3/4} \approx 0.86602$ at each step. These facts support the conjecture that all orbits of the $3x + 1$ iteration enter a bounded set, and hence fall into a finite number of periodic orbits. Heuristic stochastic models (such as those of Lagarias and Weiss [**15**] and Borovkov and Pfeifer [**4**]) predict that for an integer of size about X the 'random' character above persists for about the first $\alpha \log X$ iterates, with $\alpha = (\frac{1}{2}\log\frac{3}{4})^{-1} \approx 6.95212$; the model predicts that most integers of size near X will arrive at the periodic orbit $\{1, 2\}$ near this number of iterations. The stochastic model in [**15**] also predicts that for large n the number of steps to enter a periodic orbit should never exceed $42 \log n$. Experimentally, E. Roosendaal (private communication) has found a number n of size 7.2×10^{21} (he found $n = 72, 19\,136, 41\,637, 72\,362, 71\,195 \approx 7.2 \times 10^{21}$) which requires about $36.7 \log n$ iterations before entering the periodic orbit $\{1, 2\}$.

The present paper concerns the base B expansion of the initial sequence of the first N iterates of the $3x + 1$ map on a random starting value n, drawn from $1 \leqslant n \leqslant X$ where $X \geqslant 2^N$. This is in the region of the dynamics where most

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trajectories are decreasing at an exponential rate, before they enter a periodic orbit. It shows that, in a certain sense, the leading digits of the base B expansion of most such sequences approximately satisfy a strong form of Benford's law. Here Benford's law concerns the distribution of the initial digits in the base B expansion of an infinite sequence $\mathcal{X} = \{x_1, x_2, x_3, \dots\}$ of positive real numbers. The original version of Benford [**1**] in 1938 concerned the first few leading digits in the decimal expansion of real numbers in tables; the distribution had already been formulated by Newcomb [**20**] in 1881. An infinite sequence $\mathcal{X}$ is said to satisfy the *strong Benford's law* (to base B) if for each fixed $k \geqslant 1$, the first k digits in the B-ary expansion of $\{x_1, x_2, x_3, \dots\}$ approach limiting probabilities given by the 'B-ary Benford distribution', which we specify below. This is known to be equivalent to the condition that the associated infinite sequence $y_i := \log_B x_i$ is uniformly distributed modulo one (Diaconis [**6**, Theorem 1]). In the following we adopt this criterion as our definition of Benford's law.

This paper is motivated by work of Kontorovich and Miller [**11**], who showed that certain statistics drawn from $3x + 1$ iterates approximately obey Benford's law. They treated a version of the $3x + 1$ iteration in which the initial starting point w_0 is an odd integer, and they studied the subset of the successive odd integers $\{w_1, w_2, \dots\}$ appearing in the $3x + 1$ iteration of w_0. Here $w_i = T^{(k_i)}(w_0)$ where $k = k_i$ is the ith value where $T^{(k)}(w_0)$ is odd. They showed that for a suitable natural initial distribution on the odd integers drawn from $1 \leqslant w_0 \leqslant X$, and for a suitable number k of iterates (growing slowly with X), as $X \to \infty$ the distribution of the B-ary digits of the ratios w_k/w_0 approached the B-ary Benford distribution, provided that B was not a power of 2. More precisely, they obtained the Benford distribution in a double limit, in which $X \to \infty$ with k held fixed, and after this taking $k \to \infty$. They also gave results of numerical simulations indicating that the distribution of the odd $3x + 1$ iterates $\{w_1, w_2, \dots, w_k\}$ starting from an odd w_0 themselves should approximately satisfy Benford's law, for all integer bases B not a power of 2. In the case where B is a power of 2, they showed that a double limiting distribution exists, but is not the B-ary Benford distribution.

The main result of this paper, Theorem 2.1 in § 2, establishes in a quantitative form the assertion that most initial sequences of the first N iterates of the $3x + 1$ function approximately satisfy the strong Benford law. It applies to a finite sequences of initial $3x + 1$ iterates $\{x_1, x_2, \dots, x_N\}$, and obtains an upper bound on the discrepancy $D(\{y_1, y_2, \dots, y_N\})$ of the sequence of numbers $y_j = \log_B x_j$ for most such sequences. The discrepancy is a well-known statistic which is a measure of distance to the uniform distribution. It is defined in § 2, and relevant properties of discrepancy are treated in § 3. We obtain an explicit upper bound on the number of 'exceptional' sequences for which the discrepancy is large. We treat $3x+1$ iterates including both even and odd iterates, and our main result implies convergence to a generalized Benford's law for all bases $B \geqslant 2$, including B being a power of 2. The anomalous behavior of powers of 2 in the results of Kontorovich and Miller [**11**] is associated to their restriction to the subset of iterates that are odd integers.

The basic approach is as follows. We use the fact that the initial iterates of a large randomly chosen integer n are well approximated by a stochastic process that takes $T(n) = n/2$ or $3n/2$ with equal probability. Taking logarithms to the base B, we are reduced to studying the stochastic process which sets either

$$y_{n+1} = y_n + \theta_1,$$

or

$$y_{n+1} = y_n + \theta_2$$

with equal probability, where

$$\theta_1 = \log_B \tfrac{3}{2} \quad \text{and} \quad \theta_2 = \log_B \tfrac{1}{2}.$$

In § 4 we consider this process in its own right, for arbitrary (θ_1, θ_2). We first show that the realizations

$$\omega = \{y_n : n = 1, 2, 3, \dots\}$$

of such a stochastic process for general (θ_1, θ_2) are uniformly distributed modulo one with probability one, if and only if at least one of θ_1 or θ_2 is irrational. The main result of § 4 shows that if the numbers θ_1 and θ_2 are not simultaneously well approximable by rational numbers, as specified by a two-dimensional 'Diophantine property', then for any fixed N most initial segments of length N are close to the uniform distribution, quantitatively given by an upper bound on their discrepancy.

In § 5 we apply the results of § 4 to the $3x+1$ iteration. We show, using a result of Rhin [**22**], that $\theta_1 = \log_B \frac{3}{2}$ and $\theta_2 = \log_B \frac{1}{2}$ have suitable two-dimensional Diophantine properties for the results in § 4 to apply. Then we establish that the $3x+1$ iterates are sufficiently close to realizations of the stochastic process to obtain upper bounds on the discrepancy of sequences for most initial inputs, provided that we average over $1 \leqslant n \leqslant X$, and for N iterates we require $X \geqslant 2^N$. Putting all of these results together yields the main result, Theorem 2.1.

