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LOCAL STRUCTURE THEORY FOR CELLULAR AUTOMATA

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The mean-field theory for cellular automata (Wolfram, and Schulman and Seiden) is generalized to *the local structure theory*. The local structure theory is a sequence of finitely-parameterized models of the *statistical* features of a cellular automaton's evolution. The nth model in the sequence takes into account correlations in terms of the probability of blocks of n states. A class of measures, the n-block measures, is introduced. The local structure operator of order n maps n-block measures to n-block measures in a manner which reflects the cellular automaton map on blocks of states. The fixed points of the map on measures approximate the invariant measures of the cellular automaton.

The ability of the local structure theory to model evolution from uncorrelated initial distributions is studied. The theory gives exact results in simple cases. In more complex cases, Monte Carlo numerical experiments suggest that an accurate statistical portrait of cellular automaton evolution is obtained. The invariant measures of a cellular automaton and the stability of these measures may be obtained from the local structure theory.

The local structure theory appears to be a powerful method for characterization and classification of cellular automata. Nearest neighbor cellular automata with two states per cell are studied using this method.

1. Introduction

Cellular automata are discrete dynamical systems. A cellular automaton consists of a discrete lattice of cells, and a rule which operates on the lattice. The lattice may be infinite in extent. Each cell of the lattice has a finite number of states. The rule is deterministic and translationally invariant. It gives the state of a cell in terms of the states of cells in a finite neighborhood about the cell at the previous time step (von Neumann [19], Wolfram [22]).

Cellular automata were introduced by von Neumann [19], who used computation theory to study organic self-reproduction. He was able to show that a particular two-dimensional cellular automaton supports configurations which are capable of simulating a universal Turing machine, and capable of constructing copies of themselves on the lattice. The appeal of cellular automata is that they are simple to construct, yet potentially give rise to very complicated behavior when the rule is iterated. This phenomenon has mathematical, computational and physical interest, as von Neumann was the first to realize.

It is typically difficult to determine the nature of a cellular automaton's performance directly from a description of the rule. The "local structure theory" described in this paper is a finitely-parameterized procedure for the determination of the *statistical* features of a cellular automaton's evolution. Its ability to accurately model the evolution of an arbitrary cellular automaton is noteworthy in view of Wolfram's [24] conjecture that no finite computational procedure may be given to effectively predict the behavior of a chaotic cellular automaton.

The local structure theory may be viewed as a generalization of the mean-field theory for cellular automata (Wolfram [22], Schulman and Seiden [18]). The mean-field theory is a model of cellular automaton evolution which makes the assumption

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that iterative application of the rule does not introduce correlations between the states of cells in different positions, so that if an initial configuration were uncorrelated, it would remain uncorrelated under cellular automaton evolution. This assumption is generally not valid, but allows the derivation of a simple formula for an estimate of the limit density of each possible state of a cell. In some cases (Wolfram [22]), the mean-field theory does well in predicting the limit density, as ascertained by comparison with Monte Carlo simulations of the rule. In the case of interesting and complex rules, the mean-field theory performs quite poorly (Schulman and Seiden [18]).

The most striking feature of cellular automata is that correlations between the states of cells develop as the automata evolve. The mean-field theory fails to predict statistical features since it assumes that correlations are never generated during cellular automaton evolution. By contrast, the local structure theory takes correlation explicitly into account. It has the potential to capture detailed statistical features of cellular automaton evolution. Recently, Wilbur et al. [20] have shown that cellular automaton evolution may be approximated by a Markov process. This work demonstrates the value of expressing the intuitive notion of "correlation" in terms of block probabilities. Their method may be directly related to the local structure theory.

Empirical study of a number of cellular automaton rules demonstrates the potential of the local structure theory to describe the statistical features of cellular automata. The behavior of some particularly simple rules is derived analytically. These rules serve as useful checks for the empirical methods employed. Other rules have more complex behavior. Even for these rules, the local structure theory yields an accurate portrait of both small- and large-time statistics.

In this paper we initiate a classification study of cellular automata using the local structure theory. Rules which differ in construction may nonetheless lead to the same local structure approximation. It is argued that this provides a useful classification scheme for cellular automata.

2. Fundamentals

Before the local structure theory itself is discussed, some fundamental concepts and notation will be introduced. Let Z be the integers, $\ldots, -1, 0, 1, \ldots$. We construct a 1-dimensional lattice by associating with each integer i a *cell* b_i. Each cell can have any one of k states: $s_0, s_1, \ldots, s_{k-1} \in S$, where k is finite. We denote elements of S by $0, 1, \ldots, k-1$. In the following k has the value 2, though all results generalize readily. An assignment of states to the entire lattice is called a *configuration*. The collection of all configurations, S^Z, is a compact metric space under the metric

$$d(x, y) = \sum_{-\infty}^{\infty} 2^{-|i|} |x_i - y_i| \quad x, y \in S^Z. \tag{1}$$

Under this metric, two configurations are close if their central cells agree.

The set of all configurations with a specified sequence of states in particular contiguous positions is called a *cylinder set*. Cylinder sets are open in the topology imposed by the metric (1) on S^Z. All open sets may be expressed as unions of cylinder sets. A specified sequence of states, $(b_{-r}, \ldots, b_0, \ldots, b_r)$ or $(b_1, b_2, \ldots, b_n)$, depending on context, is called a *block*. (Length n)-cylinder sets may be put in one-to-one correspondence with n-blocks. The symbol B or B_n will denote either a block or the corresponding cylinder set. $|B|$ denotes the length of B; for example, $|B_n| = n$. $(B)_i$ denotes the state of the ith cell in B. The *shift operator* γ is defined by $(\gamma B)_i = (B)_{i+1}$. The collection of all n-blocks (or n-cylinders) for fixed n will be called $\mathbf{B}_n$. $\mathbf{B}_1$ is identical to the state space S. Blocks of a given size may be put in lexicographic order by taking the block itself to be the k-ary expansion of an integer. This integer gives the index of the block in the ordering. $I(B)$ denotes the integer represented by the block B.

2.1. *Cellular automata*

A *cellular automaton*, τ, of radius r is a map from $\mathbf{B}_{(1+2r)}$ into $\mathbf{B}_1$. It may be extended via the

shift operator to a map $B_{(n+2r)} \to B_n$ for arbitrary n. By infinite extension, a shift-commuting map on configurations c may be defined as

$$(\tau c)_i = \tau(c_{i-r}, \ldots, c_i, \ldots, c_{i+r}). \tag{2}$$

We may refer to either the fundamental map τ: $B_{(1+2r)} \to B_1$ or its extensions by the shift as a cellular automaton. The set of shift-commuting functions on configuration space S^Z which are continuous with respect to the metric (1) is identical with the set of cellular automata (Hedlund [12]).

We will find it convenient to name cellular automata with code numbers following Wolfram [22]. A unique number may be associated with each cellular automaton τ of radius $r = 1$ and state space of size $k = 2$. Let the states of S be labeled 0 and 1, and consider them as integers, not merely labels. The cellular automaton applied to a block B in B_3 yields a single state, hence $\tau(B)$ defines an integer, provided B is in B_3. Recall that $I(B)$ is the position of B in lexicographic order. A number $w(\tau)$ corresponding to τ is given by

$$w(\tau) \equiv \sum_{B \in B_3} \tau(B) 2^{I(B)}. \tag{3}$$

The code number $w(\tau)$ ranges from 0 to 255, and uniquely defines τ. The action of τ on 3-blocks may be decoded from $w(\tau)$; thus, *every* integer in the range $[0, 255]$ defines a distinct cellular automaton. Unique code numbers for rules of arbitrary radius and state space size are easily derived in a similar fashion.

2.2. *Truncation operators*

The truncation operators L and R map any n-block B_n to an $(n-1)$-block B_{n-1} by truncation from the left or right, respectively. That is, if $B_n = (b_1, b_2, \ldots, b_n)$ then

$$LB_n \equiv (b_2, b_3, \ldots, b_n) \tag{4}$$

and

$$RB_n \equiv (b_1, b_2, \ldots, b_{n-1}). \tag{5}$$

Observe that L and R commute. L or R applied to a 1-block yield the null-block.

2.3. *Block probability functions*

A map P_n from $\{B_n, B_{n-1}, \ldots, B_0\}$ into the reals is a *block probability function of order n* if it satisfies the *Kolmogorov consistency conditions*. There are four of these. The first,

$$P_n(B) \geq 0 \quad \text{for } |B| = 0, 1, \ldots, n, \tag{6}$$

states that P_n is non-negative on all blocks in its domain. The second condition,

$$\sum_{B \in B_m} P_n(B) = 1 \quad \text{for } m = 0, 1, \ldots, n, \tag{7}$$

states that on each collection of blocks of *fixed* size, up to a maximum n, P_n is a probability function. In particular, the probability of the null-block is 1 under all block probability functions. The next two conditions,

$$P_n(B') = \sum_{B \mid RB = B'} P_n(B) \quad \text{for } |B'| < n, \tag{8}$$

and

$$P_n(B') = \sum_{B \mid LB = B'} P_n(B) \quad \text{for } |B'| < n, \tag{9}$$

define self-consistency for a block probability function. The vertical bar under the summation, $\mid$, is read "such that". Satisfaction of both of these conditions together implies that the probability of any block in the domain of P_n is the sum of the probabilities of blocks which contain the given block at a particular position.

The set of all block probability functions P_n for a particular n is called P_n. If, in addition to being self-consistent, two block probability functions P_n and P_m $(m \leq n)$ agree on m (and smaller) blocks, they are said to be *consistent* with each other.

A consequence of the Kolmogorov consistency theorem (Denker [3]) is that if a set of self-consistent function $\{P_m\}$, $m = 1, 2, \ldots$, which are consistent with each other, is given then these functions extend to a unique shift-invariant measure on S^Z. Below, we will use this method of defining measures in terms of block probability functions by constructing a canonical map from P_n to P_m for $m > n$.

2.4. *The associated Markov matrix of a block probability function*

The Kolmogorov consistency conditions constrain the values of n-block probability functions. These constraints imply that fewer than 2^n parameters are needed to describe a generic n-block probability function (i.e. one with no excluded blocks). We will see that 2^{n-1} parameters are in fact necessary and sufficient. Let B be an n-block. To each block probability function we construct a unique 2^{n-1} by 2^{n-1} Markov matrix whose rows are indexed by RB and columns by LB. This matrix describes the transition from $(n-1)$-blocks RB to $(n-1)$-blocks LB. There are two possible paths originating at each RB. On one path we adjoin on the right of RB a cell in state 0 and drop the left-most cell of RB to obtain a block LB. The other path differs in that we adjoin a cell in state 1. For each block RB, a single parameter describes the relative probability of these two paths. Given a block probability function, the value of each of these parameters may be computed. Conversely, each way of choosing the transition probabilities leads to a block probability function. Hence, 2^{n-1} parameters, one for each of the 2^{n-1} blocks RB, are needed to describe an n-block probability function.

Powers of this Markov matrix describe the probability of a transition from a given $(n-1)$-block to an $(n-1)$-block at a distance. The eigenvalues of this Markov matrix determine the way that correlations between blocks change with distance.

3. The local structure theory

3.1. *Finite-block measures*

Though the Kolmogorov consistency theorem assures that a set of block probability functions satisfying the consistency conditions extends to a measure, it does not show how to construct such a set of functions. The *Bayesian extension process*, introduced in this section, provides such a construction. Given a block probability function P_n, the Bayesian extension process generates block probability functions P_m, $m > n$ which are consistent with P_n. The Bayesian extension process will enable us to construct a class of measures called the finite-block measures. These measures are the domain of the local structure theory. Their basic properties are discussed in this section.

It is reasonable to suppose, for at least some cellular automata, that although the repeated action of the cellular automaton produces configurations in which the states of nearby cells are correlated, this correlation dies away with increasing separation. That is, for a block $\hat{B}$ which is "long enough", the conditional probability of finding that block augmented by a cell in state s on the right (say) will not significantly depend on the state of the left-hand-most cell of $\hat{B}$. If P is a block probability function, then

$$\frac{P(\hat{B}s)}{P(\hat{B})} = \frac{P(L\hat{B}s)}{P(L\hat{B})} \tag{10}$$

or

$$P(\hat{B}s) = \frac{P(L\hat{B}s)P(\hat{B})}{P(L\hat{B})}. \tag{11}$$

This relation is anticipated to good approximation if $\hat{B}$ is long compared to the correlation length. The Bayesian extension process constructs measures for which the relation (11) is exact after some finite $|\hat{B}| = N$.

Clearly, (11) should be symmetric in form between the addition of cells to the right or left of $\hat{B}$.

The symmetry becomes evident when we let $\hat{B}s = B$ and observe that $\hat{B} = R(\hat{B}s) = RB$. Substitution of these expressions in (11) yields

$$P(B) = \frac{P(LB)P(RB)}{P(LRB)}. \tag{12}$$

We use expression (12) to define an operator $\pi(P_n)$. This operator maps an n-block probability function to an $(n+1)$-block probability function $\pi(P_n)$ which gives the probability of $(n+1)$-blocks B by

$$\pi(P_n)(B) = \frac{P_n(LB)P_n(RB)}{P_n(LRB)}, \tag{13}$$

and is identical to P_n on blocks of smaller size. It may happen that $P_n(LRB)$ is 0, in this case any block which contains LRB also has probability 0. In particular, both numerator terms LB and RB have probability 0 if LRB does. In this case we will assign the ratio (13) the value 0. Summarizing,

$$\pi(P_n)(B) \equiv \begin{cases} \dfrac{P_n(RB)P_n(LB)}{P_n(RLB)} \\ \quad \text{if } |B| = n+1 \text{ and } P_n(RLB) > 0, \\ 0 \\ \quad \text{if } |B| = n+1 \text{ and } P_n(RLB) = 0, \\ P_n(B) \\ \quad \text{if } |B| \le n. \end{cases} \tag{14}$$

We will show below that $\pi(P_n)$ is a block probability function of order $n+1$. Given this fact, it will be clear that block probability functions P_m of order $m > n+1$ may be generated by recursive application of π. The collection of functions P_m generated in this way from a block probability function P_n is called the *Bayesian extension* of P_n.

