APERIODIC ORDER AND SPECTRAL PROPERTIES

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1. Introduction

The concept of order is fundamental to human culture. It not only underlies much of art and architecture, the scientific approach to the understanding of our world is based on detecting and describing order in Nature, in the form of laws of Nature described by mathematics.

Although humans have an instinctive understanding of order, it is surprisingly difficult to define precisely what order is. An example of order in Nature is provided by a perfect crystal, such as a flawless diamond, in which atoms are ordered in a periodically repeating pattern. That Nature can accommodate more complex forms of order is well known, not the least since the discovery of quasicrystals by Dan Shechtman [13], for which he received the Wolf Prize in Physics in 2011 and eventually the Nobel Prize in Chemistry in 2011, almost 30 years after his ground-breaking discovery. The characteristic feature of these materials is the fact that, while showing a similar degree of atomic order, they display symmetries that are incompatible with a periodic arrangement of atoms.

The theory of aperiodic order considers mathematical structures that possess order without periodicity. While the advent of quasicrystals has provided additional physical context to the research, it dates back to the beginning of the twentieth century, with the work of Harald Bohr on almost periodic functions [4, 5]. It has since developed into a fascinating field of modern mathematics, with links to many areas of mathematics such as dynamical systems, harmonic analysis, spectral theory, number theory, to name but a few. For a gentle introduction to the field, we refer to [2]; a more comprehensive introductory account is given in [1].

Apart from the visual attraction of aperiodic tilings, an attractive aspect of the field is the fact that one can make seemingly simple statements which are easy to understand but turn out to be very difficult to prove (similar to, say, Goldbach’s conjecture in number theory, which states that every even number can be written as the sum of two prime numbers). An example of such a question is whether there exists a planar shape that can tile the entire plane without gaps or overlaps (like in a puzzle), but does not admit any periodic tilings. The answer to this question is still open, although there has been some recent progress towards an answer by the Australian mathematician Joan Taylor; see [14] as well as [1, Ex. 6.6] and references therein.

In this exposition, we introduce the general idea behind aperiodic order by means of simple but instructive examples, and provide a hint of why spectral properties are of interest in this context. In doing so, we will gloss over any technical details; we refer to [1] for a proper mathematical treatment.
2. Point sets

We introduce the notion of periodic and aperiodic order by considering simple examples of point sets on the line, that is, in one dimension of space. Sometimes we would like to distinguish different types of points, say by assigning a colour to each point; each point is then characterised by its position \( x \in \mathbb{R} \) on the real line and by its colour. We start with a simple case where all points are located at integer positions along the line. Imagine placing a red point at any integer position of the real line to obtain the point set \( P_0 \) of red points at all positions \( n \in \mathbb{Z} \), which looks like

where the small vertical line denotes position \( n = 0 \). This point set, which you have to imagine to continue indefinitely in both directions, is periodic with period 1, because shifting all positions by 1 reproduces the same point set, so \( P_0 + 1 = P_0 \) (where the notation means adding 1 to the position of each point in the coloured point set \( P_1 \)). Of course, if shifting by 1 maps the point set onto itself, so does shifting by 2, or indeed by any integer \( n \in \mathbb{Z} \), so the set of periods of \( P_0 \) is \( \text{per}(P_0) = \mathbb{Z} \). This reasoning holds true for any periodic point set; so once a point set possesses a period, it automatically possesses an infinite set of periods, which forms a lattice, consisting of all integer linear combinations of a set of fundamental periods.

Here, we are in one dimension, and the fundamental period (which is the smallest non-trivial period, where 0 is deemed to be a trivial period) is 1.

Now, let us take every point at a position \( n \) with \( n \equiv 1 \pmod{4} \) (which means that dividing \( n \) by 4 gives a remainder of 1) and change its colour to blue, and call the corresponding point set \( P_1 \). The result is

where again you have to imagine the point set to continue in both directions, so we have changed the colour of infinitely many points. What is the periodicity of the new point set? We now need to shift \( P_1 \) by multiples of 4 to respect the positions and the colourings of points, so \( \text{per}(P_1) = 4\mathbb{Z} \).

