# *Stability of Vertices in Random Boolean Cellular Automata*

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## ABSTRACT

Based on computer simulations, Kauffman (*Physica D*, **10**, 145–156, 1984) made several generalizations about a random Boolean cellular automaton which he invented as a model of cellular metabolism. Here we give the first rigorous proofs of two of Kauffman's generalizations: a large fraction of vertices stabilize quickly, consequently the length of cycles in the automaton's behavior is small compared to that of a random mapping with the same number of states; and reversal of the states of a large fraction of the vertices does not affect the cycle to which the automaton moves.

## 1. INTRODUCTION

As a model of cellular metabolism, Kauffman [5–7] introduced a random Boolean cellular automaton, which will be described formally below. On the basis of extensive computer simulations, he made several empirical generalizations about the behavior of this model. Here we prove two of Kauffman's generalizations. To our knowledge, these are the first rigorous results proved about Kauffman's model.

Let $D = D(n)$ be a directed graph (digraph) on the vertex set $[n] = \{1, 2, \ldots, n\}$, each vertex of which has indegree two, and let $b = (b_1, \ldots, b_n)$ be a vector consisting of $n$ two-argument Boolean functions. Define a function $\varphi = \varphi(D, b)$ on the space $\{0, 1\}^n$ of all 0–1 vectors of length $n$ by putting for every $x = (x_1, \ldots, x_n) \in \{0, 1\}^n$

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$$\phi(x) = y = (y_1, \ldots, y_n)$$

where $y_i = b_i(x_i', x_i'')$ and $x_i', x_i''$ denote the two inneighbors of $x_i$ in $D$. Sometimes we shall write the value of vertex $v$ of $\varphi(x)$ as $\varphi(x)(v)$. Now introduce discrete "time" $t$ by defining $\varphi_1 = \varphi$, $\varphi_{t+1} = \varphi(\varphi_t)$. Since the space of all possible states is finite, for every initial vector $x$, the system must end up in a cycle, i.e., there is a natural number $c$ such that

$$\exists T, \quad \forall t > T: \quad \phi_{t+c}(x) = \phi_t(x) .$$

The smallest possible $c$ and $T$ with this property we denote by $c(D, b, x)$ and $T(D, b, x)$.

In this article we estimate the value of $c(\tilde{D}, \tilde{b}, \tilde{x})$ where $\tilde{D}$ is picked at random from the family of all $\binom{n-1}{2}^n$ 2-indegree regular digraphs $D$ on $n$ vertices, $\tilde{b}$ is chosen from all $16^n$ possible vectors $b$, and an initial state $\tilde{x}$ is picked at random from all $2^n$ possibilities $x$. Thus $(\tilde{D}, \tilde{b}, \tilde{x})$ with superior tildes denotes a random Boolean cellular automaton, while $(D, b, x)$ without tildes denotes a particular one of these.

Kauffman [5–7] performed numerical simulations of this model. He summarized his results as follows [7, pp. 151–152]:

"1) Simulation results with $n$ ranging up to 8,000 reveal that median state cycle lengths increase roughly as $n^{1/2}$. Thus, an automaton with 10,000 binary variables and $2^{10,000} \approx 10^{3000}$ states, typically settles down and cycles among a mere 100 states. That is, dynamical behavior is localized to attractors occupying a small subvolume e.g. $10^{-2998}$ of the state space.

"2) The number of distinct state cycles also increases approximately as $n^{1/2}$. Hence an automaton with 10,000 binary variables would typically have on the order of 100 state cycle attractors, each lying in its distinct basin of attraction.

"3) A large fraction of the binary variables, 60%–80% typically fall to fixed active (1) or inactive (0) values and maintain the same values on all state cycles. Consequently, states on any state cycle are similar to one another and states on different state cycles are less, but again fairly similar to one another. Typical mean Hamming distances between members of distinct state cycles is about 1–10%.

"4) Each state cycle is typically stable to 80–95% of the possible minimal perturbations, reversing the value of any single variable at a time.

