Role of initial conditions in the classification of the rule space of cellular automata dynamics

Avinash Dhar,* Porus Lakdawala,[†] Gautam Mandal,[‡] and Spenta R. Wadia[§] Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay-400005, India (Received 22 September 1994)

In the qualitative classification of cellular automata (CA) rules by Wolfram [Rev. Mod. Phys. 55, 601 (1983)], there exists a class of CA rules (called class 4) which exhibit complex pattern formation and long-lived dynamical activity (long transients). These properties of class 4 CA's has led to the conjecture that class 4 rules are universal Turing machines, i.e., they are bases for computational universality. We describe the embedding of a "small" universal turing machine, due to Minsky [Computation: Finite and Infinite Machines (Prentice Hall, Englewood Cliffs, NJ, 1967)], into a cellular automaton rule table. This produces a collection of $(k = 18, r = 1)$ cellular automata, all of which are computationally universal. However, we observe that these rules are distributed among the various Wolfram classes. More precisely, we show that the identification of the Wolfram class depends crucially on the set of initial conditions used to simulate the given CA. This work, among others, indicates that a description of complex systems and information dynamics may need a new framework for nonequilibrium statistical mechanics.

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Recently, cellular automata have become paradigms for complex "lifelike" systems. Among other things, they provide an ideal substratum to simulate artificial, biological environments [1]. In this sense, they might provide a suitable, abstract setting for discussions of biological complexity.

In this paper we investigate the connection between a certain class of cellular automata (CA) (technically called class 4) and the notion of universal computation. Our main result is that the CA rule-based classification proposed by Wolfram seems to be inadequate. Any quantitative classification scheme would have to take into account the space of initial configurations. We believe that this phenomenon may have implications for nonequilibrium statistical mechanics.

Our paper is organized as follows. In Sec. II we collect for completeness the definiton of a cellular automaton and the Wolfram classes. In Sec. III, we briefly review the studies of Langton et al. on the connection between cellular automata and phase transitions in statistical mechanics. Section IV contains a brief review of universal Turing machines (UTM) as well the construction of Minsky's "small UTM. " Section ^V contains the main result. We then conclude with some observations and remarks.

I. INTRODUCTION **II. THE WOLFRAM CLASSES**

Cellular automata (CA) are discrete (both in space and time) dynamical systems. More formally, consider variables sitting at the sites of a one-dimensional lattice. The variables take values from a finite set S . The evolution of the CA proceeds through discrete time steps by a local rule, which is specified by the function

$$
x_i^{t+1} = f(x_{i-r}^t, \dots, x_i^t, \dots, x_{i+r}^t),
$$
\n(1)

where x_i^t denotes the value of the variable at the latticesite i at time t . A CA whose lattice variables take one of k possible values and whose evolution rule depends on at most r neighbors of a given site is called a (k, r) CA. Moreover, one isolates a special state s in S , called the quiescent or stable state, as the one that is preserved by the evolution, i.e., $f(s, \ldots, s) = s$. All CA's considered here have a stable state. The function f specifying the CA rule is conventionally called the rule table, the $(2r +$ CA rule is conventionally called the rule table.
 $(x_{i-r}^t, \ldots, x_{i+r}^t)$ is called a template.

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The qualitative features of the space of CA rules can be studied by observing their space-time histories obtained by the evolution of cellular automata on a computer. Such studies were made by many authors, in particular, by Toffoli [2], Wolfram [3, 4], Margolus [5], and Vichniac [6]. Wolfram isolated four qualitative classes of behavior (now known as the Wolfram classes). They are as follows.

 (1) Class 1 — evolution leads to a homogeneous (stable) configuration.

 (2) Class 2 — evolution leads to periodically repeating patterns, in a largely quiescent background.

^{*}Electronic address: adhar@theory.tifr.res.in

[~]Electrnoic address: por us @theory. tifr.res. in

 $~^{\ddagger}$ Electronic address: manda@theory.tifr.res.in

Electronic address: wadia@theory.tifr.res.in

site.

