Aperiodic structures, notions of order and disorder

Shelomo I Ben-Abraham
Ben-Gurion University, Beer-Sheba, Israel
and
Alexander Quandt
University of Greifswald, Greifswald, Germany

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Outline

Motivation
Aperiodic heterostructures
Two-dimensional Prouhet-Thue-Morse and paperfolding structures
Order and disorder
Symbolic complexity and entropy
Motivation

Applications:
quasiregular (layered) heterostructures,
photonic and phononic metamaterials
(as optical and acoustical bandpass filters
and much more)

Materials:
GaAs-AlGaAs,
other III-V and II-VI semiconductors,
Ge, Si, porous Si,
modulation by waves
GaAs-AlAs slab
How to produce such a structure?
MBE (Molecular Beam Epitaxy)

**Fig. 1:** A typical MBE system.
Sheer intellectual curiosity: properties of multidimensional substitution systems; fundamental questions about determinism, order vs. disorder, complexity, entropy
What are we doing?

- Construct and study double-sided versions of Fibonacci (F), Prouhet-Thue-Morse (PTM), paperfolding (PF), period doubling (PD) and Golay-Rudin-Shapiro (GRS) sequences. Their spectral properties and complexities are all well known but not so for higher dimensions.

The recursion equations for the 1D double-sided PTM sequence are

\[ a(-2x) = a(x), \]
\[ a(-2x + 1) = -a(x), \quad x \in \mathbb{C}^*, \]
\[ a(0) = -1, \quad a(1) = 1. \]

For the 1D PF sequence we have

\[ a(2x+1) = a(x), \quad a(4x) = 1, \quad a(4x+2) = -1, \quad x \geq 0 \]
\[ a(2x) = a(x), \quad a(4x-1) = -1, \quad a(4x-3) = 1, \quad x \leq 0 \]
\[ a(0) = 1, \quad x \in \mathbb{C}^*, \]

This can be readily generalized to nD.
For a start (and for a current experiment) we stay in 2D. Choose an expanding matrix $M$, a shift vector $s = (1,0)$ and an entry $x \in \mathbb{C}^2$.

The recursion is

\[
a(Mx) = a(x), \\
a(Mx + s) = -a(x), \quad x \in \mathbb{C}^2, \\
a(0,0) = -1.
\]

For the present example we choose

\[
M = \begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix}.
\]
Patch of 2D PTM after 13 iterations containing $2^{13} = 8192$ points. This example is chiral and anorthotropic and has a fractal boundary.
To construct a *periodic* 2D PTM structure just change the matrix $M$ to

$$M = \begin{pmatrix} 0 & -2 \\ 1 & -1 \end{pmatrix}.$$
Patch of 2D PTM after 13 iterations containing $2^{13} = 8192$ points. This example is periodic and anorthotropic and has a fractal boundary.
For the 2D paperfolding sequence the recursion is

\[ a(Mx+s) = a(x) \, , \, a(M^2x) = 1 \, , \, a(M^2x+Mx) = -1 \, , \]

\[ a(0,0) = 1 \, , \, x \in \mathbb{C}^2 \, , \]

with the same matrix \( M \) :

\[
M = \begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix}.
\]
Patch of 2D PF after 9 iterations containing 19683 points. This example is anorthotropic and has an extremely fractal boundary.
A 3D example
“order ↔ disorder”
“cold ↔ hot”
Intuitive but undefined, subjective, context dependent
Quantify “cold ↔ hot” by temperature (energy, frequency)
Quantify “order ↔ disorder” by entropy (negentropy = information)
???
???
determinism ↔ order ???
Entropy is insufficient to characterize such structures. More revealing and detailed is symbolic complexity: a function $p_S(n)$ counting the number of words of length $n$ in a sequence $S$:

- $p_{1010\ldots}(n) = 2$ for all $n$,
- $p_{\text{Fibonacci}}(n) = n + 1$ for all $n$,
- $p_{\text{RS}}(n) = 8(n - 1)$ for $n \geq 8$,
- $p_{\text{Champernowne}}(n) = 2^n$ for all $n$.

Entropy:

$$H(S) := \lim_{n \to \infty} \frac{\ln p_{S(n)}}{n}$$
Eventually we computed the symbolic complexity of our examples. We started with lattice animals (polyominoes) and learned a few things, such as: the generic example of PTM is chiral and anorthotropic. Yet the numeric effort is disproportional. So we compromised and computed the rectangle complexity. To gain rapid insight we focused on lines, i.e. rows and columns. This explicitly confirmed the chirality and anorthotropy. The recursion makes the boundary fractal. The complexity is approximately quadratic, polynomial at most; hence the entropy is zero. The PF example is similar but it is not chiral and its complexity is roughly linear.
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<th>( p_c(1, N) )</th>
<th>( p_t(N) )</th>
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*) The entries for \( N = 1 \) are exceptional since rows and columns are the same: \((1, 1)\).
Conclusions and outlook

The complexity of 2D PTM is at most polynomial, probably so for \( nD \) \((n > 2)\), hence the entropy vanishes: \( H=0 \).

The complexity of 2D PF is roughly linear, it seems to satisfy \( p=8(n-8) \) (needs proof!); the entropy vanishes: \( H=0 \).

We proceed to other instances of PTM and PF, other 2D sequences, to 3D etc.
Challenges

Find (define?) canonical prototypes for these 2D (nD) sequences.

Find formulas for the 2D (nD?) complexities.

When is the entropy of a deterministic structure zero? Is entropy a measure of randomness? Champernowne is a counterexample!

A vexing puzzle!
감사합니다！

谢谢！

Gracias!

Thank you!

Obrigado!

Merci!

Grazie!

شكراً!

חֵלֶק!

Danke!

Ευχαριστώ!