The main result is established here for the $3X+1$ function, but the methods used apply equally well to number-theoretic maps of a similar nature, such as the $Qx+1$ function, for odd Q, with $T_Q(n) = n/2$ or $(Qn+1)/2$ according to whether n is even or odd. Results analogous to Theorem 2.1 should hold for the distribution of the first N iterates of such functions. For $Q \geqslant 5$ it is expected that most initial values of the $Qx+1$ iteration never enter a periodic orbit, but diverge to $+\infty$. It seems possible that the infinite sequence $\{x_n : n \geqslant 0\}$ of a divergent orbit might actually satisfy a strong Benford's law. However, at present there seems no approach to address this question; even the existence of a divergent orbit for the $Qx+1$ function, for any $Q \geqslant 5$, remains an open problem.

There has been other work showing that the iterates of certain dynamical systems satisfy Benford's law, see Berger, Bunimovich and Hill [**3**] and Berger [**2**]. For various properties of Benford's law, see Hill [**9**, **10**]. Finally we observe that the approach of Kontorovich and Miller [**11**] to Benford's law for $3x+1$ iterates introduced several ideas to this problem, including approximation to a stochastic process (not the one studied here), as well as a relation to Diophantine properties of certain constants. Their approach starts from a structure formula for odd iterates of the $3x+1$ function given by Sinai [**24**] and extended in Kontorovich and Sinai [**12**] to a wider class of maps. Their main result (see [**11**, Theorem 5.3]) for the $3x+1$ function establishes the uniform distribution in a double limit of $y_i := \log_B(w_i/w_0)$ for any real base B such that $\log_B 2$ satisfies a one-dimensional Diophantine property, as defined in § 4.

NOTATION. We let $\lfloor x \rfloor$ denote the largest integer that does not exceed x, and we let $\{\{x\}\} := x - \lfloor x \rfloor$ denote the fractional part of x, with $0 \leqslant \{\{x\}\} < 1$. Finally, $\|x\| = \min_{n \in \mathbb{Z}} |n - x|$ denotes the distance of x from its nearest integer.

2. *Main result*

Benford's law concerns the distribution of the initial digits in the base B expansion of an infinite sequence $\mathcal{X} = \{x_1, x_2, x_3, \dots\}$ of positive real numbers. An infinite sequence is said to satisfy the *strong Benford's law* (*to base* B) if the associated infinite sequence $\mathcal{Y} = \{y_1, y_2, y_3, \dots\}$ given by the base B logarithms $y_i := \log_B x_i$ is uniformly distributed modulo one. Suppose that the numbers x_n have B-ary expansion

$$x_n = B^{M_n}\left(\sum_{k=0}^{\infty} d_k^{(n)} B^{-k}\right)$$

with $1 \leqslant d_0^{(n)} \leqslant B-1$ and $0 \leqslant d_k^{(n)} \leqslant B-1$ for $k \geqslant 1$. Benford's law is the statement that

$$\mathrm{Prob}[d_0^{(n)} = d] = \log_B(d+1) - \log_B d$$

for $1 \leqslant d \leqslant B-1$, in which the 'probability' is interpreted as a limiting frequency in the first N values of x_n as $N \to \infty$. More generally the *strong Benford probability* of observing a given block of K digits $[d_0 d_1 \cdots d_{K-1}]$, with $d_0 \neq 0$, is given by

$$\mathrm{Prob}[d_0^{(n)} d_1^{(n)} \cdots d_{K-1}^{(n)} := d_0 d_1 \cdots d_{K-1}] = \log_B(r + B^{-K+1}) - \log_B r,$$

where

$$r = \sum_{j=0}^{K-1} d_j B^{-j}. \tag{2.1}$$

The departure from uniform distribution modulo one of a finite set $\mathcal{Y}$ can be measured using the discrepancy.

DEFINITION 2.1. The *discrepancy* $D(\mathcal{Y})$ of a finite set $\mathcal{Y} = \{y_1, y_2, \dots, y_N\}$ of real numbers is defined as follows. For $0 \leqslant \alpha \leqslant \beta \leqslant 1$ set

$$Z(\mathcal{Y}; \alpha, \beta) := \frac{1}{N}\#\{i : \alpha \leqslant \{\{y_i\}\} \leqslant \beta\}, \tag{2.2}$$

in which $\{\{y\}\} = y - \lfloor y \rfloor$ is the fractional part of y, and then let

$$D(\mathcal{Y}; \alpha, \beta) := Z(\mathcal{Y}; \alpha, \beta) - (\beta - \alpha). \tag{2.3}$$

The (normalized) discrepancy $D(\mathcal{Y})$ is then

$$D(\mathcal{Y}) := \sup_{0 \leqslant \alpha \leqslant \beta \leqslant 1} |D(\mathcal{Y}; \alpha, \beta)|. \tag{2.4}$$

It is also given by

$$D(\mathcal{Y}) = \sup_{0 \leqslant \alpha \leqslant 1} D(\mathcal{Y}; 0, \alpha) - \inf_{0 \leqslant \alpha \leqslant 1} D(\mathcal{Y}; 0, \alpha). \tag{2.5}$$

One has $0 \leqslant D(\mathcal{Y}) \leqslant 1$; smaller values of $D(\mathcal{Y})$ correspond to more uniformly spaced sets $\mathcal{Y}$ modulo one. No finite distribution can be perfectly uniform, so there is a nonzero lower bound on the discrepancy of all sequences of length N. This minimal value of the discrepancy is attained by equally spaced elements $y_i = i/N$ for $0 \leqslant i \leqslant N-1$, with $D(\mathcal{Y}) = 1/N$. This notion of discrepancy is *translation-invariant*; that is, for any real y_0, one has

$$D(\mathcal{Y} + y_0) = D(\mathcal{Y}). \tag{2.6}$$

Some authors treat instead a (normalized) non-translation invariant discrepancy

$$D^*(\mathcal{Y}) := \sup_{0 \leqslant \alpha \leqslant 1} |Z(\mathcal{Y}; 0, \alpha) - \alpha|.$$

This is related to $D(\mathcal{Y})$ by the inequalities $D^*(\mathcal{Y}) \leqslant D(\mathcal{Y}) \leqslant 2D^*(\mathcal{Y})$.

Our definition of discrepancy follows Kuipers and Niederreiter [**13**] and Drmota and Tichy [**7**]. A few authors (Montgomery [**19**]) study an unnormalized discrepancy that does not divide by N; this version of the discrepancy takes values between 0 and N.

The main result of this paper is an upper bound on discrepancy of the base B logarithms of most initial $3x + 1$ sequences.

THEOREM 2.1. *Let $B \geqslant 2$ be a fixed integer base. For each $N \geqslant 1$ and each $X \geqslant 2^N$, most initial seeds x_0 in $1 \leqslant x_0 \leqslant X$ have first N initial $3x + 1$ iterates $\{x_k : 1 \leqslant k \leqslant N\}$ that satisfy the discrepancy bound*

$$D(\{\log_B x_k : 1 \leqslant k \leqslant N\}) \leqslant 2N^{-1/36}. \tag{2.7}$$

The set $\mathcal{E}(X, B)$ of exceptional initial seeds x_0 in $1 \leqslant x_0 \leqslant X$ that do not satisfy this bound has cardinality

$$|\mathcal{E}(X, B)| \leqslant c(B)N^{-1/36}X, \tag{2.8}$$

where $c(B)$ is a positive constant depending only on B.