(3) Class 3 – evolution leads to "chaotic" patterns, created by rapidly changing states of any given lattice

(4) Class 4 – evolution leads to complex patterns, generated by mobile interacting structures which are relatively long lived.

To obtain a feel for the qualitative aspects of the classification we suggest that the reader consult the large number of space-time histories given in [3, 4]. It is important to note that this classification is based on the evolution of a given rule from a randomly chosen initial configuration. Wolfram further conjectured that the rules belonging to class 4 possess the capacity to perform universal computation [4]. For a precise definition of the notion of universal computation see Sec IV.

III. PHASE TRANSITIONS AND CLASS 4

There have been numerous attempts in the past few years either to provide a quantitative basis for Wol fram's classification or to propose alternative classification schemes. We note two such attempts. The first is due to Cullick and Yu [7, 8], who have tried to use a computation theoretic approach as a basis for classification. It is a remarkable fact that their classification coincides with Wolfram's for the $(k = 2, r = 2)$ totalistic CA's [7]. An important fact, which is of relevance to our discussion, is that in this classification all CA's which are computationally universal belong to class 4. In this classification, the diferent classes are statements about all initial conditions for the given rule.

The other attempt at trying to provide a quantitative understanding of the Wolfram classes that we would like to discuss is due to Langton and co-workers [9, 10], who made a statistical study of the rule spaces of various (k, r) CA rules. They used various information theoretic quantities like the Shannon entropy and mutual information. For definitions of Shannon entropy and mutual information see, for example, [11]. In what follows, we briefly describe this work. For details, we refer the reader to the original sources.

For a given rule table, Langton introduced a parameter, λ , defined as the fraction of templates in the ruletable which are mapped to a nonquiescent state. It is intuitively quite clear that rules with a low value of λ (close to 0) belong to either class 1 or 2, while those with a high value of λ (close to 1) belong to class 3. The "complex" class 4 rules are expected to occur at intermediate values of the λ parameter. Consider a collection of randomly generated rules, one at each value of λ , spanning the interval [0, 1]. We will call such a collection a lambda string. If we now think of the rule space as an abstract space where each point represents a CA rule, then a particular lambda string might be thought of as a curve through the rule space. What Langton noticed was that, while along most curves (or equivalently, lambda strings) the transition from class 2 rules to class 3 rules was discontinuous (sharp), there did occur some curves in the rule space along which the transition from class 2 to class 3 was smooth. These curves in fact "passed

through" class 4 rules. In more quantitative terms, the Shannon entropy, when calculated over lambda strings of the former type, showed a jump at some value of λ (which depended on the chosen string), from values quite close to 0 to values near 1. The value of the mutual information at different points on such curves did not differ substantially from 0. However, for lambda strings of the latter type, the entropy showed a relatively smooth transition from values near 0 to values near 1. The mutual information, on the other hand, showed a sharp peak for these lambda strings. Langton concluded that the structure of the rule space appeared to be as follows.

There is an "ordered phase" of class 1 and 2 CA rules, separated, in general, from the "disordered or chaotic phase" of class 3 rules by a "first order" transition. However, in the vicinity of this phase boundary lie pockets of "complex" class 4 rules. If the rule space is traversed across these pockets of complex rules, the order-to-chaos transition is a "second order" transition.

The order of the phase transition is to be understood, by treating the Shannon entropy in analogy with the usual entropy in statistical mechanics and the mutual information, with the derivative of the entropy.

IV. MINSKY'S "SMALL" UTM

We briefly review here the definition of a Turing machine. For details, the reader may refer any standard text on computation theory, such as [12, 13].

^A Turing machine (TM) consists of a "head" which moves along an infinite "tape" consisting of cells. The cells on the tape can each carry a symbol from a finite set Q. There is a special symbol in Q called the blank. Initially, all except for a finite number of cells on the tape carry the blank. The head of the TM, on the other hand, can exist at each instant in one of a finite number of states chosen from some finite set T . T contains a special state called the start state. Initially, the head of the TM is in the start state. At a given instant of time, the head resides at a particular cell on the tape. Depending on the tape-symbol that is "read" by the head and also on the particular state that the head is currently in, the following transformations are allowed.