Intuitively, Bayesian extension works by making a "best estimate" of $(n+1)$-block probabilities in terms of n-block probabilities. In fact, Bayesian extension constructs the block probability functions P_m, $m \ge n$, of maximum entropy which are consistent with a given probability function P_n (Gutowitz et al., in preparation).

A trivial but important example of Bayesian extension is the estimation of the probability of a sequence of flips of a biased coin from knowledge of the probability p of a head (1), and $1-p$ of a tail (0). These probabilities correspond to a block probability function P in $\mathbf{P}_1$ specified by $P(1) = p$ and $P(0) = 1-p$. The probability of a 2-sequence of flips b_1b_2 can be found by Bayesian extension of P:

$$\begin{aligned} \pi(P(b_1b_2)) &= \frac{P(Rb_1b_2)P(Lb_1b_2)}{P(RLb_1b_2)} \\ &= P(b_1)P(b_2). \end{aligned} \tag{15}$$

The denominator is the probability of a null block which is 1. A simple induction shows that the probability of a block B of arbitrary length computed by recursive application of π is $p^{\#1(B)}(1-p)^{\#0(B)}$, where #1 and #0 are the number of 1's and 0's, respectively, in B. This result connects the local structure theory to the mean-field theory (section 3.8).

Bayesian extension has a concrete interpretation. Imagine an urn of infinite capacity containing oriented n-cell "dominos" labeled with 0's and 1's. The probability of drawing from the urn an n-domino labeled in a particular way is given by a block probability function P_n. The probability of a smaller block of labels occurring at a particular place in a drawn n-domino is also given by P_n. An $(n+1)$-domino may be constructed by drawing an n-domino, and then drawing a second domino from the urn until the right-most $n-1$ labels of the first n-domino match the left-most $n-1$ labels of the second n-domino. The middle $n-1$ labels of the two dominos are fused, producing an $(n+1)$-domino. The probability that a particular $(n+1)$-domino may be constructed by drawing from the urn according to the above procedure is given by $\pi(P_n)$. Longer dominos may be constructed in the same manner. The probability that a particular domino may be constructed in the appropriate number of successful draws from the urn is com-

puted by recursive application of π to P_n. Equivalently, these probabilities may be found using the Markov matrix associated with the block probability function.

We will now show that the functions P_m generated by Bayesian extension satisfy the Kolmogorov consistency conditions and are therefore block probability functions.

Theorem. If a function P_n satisfies the Kolmogorov consistency conditions (6)–(9) for blocks up to size n, then $\pi(P_n)$ satisfies the Kolmogorov consistency conditions for blocks up to size $n+1$.

Proof. $\pi(P_n)$ satisfies the Kolmogorov consistency conditions on blocks of length n or less because its values on these blocks are identical with those of P_n; and P_n, a block probability function, satisfies the consistency conditions by definition. We will show that condition (9) is satisfied by $\pi(P_n)$ on blocks B of length $n+1$, and use this fact to show that conditions (6)–(8) are also satisfied for $\pi(P_n)$ on $(n+1)$-blocks. Let B' be an n-block, B an $(n+1)$-block. We need to verify that

$$\sum_{B \mid LB = B'} \pi(P_n)(B) = P_n(B'). \tag{16}$$

By definition

$$\sum_{B \mid LB = B'} \pi(P_n)(B) = \sum_{B \mid LB = B'} \frac{P_n(RB)P_n(LB)}{P_n(RLB)}. \tag{17}$$

By substitution of B' for LB, (17) becomes

$$\sum_{B \mid LB = B'} \frac{P_n(RB)P_n(B')}{P_n(RB')}. \tag{18}$$

Removing constants from the sum, (18) becomes

$$\frac{P_n(B')}{P_n(RB')} \sum_{B \mid LB = B'} P_n(RB). \tag{19}$$

Define a new variable $\hat{B} = RB$. Then, $LB = B'$ implies $L\hat{B} = RB'$. Thus, the sum (19) over $(n+1)$-blocks B may be written as a sum over n-blocks. Eq. (19) becomes

$$\frac{P_n(B')}{P_n(RB')} \sum_{\hat{B} \mid L\hat{B} = RB'} P_n(\hat{B}). \tag{20}$$

The value of this sum is $P_n(RB')$ by the consistency hypothesis for P_n. Hence

$$\sum_{B \mid LB = B'} \pi(P_n)(B) = P_n(B'). \tag{21}$$

as we wished to verify.

An identical argument holds with L exchanged for R, which establishes condition (8). Condition (6) is immediate. To see that condition (7) holds, we evaluate

$$\sum_{B \in \mathcal{B}_{n+1}} \pi(P_n)(B) = \sum_{B' \in \mathcal{B}_n} \left[\sum_{B \mid LB = B'} \frac{P_n(RB)P_n(LB)}{P_n(RLB)} \right]. \tag{22}$$

By the proof of (9), the inner sum is $P_n(B')$. By the consistency hypothesis for P_n, the outer sum is 1. Hence $\pi(P_n)$ is in P_{n+1}.

We have just shown that $\pi(P_n)$ satisfies the Kolmogorov consistency conditions. Inductively, all block probability functions constructed by recursive application of π to P_n are consistent with P_n and satisfy the Kolmogorov consistency conditions.

We thus have extended P_n to a collection of functions which allows us to assign probabilities to blocks of arbitrary length in a canonical fashion.

The Kolmogorov consistency theorem (Denker [3]) says that we can use this collection of functions on finite blocks to define a *measure* on the set of all infinite configurations, S^Z. We will call such a measure, constructed from a block-probability function P_n by a Bayesian extension, a

finite-block measure, or, if n is specified, an *n-block measure*. A finite-block measure constructed by Bayesian extension of a block probability function P_n will be denoted $\mathrm{Bay}(P_n)$. Recall that a cylinder set is a set of configurations which have a particular block B at a particular position in the configuration. A finite-block measure assigns to each cylinder set B a value equal to the probability of the associated block B. This probability is determined by Bayesian extension from blocks of length n up to blocks of length $|B|$.

A finite-block measure is *shift-invariant*: cylinder sets receive the same measure regardless of where the origin of configurations is chosen. Let M be the set of all shift-invariant measures on S^Z and M_n be the set of all n-block measures. Then $M_n \subset M$ for each n, and $M_m \subset M_n$ if $m \leq n$.

The difference between the probability of the blocks 1 and 0 will be called the *bias* of a measure. 1-block measures are those based on the generation of block probabilities by flips of a biased coin. Such measures will be called *uncorrelated*. The unbiased, uncorrelated measure is called the *standard* measure.

3.2. *The scramble operator*

The *scramble operator* of order n, denoted as σ_n, is a map from M, the set of shift-invariant measures on configuration space to M_n, the set of n-block measures. The scramble operator first maps a measure μ in M to a block probability function by integrating the measure over n-cylinders, then it extends this function to a finite-block measure by Bayesian extension. Recall that if P_n is a block probability function then $\mathrm{Bay}(P_n)$ is the corresponding n-block measure. We define an "inverse" operation $\mathrm{Blk}_n(\mu)$ which defines a block probability function in terms of a measure,

$$\mathrm{Blk}_n(\mu)(B) = \int_B \mathrm{d}\mu \quad \text{for } |B| \leq n. \tag{23}$$

The scramble operator of order n, σ_n, is defined as

$$\sigma_n(\mu) = \mathrm{Bay}\left(\mathrm{Blk}_n(\mu)\right). \tag{24}$$

$\sigma_n(\mu)$ is an approximation to an arbitrary shift-invariant measure μ by an n-block measure. Elementary properties of the scramble operator are that $\sigma_n\sigma_m = \sigma_m$ for $m \leq n$, and $\sigma_n\mu = \mu$ if μ is an n-block measure. Note that σ_n is *not* a linear operator because $\mathrm{Bay}(P_n)$ is not, according to (14).

We now show that the sequence $\{\sigma_n\mu\}$ converges to μ in the weak topology on measures. We will say that a sequence $\{\mu_n\}$ *converges weakly* to μ if $\lim_{n\to\infty} \int f \,\mathrm{d}\mu_n = \int f \,\mathrm{d}\mu$ for all continuous functions f: $S^Z \to \mathbb{R}$ (Parthasarathy [17]). We say that a function on S^Z is *approximable* if it may be uniformly approximated by functions constant on cylinder sets. Since S^Z is compact and totally disconnected, each continuous function on S^Z is approximable. Hence convergence with respect to the set of approximable functions is equivalent to convergence in the weak topology.

Theorem. Let μ be a measure in M, and let f be an approximable function from S^Z into $\mathbb{R}$. Then, the sequence $\{\mu_n\} = \{\sigma_n\mu\}$ converges to μ for all $\mu \in M$.

Proof. Given $\epsilon > 0$, let f_ϵ be an approximation to f which satisfies

$$|f - f_\epsilon| < \frac{\epsilon}{2} \tag{25}$$

and is constant on cylinder sets of length $N(\epsilon)$. We will show that

$$\left| \int f \,\mathrm{d}\mu_{N'} - \int f \,\mathrm{d}\mu \right| < \epsilon \tag{26}$$

for all $N' \geq N(\epsilon)$. By the triangle inequality,

$$\left| \int f \,\mathrm{d}\mu_{N'} - \int f \,\mathrm{d}\mu \right| \leq \left| \int f \,\mathrm{d}\mu_{N'} - \int f_\epsilon \,\mathrm{d}\mu_{N'} \right| + \left| \int f_\epsilon \,\mathrm{d}\mu_{N'} - \int f_\epsilon \,\mathrm{d}\mu \right| + \left| \int f_\epsilon \,\mathrm{d}\mu - \int f \,\mathrm{d}\mu \right|. \tag{27}$$

We evaluate the first tem on the right-hand side of

(27),

$$\left|\int f\,\mathrm{d}\mu_{N'} - \int f_\epsilon\,\mathrm{d}\mu_{N'}\right| \le \int |f - f_\epsilon|\,\mathrm{d}\mu_{N'}$$
$$< \epsilon/2 \int \mathrm{d}\mu_{N'} = \epsilon/2. \qquad (28)$$

The third term evaluates in the same way to $\epsilon/2$. It remains to evaluate the second term. f_ϵ is constant on cylinder sets. Let B be a cylinder set of length N' and $f_\epsilon(B)$ be the value of f_ϵ on B. We have

$$\int_B f_\epsilon\,\mathrm{d}\mu_{N'} = f_\epsilon(B)\int_B \mathrm{d}\mu_{N'},$$
$$\int_B f_\epsilon\,\mathrm{d}\mu = f_\epsilon(B)\int_B \mathrm{d}\mu. \qquad (29)$$

By definition of σ_n, $\mu_{N'} = \sigma_{N'}(\mu)$ agrees with μ when integrated over cylinders of size $N'(\epsilon)$. By (29),

$$\int_B f_\epsilon\,\mathrm{d}\mu_{N'} = \int_B f_\epsilon\,\mathrm{d}\mu. \qquad (30)$$

We may decompose the integrals in the second term of (27) into a sum of integrals over each B in $B_{N'}$. By eq. (30), each of these vanishes. Hence,

$$\left|\int f\,\mathrm{d}\mu_{N'} - \int f\,\mathrm{d}\mu\right| < \epsilon \qquad (31)$$

as desired.

This theorem says that any measure on S^Z may be approximated arbitrarily well by finite-block measures.

3.3. *The cellular automaton map on measures*

A cellular automaton τ maps each configuration c in S^Z to another configuration. The inverse image under τ of a configuration is a set of configurations. We can think of τ as mapping subsets of S^Z to other subsets. This action of τ on subsets of S^Z induces an action on *measures* on S^Z. Following Lind [14] we define $(\tau\mu)(E) = \mu(\tau^{-1}(E))$ for all μ-measurable sets E. If μ is an n-block measure, then $\tau\mu$ may be explicitly computed. $\tau\mu$ assigns to a set E the measure of its inverse image. Each open set is a union of cylinder sets. The inverse image of each cylinder set in the union is again a union of cylinder sets. $\tau\mu(E)$ is the sum of the measures of the component cylinder sets in a disjoint cover of the inverse image of E. The measure of each of these cylinder sets may be found by Bayesian extension.

3.4. *The local structure operator*

The local structure operator combines the operations of scrambling and applying a cellular automaton to a measure. The local structure operator of order n for a cellular automaton τ is a map, $\Lambda_n(\tau)$, on measures defined by

$$\Lambda_n(\tau)\mu \equiv \sigma_n\tau\sigma_n\mu. \qquad (32)$$

The first application of σ_n produces an n-block measure. The application of τ produces a general measure, and the final application of σ_n reduces this to an n-block measure. In particular, $\Lambda_n(\tau)$ maps M_n, the set of n-block measures, into itself.

3.5. *Invariant measure*

The *invariant* or *limit* measure, μ^*, of a cellular automaton τ is defined as $\lim_{t\to\infty}\tau^t\mu$. If a measure invariant under a cellular automaton τ were a finite block measure of order n or less, then this measure would also be invariant under $\Lambda_n(\tau)$. For let μ be a finite block measure of order n invariant under τ. $\sigma_n\mu = \mu$ since σ_n is the identity on n-block measures. $\tau\mu = \mu$ by hypothesis. Hence, $\Lambda_n(\tau)\mu = \sigma_n\tau\sigma_n = \mu$.