This result implies approximation to base B Benford's law, as follows. Let $\mathcal{X} = \{x_1, \ldots, x_N\}$ be a set of positive real numbers, and set $y_i = \log_B x_i$ and $\mathcal{Y} = \{y_1, \ldots, y_N\}$. Let $1 \leqslant r < B$ be a B-ary rational as in (2.1) with $1 \leqslant r < B$. Requiring that the first K digits of x_n match the digits of r is clearly equivalent to having $\{\{y_n\}\}$ lie in the interval $[\log_B r, \log_B(r + B^{-K+1}))$. From the definition of discrepancy, we have that

$$\left| \frac{1}{N} \#\{1 \leqslant i \leqslant N\colon \log_B r \leqslant \{\{\log_B x_i\}\} < \log_B(r+B^{-K+1})\} - \log_B\left(\frac{r + B^{-K+1}}{r}\right) \right|$$

is bounded above by $D(\{y_1, y_2, \ldots, y_N\})$, independent of K. Theorem 2.1 provides an upper bound for this discrepancy for the initial iterates of most $3x+1$ sequences.

3. *Discrepancy and exponential sums*

We will use standard criteria for uniform distribution of an infinite sequence $\mathcal{Y} = \{y_1, y_2, \ldots\}$ in terms of exponential sums and of the discrepancy of its initial segments [**19**, Chapter 1].

For an infinite sequence $\mathcal{Y} = \{y_1, y_2, \ldots\}$ we let $\mathcal{Y}_N$ denote the first N elements of $\mathcal{Y}$. For integers k, we associate to $\mathcal{Y}_N$ the 'Fourier coefficients'

$$\hat{U}_N(k, \mathcal{Y}) = \hat{U}(k, \mathcal{Y}_N) := \sum_{j=1}^{N} e^{2\pi i k y_j}. \tag{3.1}$$

PROPOSITION 3.1. *For an infinite sequence $\mathcal{Y} = \{y_1, y_2, \ldots\}$ of real numbers, the following conditions on $\mathcal{Y}$ are equivalent.*

(1) *The sequence $\mathcal{Y}$ is uniformly distributed modulo one.*

(2) (*Weyl's criterion.*) *For each nonzero integer k we have*

$$\lim_{N\to\infty} \frac{1}{N} |\hat{U}_N(k,\mathcal{Y})| = 0. \tag{3.2}$$

(3) *For any properly Riemann integrable function F on* $[0,1]$,

$$\lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} F(y_j) = \int_0^1 F(t)\, dt. \tag{3.3}$$

(4) *The discrepancy $D(\mathcal{Y}_N)$ satisfies*

$$\lim_{N\to\infty} D(\{y_1, y_2, \ldots, y_N\}) = 0. \tag{3.4}$$

Proof. Here conditions (1)–(3) are Weyl's criterion in [**19**, p. 1], and the equivalence of conditions (1) and (4) appears in [**19**, p. 2]. □

We will need a quantitative relation between exponential sums $\hat{U}_N(k,\mathcal{Y})$ and discrepancy, given by the Erdős–Turan inequality.

Proposition 3.2 (Erdős–Turan inequality). *For any positive integer $K \geqslant 1$,*

$$D(\{y_1, y_2, \ldots, y_N\}) \leqslant \frac{1}{K+1} + 3\sum_{k=1}^{K} \frac{1}{k} \left| \frac{1}{N} \sum_{n=1}^{N} e^{2\pi i k y_n} \right|. \tag{3.5}$$

Proof. This is a weak form of the Erdős–Turan inequality. A short proof of it is given by Montgomery [**19**, p. 8] (after normalizing the discrepancy). For a stronger form, see Kuipers and Neiderreiter [**13**, Chapter 2, Theorem 2.5]. □

We will also need the following simple bound on the change in discrepancy under perturbation.

Proposition 3.3. *If $|y_i - \tilde{y}_i| \leqslant \epsilon$ for $1 \leqslant i \leqslant N$, then*

$$|D(\{y_1, y_2, \ldots, y_N\}) - D(\{\tilde{y}_1, \tilde{y}_2, \ldots, \tilde{y}_N\})| \leqslant 2\epsilon. \tag{3.6}$$

Proof. Let $\mathcal{Y}$ and $\mathcal{Y}'$ denote the sets in the Proposition. Suppose first that the discrepancy $D(\mathcal{Y})$ is attained on an interval $J = [\alpha, \beta]$ with $Z(\mathcal{Y}; J) - |J| > 0$. If $\alpha > \epsilon$ and $\beta < 1-\epsilon$, then with $J' = [\alpha-\epsilon, \beta+\epsilon]$ we see that $J(\mathcal{Y}'; J') \geqslant Z(\mathcal{Y}; J)$, and it follows that

$$D(\mathcal{Y}') \geqslant Z(\mathcal{Y}'; J') - |J'| \geqslant Z(\mathcal{Y}; J) - |J| - 2\epsilon = D(\mathcal{Y}) - 2\epsilon.$$

If $\alpha < \epsilon$ or $\beta > 1-\epsilon$ we would still like to consider $J' \subset [0,1]$ which is the image (mod 1) of the interval $[\alpha-\epsilon, \beta+\epsilon]$. The only issue is that J' now consists of two intervals, one near 0 and the other near 1. However, the complement J'^{c} is a genuine interval and we have $|J'^{\mathrm{c}}| - Z(\mathcal{Y}'; J'^{\mathrm{c}}) = Z(\mathcal{Y}'; J') - |J'| \geqslant D(\mathcal{Y}) - 2\epsilon$. Thus we have again $D(\mathcal{Y}') \geqslant D(\mathcal{Y}) - 2\epsilon$.

In the remaining case where the discrepancy $D(\mathcal{Y})$ is attained on an interval $J = [\alpha, \beta]$ with $|J| - Z(\mathcal{Y}; J) > 0$, we consider $J' = [\alpha+\epsilon, \beta-\epsilon]$ if $\beta - \alpha > 2\epsilon$, and J' to be the empty interval otherwise. We deduce in this case also that $D(\mathcal{Y}') \geqslant D(\mathcal{Y}) - 2\epsilon$.

Since $\mathcal{Y}$ and $\mathcal{Y}'$ are interchangeable in the argument, we obtain $D(\mathcal{Y}) \geqslant D(\mathcal{Y}') - 2\epsilon$, completing the proof. □

In the sequel we will obtain bounds on exponential sums and from this derive bounds on the discrepancy using the Erdős–Turan inequality. We will approximate the values $y_i = \log_B x_i$ of the $3x+1$ iterates of a randomly drawn initial value x_0 by the values of a stochastic process, of a type which we analyze in the next section.