(1) The present tape symbol may or may not be altered to a new symbol.

(2) The present head state may or may not be altered to a new state.

(3) The head will move one cell either to its right or left, or else the TM will halt.

The definition of a particular TM consists in specifying Q, T and the state-symbol transition table.

As was mentioned before, the tape of the TM would initially have all cells "blank" except for a finite number. These nonblank cells can be thought of as encoding the "program" or "algorithm" which controls the evolution of the TM. A universal Turing machine (UTM) is defined to be a TM which can simulate any other TM, if supplied with an appropriate program which encodes the

description of the TM to be simulated.

We now give the description of a four-symbol, sevenstate UTM due to Minsky $[12]$. The set of symbols is $Q = \{q_0, q_1, q_2, q_3\}$ and the the set of states is $T =$ $\{t_0, t_1, t_2, t_3, t_4, t_5, t_6\}$. q_0 denotes the blank symbol, while t_1 is the start state. The transition table for this TM is given below (see Table I). If the combination of the tape symbol and the head state at a particular instant is (q_i, t_k) , the corresponding entry in the table gives the appropriate transformation for the TM. Here r denotes "move to the right," l denotes "move to the left," while h denotes "halt." The proof that this TM is indeed computationally universal can be found in [12].

V. UNIVERSAL COMPUTATION AND CLASS 4

Universal computation is, by definition, the domain of performance of a universal Turing machine. A universal cellular automaton (UCA) is one which simulates, at every time step, a UTM. A CA which has been proven to be universal is the well known Game of Life, due to Conway [14]. In general, it is difficult to decide whether a given CA is a UCA. It is in fact easier to construct CA's which are universal. Small UCA's are obtained by "embedding" a small universal Turing machine into a CA rule. Of these methods, which by now are quite well known, we describe one a little later.

From the discussion in Secs. II and III, it appears that the class 4 CA rules bring together two rather disparate looking themes $-$ that of phase transitions from statistical mechanics and universal computation from computation theory. However, at present it can hardly be said that the connection between these two themes is clear.

The aim of the present investigation is to provide a somewhat better understanding of the connection between class 4 CA's and universal computation. In a sense this work may be thought of as an effort in a direction, complementary, to that of Langton et al. in addressing the above question.

The idea employed in the present work is quite simple and is as follows. Using a well-known construction of a "small" UTM due to Minsky [12] we construct a rather large collection of $(k = 18, r = 1)$ CA rules, all of which are universal. We then perform a Wolfram classification of the CA rules within this subspace of the rule-space. Surprisingly, one finds that even within the subspace of UCA's there are rules which seem to belong to each of the Wolfram classes (except class 1).

We now describe this result in greater detail. First we demonstrate a simple and very well-known way [15] of embedding any TM into a CA.

An embedding of a TM into a CA requires the following.

(1) The specification of a mapping between the states and symbols of the TM and the states of the CA, which would allow us, at every time step, to transform a TM tape-head configuration into the corresponding CA configuration.

(2) The specification of the rule table of the CA which is consistent with the state-symbol transition table of the TM with respect to the above mapping.

To construct the embedding, think of the CA lattice as the tape of the TM. The lattice variables should thus carry the tape symbols of the TM. Moreover, they should also carry information about the position and the state of the TM head. This can be done by introducing CA states corresponding to the different head states of the TM, along with the information that the head is currently reading the cell to either its immediate right or left, specified by the symbols L, R . The map required in (1) above can now be chosen as follows: The set of states S of the CA consists of tape symbols as well as ordered pairs of the head states and L or R, i.e., $S = Q \cup (T \times \{L, R\}).$ The number of CA states is evidently $|S| = |Q| + 2|T|$. With this map between the CA states and the TM symbol and states, it is not hard to construct a CA rule table, with nearest-neighbor interaction, which simulates the transition table of the TM. We can also construct an embedding in which the CA states are just the TM states and symbols, along with the prescription that the "head" variable always reads the cell which, say, is to its immediate right. This leads to a CA rule table with a next-nearest-neighbor interaction.

