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Exact quantification of the complexity of spacewise pattern growth in cellular automata

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Abstract

We analyze the two possible ways of simulating complex systems with cellular automata: by using the familiar *timewise* updating or by using the complementary *spacewise* updating. Both updating algorithms operate on identical sets of *initial conditions* defining the state of the automaton. While timewise growth generally probes just vanishingly small sets of initial conditions producing statistical *samples* of the asymptotic attractors, spacewise growth operates with much restricted sets which allow one to simulate them all, exhaustively. Our main result is the derivation of an exact analytical formula to quantify precisely one of the two sources of algorithmic complexity of spacewise detection of the complete set of attractors for elementary 1D cellular automata with generic non-periodic architectures of any arbitrary size. The formula gives the total number of initial conditions that need to be investigated to locate rigorously all possible patterns for any given rule. As simple applications, we illustrate how this knowledge may be used (i) to uncover missing patterns in previous classifications in the literature and (ii) to obtain surprisingly novel patterns that are totally unreachable with the time-honored technique of artificially imposing spatially periodic boundary conditions.

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(Some figures in this article are in colour only in the electronic version)

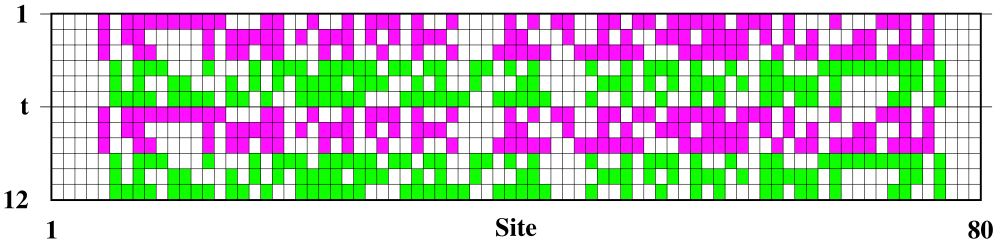

Figure 1. Static period-6 glider supported by rule 20. Its minimal width is 73 sites. As indicated by the two colors, the period-6 displays an inner 'helicoidal' flip symmetry repeating at every three time steps. This structure is missing in the table on page 285 of a recent book by Wolfram [8].

1. Introduction

One of the key sources of the complexity, or computational workload, needed to locate exhaustively all possible asymptotic behaviors of complex systems when simulated by cellular automata is defined by the number of initial conditions that must have their dynamical evolution simulated explicitly [1–4]. Such simulations may be performed in one of two complementary ways: either by using the familiar *timewise* updating [5–8], or by using the complementary *spacewise* updating [9]. The familiar timewise updating algorithm starts with the selection of a convenient spatial dimension, say L cells, and by imposing *periodic boundary conditions* [5–8]. For each possible initial state of the L cells, the time evolution of the automaton is then calculated at successive times $t = 0, 1, 2, \ldots$. Obviously, this procedure can detect no attractors with a spatial dimension larger than L cells. Therefore, to find all asymptotic attractors one needs to repeat the search for progressively larger and larger spatial dimensions, $L \to \infty$, the so-called 'thermodynamic limit'. This process leads very rapidly to an impracticably high number of calculations. In contrast, as explained below, the growth in the number of initial conditions that need to be investigated by the spacewise algorithm is considerably smaller allowing one to probe them all exhaustively. Thus, the number of initial conditions is an important indicator that characterizes the computational workload required to generate all asymptotic attractors efficiently, with minimal computational effort.

The purpose of this paper is to derive an exact analytical formula, equation (9) below, giving the total number $n(k)$ of initial conditions that one needs to investigate in order to find rigorously all possible temporally periodic patterns of a given period k. For the spacewise algorithm, the number $n(k)$ characterizes the complexity of one of the two key bottlenecks that one needs to face when computing and classifying all possible static gliders supported by elementary 1D totalistic (deterministic) cellular automata. Of course, $n(k)$ is independent of the automaton rule and is a convenient measure of computational complexity for both timewise and spacewise algorithms.