3.6. *The basic hypothesis of the local structure theory*

The basic hypothesis of the local structure theory is that the local structure operator $\Lambda_n(\tau)$ approximates the action of τ on a measure, and does so increasingly well as $n \to \infty$. In particular,

we hypothesize that $\Lambda_n(\tau)$ acts dynamically on measures approximately as τ does. In the experiments described below we demonstrate that the evolution of block probabilities under the local structure operator of small order for a given rule closely approximates the evolution of block probabilities under the rule itself.

If the cellular automaton has a large time limit measure, and the close approximation of the dynamics of $\Lambda_n(\tau)$ to the dynamics of τ continues to large time, then we can expect that $\Lambda_n(\tau)$ should also possess a limit measure, and that the limit measure of $\Lambda_n(\tau)$ should approximate that of τ. Below we demonstrate empirically that some cellular automata do indeed possess limit measures. We will see that cellular automata typically do not have finite-block limit measures. Nonetheless, the limit measures of the rules studied are well-approximated by the fixed points of the corresponding local structure operators of low order.

Close dynamic approximation of τ by $\Lambda_n(\tau)$ implies that if τ has a single invariant measure then $\Lambda_n(\tau)$ will also have a single invariant measure. More generally, one might expect the number of parameters which specify the set of invariant measures of a rule τ to be the same as for the set of invariant measures of $\Lambda_n(\tau)$, for n sufficiently large.

A matter of concern is the *stability* of the invariant measures of τ with respect to perturbation as compared to the stability of invariant measures of $\Lambda_n(\tau)$. This question is of particular importance in view of the use of cellular automata as models of physical systems. Let $\mu(F(x(t)))$ be an invariant measure of a dynamical system stepped forward by the vector field $F(x(t))$. Following Eckmann and Ruelle [4], the *natural* or *physical* measure of $F(x(t))$ is $\lim_{\epsilon \to 0} \mu(F(x(t)) + \epsilon\omega(t))$ where $\omega(t)$ is a suitable noise operator. They suggest that the natural measure represents experimental time-averages. Heuristically, the scramble operator of order n may be thought of as an n-block noise generator, obliterating features of a measure contained in the probability of blocks of size greater than n. In this interpretation, it is reasonable that only the natural measures of a cellular automaton could be approximated by invariant measures of the local structure operator. Below we will study a few examples in which the measures invariant under a cellular automaton in local structure approximation correspond to measures obtained by time-averaging or perturbation of empirical measures.

3.7. *Implementation of the local structure theory*

We noted above that $\Lambda_n(\tau)$ maps the set of n-block measures into itself. Since n-block measures are finitely parameterized, and π is a rational function in block probabilities, the action of $\Lambda_n(\tau)$ can be computed from a finite system of rational recursion equations. Hence, we can numerically investigate the ability of the local structure theory to approximate a cellular automaton. In particular, we will test whether the fixed point parameters (block probabilities) of $\Lambda_n(\tau)$ extend to a measure which approximates the true limit measure of the cellular automaton τ.

To find the evolving n-block measures of $\Lambda_n(\tau)$ numerically, we repeatedly calculate the action of τ on an n-block measure by the following steps:

1) Find the inverse image under τ of each block of length n. For each n-block this is a set of $(n + 2r)$-blocks.

2) Compute the probability of each of the $(n + 2r)$-blocks using Bayesian extension.

3) For each n-block, sum the probabilities of the blocks in its inverse image, and take the sum as the probability of the n-block at the next generation. Repeated application of these steps locates a fixed point of $\Lambda_n(\tau)$.

In the experiments described below, we study the various aspects of the relationship between a rule τ and its local structure approximations using the procedure outlined above.

In this paper we will be primarily concerned with $r = 1$ cellular automata. To accomplish the program above, we need to compute the conditional probability of $(n + 2)$-blocks given a specification of n-block probabilities. Let B be an $(n +$

2)-block and B' an n-block. Bayesian extension of an n-block probability function gives the probability of the $(n+2)$-block B as

$$\frac{P_n(R^2B)P_n(RLB)P_n(L^2B)}{P_n(R^2LB)P_n(L^2RB)}. \tag{33}$$

Let $\delta(\tau(B), B')$ take the value 1 if $\tau(B)$ is the n-block B', and 0 otherwise. Let P_n^t be an n-block probability function at time t. The evolution of P_n^t is given by a system of non-linear recursion equations

$$P_n^{t+1}(B') = \sum_{B\in\mathcal{B}_{n+2}} \left[\delta(\tau(B), B') \times \frac{P_n^t(R^2B)P_n^t(RLB)P_n^t(L^2B)}{P_n^t(R^2LB)P_n^t(L^2RB)}\right]. \tag{34}$$

Probabilities of blocks of length smaller than n at time t are found using the Kolmogorov consistency conditions.

3.8. *The mean-field theory as a special case*

Before turning to specific empirical results, we will discuss the relationship of the mean-field theory and the local structure theory.

An approximation is typically called a mean-field theory if the assumption is made that the state of a particular member of a collection depends only on an average of the states of other members of the collection. Let p_t be the probability of the state 1 at time t. In the mean-field theory it is assumed that the probability of larger blocks may be computed in terms of p_t. That is, it is assumed that no correlations are introduced by the evolution of the cellular automaton. The probability of a block B at time t is given by: $p_t^{\#1(B)}(1-p_t)^{\#0(B)}$, where $\#1(B)$ and $\#0(B)$ are the number of 1's and 0's, respectively, in a block B. The mean-field theory approximates the probability of a 1 at a time t by the sum of the probabilities at the previous time of the blocks which map to 1. Explicitly,

$$p_{t+1} = \sum_{B\in\mathcal{B}_{(1+2r)}} \tau(B)(p_t)^{\#1(B)}(1-p_t)^{\#0(B)}. \tag{35}$$

This is identical to the local structure theory of order 1. To see this, put $B'=1$ in eq. (34). We may replace $P_n^{t+1}(B')$ in (34) by p_{t+1}. Also, since $\tau(B)$ is an integer, either 0 or 1, $\tau(B)$ replaces $\delta(\tau(B), B')$. Now, since P_n is a 1-block measure, parameterized by p,

$$P_n^t(R^2B) = \begin{cases} p_t & \text{if } B_{-1}=1, \\ (1-p_t) & \text{if } B_{-1}=0; \end{cases}$$

$$P_n^t(RLB) = \begin{cases} p_t & \text{if } B_0=1, \\ (1-p_t) & \text{if } B_0=0; \end{cases} \tag{36}$$

$$P_n^t(L^2B) = \begin{cases} p_t & \text{if } B_1=1, \\ (1-p_t) & \text{if } B_1=0. \end{cases}$$

Further, since the probability of the null-block is 1,

$$P_n^t(R^2LB)=1, \quad \text{and} \quad P_n^t(L^2RB)=1. \tag{37}$$

Using these substitutions, the local structure recursion equations (34) reduce to the mean-field equation (35).

This simple case illustrates the fact that some of the recursion equations (34) are redundant; a fact which may be traced back to the existence of *two* consistency conditions (8) and (9) which establish a relation between different partial sums of probabilities. A count on the number of independent equations was given in section 2.4.

4. Rule-specific results

We will investigate the statistical behavior of a number of $r=1$, $k=2$ cellular automata. These rules have been widely studied (see Wolfram [26] and references therein). The rules chosen form a

sequence of roughly increasing statistical complexity. For each rule, we examine the correspondence between the exact behavior of the rule as determined by Monte Carlo experiments and the behavior of the local structure theory approximations to the rule. When possible, we take advantage of special features of a rule to perform an analytical treatment of a rule and the local structure theory for the rule.

Since the local structure theory is a statistical theory, while cellular automata themselves are deterministic, it is evident that local structure theory represents in some sense the average behavior of a cellular automaton. In the following, we consider several ways in which the average behavior of a cellular automaton can be discovered using Monte Carlo techniques. In some cases (e.g. rule 90), time-averaging suffices to set up a correspondence between space-averaged Monte Carlo statistics and the local structure theory. For rules with very little mixing (e.g. rule 180), complex dynamics are present in Monte Carlo simulations. These persist after time-averaging but do not persist after stochastic perturbation of the evolution. Nevertheless, the local structure theory of sufficiently high order indicates the presence of the complex dynamical behavior. In the case of a cellular automaton with chaotic dynamics (e.g. rule 22), the mixing properties of the rule itself are sufficient to permit correspondence of local structure theory and Monte Carlo statistics.

4.1. *Monte Carlo techniques*

The local structure theory is a theory of the behavior of cellular automata in the infinite size limit. Any Monte Carlo experiment, on the other hand, is subject to finite size constraints. In particular, the choice of boundary conditions may strongly affect the outcome of statistical experiments (Martin et al. [15], Falk [5]). When it was necessary to eliminate boundary effects, we employed "triangular" boundary conditions. That is, we only computed statistics on the basis of the central $N - 2rt$ cells of a configuration, where N is the length of the configuration, r the radius of the rule, and t the number of times the rule has been applied.

In all experiments, initial configurations of length $N = 6000$ with triangular boundary conditions were pseudorandomly generated to be uncorrelated and to have a specified density. We then applied the cellular automaton to these configurations, for a number of iterations much smaller than the length of the initial configuration. At each generation, block probabilities were computed by counting occurrences of blocks in the configuration. When quoted, standard errors of the mean of block probabilities are relative to the number of configurations (samples) used to derive the given statistic.

4.2. *Linear rules*

Linear rules are particularly simple. They have been extensively studied (Falk [5], Hedlund [12], Lind [14], Martin et al. [15]). There are 8 linear rules among the $r = 1$, $k = 2$ cellular automata. These include the rule 0 which maps all 3-blocks to 0, the identity (204), the left shift (170) and the right shift (240). The non-trivial linear rules are rules 60, 90, 102, 150. By interchange of the state labels 0 and 1, we obtain rules 255, 195, 165 and 153 from the linear rules 0, 60, 90, and 102, respectively (see table I). These additional rules are non-linear, but since they are related by a trivial automorphism to linear rules, they may also be analyzed by the methods outlined below.

For non-trivial linear rules every block has predecessors. In addition, the number of blocks of length $(n + 2r)$ in the inverse image of an n-block is the same for all n-blocks. To see this, let N be the set of $(n + 2r)$-length predecessors of the 0 n-block under a non-trivial linear rule τ. If B' in B_{2r+n} is a predecessor of a block B in B_n then, by linearity, every other predecessor of B may be expressed as $B' + n$, where n is in N. Thus, the number of predecessors of every block is simply the number of elements in N, which is $k^{n+2r}/k^n = k^{2r}$.

Under the standard measure, the probability of each block of a given length is the same. Since there are the same number of blocks in the inverse image of each block of the given length, the standard measure is invariant under the action of non-trivial linear rules.

4.2.1. *Invariant measure of* $\Lambda_n(\tau)$

We observed above (section 3.5) that if a cellular automaton has an n-block measure as an invariant measure, then this measure is also invariant under the local structure operator of order $m \geq n$. Since the standard measure is a 1-block measure, the local structure operators of all orders for linear rules have the standard measure as a fixed point.

4.2.2. *Stability of the standard measure*

The *stability* of the standard measure under linear rules is a more subtle matter than its invariance. For linear rules, the number-theoretic properties of the generation number strongly influence the statistics at that time. Let us focus on rule 90, for which the state of a cell at a time t is the sum modulo 2 of the states of its nearest neighbors at the previous time. Lind [14] proved that if τ is rule 90, $\lim_{t\to\infty}\tau^t\mu$ does not converge to the standard measure if it did not begin there. This is due to statistical anomalies which occur at generation numbers which are a power of 2. Lind shows further, however, that $\lim_{T\to\infty}(1/T)\sum_{t=1}^{T}\tau^t\mu$ converges to the standard measure, *independent* of the density of the initial measure μ. This result suggests that the standard measure is the "physical measure" of rule 90 in the language of Eckmann and Ruelle [4]. It is the unique invariant measure which emerges when the statistics of evolution are time-averaged.

The Monte Carlo experiment of fig. 1 illustrates Lind's results. In this experiment 50 configurations of length 6000 were pseudorandomly generated so as to be uncorrelated and to have density 0.75. The evolution of these configurations under rule 90 was followed for 512 generations, with triangular boundary conditions imposed. The

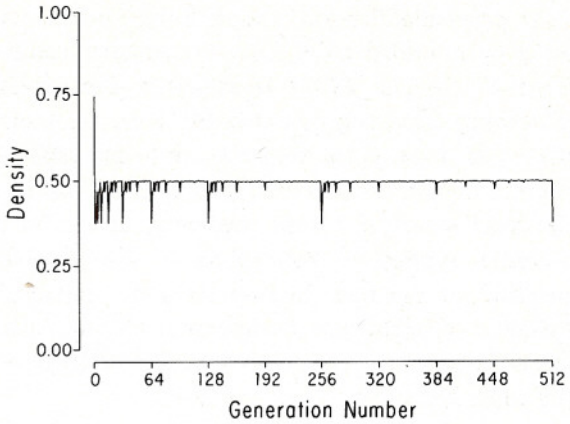

Fig. 1. Evolution of linear rule 90 on initial configurations of length 6000 with triangular boundary conditions. 50 configurations were generated pseudorandomly to have a density of 1's of 0.75. The average density was computed over the set of configurations at each iteration 0–512.

density was computed at each generation. The departures from the standard measure at power of 2 generations described by Lind are clearly seen in this figure. Aside from the rare departures, the empirical density conformed with the local structure prediction of 0.5. In this experiment, time-averaging of statistics would have produced a limiting density of 0.5, as Lind proved to be the case for the infinite cellular automaton. At very high initial bias additional, more complicated departures occur (not shown), but these also do not survive time-averaging.