4. *Stochastic process*

We study the following family of stochastic processes. We suppose that we are given two real numbers $(\theta_1 \theta_2)$, and an initial value y_0. The discrete stochastic process $\mathcal{P}(\theta_1, \theta_2, y_0)$ has realizations of the form

$$\omega = (y_1, y_2, y_3, \dots) \tag{4.1}$$

in which the y_i are generated from the initial value y_0 by choosing

$$y_{n+1} = y_n + \theta_1 \text{ with probability } \tfrac{1}{2} \quad \text{and} \quad y_{n+1} = y_n + \theta_2 \text{ with probability } \tfrac{1}{2}, \tag{4.2}$$

where each step is an independent Bernoulli trial. We think of the y_i as given modulo one, in which case this process is a Bernoulli mixture of two rotations of the circle.

Theorem 4.1. *If at least one of θ_1 or θ_2 is irrational, then for any fixed initial value y_0 the process $\mathcal{P}(\theta_1, \theta_2, y_0)$ has a probability one subset of realizations $\omega = (y_1, y_2, \dots)$ that are uniformly distributed modulo one. Equivalently, with probability one,*

$$\lim_{N \to \infty} D(\{y_1, \dots, y_N\}) = 0. \tag{4.3}$$

Note that if θ_1 and θ_2 are both rational numbers, then the values y_i can only take a finite number of distinct values modulo one and no realization ω is uniformly distributed modulo one. We also remark that Theorem 4.1 may be easily generalized to cover Bernoulli mixtures of K rotations of the circle.

Theorem 4.1 will be derived using exponential sums. We first study finite initial segments of length N of such a stochastic process $\mathcal{P}(\theta_1, \theta_2, y_0)$. We let

$$\omega_N := (y_1, y_2, \dots, y_N)$$

denote such an initial segment, and write $\mathbb{E}_{\omega_N}[f(\omega_N)]$ for the expected value of a random variable over the process restricted to these initial segments. We begin by calculating the second moment of the individual Fourier coefficients $\hat{U}_N(k, \omega)$ of ω_N.

Lemma 4.1. *For each $N \geqslant 1$ and each $k \in \mathbb{Z}$*

$$\mathbb{E}_{\omega_N}[|\hat{U}_N(k,\omega)|^2] = N + 2\,\mathrm{Re}\biggl(\sum_{r=1}^{N} (N-r) \biggl(\frac{e^{2\pi i k \theta_1} + e^{2\pi i k \theta_2}}{2}\biggr)^r\biggr). \tag{4.4}$$

If at least one of θ_1 or θ_2 is irrational, then for each non-zero integer k and each $N \geqslant 1$

$$\mathbb{E}_{\omega_N}[|\hat{U}_N(k,\omega)|^2] \leqslant \biggl(1 + \frac{8}{|2 - e^{2\pi i k\theta_1} - e^{2\pi i k \theta_2}|}\biggr) N \leqslant \biggl(1 + \frac{1}{\|k\theta_1\|^2 + \|k\theta_2\|^2}\biggr) N, \tag{4.5}$$

where $\|\xi\| = \min_{n \in \mathbb{Z}} |\xi - n|$ denotes the distance between ξ and its nearest integer.

Proof. Observe that

$$|\hat{U}_N(k,\omega)|^2 = \left|\sum_{j=1}^{N} e^{2\pi i k y_j}\right|^2 = N + 2\,\mathrm{Re}\Big(\sum_{1\leqslant j<\ell\leqslant N} e^{2\pi i k(y_\ell - y_j)}\Big).$$

If we write $r = \ell - j$, then $y_\ell - y_j$ is a sum of r random variables each taking the values θ_1 or θ_2 with equal probability. Thus,

$$\mathbb{E}_{\omega_N}[e^{2\pi i k(y_\ell - y_j)}] = \left(\frac{e^{2\pi i k\theta_1} + e^{2\pi i k\theta_2}}{2}\right)^{\ell - j}.$$

Since for $1 \leqslant r \leqslant N$ there are $N - r$ pairs $1 \leqslant j < \ell \leqslant N$ with $\ell - j = r$, we conclude that

$$\mathbb{E}_{\omega_N}[|\hat{U}_N(k,\omega)|^2] = N + 2\,\mathrm{Re}\Big(\sum_{r=1}^{N}(N-r)\Big(\frac{e^{2\pi i k\theta_1} + e^{2\pi i k\theta_2}}{2}\Big)^r\Big).$$

This proves (4.4).

For any $z \neq 1$ we note that

$$\sum_{r=1}^{N}(N-r)z^r = \frac{(N-1)z - Nz^2 + z^{N+1}}{(1-z)^2},$$

and so, if $|z| \leqslant 1$ and $z \neq 1$ we get that

$$\left|\sum_{r=1}^{N}(N-r)z^r\right| \leqslant \frac{N|z-z^2| + |z - z^{N+1}|}{|1-z|^2} \leqslant \frac{2N}{|1-z|}. \tag{4.6}$$

If at least one of θ_1 or θ_2 is irrational, then for non-zero k we have that $e^{2\pi i k\theta_1} + e^{2\pi i k\theta_2} \neq 2$, and, of course $|e^{2\pi i\theta_1} + e^{2\pi i\theta_2}| \leqslant 2$. Combining (4.4) and (4.6) with $z = (e^{2\pi i k\theta_1} + e^{2\pi i k\theta_2})/2$, we obtain that

$$\mathbb{E}_{\omega_N}[|\hat{U}_N(k,\omega)|^2] \leqslant \left(1 + \frac{8}{|2 - e^{2\pi i k\theta_1} - e^{2\pi i k\theta_2}|}\right)N.$$

For $|\xi| \leqslant \frac{1}{2}$ note that $\sin^2(\pi\xi) \geqslant 4\xi^2$ and so

$$\begin{aligned}|2 - e^{2\pi i k\theta_1} - e^{2\pi i k\theta_2}| &\geqslant 2 - \cos(2\pi k\theta_1) - \cos(2\pi k\theta_2)\\ &= 2(\sin^2(\pi k\theta_1) + \sin^2(\pi k\theta_2)) \geqslant 8(\|k\theta_1\|^2 + \|k\theta_2\|^2),\end{aligned}$$

which completes the proof of (4.5). □

Proof of Theorem 4.1. We suppose that at least one of θ_1 or θ_2 is irrational. We claim that for each nonzero k the following holds:

$$\mathrm{Prob}_\omega\left[\lim_{N\to\infty}\frac{1}{N}|\hat{U}_N(k,\omega)| = 0\right] = 1. \tag{4.7}$$

Thus, for each fixed non-zero integer k, there is a probability one set of ω such that $\lim_{N\to\infty} N^{-1}|\hat{U}_N(k,\omega)| = 0$. Since the set of non-zero integers k is countable, it follows that the set of all ω for which $\lim_{N\to\infty} N^{-1}|\hat{U}_N(k,\omega)| = 0$ holds simultaneously for all non-zero integers k still has probability one. (Its complement is a countable union of sets of measure zero.) Now by Weyl's criterion (Proposition 3.1(2)) all such ω are uniformly distributed modulo one. Proposition 3.1(4) then yields (4.3) with probability one.