As mentioned, the key distinction between the timewise and spacewise algorithms is that while timewise growth implies generally the necessity of dealing statistically with an exponentially growing number of initial conditions [5–8], in spacewise growth small numbers of initial conditions suffice to obtain explicitly patterns that are virtually unreachable otherwise. In other words, for a given period k, while it is computationally hopeless to investigate typical patterns exhaustively for increasingly larger sets of *spatial initial conditions timewisely*, it is perfectly feasible to simulate all *temporal initial conditions spacewisely*. The reason for this is a strong length-asymmetry between the temporal and spatial widths of typical patterns, as observed recently during a systematic computer search [10]. For example, the pattern in figure 1 has temporal period 6 and spatial range 73 plus 4 empty sites needed for the

Table 1. The number $n(k)$ of independent initial conditions that need to be spatially grown to ascertain unambiguously the periodicity, as a function of the period k. The 'defect' $\delta(k) \equiv 2n(k-1) - n(k)$ measures the difference between a perfect doubled growth as the period increases.

k	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$n(k)$	1	1	2	3	6	9	18	30	56	99	186	335	630	1161	2182
$\delta(k)$	–	1	0	1	0	3	0	6	4	13	12	37	40	99	140

pattern to remain stable. In table 1, $n(6) = 9$; the spacewise search which uncovered this pattern had to investigate a total of nine initial conditions, plus the possible ambiguities in the spacewise algorithm (see below). In contrast, a search of this pattern by an exhaustive timewise search on a spatial lattice of size 77 would have required to investigate a total of $n(77) = 1962\,541\,914\,958\,813\,595\,274 \simeq 10^{21}$ initial conditions.

Thus, instead of conducting a timewise search with *large* sets of spatial initial conditions, the classification of asymptotic attractors can be more efficiently performed by following the 'orthogonal' route, i.e. conducting a spacewise search with *small* sets of temporal initial conditions. As we show below, even for relatively small sets of initial conditions, the spacewise algorithm leads to new and unexpected results. First, it allows one to uncover a pattern missing in previous classifications in the literature. Second, it allows one to locate some surprising patterns that are totally inaccessible with the time-honored technique of artificially imposing spatially periodic boundary conditions on the lattice. Third, for each k, spacewise search provides rigorously exhaustive results, not just probabilistic estimates of a full classification.

The spacewise algorithm applies equally well to periodic as well as to non-periodic lattice topologies and, therefore, is free from unnecessarily restrictive spatially periodic boundary conditions familiar from timewise growth. Nowadays, applications of non-periodic architectures include the adequate selection of bifurcation strategies for spatially localized evolving agents competing for spatially localized resources [11], synchronization of replicas of extended systems with long-range interactions [12, 13], among others [1].

As an illustrative application of spacewise updating considering complete sets of initial conditions, we re-investigate the paradigmatic 'class-4' rules 20 and 52, the pair of totalistic binary rules involving five adjacent neighbors and conjectured to produce exceedingly intricate dynamical evolutions [9, 10, 14–16]. Such a class of rules attracts much attention as capable of mimicking universal Turing machines. For instance, there is an excruciatingly elaborate paper claiming that one elementary automaton of class 4, rule 110, should be capable of emulating universal Turing machines [17].

In the next section, we review briefly the spacewise updating algorithm. Section 3 contains the derivation of $n(k)$, equation (9), giving the total number of initial conditions that need to be tested for a given temporal period k. Then, by considering explicitly the $n(k)$ initial conditions up to $k = 15$, section 4 reports novel patterns that are not listed in catalogs presently available in the literature. In addition, section 4 also shows that non-periodic lattice architectures can support rich *spatial transients* before entering spatially periodic regimes. Spatial transients are exclusive signatures found with spacewise growth, being not accessible when imposing periodic boundary conditions. Finally, section 5 summarizes our conclusions and lists a few open questions.

2. The spacewise updating algorithm

For completeness, this section reviews briefly the spacewise algorithm that is used below. A complete description is available elsewhere [9].