As the next step, let us look at all points at positions \( n \) with \( n \equiv 7 \pmod{16} \). As you can easily convince yourself, all these points are currently red, so let us change them to blue to obtain the next point set, which we call \( P_2 \). The result is

and is still periodic, but now only under shifts by multiples of 16, so \( \text{per}(P_2) = 16\mathbb{Z} \).

We can continue this game, for example by defining \( P_{k+1} \) as the point set obtained from \( P_k \) by changing the colour of all points at positions \( n \equiv (2 \cdot 4^k - 1) \pmod{4^{k+1}} \). All these points are still red in \( P_k \), so will then become blue. The resulting point set \( P_{k+1} \) is then periodic under shifts by multiples of \( 4^{k+1} \). In this way, we obtain point sets \( P_k \) for all integer \( k \geq 0 \), which are periodic with \( \text{per}(P_k) = 4^k\mathbb{Z} \). With increasing \( k \), the periods get sparser and sparser (indeed, in order to actually see this happening even for the next step \( k = 3 \) you would need to consider a longer part of the point set than we displayed above, because
this step affects points at positions \( n \equiv 31 \text{ mod } 64 \) only), and if we kept on performing this process indefinitely and consider the limiting case where \( k \) becomes infinite, we eventually end up with a point set \( P \) that no longer has any periods at all.

Such a point set that does not admit any non-trivial period is called non-periodic. In fact, our point set \( P \) is not just non-periodic, but actually \emph{aperiodic} in the sense of [1], which is a somewhat stronger statement. A proper explanation of the difference between the notions of non-periodicity versus aperiodicity requires a more careful definition of limits of shifted point sets, but the main point of the distinction is to eliminate certain ‘trivial’ situations. An example is the case where you take our original single-colour point set \( P_0 \) and change the colour of a single point, say the point at 0. The resulting point set is non-periodic, because any non-zero shift moved the blue point at 0 to another position and hence changes the point set, because there is no other blue point in the entire point set. However, if you keep shifting the blue point further and further away, the point set will look more and more like the original point set \( P_0 \) around the origin, and in the limit where the blue point has been moved off to infinity, the periodicity of the point set is restored. This point set would not be considered as aperiodic, because periodicity is violated only locally, not globally. Because, in our construction of the point sets \( P_k \), we change the colour of infinitely many points in each step, this is not the case here, and \( P \) possesses the stronger aperiodicity property.

Although the point set \( P \) is aperiodic, it is clearly ordered in some sense, because it is built from an explicit construction which determines the colour for each position uniquely. Even if you did not know where the origin was located, you can still recognise this order. For instance, if you pick a red point which is located between two blue points, you know immediately that every second point along either direction will be red as well, because all points at even positions stay red in our construction. This also shows that you can never find two blue points next to each other. However, like for the simple periodic set \( P_0 \), if you do not know where the origin is located, you actually cannot decide where the origin would have been from looking at an arbitrarily large finite part of the set, because any local arrangements of colours repeat indefinitely often along the line, just not periodically. This property is called repetitivity and arises here as a consequence of the systematic way we used to perform the colour changes, which affected points in the same way anywhere along the line.

So our point set \( P \) is an example of a structure that is both ordered and aperiodic. It is closely related to a class of sequences known as Toeplitz sequences [16]. The theory of aperiodic order is concerned with understanding such point sets and analysing their properties.