To prove (4.7) it suffices to show that for each $1 \geqslant \delta > 0$,

$$P_\delta := \mathrm{Prob}_\omega \left[\limsup_{N\to\infty} \frac{1}{N} |\hat{U}_N(k,\omega)| \geqslant \delta \right] = 0. \tag{4.8}$$

For $j \geqslant 1$ set $N_j := \lfloor 1/(1-\delta/2)^j \rfloor$. If $N_j \leqslant N < N_{j+1}$ is such that $|\hat{U}_N(k,\omega)| \geqslant \delta N$, then we see that

$$\begin{aligned} |\hat{U}_{N_j}(k,\omega)| &\geqslant |\hat{U}_N(k,\omega)| - \left| \sum_{\ell=N_j+1}^{N} e^{2\pi i k y_\ell} \right| \geqslant \delta N - (N - N_j) \\ &\geqslant N_j - \left(\frac{1-\delta}{1-\delta/2} \right) N_j \geqslant \frac{\delta}{2} N_j. \end{aligned}$$

Therefore, for any $B \geqslant 1$,

$$P_\delta \leqslant \mathrm{Prob}_\omega \left[\limsup_{j\to\infty} \frac{1}{N_j} |\hat{U}_{N_j}(k,\omega)| \geqslant \frac{\delta}{2} \right] \leqslant \sum_{j=B}^{\infty} \mathrm{Prob}_\omega \left[|\hat{U}_{N_j}(k,\omega)| \geqslant \frac{\delta N_j}{2} \right]. \tag{4.9}$$

Now

$$\mathrm{Prob}_\omega \left[|\hat{U}_{N_j}(k,\omega)| \geqslant \frac{\delta N_j}{2} \right] \leqslant \left(\frac{\delta N_j}{2} \right)^{-2} E_\omega[|\hat{U}_{N_j}(k,\omega)|^2],$$

and by Lemma 4.1 this gives

$$\mathrm{Prob}_\omega \left[|\hat{U}_{N_j}(k,\omega)| \geqslant \frac{\delta N_j}{2} \right] \leqslant \frac{4}{\delta^2} \left(1 + \frac{1}{\|k\theta_1\|^2 + \|k\theta_2\|^2} \right) \frac{1}{N_j}.$$

We use this in (4.9), and obtain that for any $B \geqslant 1$,

$$P_\delta \leqslant \frac{4}{\delta^2} \left(1 + \frac{1}{\|k\theta_1\|^2 + \|k\theta_2\|^2} \right) \sum_{j=B}^{\infty} \frac{1}{N_j}.$$

Since the N_j grow exponentially, letting $B \to \infty$ we may conclude that $P_\delta = 0$. This establishes (4.8), and (4.7) and the theorem follow. □

For general non-rational pairs (θ_1, θ_2) the convergence rate to zero in (4.3), or equivalently (4.7), can be arbitrarily slow. To obtain explicit bounds on the convergence rate in (4.3) one must impose restrictions on the Diophantine approximation properties of the numbers θ_1 and θ_2. The following definition has been much used in connection with 'small divisors' problems in dynamical systems (cf. Herman [**8**] and Yoccoz [**26**, **27**]) and in number theoretical dynamics (cf. Marklof [**16**]).

DEFINITION 4.1. A real number θ is said to be *Diophantine with exponent* α if there is a positive constant $C(\theta)$ such that for all integers $k \geqslant 1$

$$\|k\theta\| \geqslant C(\theta)|k|^{-\alpha}. \tag{4.10}$$

Any real number that is Diophantine with some positive exponent α is irrational; necessarily $\alpha \geqslant 1$. For any $\alpha > 1$, the set of real numbers that are Diophantine with exponent α has full Lebesgue measure. In fact, the exceptional set of real numbers that are not Diophantine with a given exponent $\alpha > 1$ has Hausdorff dimension $f(\alpha)$ with $f(\alpha) < 1$. *Liouville numbers* are those real numbers that are not Diophantine for any finite exponent, and they form an uncountable set of Hausdorff dimension zero. The set of real numbers that are Diophantine with exponent $\alpha = 1$ comprise the *badly approximable numbers*, and these form a set of Hausdorff dimension one but Lebesgue measure zero.

In this paper we use the following generalization of this notion to simultaneous approximation, which is the complement of the notion of d-dimensional very well approximable vectors appearing in [**23**].

DEFINITION 4.2. The vector $(\theta_1, \theta_2, \ldots, \theta_d)$ of real numbers is said to be *d-dimensional Diophantine with exponent α* if there is a positive constant $C(\theta_1, \theta_2, \ldots, \theta_d)$ such that for all integers $k \geqslant 1$,

$$\max(\|k\theta_1\|, \|k\theta_2\|, \ldots, \|k\theta_d\|) \geqslant C(\theta_1, \theta_2, \ldots, \theta_d) k^{-\alpha}. \tag{4.11}$$

This notion has been used in the dynamical system context by Marklof [**17**, **18**]. Here we use the case $d = 2$. The multidimensional notion is less restrictive than the case $d = 1$ in the sense that if any θ_i is one-dimensional Diophantine with exponent α, then the vector $(\theta_1, \ldots, \theta_d)$ will be d-dimensional Diophantine with the same or smaller exponent.

The next result gives bounds on the expected size of the discrepancy of a finite initial segment of this stochastic process, under suitable Diophantine conditions on (θ_1, θ_2).

