A diffraction abstraction

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Abstract For some time now, I have been trying to understand the complexity of integer sequences from a variety of different viewpoints and, at least at some level, trying to reconcile these viewpoints. However vague that sounds—and it certainly is vague to me—in this short note, I hope to explain this sentiment.

1 Introduction

My interest in the complexity[1] of integer sequences is rooted in some classical results from the first part of the twentieth century concerning power series. These start with a result of Fatou [12], that a power series $F(z) \in \mathbb{C}[[z]]$ whose coefficients take only finitely many values is either rational or transcendental over $\mathbb{C}(z)$. Szegő [16] generalised Fatou's result to give, under the same assumptions, that $F(z)$ is either rational or has the unit circle as a natural boundary. Completing this picture in a certain sense, Carlson [9] then showed that if $F(z) \in \mathbb{Z}[[z]]$ converges in the unit disc, the same conclusion holds—either $F(z)$ is rational or it has the unit circle as a natural boundary. I use the word 'completing' as Carlson's theorem cannot be extended without adding more restrictive assumptions—there are irrational integer power series with a smaller radius of convergence that are meromorphic, such as the algebraic function

$$\frac{1}{\sqrt{1-4z}} = \sum_{n\geqslant 0} \binom{2n}{n} z^n.$$

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[1] I mean complexity in the standard dictionary definition: the state or quality of being intricate or complicated.

Of course, one would like to know more about the behaviour of these power series as z approaches the unit circle. Towards addressing this, a beautiful result of Duffin and Schaeffer [11] states that a power series that is bounded in a sector of the unit disc and has coefficients from a finite set is necessarily a rational function. As well, this result cannot be extended to full generality—there are integer power series converging in the unit disc that are bounded in certain sectors, such as the series

$$\sum_{n\geqslant 0}(1-z)^n z^{n!},$$

which is bounded in the sector $\arg(z)\in[-\pi/4,\pi/4]$. One of the 'takeaways' for me from these results is the importance of asymptotics in relation to the complexity of integer sequences.

It is worth pointing out that these results occurred during an historically interesting time for integer sequences. Up to the year 1909, problems of probability were classified as either 'discontinuous' or 'continuous' (also called 'geometric'). Towards filling this gap, in that year, Borel [8] introduced what he called countable probabilities (probabités dénombrables). In this new type of problem, one asks probabilistic questions about countable sets. As a—now common—canonical example, Borel considered properties of the frequency of digits in the digital expansions of real numbers. A central concept in Borel's approach is that of normality. A real number x is called simply normal to the base k (or k-simply normal) if each of $0,1,\dots,k-1$ occurs in the base-k expansion of x with equal frequency $1/k$. This number x is then called normal to the base k (or k-normal) provided it is k^m-simply normal for all positive integers m, and the number x is just called normal if this is true for all integers $k\geqslant 2$. Borel's use of the word 'normal' is well-justified; he showed, in that 1909 paper, that almost all real numbers, with respect to Lebesgue measure, are normal. The question he left was to determine if the decimal expansion of $\sqrt{2}$ is normal. It is now customary to attribute the following broader question to Borel: *Is the base expansion of an irrational algebraic real number normal?* It is not at all an exaggeration to say that nothing substantial is known now, 110 years later.

The strength of Borel's approach, as well as the difficulty, rests upon considering large blocks of a bounded integer sequence, the sequence of digits of a base expansion of a real number. But what if we relax this a bit and consider only the two-point correlations? This brings us squarely into the realm of diffraction.

In classical Fraunhofer (far-field) diffraction, monochromatic light waves from a (far) point source come into contact with an object, are scattered (diffracted) and then meet a (far) screen. The image left on the screen is (essentially) the Fourier transform of the object. The present situation concerns the specific case of a sequence of integers. For a bounded sequence w of integers, one arrives at the diagram

$$\omega:=\sum_{n\in\mathbb{Z}} w(n)\,\delta_n \xrightarrow{\;\circledast\;} \gamma_\omega:=\omega\circledast\omega=\sum_{m\in\mathbb{Z}}\eta(m)\,\delta_m \xrightarrow{\;\mathscr{F}\;} \widehat{\gamma}_\omega=\widehat{\omega\circledast\omega}$$