### 3. Substitution and inflation

You may wonder why we used the rather specific way of changing colours in our construction of the point sets \( P_k \) above. Clearly, there are lots of ways to produce aperiodic point sets in a similar way. The reason why we chose this particular approach is that the point set \( P \) is a nice and simple example of a set that can also be obtained in a different way, namely by what is known as a substitution or inflation rule (where the latter is commonly used for the geometric interpretation which will be discussed later). To see this, let us denote the sequence of the two coloured points by letters \( r \) (for red) and \( b \) for blue, and consider the rule \( S \) that
maps \( r \mapsto rb \) and \( b \mapsto rr \). Applying this rule repeatedly, starting from a single letter, gives
\[
\begin{align*}
s &\mapsto rb \\
rb &\mapsto rbrr \\
rbrr &\mapsto rbrrrb \\
rbrrrb &\mapsto rbrrrbrrb \\
rbrrbrrbrrbrrbrr &\mapsto \ldots 
\end{align*}
\]
where, in each step, every letter is replaced by a pair of letters according to the rule \( S \). You can continue to do this as long as you like, producing longer and longer words in the two letters \( r \) and \( b \), and in the limit you obtain an infinite word, \( v \) say, that is mapped onto itself under the rule, so \( Sv = v \). This word is thus invariant under the application of the rule \( S \), and in this sense possesses a symmetry under this operation, sometimes referred to as an inflation symmetry. The surprising result is that the infinite sequence \( v \) you obtain in this way will exactly reproduce the sequence of colours in \( P \), starting with the red point at position \( n = 0 \).

To mathematically prove why this is so requires some work; if you are interested, you can find the argument in [1, Chapter 4.5.1], where this example is referred to as the period doubling substitution.

You may ask what happens to the ‘left’ part of the point set \( P \), consisting of all points at negative positions \( n < 0 \). In fact, you can obtain this in a very similar fashion, starting from a two-letter seed and keeping track of the origin as follows
\[
\begin{align*}
r|r &\mapsto rb|rb \\
rbrr &\mapsto rbrrrb \\
rbrrrb &\mapsto rbrrrbrrb \\
rbrrbrrbrrbrrbrrbrr &\mapsto \ldots 
\end{align*}
\]
which you can again continue indefinitely. Considering every second word, starting from the seed \( r|r \), you find that the words grow into a bi-infinite word \( w \) which coincides with \( v \) on the ‘right’ of the origin, and which satisfies \( S^2 w = w \). It produces precisely the sequence of colours of the point set \( P \). Note that, if you had chosen the other word obtained by using an odd number of applications of \( S \) on \( r|r \), the only difference would be that the point at position \( n = -1 \) is blue rather than red, all other colours remain the same.

Substitution rules like \( S \) have been studied extensively, and produce many well-known examples of interesting sequences. The most famous such sequence is named after Leonardo of Pisa, also known as Fibonacci, who introduced it in his book Liber Abaci already in 1202, although it was apparently familiar to Indian mathematicians even earlier. It was motivated by studying the evolution of a rabbit population, with the rule that, in one step, any adult rabbit produces one offspring, and any juvenile rabbit matures to an adult rabbit. This is, of course, a very simplified model in which rabbits live and (asexually) reproduce eternally, and the total population grows exponentially! Let us denote the adult rabbits by \( \ell \) (for large) and the young rabbits by \( s \) (for small), the Fibonacci rule \( F \) is \( \ell \mapsto \ell s \) and \( s \mapsto \ell \). Applying the rule repeatedly, starting with a single adult, gives
\[
\begin{align*}
\ell &\mapsto \ell s \\
\ell s &\mapsto \ell s l \\
\ell s l s &\mapsto \ell s l s l s \\
\ell s l s l s &\mapsto \ell s l s l s l s \\
\ell s l s l s l s &\mapsto \ldots 
\end{align*}
\]
which, when repeating the process indefinitely, produces an infinite word \( v \) which satisfies \( Fv = v \) and is known as the Fibonacci sequence.