THEOREM 4.2. *Suppose that the pair (θ_1, θ_2) is two-dimensional Diophantine with exponent α. Then there is a constant $C_2(\theta_1, \theta_2)$ such that for all $N \geqslant 1$,*

$$\mathbb{E}_{\omega_N}[D(\{y_1, y_2, \ldots, y_N\})] \leqslant C_2(\theta_1, \theta_2) N^{-2(1+\alpha)^{-1}}. \tag{4.12}$$

Proof. The Erdős–Turan inequality (Proposition 3.2) gives that for any K,

$$\mathbb{E}_{\omega_N}[D(\{y_1, \ldots, y_N\})] \leqslant \frac{1}{K+1} + 3\sum_{k=1}^{K} \frac{1}{kN} \mathbb{E}_{\omega_N}[|\hat{U}_N(k,\omega)|]. \tag{4.13}$$

By the Cauchy–Schwarz inequality, (4.5), and the definition of the two-dimensional Diophantine property, we have that

$$\mathbb{E}_{\omega_N}[|\hat{U}_N(k,\omega)|] \leqslant (\mathbb{E}_{\omega_N}[|\hat{U}_N(k,\omega)|^2])^{1/2} \leqslant (1 + C(\theta_1, \theta_2)^{-2} k^{2\alpha})^{1/2} \sqrt{N}. \tag{4.14}$$

Using this in (4.13) we obtain that for an appropriate constant $C_1(\theta_1, \theta_2)$,

$$E_{\omega_N}[D(\{y_1, \ldots, y_N\})] \leqslant \frac{1}{K+1} + C_1(\theta_1, \theta_2) \frac{K^\alpha}{\sqrt{N}}.$$

Choosing $K = N^{2(1+\alpha)^{-1}}$ we obtain the theorem. □

REMARK. The stochastic process studied in this section can be reformulated in terms of the iterates of a skew-product dynamical system, as defined by Cornfeld, Fomin and Sinai [**5**, Chapter 10] and Petersen [**21**]. Let $\Sigma = \{0,1\}^{\mathbb{N}}$ denote the set of all zero–one sequences $\mathbf{s} = (s_0, s_1, s_2, \ldots)$, with the product topology, which is a compact space with natural invariant measure, and let $S : \Sigma \to \Sigma$ be the shift operator $S(s_0, s_1, s_2, \ldots) = (s_1, s_2, s_3, \ldots)$. The skew-product dynamical system $T : \Sigma \times \mathbb{T} \to \Sigma \times \mathbb{T}$ over the base Σ, with fibers $\mathbb{T} = \mathbb{R}/\mathbb{Z}$, is defined by

$$T(\mathbf{s}, x) := (S(\mathbf{s}), x + f(s_0) \pmod 1),$$

with $f(0)=\theta_1, f(1)=\theta_2$, respectively. Here the initial condition is $(\mathbf{s}^{(0)}, x_0)$, with $\mathbf{s}^{(0)} \in \Sigma$ being a random starting point. The invariant measure on $\Sigma \times \mathbb{T}$ is the product measure, using Lebesgue measure on $\mathbb{T}$, and T is ergodic with respect to this measure if at least one of θ_1 and θ_2 is irrational. The initial result of this section (Theorem 4.1) shows weak convergence of almost all orbits to Lebesgue measure on $\mathbb{T}$ for the dynamical system. This result is true in great generality for ergodic skew products. However, the detailed result on rate of convergence to Lebesgue measure (Theorem 4.2) relies on specific properties of this dynamical system.

5. *Application to the $3x+1$ map*

We can describe the $3x+1$ iteration applied to an integer m in terms of the parity of its iterates. We set $T^{(0)}(m)=m$ and define the *parity sequence* $\{b_k(m) : k \geqslant 0\}$ with each $b_k(m) \in \{0,1\}$ by

$$b_k(m) \equiv T^{(k)}(m) \pmod 2. \tag{5.1}$$

PROPOSITION 5.1. *We have the following.*
(1) *The kth iterate $T^{(k)}(m)$ for $k \geqslant 1$ has the form*

$$T^{(k)}(m) = \frac{3^{b_0(m)+\ldots+b_{k-1}(m)}}{2^k} m + R_k(m) \tag{5.2}$$

in which the remainder term

$$R_k(m) := \sum_{j=0}^{k-1} b_j(m) \frac{3^{b_{j+1}(m)+\ldots+b_{k-1}(m)}}{2^{k-j}} \tag{5.3}$$

depends only on $m \pmod{2^k}$.
(2) *Each $b_k(m)$ depends only on $m \pmod{2^{k+1}}$. For each vector $(b_0, b_1, \ldots, b_{N-1}) \in \{0,1\}^N$ there is a unique residue class $m \pmod{2^N}$ such that*

$$b_k(m) = b_k \quad \text{for } 0 \leqslant k \leqslant N-1. \tag{5.4}$$

Proof. (1) This is easily proved by induction on k, see Lagarias [**14**, (2.6)].
(2) This is also proved by induction on k, see Lagarias [**14**, Theorem B]. ☐

We define $x_k(m) = T^{(k)}(m)$ and view

$$\tilde{x}_k(m) := \frac{3^{b_0(m)+\ldots+b_{k-1}(m)}}{2^k} m \tag{5.5}$$

as an approximation to $x_k(m)$. Viewing the base $B \geqslant 2$ as fixed, we set $y_k(m) := \log_B x_k(m)$ and the main result will concern the discrepancy of most sets $\mathcal{Y}_N(m) := \{y_1(m), \ldots, y_N(m)\}$. We approximate the $y_k(m)$ by

$$\tilde{y}_k(m) := \log_B \tilde{x}_k(m) = \log_B m + \left(\sum_{j=0}^{k-1} b_j(m)\right) \log_B 3 - k \log_B 2. \tag{5.6}$$

and we will study the sets $\tilde{\mathcal{Y}}_N(m) := \{\tilde{y}_1(m), \ldots, \tilde{y}_N(m)\}$ for variable m as realizations of a stochastic process of the kind treated in § 4.

The following lemma shows that the error of approximation of $\mathcal{Y}_N(m)$ by $\tilde{\mathcal{Y}}_N(m)$ is exponentially small in N for most m.

LEMMA 5.1. *Let the integer $B \geqslant 2$ be fixed. There exists an exceptional subset $E_B(N)$ of integers $1 \leqslant m \leqslant 2^N$ such that*

$$|E_B(N)| \leqslant 2^{1+(99/100)N},$$

and such that if $1 \leqslant m \leqslant 2^N$ is not in $E_B(N)$, then

$$|y_k(n) - \tilde{y}_k(n)| \leqslant 2^{1-(1/100)N} \quad \text{for } 1 \leqslant k \leqslant N, \tag{5.7}$$

for every $n \equiv m \pmod{2^N}$.

Proof. We will prove more, and show that the set $E_B(N)$ may be taken to be the set of integers $1 \leqslant m \leqslant 2^N$ such that either $m \leqslant 2^{(99/100)N}$, or $b_0(m) + \ldots + b_{N-1}(m) \leqslant (2/5)N$. Since all 2^N possible choices for the parities $b_0(m), \ldots, b_{N-1}(m)$ occur exactly once, we see that the number of m satisfying the second criterion above is less than or equal to $\sum_{j \leqslant (2/5)N} \binom{N}{j} \leqslant 2^{H(2/5)N} \leqslant 2^{(99/100)N}$, where $H(x) = -x \log_2 x - (1-x)\log_2(1-x)$ is the binary entropy function. Thus, $|E_B(N)| \leqslant 2^{1+(99/100)N}$, as desired. It remains now to show (5.7) holds for $m \notin E_B(N)$.