where ω is the (weighted) Dirac comb with weights w, $\circledast$ represents convolution, the values

$$\eta(m) := \lim_{N\to\infty} \frac{1}{2N+1} \sum_{i=-N}^{N} w(i)w(i+m)$$

are the autocorrelation coefficients and $\mathscr{F}$ is Fourier transformation. In the more general context, this diagram is commonly called a *Wiener diagram*, after the American applied mathematician Norbert Wiener, who pointed out the usefulness of the autocorrelation function for understanding X-ray diffraction patterns; see Senechal [15] and Patterson [14]. In fact, Wiener [17] instigated the use of diffraction methods on integer sequences. In his paper, "The spectrum of an array and its application to the study of the translational properties of a simple class of arithmetical functions, Part One," Wiener outlined a process whereby one uses the autocorrelation function to produce a spectral function that in a sense encodes some of the complexity of the underlying sequence. In modern day terms, he was showing, given a subset A of $\mathbb{Z}$, how to produce the diffraction measure $\widehat{\gamma_\omega}$ and then using the Lebesgue decomposition theorem to determine a sort of complexity for the set A. Recall that the Lebesgue decomposition theorem states that any regular Borel measure μ on $\mathbb{R}^d$ has a unique decomposition $\mu = \mu_{\text{pp}} + \mu_{\text{ac}} + \mu_{\text{sc}}$ where μ_{pp}, μ_{ac} and μ_{sc} are mutually singular and also $|\mu| = |\mu_{\text{pp}}| + |\mu_{\text{ac}}| + |\mu_{\text{sc}}|$. Here μ_{pp} is a pure point measure corresponding to the monotone step function part of Wiener's spectral function (the Bragg part), μ_{ac} is an absolutely continuous measure corresponding to the part of the spectral function that is the integral of its derivative, and μ_{sc} is a singular continuous measure corresponding to the continuous part of the spectral function which has almost everywhere a zero derivative. Wiener's purpose is exactly what I am aiming at, *"to extend the spectrum theory [...] to the harmonic analysis of functions only defined for a denumerable set of arguments—arrays, as we shall call them—and the application of this theory to the study of certain power series admitting the unit circle as an essential boundary."* [17]

In the remainder of this note, I will describe some examples of each (pure) type of measure with a number-theoretic flavour, then move on to an extended diffraction example before finishing our exposition with an example of a non-diffractive measure, which still gives some reasonable information, but for an unbounded sequence.

2 Three examples: diffraction measures of pure type

My current favourite three examples, illustrating each (pure) type of measure are the characteristic function on k-free integers, the Rudin–Shapiro sequence and the Thue–Morse sequence. Each of these sequences have power series generating functions having the unit circle as a natural boundary.

The k-free integers. Let $V_k \subset \mathbb{Z}$ be the set of k-free integers with fixed $k \geqslant 2$, that is, the elements of $\mathbb{Z}$ that are not divisible by a k-th power of any (rational) prime number. If one lets $w = \chi_k$ be the characteristic function on V_k and considers

$$\omega_k := \sum_{n\in\mathbb{Z}} \chi_k(n)\,\delta_n,$$

then a result of Baake, Moody and Pleasants [6] gives that the diffraction measure $\widehat{\gamma}_{\omega_k}$ is a pure point measure, which is explicitly computed in terms of elementary number-theoretic functions.

The Rudin–Shapiro sequence. In this example, one lets the sequence of weights w be the Rudin–Shapiro sequence $w_{\mathrm{RS}} : \mathbb{Z} \to \{\pm 1\}$ determined by the recurrences

$$w_{\mathrm{RS}}(4m+\ell) = \begin{cases} w_{\mathrm{RS}}(m), & \text{for } \ell \in \{0,1\}, \\ (-1)^{m+\ell}\, w_{\mathrm{RS}}(m), & \text{for } \ell \in \{2,3\}, \end{cases}$$

with initial conditions $w_{\mathrm{RS}}(0) = -w_{\mathrm{RS}}(-1) = 1$. Given this definition, using weights $w = w_{\mathrm{RS}}$, it turns out that the diffraction measure $\widehat{\gamma}_{\omega_{\mathrm{RS}}}$ is absolutely continuous with respect to Lebesgue measure; in fact, the two are equal. See Baake and Grimm [4, Section 10.2] for more details.