Recognising that each finite word in the iteration above is the concatenation of the two previous words, the number of letters of any one of these words is the sum of the number of letters of the two previous words. This produces the sequence of Fibonacci numbers \( 1, 2, 3, 5, 8, 13, 21, 34, \ldots \) satisfying the recursion relation \( f_{k+1} = f_k + f_{k-1} \), with initial conditions \( f_0 = 0 \) and \( f_1 = 1 \) (in which case the list above starts with \( f_2 = 1 \), and
The Fibonacci numbers thus give the total number of rabbits after a number of generations. Counting the numbers of adult or young rabbits, so either of the letter \( \ell \) or the letter \( s \), in each of generations again produces the same sequence, so that in a word of length \( f_{k+1} \) there are exactly \( f_k \) letters \( \ell \) (adult rabbits) and \( f_{k-1} \) letters \( s \) (young rabbits). Using this observation, it is not difficult to show that the ratio of letters \( \ell \) and \( s \) (the ratio of adult to young rabbits), as the number of generations grows, approaches the limit

\[
\lim_{k \to \infty} \frac{f_k}{f_{k-1}} = \frac{1 + \sqrt{5}}{2} = 1.6180339887\ldots
\]

which is an irrational number, conventionally denoted by \( \tau \), known as the golden ratio (and an important number in art and architecture, representing an ‘ideal’ way of dissecting an interval into two parts). The fact that \( \tau \) is irrational shows that the Fibonacci sequence \( v \) cannot be periodic. Indeed, assuming that \( v \) would repeat periodically after, say, \( N \) letters, the ratio of letters in \( v \) would have to be the same as their ratio in a finite word of length \( N \), and hence a rational number with a denominator of at most \( N \).

As for the rule \( S \), we can also produce a two-sided sequence by taking every second step in the iteration of \( F \) on the two-letter seed \( \ell | \ell \), giving

\[
\ell | \ell \xrightarrow{F^2} \ell s | \ell s \xrightarrow{F^2} \ell s l s | \ell s l s \xrightarrow{F^2} \ldots
\]

which produces a bi-infinite word \( w \) which coincides with \( v \) on the ‘right’ and satisfies \( F^2 w = w \).

There is a natural way to interpret the Fibonacci sequence as a point set on the real line, in a way that the rule \( F \) becomes an inflation rule in the following sense. Let us associate to the two letters \( \ell \) and \( s \) two interval lengths, a long one (to \( \ell \), to fit the adult rabbits in) and a short one (to \( s \), for the young rabbits). A natural way to choose the length is given by the golden ratio again, so let us choose the length of the interval \( \ell \) to be \( \tau \) and the length of the interval \( s \) to be 1 (for the mathematical reason for this choice see the discussion of geometric inflation rules in [1, Ch. 4]). Then, the geometric interpretation of the rule \( F \) is

- \( \ell \rightarrow \ell s \)
- \( s \rightarrow \ell \)

which consists of a scaling of the intervals by a factor \( \tau \), followed by the dissection of the long interval into a long and short one (according to the rule \( \ell \mapsto \ell s \), which is geometrically consistent because \( \tau^2 = \tau + 1 \)) and interpreting the scaled short interval as a long one (according to the rule \( s \mapsto \ell \)). The geometric versions of the infinite or bi-infinite words \( v \) and \( w \) become series of intervals

\[
\ell | s | \ell | \ell | s | \ell | s | s | \ell \]

which are invariant under this geometric inflation map.
4. Cut and project sets

The Fibonacci sequence, in its geometric presentation, can also be obtained in a seemingly very different way, which is sketched in Figure 1. Here, the long and short intervals are obtained by a projection of a two-dimensional periodic point lattice (the blue dots) onto a one-dimensional subspace, selecting all the points that fall within the coloured strip. Note that points within the yellow part of the strip give rise to left endpoints of long intervals, while those within the green part correspond to left endpoints of short intervals. With the chosen setup, in particular the location and width of the strip used for the selection of lattice points, the projected one-dimensional tiling turns out to be exactly the same as the one obtained from the inflation description discussed above. Note that the choice of lattice is not unique; our choice is motivated by an interesting connection to number theory, namely the Minkowski embedding of the ring $\mathbb{Z}[\tau] = \{m + n\tau \mid m, n \in \mathbb{Z}\}$; see [1, Ch. 3.4] for details.

