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Aperiodic structures and notions of order and disorder

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Abstract

Artificial aperiodic structures have been recently the subject of extensive and intensive research resulting in layered quasiregular heterostructures as well as photonic and phononic metamaterials with possible applications as optical and acoustic bandpassfilters and much more. Our main interest focuses on fundamental questions about determinism, order vs. disorder, their possible quantification, complexity and entropy and beyond. We construct a two-dimensional instance of the Prouhet-Thue-Morse system and compute its line complexity; it is at most polynomial and hence the entropy vanishes. We point out that the perfectly deterministic Champernowne sequence has entropy ln 2 and hence entropy cannot serve as an unqualified measure of disorder. Thus there remain many unanswered questions.

1. Introduction

The motivation of our research is twofold: (1) Artificial aperiodic structures, such as layered *quasiregular heterostructures*, have been the subject of intensive research activities. Considerable progress has been achieved in recent years, where some of the most promising physical realizations of structures are *photonic* or *phononic metamaterials*, mainly being applied as optical and acoustical bandpassfilters. The fabrication of such structures is mostly governed by algorithms based on substitution sequences (cf. [1, 2]).

(2) Our main interest focuses on fundamental questions about determinism, order vs. disorder, complexity, entropy and beyond. The commonplace notions of "order" and "disorder" are heavily context-dependent and rather subjective. Even though in most cases their meaning might be more or less clear, they are, in fact, not defined at all. In order to gain more insight into these fundamental issues, we undertook a study of double-sided substitution sequences and their multidimensional generalizations. The main topic of our analysis is their degrees of order vs. disorder. A rough measure is the *topological entropy*, but better insight might be provided by the *symbolic complexity*. While in for the standard one-dimensional sequences these functions are well known, little is known about their multidimensional counterparts (cf. [3-5]).

Here we present a generic instance of the two-dimensional Prouhet-Thue-Morse system (PTM) and compute its line complexity. It turns out to be at most polynomial and hence its entropy vanishes. We also briefly mention the more general notions of rectangle as well as lattice-animals (polyominoes) complexity. For comparison we also show a periodic example of 2D PTM.

2. The algorithm

To construct our multidimensional sequences we essentially apply a recursive algorithm put forward by Barbé and von Haeseler [6] but we significantly simplify it.

The recurrence equations for the one-dimensional double-sided PTM sequence with the alphabet $\{1, -1\}$ are

(1)
$$t(-2x) = t(x)\ ,$$
$$t(-2x+1) = -t(x)\ ,\quad x \in \mathbf{Z}\ ,$$
$$t(0) = -1\ ,\ t(1) = 1\ .$$

These equations can be readily generalized to n dimensions. For a start (and for a current experiment) we stay in 2D. We choose an expanding matrix $\mathbf{M}$, a shift vector $\mathbf{s}$ and an entry $\mathbf{x} \in \mathbf{Z}$. The recurrence equations then are

(2)
$$t(\mathbf{Mx}) = t(\mathbf{x})\ ,$$
$$t(\mathbf{Mx}+\mathbf{s}) = t(\mathbf{x})\ ,\quad \mathbf{x} \in \mathbf{Z}^2\ ,$$
$$t(0,0) = -1\ .$$

The particular instance of the sequence thus produced depends on the matrix $\mathbf{M}$. For the present example we choose

(3)
$$\mathbf{M} = \begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix}.$$

After 13 iterations this produces a patch shown in Fig.1. It contains $2^{13} = 8192$ points. It is chiral and anorthotropic; it should be noted that this is the generic case. The patch is also fractal; that is intrinsic to the algorithm which jumps back and forth and leaves holes to be filled in later stages.

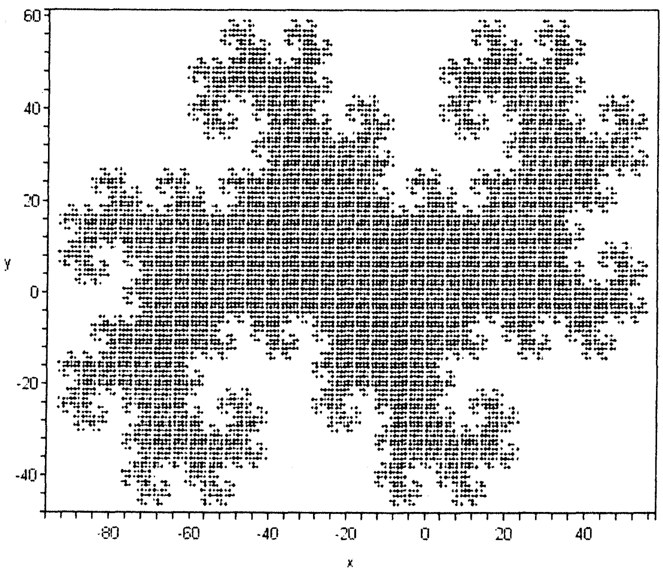

Fig.1. Patch of 2D PTM after 13 iterations containing $2^{13} = 8192$ points.
This example is generic, anorthotropic and fractal.