"5) After some such minimal perturbations, the automaton undergoes a transition from one state cycle to another. Typically, any state cycle can 'reach' only a few neighboring state cycles by such minimum perturbations. A 'reachability' matrix showing which cycles have access to which cycles therefore typically exhibits few transitions from each cycle, to a restricted number of neighboring state cycles. In addition, the 'reachability' matrix typically exhibits ergodic subsets of state cycles which can be reached by cycles outside the subset, but, once the automaton is within the ergodic subset of cycles, it is trapped and flows probabilistically among them, as driven by random minimal perturbations."

This behavior differs substantially from the behavior of a system of $2^n$ states in which each state chooses the next one at random [1, paragraph XIV.5]. It is well known that for such a system the expected length of a cycle is of the order $2^{n/2}$, far longer than the cycle length in Kauffman's simulations. Moreover, if each state is represented as a binary $n$-vector, then a change in a single element (bit) of the state vector is likely to move the system into the domain of attraction of a different cycle, again differing from Kauffman's simulations.

Although we are not able to give a full analysis of the behavior of $(\tilde{D}, \tilde{b})$, as described in Kauffman's 1)–5), we shall give rigorous mathematical arguments that explain phenomena 3) and 4). We shall deduce then (in the Corollary stated at the end of this introduction) that $\log c(\tilde{D}, \tilde{b}, \tilde{x})$ is of order less than $n$, i.e., the length of cycles of Kauffman's model is much smaller than the length of cycles in a system in which consecutive states are chosen at random.

To state our results precisely, we introduce some notation and definitions. We say that vertex $v$ of the system $(D, b)$ *stabilizes in time $l$* if $v$ does not change its value after $l$ steps independently of the value of the initial vector, i.e., either

$$\forall x, \forall t > l: \quad \phi_t(x)(v) = 1$$

or

$$\forall x, \forall t > l: \quad \phi_t(x)(v) = 0\,.$$

Moreover, we say that vertex $i$ is *weak* if the value of the initial state in this vertex does not affect the asymptotic behavior of the system, i.e., if for an initial state $x = (x_1, \ldots, x_n)$ by $\bar{x}^i$ we denote $(x_1, \ldots, 1 - x_i, \ldots, x_n)$ then

$$\exists T, \forall t > T: \quad \phi_t(x) = \phi_{t+T}(\bar{x}^i)\,.$$

Clearly, from the definition of a weak vertex, it follows that one can switch the value of such a vertex at any time without changing the cycle that the system will finally enter.

Our main results, which follow, hold for every initial state $x$, not merely for almost all initial states. In this sense, our results are stronger than the simulation results of Kauffman [5–7].

**Theorem 1.** *Let $\omega(n) \to \infty$ arbitrarily slowly. Then as $n \to \infty$, the probability tends to 1 that at least $n(1 - \omega(n)/(\log n))$ vertices of $(\tilde{D}, \tilde{b})$ stabilize after time less than $(\log n)/3$.*

**Theorem 2.** *Let $\omega(n) \to \infty$ arbitrarily slowly. Then as $n \to \infty$, the probability tends to 1 that $(\tilde{D}, \tilde{b})$ contains at least $n(1 - \omega(n)/(\log\log n))$ weak vertices.*

From Theorem 1 one can get an upper bound for $c(\tilde{D}, \tilde{b}, \tilde{x})$.

**Corollary.** *Let $\omega(n) \to \infty$ arbitrarily slowly. Then as $n \to \infty$, the probability tends to 1 that for all initial states $x$, we have*

$$c(\tilde{D}, \tilde{b}, x) \leq \exp\left(\frac{n\omega(n)}{\log n}\right).$$

We defer the proof of the corollary until after the proof of Theorem 1.

Interesting modifications of Kauffman's model, such as $K$-argument Boolean functions of $K$ inneighbors ($K \neq 2$), and an annealed version in which the Boolean functions are randomly chosen at each time step, rather than once and for all, have been proposed and insightfully analyzed by, e.g., Derrida and Pomeau [3] and Derrida and Weisbuch [4]. See Derrida [2] for a review.