This interpretation of the Fibonacci case in terms of a cut and project set (or model set, a notion that goes back to Meyer’s work on harmonious sets [10]) is another indication of the inherent order that is ‘hidden’ in the aperiodic sequence. Although it is not periodic, it is very closely related to a periodic structure, albeit in two rather than in one dimension. This is an important property, and the cut and project construction can be generalised and applied in a quite general setting. The resulting cut and project sets are now quite well understood, because the underlying higher-dimensional periodicity provides a quasiperiodic order, which is a particular case of the general notion of almost periodic order.

The fact that the Fibonacci sequence allows both an inflation and a projection description should not mislead you to assume that this happens in general. Indeed, we are looking at a very special situation here, although many of the ‘nice’ examples will be of this kind. Given an inflation rule, it does not automatically allow for an embedding into a periodic lattice.
in a higher-dimensional space; only certain inflation rules can be represented in this way at all. It turns out that the period doubling sequence discussed at the beginning does in fact have a projection description, but only in a setting where the periodic lattice lies in a more general space, which is not a finite-dimensional Euclidean space, but in general even this is not guaranteed. Conversely, given a cut and project description, the projected structure does not automatically possess an inflation symmetry. In the Fibonacci setup shown in Figure 1, this is only true if the strip is chosen appropriately.

5. Spectral properties

The one-dimensional examples discussed above should provide an intuitive idea about the type of structures that we have in mind when we talk about aperiodic order. The question then arises of how one can characterise order in such aperiodic structures. This is where spectral properties find an application, inspired by applications in crystallography, physics and materials science.

Crystalline order is defined in terms of the diffraction of a material. Diffraction is experimentally observed as the pattern of radiation (such as X-rays) that is scattered by the material. It mainly measures two-point correlations in a structure, with a point-like diffraction pattern indicating strong (crystalline) order, and diffuse scattering typically being interpreted by an absence of order. Mathematically, the quantity that is probed (in the simplest approximation of what happens in reality) is the autocorrelation. Let us consider an example. Take our point set $P$ from our first example, and interpret all red points as scatterers (for simplicity, we associate a scattering strength $u(r) = 1$ to these) and consider the blue points as empty ($u(b) = 0$). The autocorrelation for a given distance $m$ is then the average over the product of scattering strengths of points at distance $m \in \mathbb{Z}$, so

$$a(m) = \lim_{N \to \infty} \frac{1}{2N + 1} \sum_{n=-N}^{N} u(w_n)u(w_{n+m})$$

where $w_n$ denotes the letter ($r$ or $b$) at position $n$ in the bi-infinite sequence $W$. So $0 \leq a(m) \leq 1$ is the average proportion of times you find two scatterers at distance $m$ along the line.

The autocorrelation coefficients $a(m)$ can be explicitly calculated for this case, giving $a(0) = 2/3$ and

$$a(m) = \frac{2}{3} \left( 1 - \frac{1}{2^{r+1}} \right)$$

for $m = (2\ell + 1)2^r$ with $r \geq 0$ and $\ell \in \mathbb{Z}$. The diffraction is obtained from the autocorrelation by what is called a Fourier transformation, which essentially is analysing the frequency distribution of the autocorrelation [8]. This is similar to the frequency analysis of a sound. For the example at hand, the increasingly long periods of powers of 4 in the point set $P$ give rise to frequencies at rational numbers with powers of 2 in the denominator. The diffraction in this case is thus concentrated on a dense point set consisting of all integers $k \in \mathbb{Z}$, with intensity $I(k) = 4/9$, as well as all rational numbers $k = (2n + 1)/2^r$ with $n \in \mathbb{Z}$ and $r \geq 1$ (whose denominators are powers of 2), with the diffraction intensity at $k$ given by

$$I(k) = \frac{1}{9 \cdot 4^{r-1}}.$$
Here, contributions at \( k \) are represented by a disk, centred at \( k \), of an area that is proportional to the diffraction intensity \( I(k) \). See [1, Ch. 9.4.4] for details. So, despite the fact that the positions are dense in space, the decaying nature of \( I(k) \) as a function of \( r \) means that contributions above any given threshold involve a discrete set of positions only, and in any experiment you would see a discrete patterns of spots of different intensity. A sketch of the diffraction pattern, which is periodic with period 1, is shown in Figure 2. As mentioned previously, the point set \( P \) admits an interpretation as a cut and project set, so the pure point nature of the diffraction spectrum is in line with the general result [13] that such sets, under rather general assumptions, are pure point diffractive.