The Thue–Morse sequence. This example is a special case of a result of Kurt Mahler [13], who wrote "Part Two" of Wiener's above-mentioned paper [17].

Let $\{t(n)\}_{n\in\mathbb{Z}}$ be the Thue–Morse sequence defined on the alphabet $\{\pm 1\}$ by $t(0) = 1$, for $n \geqslant 1$ by the recurrences $t(2n) = t(n)$ and $t(2n+1) = -t(n)$ and extended to all of $\mathbb{Z}$ by the symmetric relation $t(-n) = t(n)$. The right half of this sequence, which starts

$$\{t(n)\}_{n\geqslant 0} = \{1,-1,-1,1,-1,1,1,-1,-1,1,1,-1,1,-1,-1,1,\ldots\},$$

is one of the most ubiquitous integer sequences and one of central importance in various areas within number theory, combinatorics, theoretical computer science and dynamical systems theory. In both theoretical computer science and dynamics one often views this sequence as the infinite iteration of the binary substitution (or morphism) ρ_{TM} defined on the two letter alphabet $\Sigma_2 := \{a,b\}$ by

$$\rho_{TM} : \begin{cases} a \mapsto ab \\ b \mapsto ba\,. \end{cases}$$

If one considers the Dirac comb

$$\omega_{\mathrm{TM}} = \sum_{n\in\mathbb{Z}} t(n)\,\delta_n,$$

then, as implied by the result of Mahler, the diffraction measure $\widehat{\gamma}_{\omega_{\mathrm{TM}}}$ is a purely singular continuous measure. Indeed, this was the first explicit example of such a measure, and appeared in Mahler's first published paper!

3 An extended diffraction example: the Thue–Morse sequence

Standing at the intersection of number theory, dynamics and theoretical computer science, the most widely interesting of these examples is that of the Thue–Morse sequence. Fortunately for us, it is also an example where much is known. In this section, I highlight a few of the known results concerning this sequence and provide some questions on further relationships.

Before continuing, we note that in this instance, the existence of the autocorrelation measure $\gamma_{\omega_{\mathrm{TM}}}$ is guaranteed by an application of Birkhoff's ergodic theorem; see Baake and Grimm [4, Section 10.1] for all details regarding measures associated to the Thue–Morse sequence. As well, the autocorrelation coefficients satisfy $\eta_{\mathrm{TM}}(-m) = \eta_{\mathrm{TM}}(m)$, so that one can determine the coefficients via the one-sided limit

$$\eta_{\mathrm{TM}}(m) = \lim_{N\to\infty} \frac{1}{N} \sum_{i=0}^{N-1} t(i)t(i+m),$$

for all $m \in \mathbb{N}$. Using the recursions defining t, with some rearrangement, we arrive at the recursions

$$\eta_{\mathrm{TM}}(2m) = \eta_{\mathrm{TM}}(m) \quad \text{and} \quad \eta_{\mathrm{TM}}(2m+1) = -\frac{1}{2}\big(\eta_{\mathrm{TM}}(m) + \eta_{\mathrm{TM}}(m+1)\big),$$

for $m \geqslant 0$. Along with the fact that $\eta_{\mathrm{TM}}(0) = 1$, these recurrences specify a sequence $\{\eta_{\mathrm{TM}}(m)\}_{m\geqslant 0}$, which is 2-regular in the sense of Allouche and Shallit [2]. This presumably generalises, the moral result being that the autocorrelation coefficients of a k-automatic sequence should be k-regular. This added structure is useful and can be harnessed (as it is in the case for the Thue–Morse sequence) to help decide whether a given diffraction measure is continuous. See the monograph [1] for background and details on automatic sequences.