To construct a periodic 2D PTM structure just change the matrix **M** to

(4) $$\mathbf{M} = \begin{pmatrix} 0 & -2 \\ 1 & -1 \end{pmatrix}.$$

After 13 iterations this produces a patch shown in Fig.2. It contains $2^{13} = 8192$ points. It is also chiral and anorthotropic and fractal..

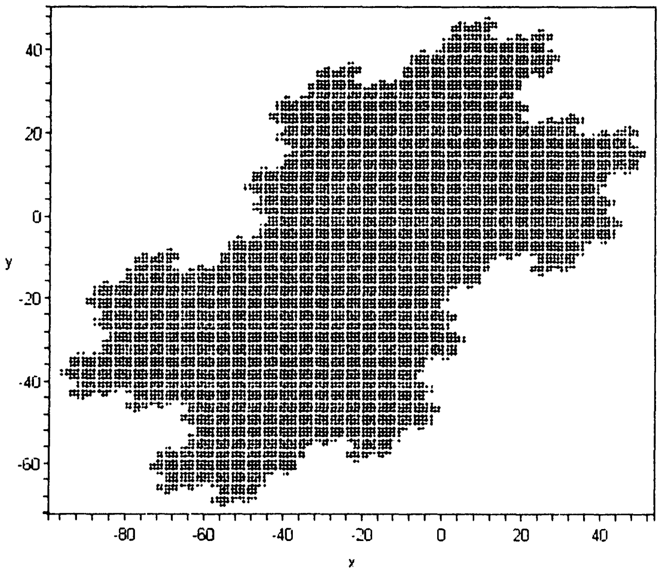

Fig.2. Patch of 2D PTM after 13 iterations containing $2^{13} = 8192$ points.
This example is periodic, anorthotropic and fractal.

As an illustration of the possibility to generalize to higher dimensions we show in Fig.3 a three-dimensional example.

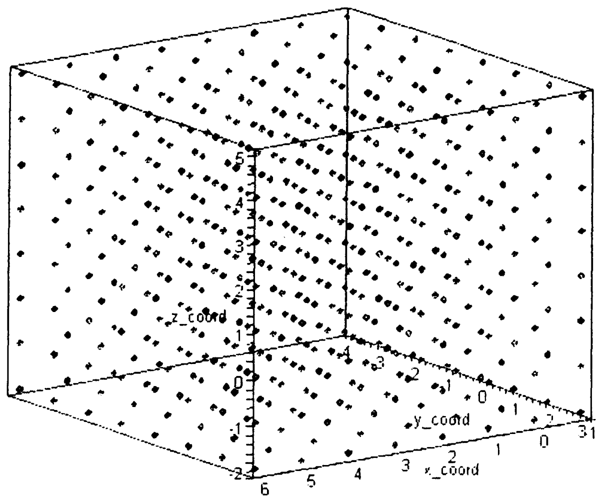

Fig.3. A 3D example of PTM.

3. Determinism, order and disorder

Physicists, chemists and material scientists often loosely speak of "order" and "disorder". In most cases it is more or less clear what is meant. Yet, these terms, while being rather intuitive, are strongly context-dependent and, in fact, not defined at all. They somewhat resemble the notions of "hot" and "cold". Yet hot electrons are quite different from hot tea or a hot onsen (with apologies for the double adjective). Cold atoms are not the same as cold weather, and even that is different in Ouagadougou, Kyoto and Oymekon. Hence, "cold and hot" have been quantified long ago. They can be given a precise meaning by defining temperature, which, of course, can be equivalently measured in units of energy, frequency or wave number.

The concept of entropy as a measure of disorder was invented in the 19th century by Clausius and interpreted in statistical terms by Boltzmann and later introduced into the mathematical literature by Kolmogorov. We note in passing that there are several slightly different definitions of entropy. Strictly speaking, here we deal with *topological entropy*. Again, instead of entropy one might use the concept of information equivalent to negentropy invented by Shannon.

Unfortunately, it turns out that entropy is insufficient to characterize the structures in question. More revealing and detailed is *symbolic complexity*, a function $p_S(n)$ counting the number of words of length n in a given sequence S [7-10].