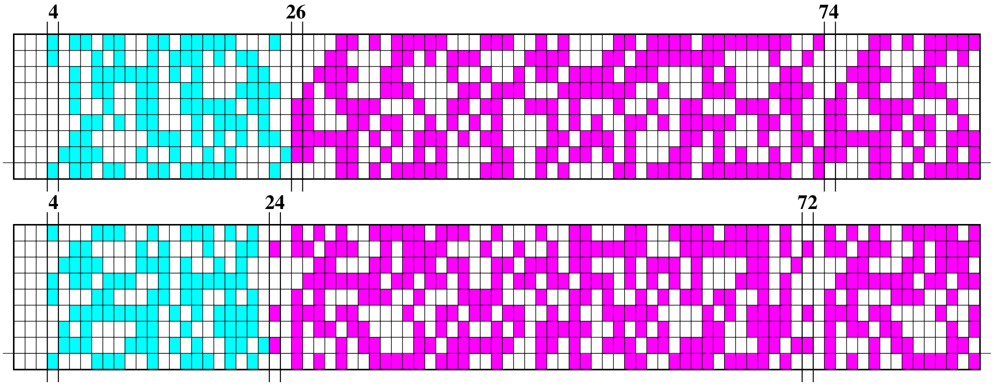

Figure 2. A pair of patterns for rule 20, generated by growing sidewise to the right the initial seeds seen vertically in column 4. Both patterns have spatial period 48 and emerge after rather distinct *spatial* transients and initial seeds. Both are time-periodic with period 8. Transients like these cannot be obtained using timewise updating in lattices with periodic boundary conditions.

Consider a general automaton with an indefinite number of sites, represented as a rectangular matrix of indefinite size and with individual sites distributed along horizontal rows. As usual, the temporal evolution is recorded vertically downward. Denote by $\sigma(t, i)$ the binary *state* of the automaton at site i at time t. For the pair of rules to be discussed below, rules 20 and 52, the state of any site i at time $t + 1$ is given by a function which depends on the sum Σ of the states at time t of the site i and its nearest and next-nearest neighbors. This sum is formally defined by the expression

$$\Sigma \equiv \sigma(t, i-2) + \sigma(t, i-1) + \sigma(t, i) + \sigma(t, i+1) + \sigma(t, i+2), \tag{1}$$

and the state i at $t + 1$ is synchronously updated (timewisely) as follows:

$$\sigma_i(t+1) = \begin{cases} 1, & \text{if} \quad \Sigma \in \mathbb{I}, \\ 0, & \text{otherwise}, \end{cases} \tag{2}$$

where for rule 20 the set $\mathbb{I}$ contains two integers, $\mathbb{I} = \{2, 4\}$, while for rule 52 it contains three: $\mathbb{I} = \{2, 4, 5\}$.

Two distinct sets of initial conditions are involved in the automaton update. In timewise update, one needs initial conditions for a single line of sites. But in spacewise update one needs to know the state of a *block* of neighboring sites. The *width* of the block depends on the range of the specific rule governing the dynamics. The *depth* of the block equals the temporal period k of the patterns that one is looking for. In the simplest case, when considering *interfaces* [9], all states take a fixed value, say 0, while only the rightmost column will contain non-quiescent values. We then refer to this active column as the 'seed' needed to attempt to grow a pattern.

In a nutshell, the algorithm for the spacewise growing of patterns works as follows. Given an automaton with all states defined up to a certain column, imposing temporal periodicity with period k is equivalent to *fixing* the configuration of the line $k + 1$. This fact can be used to determine the state of the column at the end of the range of the rule for lines $k, k-1, k-2, \ldots$, operating backward, all the way up to the starting state of the periodic pattern. The value found at line 1 in this column is then transferred (because of the periodicity) to line $k + 1$ and the process is repeated for the following column. As illustrated in figures 2 and 3, one usually starts with the automaton homogeneously filled with a quiescent state up to a certain column, inserts a seed for the spatial growth and proceeds from this seed by adding new columns as