Since the Thue–Morse sequence is an automatic sequence, its generating function is a Mahler function. A Mahler function is a function $F(z) \in \mathbb{C}[[z]]$ for which there exist integers $d \geqslant 1$ and $k \geqslant 2$ and polynomials $p_0(z), \ldots, p_d(z)$ such that

$$p_0(z)F(z) + p_1(z)F(z^k) + \cdots + p_d(z)F(z^{k^d}) = 0.$$

That is to say, the function $F(z)$ behaves predictably under the map $z \mapsto z^k$. The generating function of the (one-sided) Thue–Morse sequence,

$$T_{\pm}(z) := \sum_{n\geqslant 0} t(n) z^n,$$

satisfies the Mahler-type functional equation

$$T_{\pm}(z) - (1-z)T_{\pm}(z^2) = 0.$$

The simplicity of this functional equation allows one to write $T_{\pm}(z)$ as the infinite product

$$T_\pm(z)=\prod_{j\geqslant 0}\left(1-z^{2^j}\right).$$

It is evident by examining this product that as z radially approaches 1 from the origin, $T_\pm(z)$ is extremely flat. Indeed, de Bruijn [10] showed that as $z\to 1^-$, we have

$$T_\pm(z)=C_{\rm TM}(z)\cdot(1-z)^{1/2}\cdot 2^{-\log_2^2(1-z)/2}\cdot(1+o(1)). \tag{1}$$

Here $\log_2^2(y)=(\log(y)/\log(2))^2$ is the square of the binary logarithm and $C_{\rm TM}(z)$ is a positive oscillatory term, which in $(0,1)$ is bounded away from 0 and infinity, is real-analytic, and satisfies $C_{\rm TM}(z)=C_{\rm TM}(z^2)$.

These asymptotics of $T_\pm(z)$ are reflected in the scaling behaviour of the distribution function of the Thue–Morse measure. Indeed, consider

$$\widehat{\gamma}_{\omega_{\rm TM}}=\mu_{\rm TM}*\delta_{\mathbb{Z}},$$

where

$$\mu_{\rm TM}(x)=\prod_{\ell\geqslant 0}\left(1-\cos(2^{\ell+1}\pi x)\right),$$

and where this limit is taken in the vague topology. Setting $F_{\rm TM}(x):=\mu_{\rm TM}([0,x])$, Baake and Grimm [5] have shown that there are positive constants c_1 and c_2 such that for small x, we have

$$c_1\,x^{2+\alpha}\,2^{-\log_2^2(x)}\leqslant F_{\rm TM}(x)\leqslant c_2\,x^{\alpha}\,2^{-\log_2^2(x)}, \tag{2}$$

where $\alpha=-\log_2(\pi^2/2)$. Presumably inequality (2) holds with equal exponents of x on each side, but at the moment this remains an open question. A sort of heuristic for this is the validity of (1).

In this setting, one should view the function $T_\pm(z)$ as an exact "error term" in the following way. Let A_{01} be the set of nonnegative integers that have an odd number of ones in their binary expansion and denote by $T_{01}(z)$ the generating function of the characteristic function of A_{01}. Note that the set A_{01} has density $1/2$ in the nonnegative integers. With these definitions, we have

$$2\left(T_{01}(z)-\frac{1}{2}\cdot\frac{1}{1-z}\right)=T_\pm(z).$$

Now, de Bruijn's result gives,

$$\left(T_{01}(z)-\frac{1}{2}\cdot\frac{1}{1-z}\right)^2=\tfrac{1}{4}\cdot C_{\rm TM}(z)^2\cdot(1-z)\cdot 2^{-\log_2^2(1-z)}\cdot(1+o(1)). \tag{3}$$

Equation (3) can be interpreted as a probabilistic (or statistical) statement about the set A_{01}.

The similarities between (2) and (3) are striking and though it is quite tempting, we refrain from making any direct conjectures, but ask the following question: *Is there a direct transformation (in general) between certain asymptotics of generat-*

ing functions and the asymptotic behaviour near zero of the associated distribution function of the diffraction measure?

4 A non-diffractive example: the Stern sequence

In the previous section, we considered an example of a bounded integer sequence, the Thue–Morse sequence. Because of this, one is able to use the setting of diffraction to consider complexity and to compare with asymptotics of the related generating function. In this section, I consider an example of an unbounded sequence, the Stern sequence. Due to this unboundedness, the traditional diffraction paradigm is not available.