In terms of complexity the entropy is defined as

$$H(S) := \lim_{n\to\infty} \frac{\ln p_S(n)}{n} \quad . \tag{4}$$

Let us quote a few simple examples of sequences with low complexity. For the sequences 1010... (abbreviated to 10), Fibonacci (F) and Golay-Rudin-Shapiro (GRS) we, respectively, have:

$$p_{1010\ldots}(n) = 2 \ \text{ for all } \ n \, , \tag{5}$$

$$p_{\mathrm{F}} = n + 1 \ \text{ for all } \ n \, , \tag{6}$$

$$p_{\mathrm{GRS}} = 8(n-1) \ \text{ for } n \geq 8 \, . \tag{7}$$

On the other hand, the perfectly deterministic Champernowne (Ch) sequence has complexity

$$p_{\mathrm{Ch}} = 2^n \ \text{ for all } \ n \, , \tag{8}$$

the same as fair Bernoulli and hence the entropy of both is $H(\mathrm{B}) = H(\mathrm{Ch}) = \ln 2$. This seems to be a paradox. It was explained by Baake: the structure of Ch is by construction such that all permutations of any length n must appear in it [11]. The Champernowne number, i.e. the sequence Ch interpreted as the representation of a number is a *normal* number that is one where (in the given representation) all digits are uniformly distributed [12, 13]. The notion of a normal number is by itself somewhat paradoxical: a generic real number is supposed to be normal but it is hard to find one.

Thus we are confronted with a number of challenging questions. Is determinism equivalent to order and in what sense? In crystallography, according to the current consensus, long range order of structure is defined as the presence of a pure point part in the diffraction spectrum which reflects the existence of a non-vanishing two-point autocorrelation. In our opinion, this definition is not general enough. It excludes, for instance, the PTM case (cf. [14]).

On the other hand, we see that entropy cannot distinguish between genuine stochastic disorder and deterministic deviation from uniformity, at least in some cases. Moreover, entropy is blind to dimension; for instance, all Bernoulli structures on any $\mathbb{Z}^d$ have the same entropy $\ln 2$. Thus we need a more revealing global measure of deviation from uniformity as well as clear-cut measure of stochasticity versus determinism.

4. Complexity of PTM – an example

Eventually we computed the symbolic complexity of the generic example shown in Fig.1. We started by exploring *lattice animals* (alias *polyominoes*) on the structure. We quickly learned a few things. Already some animals of low order appeared only in one enantiomer and/or either in horizontal or vertical position. Thus the pattern was indeed proven to be chiral and anorthotropic.

However, the numeric effort to find animals of higher order proved to be quite disproportional. Thus we compromised and restricted our search to the complexity $p(m,n)$ of *rectangles* of size $N = m \times n$ [15, 16]. Moreover, to gain rapid insight we focused on the complexity of *lines* $p_\ell(N)$, i.e. *rows* $p_r(N, 1)$ and *columns* $p_c(1, N)$. The computed results again confirmed the anorthotropy of the pattern. The recursion makes the pattern fractal. The computed complexity up to $N = 20$ is shown in the Table. The complexity turns out to be approximately quadratic and thus polynomial at most; hence the entropy vanishes.

The result again raises some questions. Does the complexity depend on the particular instance of 2D PTM? The answer seems to be positive. If so, how does it depend on the particular class of realizations (cf. [6]), or else, on the choice of the generating matrix $\mathbf{M}$? Is there a canonical instance of 2D PTM?

Table – Symbolic complexity of 2D PTM.

N	rows $p_r(N,1)$	columns $p_c(1,N)$	total lines $p_t(N)$	N^2
1	2*	2*	2*	1
2	4	4	8	4
3	6	6	12	9
4	8	10	18	16
5	10	14	24	25
6	14	20	34	36
7	18	26	44	49
8	24	34	58	64
9	28	42	70	81
10	34	52	86	100
11	40	70	110	121
12	46	90	136	144
13	52	108	160	169
14	60	130	190	196
15	68	156	224	225
16	76	186	262	256
17	84	208	292	289
18	94	236	330	324
19	104	264	368	361
20	122	292	414	400

*) The entries for $N = 1$ are exceptional since rows and columns are the same: (1,1).

4. Conclusions and outlook

The symbolic complexity of the two-dimensional Prouhet-Thue-Morse structure is at most polynomial. This is probably so in higher dimensions as well. Hence the entropy of 2D PTM vanishes and we conjecture that this is also true for nD PTM. We are presently working on other instances of PTM, other 2D sequences and try to extend the study to higher dimensions. And, of course, we intend to extend the computation of complexity to higher N and non-trivial rectangles. We will also try other algorithms, mainly direct substitution.

Our study raises more questions than answers. Can one find put forward a canonical instance of 2D PTM (or any other multidimensional substitution system)? If so, can we find a formula for the complexity? And most important of all: improve our understanding of determinism, order, disorder, stochasticity and their proper quantification.

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