## 2. PROOF OF THEOREM 1

For vertex $v$ of a digraph $D$, let $N_0^-(v) = \{v\}$ and let $N_{i+1}^-(v)$ denote the set of all inneighbors of $N_i^-(v)$. Furthermore, set

$$S_i^-(v) = \bigcup_{j=0}^{i} N_j^-(v).$$

Then, for every vertex $v$, $|S_0^-(v)| = 1$, $|S_1^-(v)| = 3$ and

$$|S_i^-(v)| \leq \sum_{j=0}^{i} 2^j \leq 2^{i+1} - 1.$$

The following fact is crucial for our argument.

**Lemma 1.** *Let $v$ be a fixed vertex of $\tilde{D}$ such that the subgraph induced in an underlying multigraph of $\tilde{D}$ by $S_l^-(v)$ contains no cycles. Then the probability that $v$ stabilizes in at most $l$ steps is larger than $1 - 8/l$.*

*Proof.* Let $p_l$ denote the probability that $v$ does not stabilize by (up to and including) time $l$, $p_l \leq 8/l$. We shall find a recurrence formula for $p_{l+1}$. If both inputs of $v$ have stabilized in $l$ steps, then clearly $v$ stabilizes in $l+1$ steps no matter what Boolean function is placed in it. Since $S_{l+1}^-(v)$ does not contain cycles, stabilization of one input in $l$ steps is independent of stabilization in the other input. When neither of the inputs stabilizes in $l$ steps, which happens with probability $p_l^2$, then the Boolean function in $v$ must be different from tautology (all 1's as output) and contradiction (all 0's as output) and the probability of such an event equals $7/8$. Finally, when exactly one of the inneighbors of $v$ stabilizes in $l$ steps (an event with probability $2p_l(1-p_l)$), then the behavior of $v$ must be determined by the behavior of the nonstabilized inneighbor of $v$ and must not be a constant function of the nonstabilized inneighbor of $v$; hence the probability of the event that $v$ does not stabilize is the same as the probability that the value of a Boolean function of one argument depends on the argument, namely that the Boolean function is not identity or negation; this probability equals $1/2$. Thus

$$\begin{aligned} p_{l+1} &= (7/8)p_l^2 + p_l(1-p_l) \\ &= p_l - (1/8)p_l^2 \end{aligned}$$

and clearly $p_0 = 7/8$.

We show that $p_l \leq 8/l \leq 1$ for all $l \geq 8$ by induction:

$$p_{l+1} = p_l - \frac{1}{8} p_l^2 \leq \frac{8}{l} - \frac{8}{l^2} = \frac{8(l-1)}{l^2} \leq 8/(l+1). \qquad \blacksquare$$

In the proof of Theorem 1 we shall need the following fact about the structure of $\tilde{D}$.

**Fact.** With probability tending to 1 as $n \to \infty$, the number of vertices of $\tilde{D}$ which belong to cycles of length less than $(2/3)\log n$ in the underlying multigraph of $D$ is smaller than $n^{0.94}$.

*Proof of Fact.* Let $N = \lfloor (2/3)\log n \rfloor$, the greatest integer less than or equal to $(2/3)\log n$. Let $X$ be the number of vertices of $D$ contained in cycles of length $k$, $k = 2, 3, \ldots, N$, in the underlying multigraph of $\tilde{D}$. Then, for $k = 2, 3, \ldots, N$, the $k$ vertices of a $k$-cycle can be chosen in $\binom{n}{k}$ ways; from these $k$ vertices, an undirected cycle can be constructed in $(k-1)!/2$ ways if $k \leq 3$ and one way when $k = 2$; each such cycle contains $k$ vertices; and the probability that all the $k$ undirected edges in the underlying multigraph are present is the $k$th power of 2 times the probability that an arrow in either direction between two of the chosen vertices is present in $\tilde{D}$, and the latter probability is just $(n-2)/\binom{n-1}{2}$. Thus, for the expectation of $X$ we get