The other linear rules displayed behavior similar to that of rule 90 in this experiment.

4.2.3. *Stability in local structure theory approximation*

As discussed above, the standard measure must be invariant under the local structure operator of all orders for linear rules. To see if the standard measure is also stable, we used block probability functions with densities (0 to 1 in steps of 0.1) as initial data for the local structure operators (of order 1–10) for the non-trivial linear rules. The action of the operators on these data is simply stated: the standard measure was the fixed point of the local structure operators for these rules.

(The only qualification was that the initial data must be bounded away from the singular conditions $P(1) = 1$ or $P(0) = 1$, which are themselves invariant.) This suggests that the local structure theory of linear rules is insensitive to the generation-number anomalies described by Lind. Rather, the local structure theory prediction of the limit measure appears to correspond to the physical measure of the rule. In summary, the statistical behavior of linear rules as determined by the local structure theory corresponds to a time-average of the exact behavior.

4.3. *Toggle rules*

A rule may be said to be a (left or right) *toggle rule* if changing the state of the (left-most or right-most) cell in the neighborhood of the rule changes the value given by the rule. These rules were also studied by Milnor [16] who called them (left or right) permutative. Willson [18] proved that rules in a broad class which includes the toggle rules are ergodic with respect to the standard measure. In this section we compare the local structure theory predictions with this result.

Toggle rules share with linear rules the property that each block of a given size has the same number of blocks in its inverse image. To fix ideas, let b be an n-block, and τ be a right toggle rule. To find all the blocks in the inverse image of b, begin choosing states for cells at the left end of a prospective $(n + 2r)$-block, B. Since τ is a right toggle rule, no matter how the first $2r$ states are chosen, there is one and only one choice of state for the $(1 + 2r)$th cell such that B is in the inverse image of b. Indeed, once the first $2r$ choices are made, the makeup of b determines uniquely the states of the remaining cells in B. The $2r$ free choices imply that there are k^{2r} blocks in the inverse image of each n-block. As for linear rules, this implies that the standard measure is invariant both under the rule and all local structure approximations to the rule.

We note that for all $r = 1$, $k = 2$ left toggle rules, the rule number $w(\tau)$ is a positive multiple of 15. Conversely, each such rule number (except for 255) corresponds to a left toggle rule. To see this, let w_i $(0 \le i \le 3)$ be the value of the rule τ on each 3-block whose left-most cell is 1. Because τ has the left toggle property, it must have the value $(1 - w_i)$ on the corresponding block whose left-most cell is 0. Then,

$$w(\tau) = \sum_{i=0}^{3} \left[2^{i+4} w_i + (1 - w_i) 2^i\right]$$

$$= 15\left[1 + \sum_{i=0}^{3} w_i 2^i\right]. \tag{38}$$

The right toggle rules are obtained by reflection of the left toggle rules. Left toggle rules typically come in pairs, each member of the pair is mapped into the other by interchange of the 0,1 state labels (table I). Note that rules 90, 105, 150 and 165 are both left and right toggle rules (as discussed above, 90 and 150 are also linear). The left and right shifts (170 and 240) and left and right toggle rules, respectively.

4.3.1. *Stability of the standard measure under toggle rules*

Wolfram [25] submitted toggle rules to a variety of statistical tests which show that evolution under these rules tends to destroy correlation and bias in finite configurations. This is evidence that the standard measure is stable under toggle rules. We obtained further evidence for the stability of the standard measure under left toggle rules using the same experimental paradigm as employed above for linear rules. The statistical properties of a right toggle rule are the same as those of the corresponding left toggle rule. We will group with parentheses left toggle rules which are related by interchange of state labels (table I). Left toggle rules (30, 135), (45, 75), and (120, 225) had an average density of 0.5 at all times (up to 512) beyond an initial transient, regardless of initial density. Under exchange of state labels, rules 165 and 195 map to linear rules 90 and 102, respectively, and hence have the same statistical behavior (table I).

Three left toggle rules (180, 210, and 15) display behavior which is dissimilar to any of the linear rules. Rules (180, 210) will be studied in detail below. Rule 15 is effectively an $r = 0$ rule. It shifts a configuration one position to the right, and maps the state of each cell to the opposite state. If a configuration has a density p of 1's, then rule 15 applied to the configuration will produce a configuration which has a density $1 - p$ of 1's. The next application of rule 15 will return a configuration with the original density p. Thus, without time-averaging, the space-averaged density does not converge to 0.5 if it did not begin there. Time-averaging, on the other hand, will produce an invariant density of 0.5.

4.3.2. *Stability in local structure theory approximation*

We showed above that the standard measure is invariant under the exact action of toggle rules. The local structure operator (of order up to 10) for $r = 1$, $k = 2$ toggle rules (except rule 15, and its reflection, rule 85) has the standard measure as the unique stable fixed point.

The local structure operator of any order for rule 15 behaves exactly like the rule itself in the respect that given an initial block probability function with density p, the result of application of the local structure operator is a block probability function with density $1 - p$, the next with density p, etc.

4.3.3. *Rule 180*

Rule 180 (and corresponding rule 210) is nearly an $r = 0$ rule. Rule 180 simply shifts a cell state to the right, unless it is followed on the right by the pair 10 in which case it is mapped to the opposite state, and shifted to the right. Despite the simplicity of this description, rule 180 is the most statistically complex of the $r = 1$, $k = 2$ toggle rules. Examination of the behavior of this rule and its local structure theory approximations will enable us to gain some insight into the mixing properties of the local structure theory.

A consequence of the results of Willson [18] is that the standard measure is ergodic for rule 180. An intuitive interpretation of this statement is that for a "typical" configuration, (one in which space-averaged density of 1's converges to 0.5) will map to another configuration of density 0.5 under rule 180. This next configuration will map to another such configuration, etc., so that space-averages in a configuration at a given time may be exchanged with averages over samples taken from a given place in a time sequence of configurations. Ergodicity with respect to the standard measure does not preclude the existence of sets of configurations which 1) have measure 0 with respect to the standard measure, 2) are invariant under the rule (or some power of the rule), and 3) have space averages which may not be exchanged with time averages. It is also possible for a set of measure 0 to be invariant under rule 180 and yet have space- or time-averaged densities different from 0.5.

In the following we will present both Monte Carlo and analytical evidence that 1) sets of measure 0 exist on which rule 180 is dynamically complex, 2) this complexity is not stable to stochastic perturbation, and 3) the local structure theory accurately reflects this cellular automaton's behavior on sets of both positive and 0 measure.

(a) *Monte Carlo simulation of rule 180*

Fig. 2 shows the evolution of configurations of length 6000 for 64 generations under rule 180, with triangular boundary conditions imposed. Configurations were generated to be uncorrelated, and to have different densities: 0.1, 0.4, 0.5, 0.7, or 0.99. 10 configurations at each density were used. When 0.5 was not the density of the initial measure, the density underwent oscillations. The periods of the oscillations depended on the initial density. Period 2 oscillation at low density gave way at high density to a complex mix of oscillations whose periods were powers of 2. As the density of initial configurations was increased toward the high density limit $P(1) = 1$, power shifted into oscillations whose periods were even higher powers

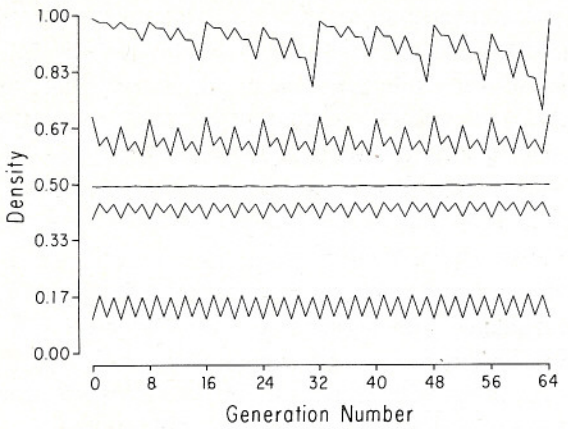

Fig. 2. Evolution of toggle rule 180 on initial configurations of length 6000 with triangular boundary conditions. Starting configurations were generated to be uncorrelated but to have different initial density. 10 configurations at each density 0.1, 0.4, 0.5, 0.7, and 0.99 were used. The average density was computed at each iteration 0–64.

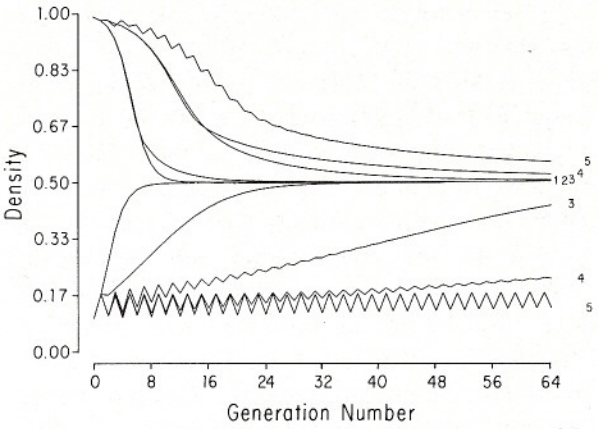

Fig. 3. Evolution according to the local structure operators of orders 1–5 for rule 180. Initial data were chosen to be uncorrelated and to have density either 0.1 or 0.99 corresponding to the Monte Carlo data of fig. 2.

of 2. There appeared to be no period-doubling bifurcations. Rather, the power expressed in high harmonics increased smoothly as the density increased.

To understand this behavior, we first consider the low density limit. At very low densities, most 1's which occur in a configuration will be isolated from other 1's by long runs of 0's. An isolated 1 maps to a pair of 1's which in turn maps to a single 1, shifted two places to the right of the original 1. This accounts for the period 2 oscillations seen at low density. At somewhat higher densities, one is lead to consider the evolution of small regions of 1's surrounded by a large number of 0's such as 11 (period 2) 111, 101, 1111, 1101 (period 4), etc. A more detailed analysis reveals that 1) a block $B = 01^{2k}01^{2a+1}01^{2b+1}\ldots 01^{2f+1}$ $(k, a, b, \ldots, f \geq 0)$, if followed by a zero, evolves in a diagonal band, independent of the remainder of the configuration, 2) the block B has a period 2^h where 2^h is the largest power 2 which is less than the length of B, and 3) all configurations can be segmented into blocks of the above form, and inert regions of 0's.

(b) *Local structure theory of rule 180*

Fig. 3 shows the evolution in response to local structure operators of all orders, 1 through 5, of uncorrelated block probabilities of initial densities 0.1 and 0.99 which may be compared with Monte Carlo data as above. The first 64 generations were studied. As was the case for other toggle rules, the local structure operators of all orders studied for rule 180 tended eventually toward the standard measure. Unlike other toggle rules, however, as the order was increased the local structure operators for rule 180 took longer to relax to the standard measure. Prior to this relaxation, they tended more to reflect the behavior of the corresponding Monte Carlo simulations.

The large-time behavior of the local structure operators of low order reflects the action of rule 180 on sets of positive measure. This is the "average" or "typical" behavior of the rule, its behavior on sets of positive measure (Willson [18]). The small-time behavior of the local structure operators only reflect the action of the rule on the measure 0 set of configurations on which it is initialized.

Whether the pattern of behavior of higher orders of theory is the same as the pattern of the low orders, with the convergence to the standard measure merely delayed, is unclear. We can construct

measures for which we can prove that the local structure theory *does not* converge to the standard measure for any sufficiently high order of theory. An example is the measure which assigns 0 probability to any configuration which contains the blocks 101 or 11, i.e. which only allows configurations with 1's isolated in runs of 0's. The square of rule 180 preserves this subset of the configuration space. Hence, on this subset, it may be regarded as an idempotent, and thus subject to exact treatment (see below).

It appears that rule 180 will not always express its average behavior in Monte Carlo experiments or at small time in the local structure theory because it is not sufficiently mixing. We now show how the Monte Carlo experiments may be modified so that the average behavior of rule 180 is expressed even though the simulations are initialized on the measure 0 set of configurations.

(c) *Stochastic perturbation*

The results of an experiment in which rule 180 was iteratively applied to configurations in the presence of a small amount of noise are displayed in fig. 4. Noise was added as follows: first the density of the current configuration was found, then each cell of the configuration was perturbed with a probability ϵ. Perturbed cells were mapped either to the same or the opposite state. Transition probabilities for this map were chosen such that the density of 1's in the configuration was not changed on the average. Noise was added in this fashion so that any effect on the outcome of the cellular automaton evolution would be due to the perturbative effect of the noise, rather than its bias.

In these experiments ϵ took on the values 0, 0.01, 0.05, and 0.1. Low levels of noise were sufficient to destroy the elaborate periodicities of the deterministic evolution within a few generations. Monte Carlo simulations in the presence of noise in the limit of large time conform with the fixed-point predictions of the local structure theory.

The action of noise may be understood as follows. At low density noise acts to disperse the

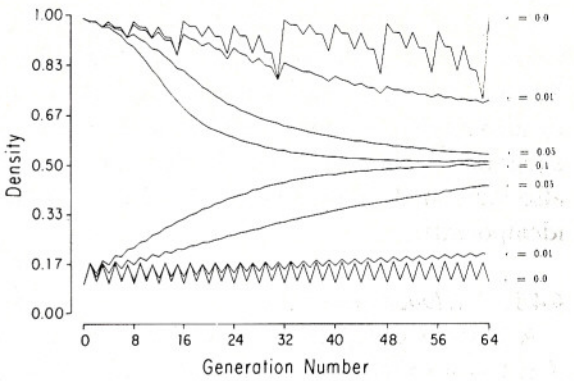

Fig. 4. Evolution under rule 180 of configurations generated as in fig. 2. In this experiment noise was added as described in the text with $\epsilon = 0$, 0.01, 0.05, or 0.1. Initial densities used were 0.1 and 0.99.