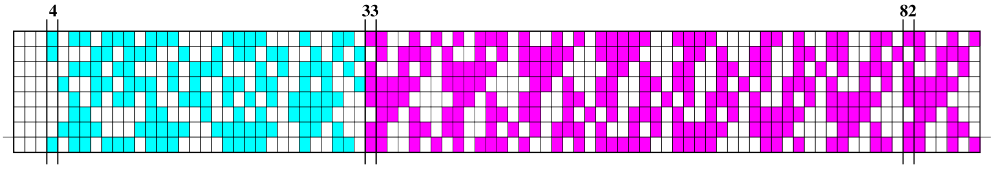

Figure 3. Pattern grown spacewise as those in figure 2, but for rule 52. It has a time period of 7 and space period of 49. The transient pattern cannot be found with timewise updating in lattices with periodic boundary conditions.

described. For details and explicit examples see [9]. A dynamical source of complexity in spacewise pattern growth arises because the growth process is not always unique: sometimes one meets *ambiguities* (equivalently, branchings or bifurcations), namely sites where there is more than one valid possibility of continuation. Complementary to such ambiguities, one sometimes faces a situation which we call *deadlock* and which is very helpful to abbreviate further consideration of the initial condition leading to it. Deadlocks reflect dead ends reached during the evolution, due to the impossibility of fulfilling the dynamical rule and advance the growth process [9]. In this context, a key question is to investigate the rate of growth for both processes, branchings and deadlocks, so as to ascertain if as the time period of the structures grows, its spacewise evolution becomes essentially unique, if it becomes blocked and how often such blockings occur, or if the branching process is finite or not.

3. The exact scaling of complexity

The complexity of the spacewise growth originates from two separate sources, (i) *the complexity of the initial conditions*, namely proliferation of the number of distinct initial conditions that need to be tested by the algorithm as the period k increases, and (ii) *the branching complexity*, i.e. the growth of the number of bifurcations that arise while updating each individual initial condition for a given k. In this section, we derive an exact analytical expression quantifying the scaling of complexity of problem (i) above.

The task is to implement spacewise updating for all possible configurations which are periodic in time with a given period k, starting on the left interface as seen in figure 2 with a non-zero k-vector which itself lies to the right of a homogeneous area of entries all equal to 0. To do this, we need a systematic way to generate the necessary initial k-vectors (but no more than the necessary vectors). These vectors have entries from the set $\mathbb{F}_2 = \{0, 1\}$. There are 2^k distinct k-vectors with entries in $\mathbb{F}_2$. The all-0 vector is of no interest here: to 'start' a spacewise updating with the all-0 vector is merely to extend the area of 0s to the left and delay the actual start of the updating. It should be noted that an isolated all-0 column may possibly appear at some stage during the updating process: see, for example, the second structure in figure 2.

If $d < k$ with $d|k$ (d is a divisor of k), then certain among the 2^k k-vectors will generate configurations with periods d (or divisors of d). Assuming an inductive situation in which such periods $d < k$ have been already investigated, we wish to exclude such k-vectors from further consideration.

Let π denote the cyclic permutation in the symmetric group S_k,

$$\pi = \begin{pmatrix} 1 & 2 & 3 & \cdots & k-2 & k-1 & k \\ 2 & 3 & 4 & \cdots & k-1 & k & 1 \end{pmatrix}, \tag{3}$$

sometimes written in 'cycle notation' as (Herstein [18], p 77)

$$\pi = (1 \quad 2 \quad \cdots \quad k-1 \quad k). \tag{4}$$

In addition, let $v = (a_1, a_2, \ldots, a_{k-1}, a_k)^T$ be a k-vector constructed such that $a_t \equiv \sigma_4(t)$, the site $i = 4$ marking arbitrarily the beginning of an interface (cf labelings in figures 2 and 3). Then π acts in an obvious way on the k-vector v, sending it to $v^\pi := (a_2, a_3, \ldots, a_k, a_1)^T$.

If the configuration starting with the k-vector $v = (a_1, a_2, \ldots, a_{k-1}, a_k)^T$ has been investigated, then all configurations starting with k-vectors whose entries are obtained from v by repeated application of π may be obtained by applying the same permutation to the rows (because we are supposing the configuration is periodic in time with period k) and are of no extra interest. We will say that two k-vectors whose entries are thus related by a power of π are *equivalent*; this affords an equivalence relation in the usual sense (Herstein [18], p 6).