$$\begin{aligned} EX &\leq 2n \cdot \left[\frac{2(n-2)}{\binom{n-1}{2}}\right]^2 + \sum_{k=3}^{N} \binom{n}{k} \cdot \frac{(k-1)!}{2} \cdot k \cdot \left(\frac{2(n-2)}{\binom{n-1}{2}}\right)^k \\ &\leq 8 + \sum_k \frac{n^k}{k!} \cdot \frac{k!}{2} \cdot \left(\frac{4}{n-1}\right)^k \leq 8 + \sum_k 4^k \cdot \frac{1}{2}\left(\frac{n}{n-1}\right)^k. \end{aligned}$$

For large $n$, since $k \leq (2/3)\log n \ll n$, we have

$$EX \leq 8 + \sum_{k=3}^{N} 4^k \leq 4^{(2/3)\log n + 2} = 16 \cdot n^{(2/3)\log 4} \leq n^{0.93}.$$

Thus, from Markov's inequality, $P(X \geq n^{0.94}) \leq n^{-0.01} \to 0$. $\blacksquare$

*Proof of Theorem 1.* Let $Y$ count vertices in $D$ which do not belong to cycles of length less than $(2/3)\log n$ in the underlying multigraph of $\tilde{D}$ and do not stabilize by time $(1/3)\log n$. Then the expectation of $Y$, due to the Lemma, can be estimated from above by

$$EY \leq n \cdot \frac{8}{(1/3)\log n} = \frac{24n}{\log n}$$

so, using Markov's inequality, we get

$$P\left(Y \geq \frac{n\omega(n)}{2\log n}\right) \leq \frac{48}{\omega(n)} \to 0.$$

Hence, due to the Fact, at least

$$n - \frac{n\omega(n)}{2\log n} - n^{0.94} \geq n - \frac{n\omega(n)}{\log n}$$

vertices stabilize in at most $(1/3)\log n$ steps. ■

*Proof of Corollary to Theorem 1.* Theorem 1 implies that, with probability $1 - o(1)$, at most $n\omega(n)/\log n$ vertices of $(\tilde{D}, \tilde{b})$ do not stabilize after time less than $(1/3)\log n$, where $\omega(n) \to \infty$ as $n \to \infty$. The maximum cycle length is bounded by the maximum number of states these nonstabilized vertices can specify, i.e., for every $x$

$$c(\tilde{D}, \tilde{b}, x) \leq 2^{n\omega(n)/\log n} \leq \exp\left(\frac{n\omega(n)}{\log n}\right). \quad ■$$

## 3. PROOF OF THEOREM 2

Let $N_0^+(v) = \{v\}$ and $N_{i+1}^+(v)$ be the set of all outneighbors of vertices in $N_i^+(v)$. Moreover, let

$$S_i^+(v) = \bigcup_{j=0}^{i} N_j^+(v).$$

This construction is analogous to that for inneighbors in the previous section. The result corresponding to Lemma 1 is:

**Lemma 2.** *Let $v$ be a vertex such that the subgraph induced by $S_l^+(v)$ in the underlying multigraph of $\tilde{D}$ contains no cycles. Then the probability $f_l$ that a change of state of $v$ affects the state of some vertex in $N_l^+(v)$ is smaller than $2/l$.*

*Proof of Lemma 2.* The probability that fixed vertex $v$ has exactly $k$ outneighbors is given by

$$\begin{aligned} P\{|N_1^+(v)| = k\} &= \binom{n-1}{k} \cdot \left(\frac{n-2}{\binom{n-1}{2}}\right)^k \left(1 - \frac{n-2}{\binom{n-1}{2}}\right)^{n-1-k} \\ &= \frac{(n-1)_k}{k!} \cdot \left(\frac{2}{n-1}\right)^k \left(1 - \frac{2}{n-1}\right)^{n-1-k} \\ &= \frac{2^k}{k!} e^{-2}\left(1 + O\left(\frac{k}{n}\right)\right). \end{aligned}$$