To clarify the procedure described rather abstractly above, we reconstruct some of the details now with reference to Minsky's UTM (see Sec. IV). In this case the set of states for the CA would be $\{q_i,(t_j,L),(t_j,R)|i=$ $0, ..., 3, j = 0, ..., 6$. We now give two examples of the evolution of the CA lattice configuration in a single time-step. From these examples it is clear how the rule

TABLE I. The symbol-state transition table of Minsky's small UTM. The entry in the table corresponds to the transformation that the TM will perform if the head is currently in the state t_i and is reading the tape cell containing the symbol q_j . I denotes a left move, r denotes a right move, h denotes halt.

	t_0	t_1	$\boldsymbol{t_2}$	t_{3}	t.	t_{5}	t_{6}
qо	(q_0, t_0, l)	$(q_2,t_1,r) \qquad (q_0,t_2,h)$		(q_2,t_4,r)	(q_2,t_2,l)	(q_3,t_2,l)	(q_2, t_5, r)
q_1	(q_1, t_1, l)	(q_3,t_1,r)	(q_3,t_2,l)	(q_1,t_6,l)	(q_3,t_4,r)	(q_3,t_5,r)	(q_1, t_6, r)
q_{2}	(q_0, t_0, l)	(q_0,t_0,l)	(q_2,t_2,l)	(q_2,t_3,l)	(q_2,t_4,r)	(q_2,t_5,r)	(q_0, t_6, r)
q_3	(q_1, t_0, l)	(q_2,t_5,r)	(q_1,t_3,l)	(q_1, t_3, l)	(q_1,t_4,r)	(q_1,t_5,r)	(q_0, t_1, r)

table for the CA can be constructed.

In the first example the UTM at the present time step has symbols \ldots q_0 q_2 q_1 q_2 ... inscribed on the tape and the head is in the state t_4 pointing at the tape cell containing q_1 . From the appropriate entry in Table 1 the UTM evolves by changing the tape cell from q_1 to q_3 and the head moves a step to the right without changing its state. In terms of the CA this evolution could be represented as follows:

$$
\cdots q_0 q_2 (t_4,R) q_1 q_2 \cdots
$$

$$
\cdots q_0 q_2 q_3 (t_4,R) q_2 \cdots
$$

In the second example the UTM performs the same evolution as in the previous example. However, in terms of the CA it could also be represented as follows:

$$
\ldots q_0 q_2 q_1 (t_4,L) q_2 \ldots
$$

$$
\ldots q_0 q_2 q_3 (t_4,R) q_2 \ldots
$$

Note, however, that this ambiguity would come into play at only the initial time step and could be removed by demanding that only one of the configurations, say the one in the first example, can be a legal initial configuration. After making this demand, the rest of the CA (or equivalently the UTM) evolution is completely unambiguous.

As a result of the prescription described above, one obtains a large class of $(k = 18, r = 1)$ CA's, all of which are computationally universal. The large class of UCA's obtained is accounted for by the fact that the embedding does not fix all the $(2r+1)$ -tuples $(x_{i-r}^t, \ldots, x_{i+r}^t)$ of the rule table to a unique value. Since the UTM contains only a single "head," the $(2r + 1)$ -tuples which contain only a single head state are uniquely determined by the definition of the UTM. However, CA lattice configurations which contain more than one head state are perfectly legal as far as the cellular automaton is concerned. For example, the following evolution is perfectly legal in

FIG. 1. Shannon entropy (H) vs λ for a generic curve in the space of UCA's. The entropy was calculated for a cell of three adjoining lattice sites. The data for computing probabilities were obtained by counting the frequency of occurrence of different configurations, between time steps 350 to 400 and further over 10 different initial conditions. Here λ is the fraction of templates not fixed by the definition of the UTM that are mapped onto the nonquiescent state.