Let $n(k)$ denote the number of inequivalent initial k-vectors that correspond to configurations of minimal period k. We will now calculate $n(k)$ exactly.

There are 2^k distinct k-vectors with entries in $\mathbb{F}_2$. This includes the zero vector $(0, \ldots, 0)^T$ which we exclude, leaving $2^k - 1$ vectors of potential interest.

Let $v = (a_1, \ldots, a_k)^T$ be a k-vector. This may be regarded as a repeating block in the (doubly) infinite periodic sequence

$$\mathcal{S} = \ldots, a_1, \ldots, a_k, a_1, \ldots, a_k, \ldots \tag{5}$$

whose period must be, by the elementary theory of such sequences, a divisor d of k. The fact that this sequence repeats after k terms corresponds to the fact that v is fixed by the kth power of the permutation π; that is, $v = v^{(\pi^k)}$.

Fix a divisor d of k. Amongst the $2^k - 1$ non-zero vectors of the form $v = (a_1, \ldots, a_k)^T$ for $a_i \in \mathbb{F}_2$, there will exist vectors which correspond to the case where $\mathcal{S}$ has minimum period d, and these vectors will be exactly those for which $v = v^{(\pi^d)}$ while $v \neq v^{(\pi^c)}$ for $1 \leqslant c < d$. Such a vector will have to be made up of k/d identical blocks each of length d, that is, of the form

$$v = (\alpha_1, \ldots, \alpha_d, \alpha_1, \ldots, \alpha_d, \ldots, \ldots, \alpha_1, \ldots, \alpha_d)^T \tag{6}$$

and such that the block $\alpha_1, \ldots, \alpha_d$ is non-zero and cannot itself be subdivided into smaller identical blocks. Each block $\alpha_1, \ldots, \alpha_d$ admits the d cyclic permutations given by powers of $\delta = (1, \ldots, d) \in S_d$ and v will be transformed into an equivalent k-vector if we apply the same power of δ to each one of the k/d blocks simultaneously. Thus, there are $n(d)d$ non-zero vectors of minimum period d. Because there are $2k - 1$ non-zero k-vectors in all, each of which corresponds to period d for some $d \leqslant k$ with $d|k$, it follows that

$$2^k - 1 = \sum_{d|k} n(d)\, d. \tag{7}$$

By Möbius inversion (Hardy and Wright [19], theorem 266; Ireland and Rosen [20], p 20), we have

$$k\, n(k) = \sum_{d|k} \mu\left(\frac{k}{d}\right)(2^d - 1), \tag{8}$$

where $\mu(k/d)$ is the Möbius function [19, 20], so that

$$n(k) = \frac{1}{k} \sum_{d|k} \mu\left(\frac{k}{d}\right)(2^d - 1). \tag{9}$$

Note that in deriving this equation, we removed all divisors d of k. This was done because results from explicit numerical computations performed with the spacewise algorithm up to

$k = 15$ seem to indicate that no new patterns arise from the divisors. Of course, for each divisor d of k one simply needs to investigate an additional $n(d)$ possibilities.

The first few values obtained from equation (9) are given in table 1. These numbers are in perfect agreement with those obtained by generating empirically with a computer all possible independent initial conditions up to $k = 22$ [9]. From table 1, one recognizes that $n(k)$ essentially doubles as k grows by one step, the defect $\delta(k) = 2n(k-1) - n(k)$ being also listed in table 1. Because the quantity $n(k)$ counts vectors of a certain type, it must be an integer, and then by equation (9) we conclude that

$$k \left| \sum_{d|k} \mu\left(\frac{k}{d}\right)(2^d - 1). \right. \tag{10}$$

In the special case that $k = p$ is a prime, this reduces to $p|(2^p - 2)$, which is a classic result of Fermat in elementary number theory (Hardy and Wright [19], theorem 70; Ireland and Rosen [20], p 33). Equation (9) above is a nice application of the powerful number-theoretical Möbius function to a problem in physics [21]. This expression gives the scaling of the complexity as a function of the period k. Equation (9) was fundamental to guarantee that all initial seeds were indeed tested during our systematic computer search for new patterns described in the next section. It was instrumental in uncovering the remarkable structures displayed in figures 1–3.