Stern's sequence $\{s(n)\}_{n\geqslant 0}$, also called Stern's diatomic sequence, is defined by the initial conditions $s(0)=0$ and $s(1)=1$ and for $n\geqslant 1$ by the recurrences $s(2n)=s(n)$ and $s(2n+1)=s(n)+s(n+1)$. The sequence starts

$$\{s(n)\}_{n\geqslant 0}=\{0,1,1,2,1,3,2,3,1,4,3,5,2,5,3,4,1,5,4,7,3,8,5\ldots\}.$$

Stern's sequence has some interesting properties, maybe the most interesting of which is that the sequence $\{s(n)/s(n+1)\}_{n\geqslant 0}$ is an enumeration of the nonnegative rational numbers, without repeats, and already in reduced form! Like the Thue–Morse sequence, the generating function of the Stern sequence

$$S(z):=\sum_{n\geqslant 0} s(n+1)z^n$$

is a Mahler function given by an infinite product. In this case,

$$S(z)=\prod_{j\geqslant 0}\left(1+z^{2^j}+z^{2\cdot 2^j}\right).$$

Due to the structure of this infinite product, one easily sees that the value $s(n+1)$ is the number of hyperbinary representations of n, that is, the number of ways of writing n as the sum of powers of two with each power being used at most twice.

As stated above, the unboundedness of the Stern sequence rules out the study of this sequence by means of traditional diffraction. Nonetheless, there is enough structure to form a measure associated to Stern's sequence. The following formulation follows my recent work [3] with Michael Baake. It was made possible due to the well-known relationship

$$\sum_{m=2^n}^{2^{n+1}-1} s(m) \,=\, 3^n, \tag{4}$$

for $n\geqslant 0$. This allowed us to define

$$\mu_n := 3^{-n} \sum_{m=0}^{2^n-1} s(2^n+m)\, \delta_{m/2^n}\,, \tag{5}$$

where δ_x denotes the unit Dirac measure at x. Here, we view $\{\mu_n\}_{n\geqslant 0}$ as a sequence of probability measures on the 1-torus—written as $\mathbb{T}=[0,1)$ with addition modulo 1—wherein we have re-interpreted the values of the Stern sequence in the interval $[2^n, 2^{n+1})$ as weights of a pure point probability measure on $\mathbb{T}$ with $\mathrm{supp}(\mu_n) = \big\{\frac{m}{2^n} : 0 \leqslant m < 2^n\big\}$.

The main result of [3] is that the sequence $\{\mu_n\}_{n\geqslant 0}$ of probability measures on $\mathbb{T}$ converges weakly to a singular continuous probability measure μ_{S}, which we call the Stern measure. Moreover, one has $\mu_0 = \delta_0$ and $\mu_n = \mathop{\ast}_{m=1}^{n} \frac{1}{3}\big(\delta_0 + \delta_{2^{-m}} + \delta_{-2^{-m}}\big)$ for $n \geqslant 1$. The weak limit as $n \to \infty$ is given by the convergent infinite convolution product

$$\mu_{\mathrm{S}} = \mathop{\ast}_{m\geqslant 1} \tfrac{1}{3}\big(\delta_0 + \delta_{2^{-m}} + \delta_{-2^{-m}}\big).$$

Its Fourier transform $\widehat{\mu}_{\mathrm{S}}$ is given by

$$\widehat{\mu}_{\mathrm{S}}(k) = \prod_{m\geqslant 1} \tfrac{1}{3}\big(1+2\cos(2\pi k/2^m)\big) = \prod_{m\geqslant 1} \tfrac{1}{3}\big(1+e^{2\pi k/2^m}+e^{-2\pi k/2^m}\big)$$

for $k\in\mathbb{Z}$. This infinite product is also well-defined on $\mathbb{R}$, where it converges compactly.

We also proved [3] that the distribution function $F_{\mathrm{S}}(x) := \mu_{\mathrm{S}}\big([0,x]\big)$ is strictly increasing and is Hölder continuous with exponent $\log_2(3/\tau)$, where $\tau := (1+\sqrt{5})/2$ is the golden mean. This implies that there is a positive constant c_3 such that

$$F_{\mathrm{S}}(x) \leqslant c_3\, x^{\log_2(3/\tau)}.$$

Here, the comparison with known asymptotics is again striking. It follows from a result of mine with Bell [7], that as $z \to 1^-$,