FIG. 2. Mutual information (M) vs. λ for a generic curve in the space of UCA's. The mutual information was calculated between two cells, each of three adjoining lattice sites. The data for computing probabilities were obtained by counting the frequency of occurrence of different configurations, between time steps 350 to 400 and further over 10 different initial conditions. Here λ is the fraction of templates not fixed by the definition of the UTM that are mapped onto the nonquiescent state.

terms of the CA:

$$
\dots (t_6, R) \quad q_2 \quad q_1 (t_4, L) \quad q_2 \dots \n\dots q_0 \quad (t_6, R) \quad q_3 (t_4, R) \quad q_2 \dots
$$

Although such configurations would make no sense in terms of the underlying Turing machine, they have to be considered while performing the Wolfram classification. It is of importance to mention that for initial configurations which contain a single head state, all rules within the space of UCA's that we are considering have

FIG. 3. The space-time history of a randomly generated UCA at $\lambda = 0.1$. The evolution is from a randomly generated initial condition on a lattice of size 60 with periodic boundary conditions. The class 2 behavior seen is consistent with the low value of mutual information observed at this value on λ in Fig. 2.

FIG. 4. The space-time history of a randomly generated UCA at $\lambda = 0.45$. The evolution is from a randomly generated initial condition on a lattice of size 60 with periodic boundary conditions. The class 4 behavior seen is consistent with the relatively high value of mutual information observed at this value of λ in Fig. 2.

the same evolution. Within the space of CA lattice configurations those which contain two or more head-states form an overwhelming majority, and if one is to select a (few) random initial configuration(s) as a basis of classification, then it would invariably be one of these.

In other words, the subspace of CA latticeconfigurations which governs the behavior of any of the UCA's as a UTM is quite distinct from the subspace of configurations which determines the Wolfram class, to which the UCA belongs.

In Figs. 1 and 2, we have shown the variation of the Shannon entropy and the mutual information over a (generic) lambda string through the subspace of UCA's. The decay of mutual information to 0 on both sides of a peak value suggests the wide variation in complexity of the rules associated with the lambda string. The spacetime histories shown in Figs. 3—⁵ corroborate this fact. We remark that we have defined λ as the fraction of templates of the rule table, not fixed by the definition of the UTM, that are mapped onto the nonquiescent state.

VI. CONCLUSIONS AND REMARKS

The main observation that emerges from our investigations is the importance of initial conditions for any study of complex systems. We point to the work of Banks, which demonstrates the dependence of computational universality on initial conditions [16] for a twostate automaton and proves that such an automaton cannot be universal starting from a uniform tape, but can be starting from a tape filled with a simple regular pattern. As far as CA's are concerned, any quantitative classifi-

FIG. 5. The space-time history of a randomly generated UCA at $\lambda = 0.7$. The evolution is from a randomly generated initial condition on a lattice of size 60 with periodic boundary conditions. The class 3 behavior seen is consistent with the low value of mutual information observed at this value of λ in Fig. 2.

cation of the rule space must also, perforce, be a statement about the space of initial conditions. We draw the reader's attention, once again, to the classification due to Cullick and Yu [3], where the definitions of the classes are statements about all initial conditions. Whether the agreement of these classes, with that of Wolfram's, for the $(k = 2, r = 2)$ totalistic rules is a mere coincidence or a necessity for small rule spaces remains unclear. Our analysis shows that the subspace of $(k = 18, r = 1)$ rules that we have considered, which would belong entirely to class 4 of the Cullick-Yu scheme, by virtue of their being computationally universal, is actually distributed among the various Wolfram classes.

Complex systems are invariably studied from one of two diferent points of emphasis. One is the view arising out of statistical mechanics and dynamical systems, where the emphasis is on the properties of the system observed at large times, i.e., the steady-state properties of the system. The second view is the one that arises from formal studies of the computational complexity classes. Here the emphasis is on the behavior of the system as a function of the input. We feel that a new framework of statistical mechanics which incorporates the second point of view is required to provide a better definition for a study of complex dynamical systems.

The observations made above seem to suggest an avenue for further exploration. One might be tempted to consider a scenario in which the classes are not well demarcated regions of the rule space, but rather, are sets with fuzzy boundaries. The measure of fuzziness attributed to the set could depend on the proportion of the space of initial configurations on which the rules (contained in the set) evolve in a complex manner.

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