11-blocks which come from isolated 1's at the previous generation. In this way new isolated 1 "seeds" are formed so that increasingly high densities may be reached. At high density, noise introduces isolated 0's in a string of 1's. Such a 0 produces a pair of 0's at the next generation. One of the daughters moves to the left and the other to the right as the rule is iterated. Not only is the density lowered by this mechanism, but the influence of the perturbation can spread over large distances.

4.4. *Idempotents*

A cellular automaton is said to be *idempotent* if $\tau^2 = \tau$. Some non-idempotent rules have a power which is idempotent. Since this power is a cellular automaton of larger radius, our discussion of idempotents may be applied to these rules as well. Though idempotent rules are dynamically simple (their evolution stops after one generation) they may have more complicated statistical behavior than the linear and toggle rules studied above. In the case of linear and toggle rules, we were able to describe the behavior of the local structure operator by counting the number of predecessors of blocks. We will apply the same method to the study of idempotents.

The $r = 1$, $k = 2$ rules which are idempotent or whose square is idempotent are listed in table I. Some rules obey the equation $\tau^3 = \tau$. The square of such a rule is idempotent. Rules which obey the equation $\tau^2 = \gamma\tau$, where γ is the shift operator, are also tabulated. Statistically, these rules are like idempotents.

4.4.1. *Excluded blocks*

A block is called an *excluded block* for a rule τ if it has no predecessors under the rule. A *basic* excluded block does not contain other excluded blocks. For example, rule 4 which maps all 3-blocks to 0 except the block 010 is an idempotent. The block 11 is a basic excluded block for rule 4.

The excluded blocks of an idempotent rule determine the structure of the limit measure of the rule. In particular, for all non-excluded blocks B, there exists a block B' such that $L^rR^rB' = B$ and $\tau(B') = B$. That is, every block is either mapped to itself under an idempotent rule or it is an excluded block for the rule. Assume a block B is not excluded. Then it has at least one predecessor B' which also has a predecessor B''. That is, 1) $\tau(B'') = B'$, and 2) $\tau(B') = B$, and 3) $\tau^2(B'') = B$. Since $\tau^2 = \tau$, we have both $\tau^2(B'') = B'$ (from 1) and $\tau^2(B'') = B$ (from 3), hence $B' = B$ where they overlap and hence $L^rR^rB' = B$.

If an idempotent rule τ has radius r, the largest possible basic excluded block has length $2r + 1$. To see this, assume the existence of a basic excluded block B of length a (fig. 5). LB and RB are not excluded, and thus, LB has a predecessor B' (of length $a + 2r - 1$) such that $L^rR^rB' = LB$, and RB has a predecessor B'' (of length $a + 2r - 1$) such that $L^rR^rB'' = RB$. Construct a block B^* of length $a + 2r$ whose left-most r elements are equal to the left-most r elements of B'', whose central a elements are equal to B, and whose right-most r elements are equal to the right-most r elements of B'. (B^* coincides with B, B', and B'' on its central a elements). Now consider $\tau(B^*)$. The right-most $a - r - 1$ elements of $\tau(B^*)$ are equal to $L^{r+1}B$, since B^* coincides with B' on the right-most $a + r - 1$ elements of B'. The left-most

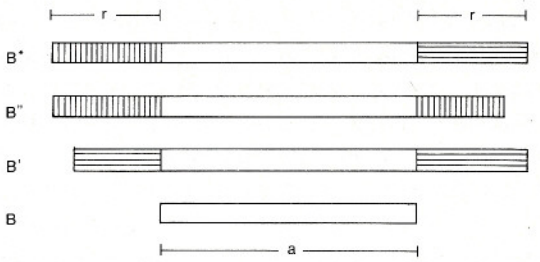

Fig. 5. The relationship among the blocks B, B', B'', and B^* used in the proof that the largest basic excluded block for an idempotent is of length $2r + 1$.

$a - r - 1$ elements of $\tau(B^*)$ are equal to $R^{r+1}B$ since B^* concides with B'' on the left-most $a + r - 1$ elements of B''. Our purpose is to show that if a is large enough then B^* is a predecessor of B, hence B is not excluded, contrary to assumption. The existence of a predecessor on the left side implies the identity of $\tau(B^*)$ and B on all but a patch of $r + 1$ cells n the extreme right side. Likewise, the existence of a predecessor on the right side implies that $\tau(B^*)$ and B can only differ on at most $r + 1$ cells on the extreme left side. But the identity forced on one side covers the potential mismatches on the other side, unless the two regions of potential mismatch overlap. Overlap only occurs if $a \leq 2r + 1$. If $a > 2r + 1$ then $\tau(B^*) = B$, that is, B has a predecessor and hence is not excluded. The bound $2r + 1$ is achieved by some $r = 1$ idempotents (e.g. the block 111 for rule 76).

These facts allow us to exactly describe the behavior of the local structure operator for idempotents. Let us compute the action of $\Lambda_n(\tau)$ on an n-block measure μ which assigns 0 to all excluded blocks. For a block B which is not excluded, $\Lambda_n(\tau)\mu(B)$ is the sum of the measures assigned by $\mathrm{Bay}_n(\mu)$ to predecessors B' of B. Such predecessors either contain excluded blocks of size n or less, (in which case $\mathrm{Bay}_n\mu$ assigns them a measure 0), or they coincide with B on their n central elements. Conversely, all blocks B'' which coincide with B on their n central elements are predecessors of B, or they contain excluded blocks (and thus are assigned a measure 0). It follows by

Kolmogorov consistency that the sum of the measures assigned to the predecessors of B by $\mathrm{Bay}_n(\mu)$ is exactly the measure of all blocks which contain B, and is thus $\mu(B)$. Any measure which assigns probability 0 to excluded blocks will be stable under $\Lambda_n(\tau)$ if n is as large as the largest basic excluded block. Thus it is also clear that if μ' is an n-block measure which assigns non-zero probability to excluded blocks, then $\Lambda_n(\tau)\mu'$ assigns 0 probability to excluded blocks. Finally, it follows that if τ is idempotent, so is $\Lambda_n(\tau)$.

4.4.2. *The number of predecessors of allowed blocks under rule 4*

For idempotents, we have found so far that for n sufficiently large, the local structure theory of order n is exact for the probability of blocks of length n. We might wish to do better still by finding an order of local structure theory at which the probability of blocks of *all* sizes is given exactly. We will now present a result which indicates that for some idempotents at least, there is no order of theory which will do this.

We noted above that the block 11 is a basic excluded block for rule 4. It is the only basic excluded block for this rule. We can use this knowledge to describe the set of all *allowed* blocks under rule 4. From this we find the action of the rule on the standard measure. If the initial measure is the standard measure, then the invariant measure will give each allowed block of a given size a probability proportional to the number of predecessors of the block. Runs of 0's of any length are allowed blocks. All other allowed blocks have isolated 1's separated by runs of 0's. Each (non-trivial) allowed block is composed of sub-blocks consisting of a pair of 1's separated by any number $k \geq 1$ of 0's. Let such blocks be denoted $10^{[k]}1$. We would like to compute the number of predecessors of these sub-blocks. Let $N(k)$ be the number of predecessors of $10^{[k]}1$. Each predecessor will be of the form $010\ldots010$. That is, each predecessor has a "core" region bounded by 0's. The core region is a $(k-2)$-block which contains no isolated 1's.

	000	001	011	100	101	110	111
000	1	1	0	0	0	0	0
001	0	0	1	0	0	0	0
011	0	0	0	0	0	1	1
100	1	1	0	0	0	0	0
101	0	0	1	0	0	0	0
110	0	0	1	1	0	0	0
111	0	0	0	0	0	1	1

Fig. 6. The transition matrix for the allowed 3-blocks under rule 4.

We can describe the blocks of this form by means of an adjacency matrix M. Each row and column of M is labeled by a 3-block which may occur in an allowed block. Thus, M is a 7×7 matrix with one row and column for each 3-block except 010. $M_{i,j}$ is 1 if the two right-most cells of the ith row block match the two left-most cells of the jth column block, otherwise $M_{i,j}$ is 0 (fig. 6). Each non-zero entry represents a transition from the left-most cell of the row block to the right-most cell of the column block. A predecessor block will begin in state 0 and follow allowed transitions such that it ends in state 0. There are two ways of doing this, namely $000 \to 000$ and $011 \to 110$. In other words, the only allowed core regions (of size 2) are 00 and 11, hence the first power of the matrix specifies $N(4) = 2$. We can find $N(5)$ by squaring M and summing the entries which connect an initial and final 0, each such path contains an allowed core region of size 3. $N(k)$ for any k is found by taking higher powers of M. Asymptotically, $N(k)$ will be given by the dominant eigenvalue of M. The characteristic polynomial of M is $\lambda^4(\lambda^3 - 2\lambda^2 + \lambda - 1)$. The non-trivial real root of this polynomial is an irrational number, approximately 1.7549.

The irrationality of the root has important consequences. If the invariant measure of rule 4 could emerge as the result of applying the local structure operator of finite order to the standard measure then the invariant measure would be a finite-block measure. If it were a finite-block measure then, eventually, $N(k)/N(k-1)$ would be a rational number. To see this, assume that the measure which results from applying rule 4 once

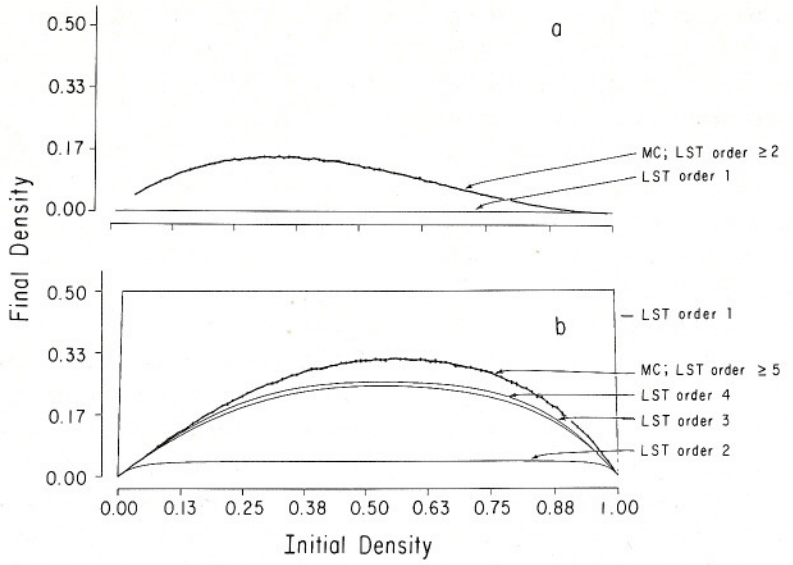

Fig. 7. Final vs. initial density for idempotent rules a) 4; and b) 108. 10 configurations of length 6000 at each initial density were used. Error bars indicate ± 2 standard errors of the mean. The step size in density was 0.01. The Monte Carlo results are compared with local structure estimates of orders 1–5. The local structure theory becomes exact for the density at order 2 for rule 4 and at order 5 for rule 108. The first order local structure theory (mean-field theory) for rule 4 predicts a final density of 0 independent for initial density.

to the standard measure were a finite-block measure of order K. We compute $N(10^{[k]}1)/N(10^{[k-1]}1)$, where k is larger than K. Since the initial measure is the standard measure, the probability of a block is proportional to the number of predecessors of the block. The probability of blocks of size k or greater is given by Bayesian extension. Hence,

$$\frac{N(10^{[k]}1)}{N(10^{[k-1]}1)} = \frac{P(10^{[k]}1)}{P(10^{[k-1]}1)} = \frac{P(10^{[k]})P(0^{[k]}1)}{P(0^{[k]})} \frac{P(0^{[k-1]})}{P(10^{[k-1]})P(0^{[k-1]}1)}. \tag{39}$$

By a second application of Bayesian extension to $P(10^{[k]})$ and $P(0^{[k]}1)$, (39) is equal to

$$\frac{P(10^{[k-1]})P(0^{[k]})}{P(0^{[k-1]})} \frac{P(0^{[k]})P(0^{[k-1]}1)}{P(0^{[k-1]})} \times \frac{P(0^{[k-1]})}{P(0^{[k]})P(10^{[k-1]})P(0^{[k-1]}1)} = \frac{P(0^{[k]})}{P(0^{[k-1]})}. \tag{40}$$

But,

$$\frac{P(0^{[k]})}{P(0^{[k-1]})} = \frac{P(0^{[k-1]})}{P(0^{[k-2]})}, \tag{41}$$

by application of Bayesian extension to $(0^{[k]})$. Hence if k is greater than K, and the limit measure is a finite-block measure, then the ratio $N(10^{[k]}1)/N(10^{[k-1]}1)$ is a rational number *independent* of k. The *irrationality* of the root of the recursion equation for $N(k)$ implies that the limit measure arising from one application of rule 4 to the standard measure cannot be a finite-block measure of any order. Counting the predecessors of blocks under an idempotent rule typically leads to a recursion equation with irrational roots. This suggests that many idempotents will not have finite-block limit measures.