Thus, since for $k \geq \log n$ this probability is of order less than $n^{-2}$, with probability $1 - o(1)$ all vertices of $\tilde{D}$ have less than $\log n$ outneighbors, and for a fixed vertex $v$ and all $k$, $0 \leq k \leq \log n$ we have

$$P\{|N_1^+(v)| = k\} = \frac{2^k}{k!} e^{-2} + O(n^{-1}\log n). \quad (*)$$

Now we find a recurrence formula for $1-f_{l+1}$ i.e., the probability that a change of the state of vertex $v$ does not affect any vertex from $N^+_{l+1}(v)$. Choose a vertex $w \in N^+_1(v)$. With probability $1/2$ the Boolean function placed in $w$ just ignores the state of $v$; and, when it is "sensitive" to it, with probability $1-f_l$ the change of state of $w$ will not be transmitted further than $l$ steps ahead. Thus, combining this with $(*)$ gives

$$
\begin{aligned}
1-f_{l+1} &= \sum_{k=0}^{\lfloor \log n \rfloor} \left(\frac{1}{2}+\frac{1}{2}(1-f_l)\right)^k P\{|N^+_1(v)|=k\} \\
&= e^{-2}\sum_k \frac{(2-f_l)^k}{k!} + O(n^{-1}(\log n)^2) \\
&= \exp(-f_l) + O(n^{-1}(\log n)^2)\,.
\end{aligned}
$$

Hence

$$f_{l+1} = 1-\exp(-f_l) + O(n^{-1}(\log n)^2)$$

where, of course, $f_0 \le 1$.

In fact, $f_l \le 2/l$ for $l \ge 2$, because

$$
\begin{aligned}
f_{l+1} &= 1-\exp(-f_l) + O(n^{-1}(\log n)^2) \\
&\le 1-1+f_l-\frac{f_l^2}{2}+\frac{f_l^3}{6} \\
&\le \frac{2}{l}-\frac{2}{l^2}+\frac{4}{3l^3} = \frac{2}{l}\cdot\frac{3l^2-3l+2}{3l^2} \\
&= \frac{2}{l+1}\left(1-\frac{l-2}{3l^3}\right) \le \frac{2}{l+1}\,.
\end{aligned}
$$

■

*Proof of Theorem 2.* Let $Z$ count the vertices $v$ which do not lie on cycles of length less than $2\log\log n$ and the state of which affects some vertices from $N^+_{\lfloor \log\log n \rfloor}(v)$. Then, due to Lemma 2,

$$EZ \le n\frac{2}{\log\log n} = \frac{2n}{\log\log n}\,.$$

Hence, Markov's inequality implies that

$$P\left\{Z > \frac{n\omega(n)}{2\log\log n}\right\} \le \frac{4}{\omega(n)} \to 0\,.$$

Moreover, from the Fact and Theorem 1 we know that, with probability $1-o(1)$, fewer than $u = 2n\omega(n)/\log n$ vertices of the system either do not stabilize in time $(1/3)\log n$ or belong to cycles of length less than $2\log\log n$. Thus, the number of vertices from which these vertices can be reached in less than $\log\log n$ steps is less than

$$u \sum_{i=0}^{\lfloor \log \log n \rfloor} 2^i \leq u \cdot 2^{\log \log n + 1} \leq \frac{n}{\log \log n}$$

provided we choose $\omega(n) \leq \log \log n$. Thus, with probability $1 - o(1)$, the system $(\tilde{D}, \tilde{b})$ contains at least

$$n - \frac{n}{\log \log n} - \frac{\omega(n)n}{2 \log \log n} \geq n - \frac{n\omega(n)}{\log \log n}$$

vertices $v$ such that changing the state of $v$ can affect only vertices which stabilize quickly and so cannot change the cycle the system enters. ■

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