4. Results of systematic computations

The behaviors of the two class-4 automata defined by equation (2) for rule 20 and for rule 52, respectively, have been investigated in detail; see for example [8]. However, as figures 2 and 3 show, rules 20 and 52 still contain interesting undetected features. Figure 2 shows two remarkable patterns for rule 20, grown from left to right from the 'seeds' $(11000000)^T$ and $(10011000)^T$ seen in column 4, by applying the spacewise updating algorithm [9]. The two different colors (shadings) in the figure represent active '1' sites, with the leftmost shading used to highlight the presence of a *spatial transient*. Numbers refer to the site position, counted from the leftmost site. The periodic patterns indicated by the shadings seen on the right-hand side are obtained after two distinct transients, indicated by the different shading on the left-hand side. Note that periodic boundary conditions preclude patterns such as those in figure 2 from being obtained with timewise updating, independently of the size of the lattice employed. Following the spatial transients in figure 2, there are spatially periodic structures of period 48 which may be used to completely fill lattices of sizes commensurate with 48, to produce coverings as discussed in [14]. Figure 3 shows analogous characteristics for rule 52. Figure 1 reports a remarkably complex static glider of temporal period 6 supported by rule 20. Its minimal width covers $w = 73$ sites, a width that coincides with that of the largest glider listed in the compilation 'All the persistent structures with period up to 15', on page 285 of Wolfram [8]. This width appears to be the largest obtained so far under rule 20. The discovery of a second glider of width 73 shows that spacewise growth can assist in locating missing gliders that have eluded previous searches. As highlighted by the two distinct colors, the temporal period-6 in figure 1 displays a curious inner 'helicoidallike' flip symmetry repeating at every three time steps.

5. Conclusions and outlook

From a theoretical point of view, we argued that the computational workload for growing patterns with the spacewise algorithm arises from two distinct sources: from the intrinsic *static* complexity introduced by the initial conditions, and from a *dynamical* branching complexity due to bifurcations inherent to the growth process. For the first process, we were able to derive an exact expression quantifying the complexity, equation (9), valid for generic periodic and non-periodic architectures of arbitrary sizes.

Concerning applications, our exhaustive investigation of the full space of initial conditions for all temporal periods up to $k = 15$ for rules 20 and 52 revealed patterns not found in previous investigations. Being exhaustive, our search now finally completes the classification of all periodic patterns with a temporal period $k \leqslant 15$. In addition, we found 'spatial transients', the remarkable novel structures illustrated in figures 2 and 3, elusive structures that cannot be found with the time-honored artifice of arbitrarily *enforcing* periodic boundary conditions. Of course, the periodic structures following spatial transients may be used *to tile* completely phase-spaces having dimensions commensurate with them and to study the spontaneous emergence of order in complex automata [14]. We are developing an explicit constructive procedure for generating recursively (as a function of k) all possible initial conditions predicted by equation (9).

In summary, the formula for $n(k)$ gives the number of initial conditions that need to be investigated spacewisely to ascertain rigorously exhaustive results. Knowledge of $n(k)$ allows one to efficiently use the spacewise algorithm [9] as an automatic filter for the detection of coherent structures in spatiotemporal systems without needing to guess or postulate *a priori* the form of such structures. It is important to emphasize the difference between knowing how many initial conditions exist and knowing which they are. Of course, the ultimate interesting question for a given automaton is to possess a complete list of the initial conditions. After predicting how many they are and thereby restricting the universe to be investigated, the next important question is to have an efficient algorithm to compute without repetitions the minimal set of initial conditions that need to be tested. Such an algorithm now exists and is reported elsewhere [22]. The formula for $n(k)$ provides an accurate estimate of the computational complexity involved in application of the spacewise algorithm to obtain exhaustive answers concerning the spatio-temporal organization of cellular automaton models of, e.g., computer networks [23–26].

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