4.4.3. *Dependence on initial conditions*

For any idempotent rule, any P_n which assigns probability 0 to excluded blocks is stable. Therefore, there is a family of stable measures,

and the limit of $\tau^t\mu$ depends on μ. This dependence on initial measure is illustrated in fig. 7. At each density in 0 to 1 steps of 0.01, we generated 10 configurations of length 6000 with uncorrelated neighbors and with the given density. We operated on these configurations with rules 4 and 108. We also generated corresponding initial data for the local structure operators for these rules. In fig. 7 the final density is plotted against the initial density, with calculations performed by both Monte Carlo and local structure theory of orders 1 to 5.

Idempotent rule 4 was discussed above. The local structure theory of order 1 for rule 4 incorrectly predicts an invariant measure density of 0 regardless of initial density. Conversely, all orders of theory greater than 1 are exact.

The square of rule 108 is an $r = 2$ idempotent. The basic excluded blocks for this rule are 1011, 1101, 1111, and 10101. The largest is a 5-block, hence the local structure operator of order 5 or greater will compute the density exactly. The local structure theory for the rule 108 has a different behavior from that of rule 4. The order 5 theory is exact, but lower orders provide reasonable approximations. As the order increases, so does the accuracy of the theory (fig. 7). This result cannot be derived from the simple combinatorial analysis described above. It encourages belief that even for complex rules the local structure operator will be a good approximation if the order is sufficiently high.

4.5. *Asymptotically trivial rules*

Rules may be said to be *asymptotically trivial* if the fraction of blocks in the mth inverse image of 0 (or 1) approaches unity as m approaches infinity. These rules are not idempotent, but successive powers are more and more like idempotents. An example is rule 32. Only the triple 101 maps to 1 under rule 32. The only predecessor of 101 is 10101, etc. This block may be said to be *asymptotically excluded*. Another example is rule 254. Rule 254 maps all triples to 1 except 000. The only predecessor of 000 is 00000, etc.

Consider the local structure theory of order 3 for rule 32. The probability assigned to the block 10101 by Bayesian extension of an order 3 block probability function must be less than or equal to the probability of a 101 block, since it contains the 101 block. Equality obtains only if $P_3(010) = P_3(101) = \frac{1}{2}$. Except in this special case, iteration of the local structure operator for rule 32 will map the P_3 to functions which assign probabilities arbitrarily close to 1 to the 000 block. This is because 101 has only the one predecessor 10101, and its probability will be progressively smaller at each application of the third-order local structure operator.

A similar argument shows that iteration of the local structure operator of order at least 3 for rule 254 maps any initial block probability function P (except $P(00\ldots00) = 1$) to $P(11\ldots11) = 1$. From these observations we conclude that the fixed-point measure of the local structure operator of suitable order for asymptotically trivial rules is the same as the limit measure of the rule itself. The asymptotically trivial rules are listed in table I.

4.6. *Summary of exact results*

We showed that for certain classes of rules: linear, toggle, idempotent and asymptotically trivial, the local structure theory is exact. In the case of linear and toggle rules we took advantage of special algebraic features of the rules. Since the limit measure for these rules is a finite-block measure of order 1, it is also a fixed point of the local structure operators of all orders. In the case of idempotent and asymptotically trivial rules, we took advantage of a special dynamical feature: the statistics do not change after a finite number of steps, or they have an asymptotically small change. For idempotents this implies that a finite order of theory applied a finite number of times to initial conditions can determine exactly the probability of a finite block under the limit measure of the rule. For asymptotically trivial rules, the theory is exact only in the limit of many applications of the local structure operator.

Table I
Some classes of rules for which the local structure theory is directly analyzable. This table lists the toggle, asymptotically trivial and idempotent rules among the $r = 1$, $k = 2$ cellular automata. For idempotent rules, each sub-table is headed by the equation obeyed by the rules in the sub-table. Within each sub-table, rules are grouped into tableaux separated by double bars. The right column of each tableau contains rules which are obtained by left-to-right reflection of rules in the left column. The bottom row of each tableau contains rules which are obtained from rules in the top row by exchange of the state labels. Some tableaux are degenerate because reflection and/or exchange of state labels fail to generate distinct rules. A blank row and/or column indicates that the corresponding row and/or column is simply copied. Asterisks indicate toggle rules which are linear.

Toggle

15	85	30	86	45	101	60*	102*	90*	
		135	149	75	89	195	153	165	

105		120	106	150*		180	166	240*	170*
		225	169			210	154		

$\tau^2 = \tau$

0		4		12	68	76		200		204	
255		223		207	221	205		236			

$\tau^2 = \gamma\tau$

2	16	10	80	34	48	42	112	138	208
191	247	175	245	187	243	171	241	174	244

$\tau^3 = \tau$

1		5		29	71	51	
127		95		71	29		

$\tau^4 = \tau^2$

8	64	19		36		72		108	
239	253	55		219		237		201	

Asymptotically trivial

32		40	96	128		136	192	160		168	224
251		235	249	254		238	252	250		234	248

These classes of rules are not mutually exclusive. By exchanging the labels of states 0 and 1 some linear rules map to non-linear rules. Rule 90 maps to rule 165, for instance. Rule 165 is both a left and right toggle rule. For rules of larger radius, this exchange of labels will lead to non-linear rules which are not toggle rules. Since the dynamics of rules do not depend on the way states are labeled, these non-linear rules may also be understood by the methods described above.

Table I contains code numbers for rules which may be approached by the methods described thus far. 100 of the 256 $r = 1$, $k = 2$ rules are listed.

4.7. *Rule 22*

We now turn to a rule that is more difficult to handle by analytical means. Rule 22 maps the triples 100, 001, and 010 to 1, and all others to 0. Monte Carlo work by others (Grassberger [6, 7, 8], Ingerson and Buvel [13], Wolfram [22]) suggests that rule 22 is among the most statistically complex $r = 1$, $k = 2$ rules. We study local structure approximations to this rule in detail. As with simpler rules, the overall strategy is to compare Monte Carlo estimates of block probabilities with those of the local structure theory. Because of its complexity, however, we will take care to establish the statistical significance of these comparisons.

4.7.1. *Initial density independence*

The result of applying rule 22 to initial configurations of various densities is shown in fig. 8. The experimental paradigm of fig. 7 was used except that configurations were subjected to repeated application of the rule until the density stabilized. At very high density, initial configurations which lead immediately to the 0 configuration were discarded. This was required to compensate for finite size effects. Only 10 configurations at each initial density were used. The density at large time is approximately 0.35, independent of the initial density. Time-averaging did not affect this result.

4.7.2. *Mixing*

We repeated the experiment of fig. 8 using periodic boundary conditions rather than triangular boundary conditions. The differences between the two paradigms were far less than the experimental error (not shown). It appears that

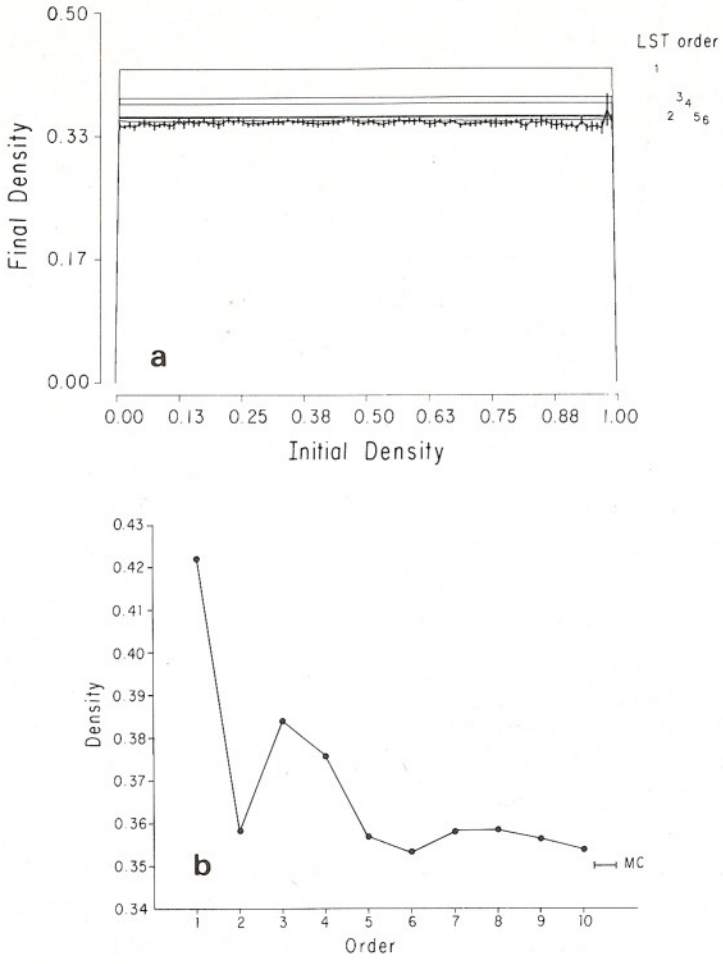

Fig. 8. a) Local structure approximations for the density of the invariant measure of rule 22. For the Monte Carlo portion of these data (line with error bars), 10 configurations at each density in the range 0 to 1, (step size 0.01) were generated pseudorandomly. Each was acted upon by rule 22 until the density stabilized. The error bars indicate ± 2 standard errors of the mean. The density of the local structure operator fixed point at each initial density, for each order of theory 1–6 is also shown. b) Fixed point density for each order of local structure theory up to 10 for rule 22. MC indicates the large time density for rule 22 according to the Monte Carlo results of Grassberger in Wolfram [26].

the limit statistics of rule 22 are independent of initial and boundary conditions, in strong contrast with rule 180 treated above. This is explained in part by the results of Grassberger [8] which show that while the correlations between sites after many iterations of rule 22 may be very long-ranged and complex, these correlations decay rapidly, roughly exponentially for distances less than 20. The influence of the boundary is diminished by the strongly mixing dynamics of the rule. Wolfram [22] studied a number of rules, comparing their behavior under periodic boundary conditions and "0" boundary conditions (fixing boundary points in the 0 state). He found no difference for chaotic rules.

4.7.3. *Local structure theory*

Fig. 8 shows the fixed point density computed from the local structure approximations to rule 22 for all orders through 6. The local structure

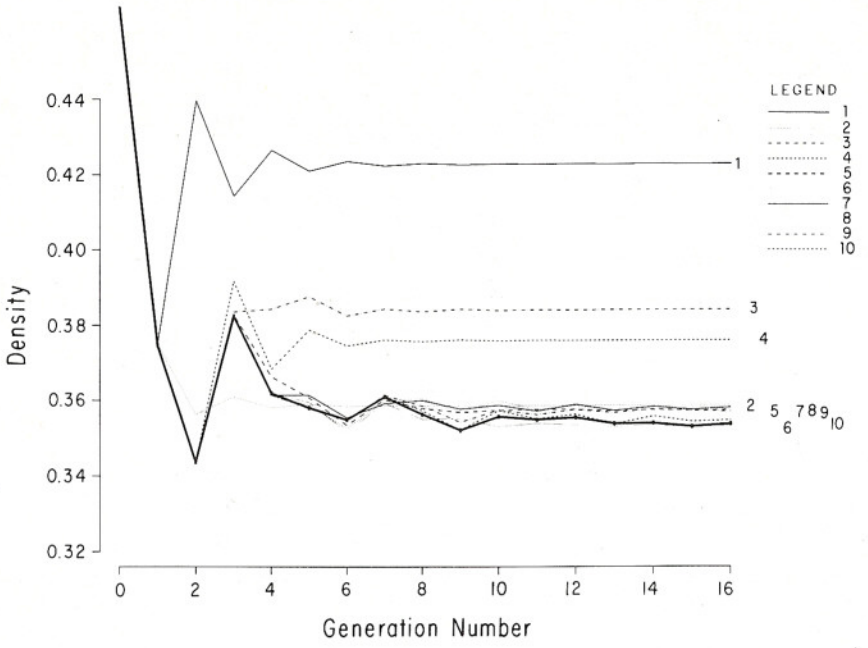

Fig. 9. Rule 22 evolution of the density with time. 1000 configurations of length 6000 with triangular boundary conditions were used. These were generated pseudorandomly to be unbiased and uncorrelated. They were acted upon by rule 22 for 16 iterations. At each iteration the average density and standard error of the mean were computed. Error bars indicate ± 2 standard errors of the mean. Also shown is the density derived from the first 16 applications of the local structure operators of order 1–10 to the standard measure. Note the expanded density scale.

approximations, like the Monte Carlo data were independent of initial density. We see further that as the order increased, the local structure estimates of the density approached the Monte Carlo estimate. Fig. 8b shows the fixed point density for the local structure theory to order 10. Also indicated is the Monte Carlo fixed point density from results of Grassberger quoted in Wolfram [26].

4.7.4. *Approach to equilibrium with standard measure initial conditions*

We studied the approach of rule 22 to a statistical equilibrium by following the evolution of unbiased, uncorrelated finite configurations. In this experiment 1000 configurations of length 6000 with triangular boundary conditions were used. After each application of the rule we computed the average density and the standard error of the mean for the density of the 1000 configurations. The evolution was followed for 16 generations. In addition, we applied the local structure operator to standard measure initial conditions, and found the density of the resulting measure at each successive application. We studied each order 1–10 of the theory, again for 16 generations. The results are shown in fig. 9.

A curious aspect of this figure is that the large-time density estimates from the third and fourth order theories were worse than the estimate from the second order. However, the third and fourth order theories did a better job than the second order theory of tracking the initial transient behavior of the Monte Carlo estimate. As the order increased beyond 4, the large-time estimate again moved toward the empirical value, and, in addition, the small-time behavior became increasing well modelled.