Suppose now that $m \notin E_B(N)$ and that $n \equiv m (\bmod 2^N)$. Proposition 5.1 gives that $b_{k-1}(n) = b_{k-1}(m)$ and $R_k(n) = R_k(m)$ for $1 \leqslant k \leqslant N$. Observe that

$$\frac{x_k(n)}{\tilde{x}_k(n)} = 1 + \frac{R_k(n)}{\tilde{x}_k(n)} = 1 + \frac{R_k(m)}{\tilde{x}_k(n)} \leqslant 1 + \frac{R_k(m)}{\tilde{x}_k(m)} = \frac{x_k(m)}{\tilde{x}_k(m)},$$

from which it follows that $y_k(n) - \tilde{y}_k(n) \leqslant y_k(m) - \tilde{y}_k(m)$. Thus, it suffices to verify (5.7) for $n = m$.

From (5.3) we see that

$$R_k(m) \leqslant \sum_{j=0}^{k-1} \frac{3^{k-j-1}}{2^{k-j}} \leqslant \left(\frac{3}{2}\right)^k.$$

Applying this bound together with $\log(1+\xi) \leqslant \xi$, we obtain that

$$y_k(m) - \tilde{y}_k(m) = \log_B\left(1 + \frac{R_k(m)}{\tilde{x}_k(m)}\right) \leqslant \frac{1}{\log B}\frac{R_k(m)}{\tilde{x}_k(m)} \leqslant \frac{1}{\log B}\frac{1}{m}3^{k-b_0(m)-\ldots-b_{k-1}(m)}. \tag{5.8}$$

Since $m \notin E_B(N)$ we have that $m > 2^{(99/100)N}$, and in addition that

$$k - \sum_{j=0}^{k-1} b_j(m) = \sum_{j=0}^{k-1}(1 - b_j(m)) \leqslant \sum_{j=0}^{N-1}(1 - b_j(m)) \leqslant N - \frac{2}{5}N = \frac{3}{5}N.$$

Thus, from (5.8) we deduce for $m \notin E_B(N)$ that

$$y_k(m) - \tilde{y}_k(m) \leqslant \frac{1}{\log B} 2^{-(99/100)N} 3^{(3/5)N} \leqslant 2^{1-(1/100)N},$$

(since $3^{3/5} < 2^{98/100}$) which proves the lemma. ☐

We wish to bound the discrepancy of most sets $\tilde{\mathcal{Y}}_N(m)$, viewed over a range $1 \leqslant m \leqslant X$, with $X \geqslant 2^N$. We will study the translated sets

$$\tilde{\mathcal{Y}}_N^*(m) := \tilde{\mathcal{Y}}_N(m) - \log_B m, \tag{5.9}$$

so that the initial element $\tilde{y}_0^*(m)$ is zero. Since the discrepancy function is translation invariant we have that

$$D(\tilde{\mathcal{Y}}_N^*(m)) = D(\tilde{\mathcal{Y}}_N(m)). \tag{5.10}$$

Note also that $\tilde{\mathcal{Y}}_N^*(m) = \tilde{\mathcal{Y}}_N^*(m+2^N)$ and so it will suffice to consider the range $1 \leqslant m \leqslant 2^N$.

Lemma 5.2. *Let $B \geqslant 2$ and $N \geqslant 1$ be fixed. Then the ensemble $\{\tilde{\mathcal{Y}}_N^*(m) \colon 1 \leqslant m \leqslant 2^N\}$ of 2^N sequences of length N is identical in distribution with the distribution ω_N of the first N elements of the stochastic process $\mathcal{P}(\theta_1, \theta_2, y_0 = 0)$, with parameters $\theta_1 = \log_B \frac{3}{2}$ and $\theta_2 = \log_B \frac{1}{2}$.*

Proof. From the definitions we see easily that $\tilde{y}_k^*(m) = \tilde{y}_{k-1}^*(m) + \theta_1$ if $b_{k-1}(m) = 1$, and that $\tilde{y}_k^*(m) = \tilde{y}_{k-1}^*(m) + \theta_2$ if $b_{k-1}(m) = 0$. Proposition 5.1(2) shows that for $1 \leqslant m \leqslant 2^N$ all possible patterns $(b_0, b_1, \dots, b_{N-1})$ occur exactly once. This corresponds exactly to independent draws in the stochastic process $\mathcal{P}(\theta_1, \theta_2, y_0 = 0)$; the 2^N possible sequences ω_N of length N of $\mathcal{P}(\theta_1, \theta_2, y_0 = 0)$ have equal probabilities and match the sequences above. □

Lemma 5.3. *For each real $B > 1$ the pair $(\theta_1, \theta_2) = (\log_B \frac{3}{2}, \log_B \frac{1}{2})$ is two-dimensional Diophantine with exponent* 7.616.

Proof. We invoke a result of Rhin [**22**] (see inequality (8) there) obtained using Padé approximation methods. There exists a positive constant C such that for integers u_0, u_1 and u_2 with $\max(|u_1|, |u_2|) \geqslant 1$ we have

$$|u_0 + u_1 \log 2 + u_2 \log 3| \geqslant C(\max(|u_1|, |u_2|))^{-7.616}. \tag{5.11}$$

Let k be a large positive integer and suppose that ℓ_1 is the nearest integer to $k\theta_1$ and that $-\ell_2$ is the nearest integer to $k\theta_2$. Thus, $|k\theta_1 - \ell_1| = \|k\theta_1\|$ and $|k \log_B 2 - \ell_2| = |k\theta_2 + \ell_2| = \|k\theta_2\|$. Note that both ℓ_1 and ℓ_2 are positive and roughly of size k. On the one hand, we see that

$$\left| \frac{\log(3/2)}{\log 2} - \frac{\ell_1}{\ell_2} \right| = \left| \frac{\ell_2 k \log_B(3/2) - \ell_1 k \log_B 2}{k\ell_2 \log_B 2} \right| \leqslant \frac{\ell_2 \|k\theta_1\| + \ell_1 \|k\theta_2\|}{k\ell_2 \log_B 2}.$$

On the other hand, we see that by (5.11),

$$\left| \frac{\log(3/2)}{\log 2} - \frac{\ell_1}{\ell_2} \right| = \left| \frac{\ell_2 \log 3 - (\ell_1 + \ell_2) \log 2}{\ell_2 \log 2} \right| \geqslant C \frac{(\ell_1 + \ell_2)^{-7.616}}{\ell_2 \log 2}.$$

Since ℓ_1 and ℓ_2 are roughly of size k, combining the above two statements immediately gives the lemma. □