Diffraction is one spectral measure attached to our point set; we shall briefly mention two other spectral measures that have been studied extensively. The first of these is the dynamical spectrum. This is related to the action of translations on our point set, and considering the space of all point sets obtained by such translations and appropriate limits of translates. The idea of associating a spectral measure to this dynamical system goes back to Koopman [9] and von Neumann [17]. For a detailed discussion of dynamical spectra for substitution-based systems we refer to [12]. It turns out that the dynamical spectrum is generally richer than the diffraction spectrum, which is due to the fact that it can detect order beyond the two-point correlations that diffraction can see. It has been known for a long time that there is a close connection between diffraction and dynamical spectra; indeed, the original proof that model sets are, under rather general assumptions, pure point diffractive [13] was based on an argument linking the two spectra in the pure point case. Recent work [3] has further elucidated the connection between the dynamical and diffraction spectra, which now is reasonably well understood.

Finally, another spectral measure motivated by physics is given by the energy spectra of Schrödinger operators describing the motion of electrons in a solid. In a periodic system, valence electrons can move ‘freely’, in what is known as a Bloch wave, whereas in a disordered system, where certain positions are energetically favourable to others, electrons would be expected to be localised at such places. Aperiodically ordered structures are somewhere in between these two, because on the one hand they have motives that keep repeating throughout the systems, while on the other hand they lack periodicity which could sustain Bloch wave solutions. Indeed, it turns out that for large classes of aperiodic models, one finds a very peculiar behaviour, in which electrons are neither localised nor can move freely, and associated to this behaviour are particularly interesting spectral properties. We refer to [6] and references therein for a recent comprehensive review of the results in this area, and to [7] for a detailed analysis of the Fibonacci case.

Although quite a bit is now known about the spectral properties of Schrödinger operators for large classes of one-dimensional examples, there is currently no satisfactory understanding of the relation between the spectral properties of these systems and the other two spectral properties discussed earlier, if indeed such a relation exists. In some respect, these spectral
measures behave in opposite ways; in diffraction and dynamical spectra, point spectra indicate order in a system, while in the Schrödinger case a periodically ordered system shows a continuous spectrum. It is our hope that further investigation of aperiodically ordered systems may shed some light on this open question.

6. Summary

In this snapshot, we limited the discussion to one-dimensional point sets (or tilings by intervals). However, aperiodic order is not limited to one dimension, quite on the contrary some of the beauty of the subject becomes apparent when considering aperiodic tilings in higher dimensions. The most famous example is Penrose’s tiling [11], of which there exist a number of variants; see [11 Ch. 6.2]. A patch of the version with two rhombic tiles is shown in Figure 3. Similar to the one-dimensional Fibonacci system discussed above, Penrose’s tiling can be described either as a two-dimensional inflation tiling or as a cut and project set, in
this case using a lattice in at least four-dimensional space. Its diffraction is pure point and shows perfect tenfold symmetry, which is incompatible with periodicity by the crystallographic restriction [1, Ch. 3.2].

A more recent, stunning example is Joan Taylor’s llama tiling shown in Figure 4, which is related to the open question mentioned at the beginning. Here, the tiles are hexagons of two different types (one of which is kept white in the figure), and the name refers to the fact that the smallest connected cluster of tiles of one colour form little a shape that is resembles the outline of a llama. For more details about this tiling, we refer to [1, Ex. 6.6].

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