The local structure operator combines the exact action of a cellular automaton on blocks of a fixed

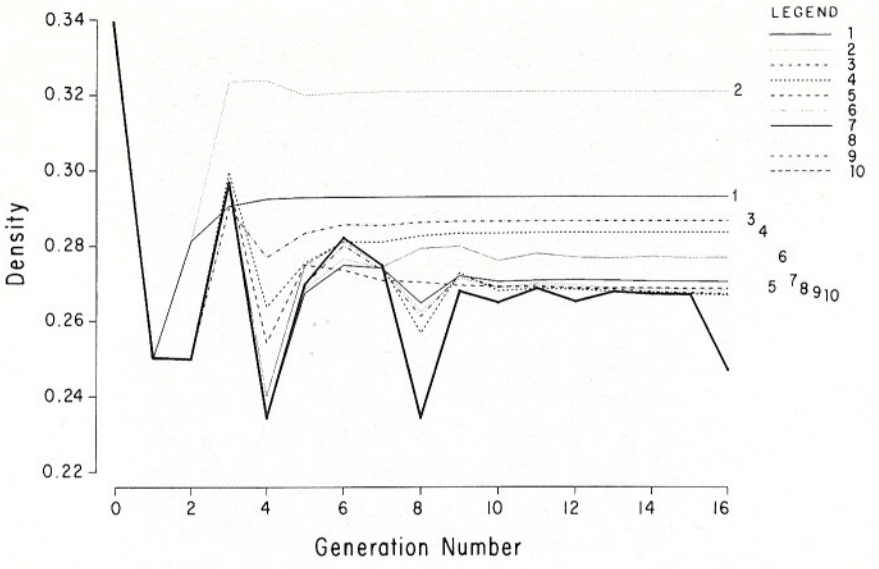

Fig. 10. Rule 18 evolution of the density with time. Experimental paradigm as in fig. 8. Note the expanded density scale.

size with an estimation of the probability of these fixed size blocks. For the first few iterations, no estimation of block probabilities is needed to determine the probability of small blocks. Small block probabilities are determined *exactly* by the local structure operator by summation of the probabilities of predecessor blocks. The local structure operator of order n is initialized with an exact specification of $(n + 2r)$-block probabilities. Each time the operator is applied, block probabilities are summed to determine the probability of blocks which are shorter by $2r$. Hence the local structure operator of order n determines the probability of blocks up to $n + 2r - 2rt$ in length at time t. In particular, the density is followed exactly by the 9th and 10th order operators to time 5.

In fig. 10 we show the results of the same experimental paradigm applied to rule 18. Here the relationship between small- and large-time local structure density estimations is more clearly revealed. The Monte Carlo density estimate underwent a sequence of fluctuations at low generation numbers. The local structure operator followed these fluctuations with increasing fidelity, and for a greater number of generations as order increased. The large-time density was not necessarily better estimated with each increase in order. The operator at each order appeared to "get stuck" at a certain iteration: it took the density at this iteration to be the final density. On one hand, the empirical distribution itself was approaching equilibrium. On the other hand, the local structure operator became an increasingly better estimator of the dynamics of the rule. These factors combined to make the local structure estimate of the invariant measure density increase in accuracy with increase in order.

4.7.5. *The invariant measure of rule 22*

The density of the invariant measure of rule 22 was found above to be approximately 0.35. Clearly this measure is not the standard measure. How then do we describe it? One way to gain a picture of this complex measure is to construct a map from configuration space S^Z to the unit square in $\mathbb{R}^2$. This can be done as follows (Halmos [11], Grassberger [6]): Let c be a configuration $\ldots c_{-1}c_0c_1\ldots$ in S^Z and x, y be the real numbers whose binary expansions are the same as the

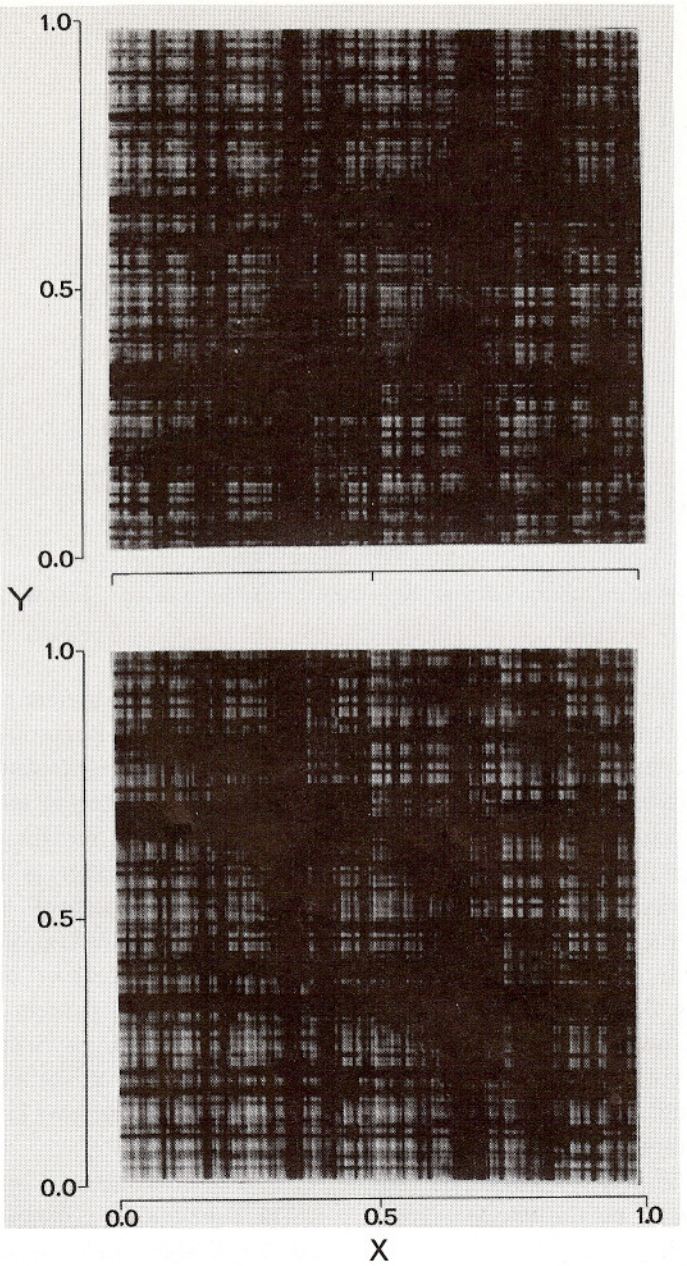

Fig. 11. The invariant measure of rule 22. Top: 400 configurations of length 6000 were generated pseudorandomly to be unbiased and uncorrelated. 16-blocks were sampled from these configurations after they had been acted upon by rule 22 for 128 generations, with triangular boundary conditions. Bottom: 13th order local structure block probability estimates. Each pixel is illuminated with an intensity proportional to the log of the probability of the associated 16-block. (Black corresponds to probability 0.)

right- and left-hand sides, respectively, of this configuration. That is: $x = 0.c_0c_1c_2\ldots$ and $y = 0.c_{-1}c_{-2}\ldots$. Each configuration maps to a point (x, y) in the unit square, and the topology of S^Z is preserved. Finite blocks may be similarly mapped to rational points in the unit square. A finite-block approximation to a measure on configuration space may be visualized by placing a symbol at the coordinates of the block illuminated with an intensity proportional to the log of the probability of the block. Using blocks of size n, there are $2^{2[n/2]}$ "pixels". The top of fig. 11 shows the result of sampling 16-blocks from 400 configurations of length 6000 generated pseudo-randomly to be unbiased and uncorrelated. The sampling occurred at the 128th generation of evolution under rule 22. Under the map described above, this sampling leads to a pattern in the unit square. This figure shows the invariant measure of rule 22 as a complicated pattern of densities and rarefactions. In the bottom of fig. 11 we show the 16-block probabilities of the invariant measure of the 13th order local structure operator. The local structure data look very much like the Monte Carlo data. In section 4.7.9, we present a quantitative analysis of the similarity of these data.

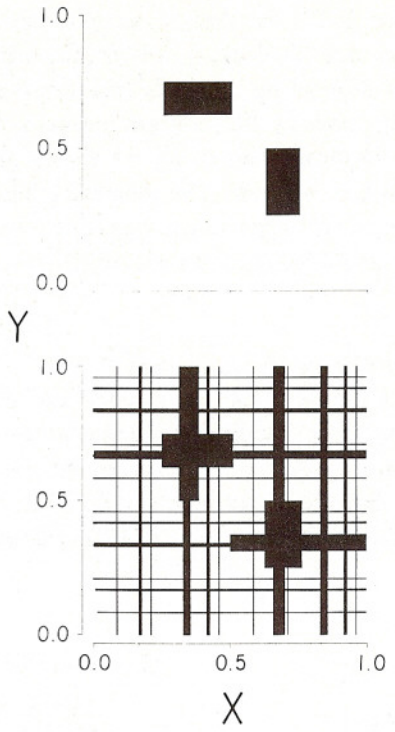

Fig. 12. Asymptotically excluded block for rule 22. Top: The shaded region contains all 16-blocks which have the block 10101 at the central positions. Bottom: All 16-blocks which have the block 10101 at any position within the block.

4.7.6. *Excluded blocks*

As discussed above, the excluded blocks of an idempotent rule completely determine the structure of the invariant measures of the rule. Asymptotically trivial rules exclude blocks in the sense that the probability of the block rapidly decreases as the rule is iterated. We will see to what extent these kinds of block exclusions help explain the pattern shown in fig. 11.

The block 10101 has only one predecessor under rule 22: the block 0101010. This block in turn has only one predecessor, etc. All other 5-blocks have more than one predecessor. Unless the probability of the configuration ...010101010... is 1, any block which contains the 5-block 10101 will have rapidly diminishing probability as rule 22 operates, regardless of its initial probability. We wish to locate in the unit square the 16-blocks which contain 10101. We first place the 10101 block so that the origin is between the first 0 and the second 1 of the block. That is, x is 0.01 in binary and y is 0.101. The first digit determines which quadrant the block is in. Since the first digit of x is 0 and the first digit of y is 1, it is in the upper left quadrant. Continuing this process through further subdivisions, we locate the set of blocks shown at the top of fig. 12. Also shown in fig. 12 is the area obtained by interchanging x and y in the preceding discussion. The block 10101 maps to itself under this interchange.

Halmos [11] points out that the action of the shift on configuration space corresponds to the baker's transformation on the unit square representation of configuration space. That is, if we shift

the block 10101 so that it occupies all possible positions in a 16-block, we obtain the area shown at the bottom of fig. 12. This area covers much of the blank space in the invariant measure of rule 22 (fig. 11). Examination of fig. 11 shows that some blank area is left over. The remaining blank areas indicate other blocks which are exactly or asymptotically excluded, such as 101100101.

4.7.7. *Higher order parameters*

Earlier (section 2.4) we pointed out that 2^{n-1} parameters are required to describe an n-block probability function. A convenient parameterization for the experiments described below is simply the probability of all blocks of length less than or equal to n whose left-most and right-most cell is 1. There are 2^{n-1} such parameters, and each is independent of the others. The parameters may be ordered according to the corresponding blocks themselves as binary expansions. In this order, the ith parameter is the probability of the block $(2i-1)$ in binary. In the following we shall use both Monte Carlo methods and the local structure theory to estimate the value of each of these parameters.

In the Monte Carlo experiment, we began with 100 configurations of length 6000, and applied rule 22 to these. At each generation we sampled 7-blocks from each configuration. From the counts on 7-blocks, we computed the value of each of the 64 independent 7-block parameters.

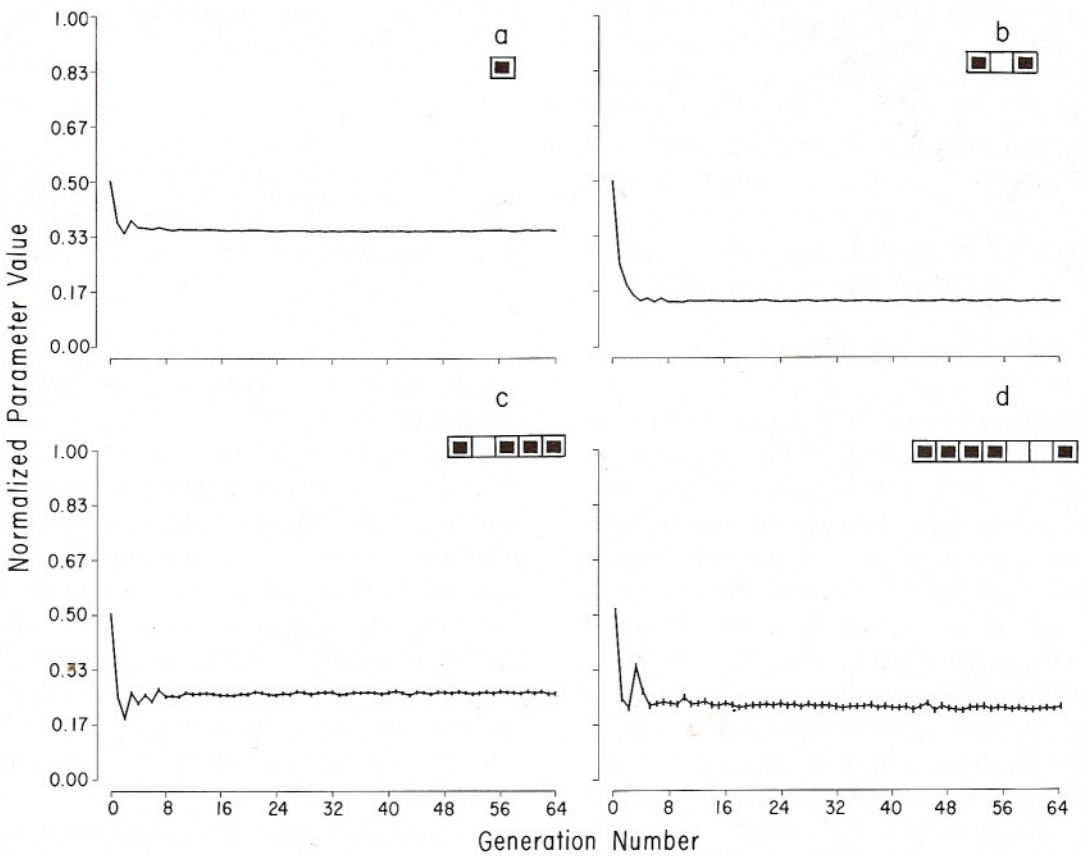

Fig. 13. The evolution of representative parameters a) 1; b) 3; c) 12; and d) 61 under rule 22. These parameters are the probability of a 1, 101, 10111, and 1111001 block respectively. Each parameter is scaled up by 2^n, where n is the size of the corresponding block. The sampling method is described in the text. The error bars indicate ± 2 standard errors of the mean.