$$S(z) = \frac{C_{\mathrm{S}}(z)}{(1-z)^{\log_2 3}} \cdot (1+o(1)),$$

where, as in the case of the Thue–Morse sequence, $C_{\mathrm{S}}(z)$ is a positive oscillatory term, which in $(0,1)$ is bounded away from 0 and infinity, is real-analytic, and satisfies $C_{\mathrm{S}}(z) = C_{\mathrm{S}}(z^2)$. It is worth noting here, that while the constant 3 essentially comes from (4), the maximal values of the Stern sequence between 2^n and $2^{n+1}-1$ are proportional to τ^n, in fact, they are Fibonacci numbers. So here, the exponent in the scaling of the distribution function is the binary logarithm of the ratio of the average value $3/2$ and of the averaged maximum $\tau/2$.

5 Concluding remark

In this note (and the talks from whence it came), I discussed generating functions and measures associated to a few paradigmatic integer sequences. For the Thue–Morse sequence, I discussed the related diffraction measure and asked whether the asymptotics of the generating function near the unit circle are related to the scaling behaviour of the distribution function of the measure close to zero. Also, I used the example of the Stern sequence to define a measure (not a diffraction measure) for an unbounded integer sequence and again related properties of the distribution function of that measure to the asymptotics of the generating function of the Stern sequence near the unit circle. I find the similar structures of the asymptotics in these situations compelling and worthy of further study.

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References

1. J.-P. Allouche and J. Shallit, Automatic sequences, Cambridge University Press, Cambridge (2003).
2. J.-P. Allouche and J. Shallit, *The ring of k-regular sequences*, Theoret. Comput. Sci. **98** (1992), no. 2, 163–197.
3. M. Baake and M. Coons, *A natural probability measure derived from Stern's diatomic sequence*, Acta Arith. **183** (2018), no. 1, 87–99. arXiv:1706.00187
4. M. Baake and U. Grimm, Aperiodic Order. Vol. 1: A Mathematical Invitation. Cambridge University Press, Cambridge (2013).
5. M. Baake and U. Grimm, *Scaling of diffraction intensities near the origin: some rigorous results*, J. Stat. Mech. (2019), 054003. arXiv:1905.04177
6. M. Baake, R. V. Moody, and P. A. B. Pleasants, *Diffraction from visible lattice points and kth power free integers*, Discrete Math. **221** (2000), no. 1–3, 3–42. arXiv:9906132
7. J. P. Bell and M. Coons, *Transcendence tests for Mahler functions*, Proc. Amer. Math. Soc. **145** (2017), no. 3, 1061–1070. arXiv:1511.07530
8. E. Borel, *Les probabilités dénombrables et leurs applications arithmétiques*, Palermo Rend. **27** (1909), 247–271.
9. F. Carlson, *Über ganzwertige Funktionen*, Math. Z. **11** (1921), no. 1–2, 1–23.
10. N. G. de Bruijn, *On Mahler's partition problem*, Nederl. Akad. Wetensch., Proc. **51** (1948), 659–669, Indagationes Math. **10**, 210–220 (1948).
11. R. J. Duffin and A. C. Schaeffer, *Power series with bounded coefficients*, Amer. J. Math. **67** (1945), 141–154.
12. P. Fatou, *Séries trigonométriques et séries de Taylor*, Acta Math. **30** (1906), no. 1, 335–400.
13. K. Mahler, *The spectrum of an array and its application to the study of the translation properties of a simple class of arithmetical functions. Part Two: On the translation properties of a simple class of arithmetical functions.*, J. Math. Phys., MIT **6** (1927), 158–163.
14. A. L. Patterson, *Experiences in crystallography–1924 to date*, in Fifty Years of X-Ray Diffraction, P. P. Ewald (Editor), Oosthoek, Utrecht, 1962, pp. 612–622.
15. M. Senechal, Quasicrystals and geometry, Cambridge University Press, Cambridge (1995).

16. G. Szegő, *Tschebyscheffsche Polynome und nichtfortsetzbare Potenzreihen*, Math. Ann. **87** (1922), no. 1–2, 90–111.
17. N. Wiener, *The spectrum of an array and its application to the study of the translation properties of a simple class of arithmetical functions. Part One: The spectrum of an array.*, J. Math. Phys., MIT **6** (1927), 145–157.