Proof of Theorem 2.1. We view the integer $B \geqslant 2$ and $N \geqslant 1$ as fixed. Consider the realizations ω_N of the stochastic process $\mathcal{P}(\theta_1, \theta_2, y_0 = 0)$ with $\theta_1 = \log_B \frac{3}{2}$ and $\theta_2 = \log_B \frac{1}{2}$. By Lemma 5.3 and Theorem 4.2 we obtain that (with $\alpha = 7.616$)

$$\mathbb{E}_{\omega_N}[D(\{y_1, \dots, y_N\})] \leqslant CN^{-2(1+\alpha)^{-1}} \leqslant CN^{-1/18},$$

for an appropriate positive constant C. Using Markov's inequality that $\mathrm{Prob}[Y \geqslant a] \leqslant \mathbb{E}[Y]/a$ for a nonnegative random variable Y, we deduce that

$$\mathrm{Prob}[D(\{y_1, \dots, y_n\}) \geqslant N^{-1/36}] \leqslant CN^{-1/36}.$$

Invoking Lemma 5.2 we conclude that the exceptional set of m with $1 \leqslant m \leqslant 2^N$ such that $D(\tilde{\mathcal{Y}}_N(m)) \geqslant N^{-1/36}$ has cardinality at most $CN^{-1/36}2^N$. By Lemma 5.1, we know that for most $1 \leqslant m \leqslant 2^N$ the sets $\mathcal{Y}_N(m)$ and $\tilde{\mathcal{Y}}_N(m)$ are very close term by term, and by Proposition 3.3 for such m the discrepancies $D(\mathcal{Y}_N(m))$ and $D(\tilde{\mathcal{Y}}_N(m))$ are very nearly equal. Thus, we may deduce that the exceptional set of m with $1 \leqslant m \leqslant 2^N$ such that

$$D(\mathcal{Y}_N(m)) \geqslant N^{-1/36} + 2^{2-(1/100)N}$$

has cardinality at most

$$CN^{-1/36}2^N + 2^{1+(99/100)N}.$$

This easily gives the conclusion of the theorem for $X = 2^N$.

It remains to treat the case $X > 2^N$. Suppose $\ell 2^N < X \leqslant (\ell+1)2^N$, for some $\ell \geqslant 1$. Since the discrepancies $D(\tilde{\mathcal{Y}}_N(m))$ are periodic (mod 2^N) we see that the exceptional set of $m \leqslant X$ with large discrepancy contains no more than $\ell + 1$ times the number of exceptional $m \leqslant 2^N$. This completes the proof. □

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References

1. F. Benford, 'The law of anomalous numbers', *Proc. Amer. Philos. Soc.* 78 (1938) 551–572.

2. A. Berger, 'Multi-dimensional dynamical systems and Benford's law', *Discrete Contin. Dyn. Syst.* 13 (2005) 219–237.

3. A. Berger, L. Bunimovich and T. Hill, 'One-dimensional dynamical systems and Benford's law', *Trans. Amer. Math. Soc.* 357 (2005) 197–219.

4. K. Borovkov and D. Pfeifer, 'Estimates for the Syracuse problem via a probabilistic model', *Theory Probab. Appl.* 45 (2000) 300–310.

5. I. P. Cornfeld, S. V. Fomin and Ya. G. Sinai, *Ergodic theory* (Springer, New York, 1982).

6. P. Diaconis, 'The distribution of leading digits and uniform distribution mod 1', *Ann. Probab.* 5 (1977) 72–81.

7. M. Drmota and R. F. Tichy, *Sequences, discrepancies and applications*, Lecture Notes in Mathematics 1651 (Springer, New York, 1997).

8. M-R. Herman, 'Sur la conjugaison différentiable des difféomorphismes du cercle à des rotations', *Publ. Math. Inst. Hautes Études Sci.* 49 (1979) 5–233.

9. T. Hill, 'Base-invariance implies Benford's law', *Proc. Amer. Math. Soc.* 123 (1995) 187–195.

10. T. Hill, 'A statistical derivation of the significant digit law', *Statist. Sci.* 86 (1996) 358–363.

11. A. V. Kontorovich and S. J. Miller, 'Benford's law, values of L-functions and the $3x+1$ problem', *Acta Arith.* 120 (2005) 269–297.

12. A. V. Kontorovich and Ya. G. Sinai, 'Structure theorem for (d, g, h)-maps', *Bull. Braz. Math. Soc.* 33 (2002) 213–224.

13. L. Kuipers and H. Niederreiter, *Uniform distribution of sequences* (Wiley, New York, 1974).

14. J. C. Lagarias, 'The $3x+1$ problem and its generalizations', *Amer. Math. Monthly* 92 (1985) 3–23.

15. J. C. Lagarias and A. Weiss, 'The $3x + 1$ problem: two stochastic models', *Ann. Appl. Probab.* 2 (1992) 329–361.

16. J. Marklof, 'Pair correlation densities of inhomogeneous quadratic forms', *Ann. of Math.* (2) 158 (2003) 419–471.

17. J. Marklof, 'Pair correlation densities of inhomogeneous quadratic forms II', *Duke Math. J.* 115 (2002) 409–434; Correction, *Duke Math. J.* 120 (2003) 227–228.

18. J. Marklof, 'Mean square value of exponential sums related to the representation of integers as sums of squares', *Acta Arith.* 117 (2005) 353–370.

19. H. L. Montgomery, *Ten lectures on the interface between analytic number theory and harmonic analysis*, CBMS Regional Conference Series 84 (American Mathematical Society, Providence, RI, 1994).

20. S. Newcomb, 'Note on the frequency of use of the different digits in natural numbers', *Amer. J. Math.* 4 (1881) 39–40.

21. K. R. Petersen, *Ergodic Theory*, corrected reprint (Cambridge University Press, Cambridge, 1989).

22. G. Rhin, 'Approximants de Padé et mesures effectives d'irrationalité', *Séminaire de Théorie des Nombres*, Paris, 1985–1986, Progress in Mathematics 71 (Birkhäuser, Boston, MA, 1987) 155–164.

23. W. Schmidt, 'Approximation by algebraic numbers', *Enseign. Math.* 17 (1971) 187–253.

24. Ya. G. Sinai, 'Statistical $(3x + 1)$ problem. Dedicated to the memory of Jürgen K. Moser', *Comm. Pure Appl. Math.* 56 (2003) 1016–1028.

25. G. J. Wirsching, *The dynamical system generated by the* $3n + 1$ *function*, Lecture Notes in Mathematics 1681 (Springer, New York, 1998).

26. J.-C. Yoccoz, 'Conjugaison différentiable des difféomorphismes du cercle dont le nombre de rotation vérifie une condition diophantienne', *Ann. Sci. École Norm. Sup.* (4) 17 (1984) 333–359.

27. J.-C. Yoccoz, 'Analytic linearization of circle diffeomorphisms', *Dynamical systems and small divisors*, Certraro, 1998, Lecture Notes in Mathematics 1784 (Springer, New York, 2002) 125–173.

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