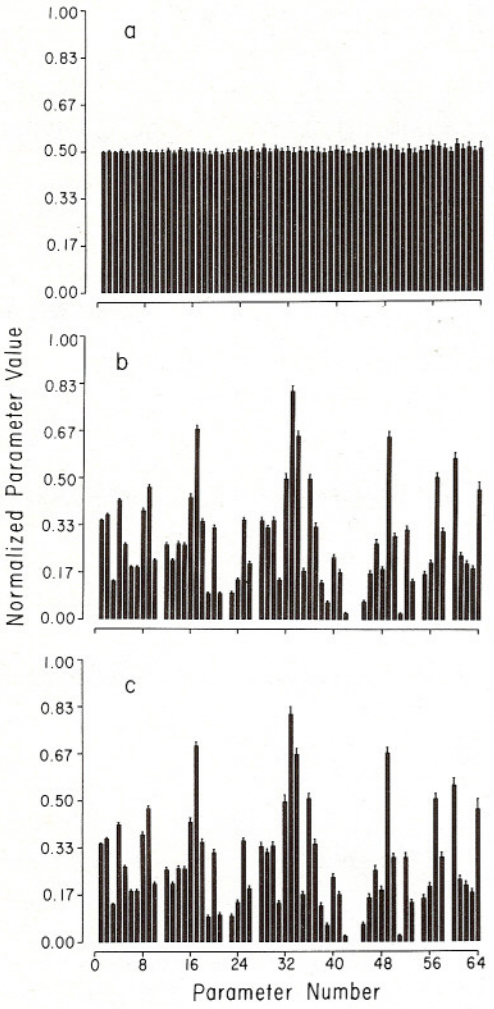

Fig. 14. Monte Carlo estimates of all 64 7-block parameters at times a) 0; b) 64; and c) 1024. The parameters are scaled by 2^n where n is the size of the corresponding block. The error bars indicate 2 standard errors of the mean.

The evolution of representative parameters 1, 3, 12, and 61 under rule 22 is shown in fig. 13. These parameters are the probabilities of a 1, 101, 10111, and 1111001 block, respectively. In this figure, each parameter is scaled up by a factor of 2^n where n is the size of the corresponding block. All parameters shown exhibit the same rough time scales in their course toward equilibrium. It appears that equilibrium is reached after only a few (approximately 10) generations, independent of the block size.

All 64 n-block parameter means are examined in fig. 14. Fig. 14a, $t = 0$, shows the result of sampling from configurations before they have been acted upon by the cellular automaton. The scaled mean for all parameters is close to 0.5 as expected for unbiased, pseudo-random generation of configurations. All standard errors are small as compared to the parameter mean. In fig. 14b the scaled value of each parameter after evolution for 64 time steps by rule 22 is displayed. These parameter values are close to the equilibrium values. In fig. 14c, the same parameter values at time 1024 are shown. Each parameter represents an average over a particular region of the pattern in fig. 11. The size of the region concerned decreases as the parameter index increases.

4.7.8. *The t-test*

We would like to determine how well each of the 64 7-block parameters is estimated by the local structure theory. The significance of a discrepancy between a Monte Carlo and a local structure parameter estimate may be assessed by computing the *t-test* (Crow [2]) for this estimate,

$$t = \left| \frac{\sqrt{N}\,(\bar{x} - c)}{s} \right|, \tag{42}$$

where $\bar{x}$ and s are the mean and standard deviation (*not* the standard error of the mean), respectively, of the Monte Carlo estimate and c is the local structure estimate for the same parameter. N is the number of samples. The smaller the value of t, the less the certainty that the Monte Carlo and local structure estimates are actually different. If the true value of a particular block probability is different from the local structure estimate we should expect the t-test to increase with increasing amounts of Monte Carlo sampling. Thus the magnitude of the t-test has meaning only relative to a given amount of Monte Carlo sampling. We will calibrate t-tests derived from local structure

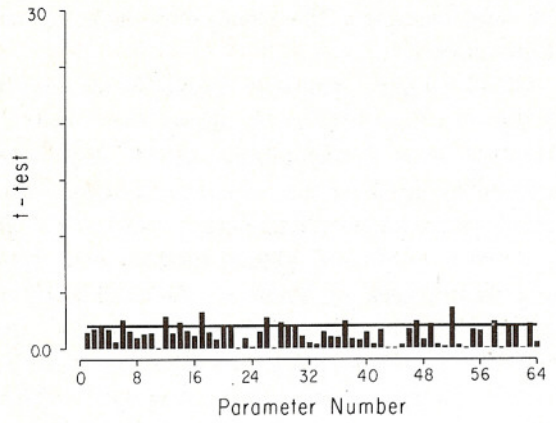

Fig. 15. Comparison of rule 22 generation 64 block parameters (fig. 14b) with the same parameters at generation 1024 (fig. 14c) using the t-test. The scale is the same as the second column of fig. 16. The horizontal solid bar indicates a t-value of 2.

estimates against t-tests from the internal comparison of portions of Monte Carlo data.

If block statistics are close to their equilibrium value by generation 64, then the value of each parameter computed at that generation time should be a good estimate of the value of the same parameter at a larger time. We took generation 64 block parameter estimates (fig. 14b), and the means and standard deviations of Monte Carlo estimates of the same parameters at generation 1024 (fig. 14c). We then computed the t-value for each parameter using the time step 64 value as the estimate c in the t-value (fig. 15). Almost all 64 t-values for the comparison of generation 64 parameters with generation 1024 are comparable with 2. Most are less than 2. Following traditional t-test usage (Crow [2]), we will consider a t-value of 2 to be small.

4.7.9. *Estimation of equilibrium 7-block parameters*

We are now in a position to quantify the similarity of Monte Carlo and local structure estimates such as those in fig. 11. From the fixed point of the local structure operator at each order 1–10, the value of each of the 64 parameters discussed above was found. These parameter values were used to compute t-values relative to

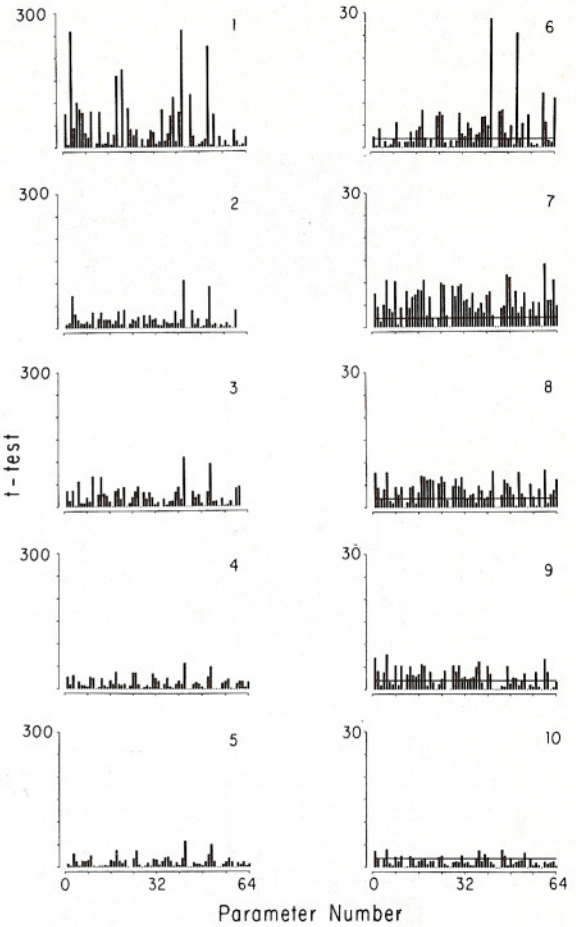

Fig. 16. Dependence on the order of the ability of the local structure theory to predict the values of the empirical 7-block parameters. First column: t-tests for block parameter estimates derived from the fixed points of the local structure operator for rule 22 of orders 1 through 5. Abscissa: 50/tick. Second column: orders 6–10. Abscissa: 5/tick. The horizontal solid bars in this column indicate a t-value of 2.

the generation 1024 Monte Carlo results. In the first column of fig. 16 t-values computed in this fashion from the local structure theory of orders 1 through 5 are displayed. Here each tick mark on the abscissa represents an increment of 50 in the value of t. Note that the t-value is quite large for some parameters, indicating that the local structure estimates of low order are significantly *different* from the empirical values. Note also, however, that as the order of the local structure theory

increases, there is an overall improvement in the goodness of fit of the local structure estimates. In the second column of fig. 16, results for the local structure theory of orders 6–10 are displayed. The same format is used but for an order of magnitude increase in the scale, so that each tick mark represents 5 in t-value. The overall improvement with order in the local structure estimates continues; by order 10 all t-values are comparable with 2. We conclude that in these experiments, 10th order theoretical parameter estimates cannot be resolved with statistical significance from empirical parameter estimates at the given level of sampling.

5. Conclusions

An important property of some cellular automata is their capacity for self-organization. A simply described rule, operating iteratively from a simple initial distribution of block probabilities, may give rise to very complex distributions at large time. Moreover, for many of these rules, the details of the complex distribution obtained do not depend on the structure of the initial distribution – only on the rule and the type of lattice on which it evolves. The capacity to generate stable complex structure from modest starting materials is characteristic of living systems. If cellular automata are to be used as models of physical or biological systems, an effective means of analyzing the statistical properties of particular rules is needed. The local structure theory is a step toward satisfying this need.

The fundamental assumption of the local structure theory is that the action of a cellular automaton on an arbitrary measure may be understood through the study of its action on finite-block measures. Finite-block measures are finitely described. This gives them a tremendous theoretical and practical advantage over general measures. On the theoretical side, the simplicity of construction of the finite-block measures allows the explicit computation of measure-theoretic functions of interest, such as the entropy (Gutowitz et al., in preparation). On the practical side, the action of a cellular automaton on a finite-block measure may be found approximately by means of a system of rational equations.

We have seen that the local structure theory is an accurate model of several aspects of cellular automaton evolution. The dependence on initial conditions and convergence properties are well modeled by the theory. It appears that, even for complex rules, the stable invariant measures of a cellular automaton may be estimated to arbitrary resolution.

For linear, toggle, idempotent and asymptotically trivial rules, proof of the accuracy of the local structure theory is possible. For more general rules, we have relied on empirical studies to demonstrate the power of the theory. There seems to be no fundamental barrier to accurate local structure approximation of the limit measure of cellular automata.

We have performed the detailed statistical analysis described above on a variety of complex rules (unpublished). We have always found the local structure theory to perform as in the case of rule 22. At a computationally accessible order of the theory, an accuracy is achieved which rivals extensive brute force calculations.

We wish to point out that all theoretical results are presented here in no more generality than needed to describe the empirical results. Generalizations in a variety of directions are readily at hand. The same formalism applies to rules of arbitrary radius, state space size, and lattice dimension. Generalization to probabilistic cellular automata (Wolfram [22], Grinstein [9]) or cellular automata which are more than first order in time may be made with little formal overhead.

We are using a statistical method to study a deterministic system. The interplay of these aspects may reveal special features of a cellular automaton. When possible we have related the algebraic properties of a cellular automaton to the behavior

of its local structure approximations. Extending these ideas, we see that the local structure theory of orders greater than 1, unlike the mean-field theory, takes into account both the nature of the cellular automaton rule and the structure of the lattice on which it operates. On one hand this puts restrictions on the manner in which local structure theories may be built for different lattices. On the other hand, it opens up the possibility of distinguishing the particular influences of rule and lattice structure. We will show in a subsequent paper (Gutowitz and Victor [10]) that local structure theories may be developed for cellular automata on lattices of higher dimension.

Wolfram ([22, 23]) suggested, largely on empirical grounds, that cellular automata can be classified in terms of four "universality classes". He used a variety of methods from computation and dynamical systems theory to arrive at this classification. To these methods we may add the local structure theory. Rules may be said to be equivalent if they have the same limit measures. This "equivalence in limit measure" is a refinement of Wolfram's classification scheme. We have seen that for some rules limit measures may be described exactly. For most rules, however, the complete specification of invariant measure needed for a measure-theoretic classification may well be unfeasible to obtain. In lieu of a complete specification of invariant measures, rules might be classified according to their local structure theory approximations.

The local structure theory provides an analytic alternative to Monte Carlo methods in the study of cellular automaton rules. Its usefulness may extend beyond the study of cellular automata into the general theory of dynamical systems. Presently, it is one of the few analytic methods for the computation of the invariant measures of a class of chaotic systems.

Acknowledgements

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