

On Forcing Functions in Kauffman's Random Boolean Networks

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The phase transition between frozen and chaotic behavior in Kauffman's cellular automata on a nearest neighbor square lattice does not agree with the percolation threshold of the forcing functions.

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In cellular automata⁽¹⁾ the value at time $t + 1$ of a "spin" or other local variable depends deterministically on the values at time t of the spin values for K neighbors in the lattice; for example, $K = 4$ on the square lattice with nearest neighbor connections, if we ignore the direct influence of a spin on itself. If each spin has only two orientations, it is also called a Boolean variable and takes the values TRUE or FALSE. We have $M = 2^K$ different configurations for the K Boolean neighbors, and thus 2^M possible rules for how to change a spin; this amounts to 65,536 different functions for cellular automata with $K = 4$.

The Kauffman model⁽²⁾ is a random mixture of these $2^{(2^K)}$ cellular automata rules: at each lattice site one chooses randomly which of the 2^M rules applies to it, and then sticks with that initial choice for the whole evolution. The model was invented⁽²⁾ to simulate the genetic aspects of life, with the single spins corresponding to genes, each of which can be turned on or off. Turning off a gene can be caused by repressor molecules influenced by K other genes. The time evolution of this irreversible Kauffman automaton may or may not lead to periodic oscillations of the spins, which

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we call limit cycles. Different limit cycles may represent different types of living cells. To be a good model for life, the Kauffman model should be rather stable against "mutations," i.e., a random change of a few spin orientations should lead to limited damage only, with the total number of spins changed by this mutation approaching for $t \rightarrow \infty$ a limit proportional to the initial changes. Cases with such built-in damage limitation are called "frozen,"⁽³⁾ as opposed to the "chaotic" case, where small perturbations may lead to a large final change independent of the small amount of initial change.⁽³⁾

Much early research⁽²⁾ concentrated on infinite ranges of connection, where the K neighbors are chosen randomly from all the sites of the system, independent of their distance. For large systems, this "infinite-dimension" limit can be solved exactly^(3,4) since then it does not matter if the rules stay fixed throughout the time development or change after every time step.⁽⁴⁾ More recently,^(3,5) on the square lattice with only nearest neighbor connections a transition from frozen to chaotic behavior was observed numerically at a threshold $p_c \simeq 0.26$ if the Boolean rules for each site are chosen randomly such that a fraction p gives TRUE and a fraction $1 - p$ gives FALSE. For $p < p_c$ one observes frozen behavior; for $p > p_c$ one sees chaos with an unlimited growth of small perturbations, with limit cycle periods increasing exponentially with system size, and with percolation of an infinite cluster of oscillating spins.^(3,5)

For these numerical investigations with finite connection range one would like to have a theoretical criterion, independent of the time development, where the transition to chaos will occur. It has long been suggested^(2,6) that forcing functions play a crucial role in preventing chaotic behavior. A rule for cellular automata is called forcing, or canalizing, if at least one of its K arguments has the property that the result of the function is already fixed if this argument has one particular value, regardless of the values for the $K - 1$ other arguments. For example, the Boolean AND function for $K = 2$ is forcing, since it is always FALSE if the first argument is FALSE. On the other hand, the Boolean EQUIVALENCE function is not forcing, since we need to know both arguments to decide if they are equal, i.e., if EQUIVALENCE is TRUE. Particularly important for $p \rightarrow 1$ is the TAUTOLOGY forcing function, which is always TRUE independent of its arguments; the forcing function CONTRADICTION, which always gives FALSE, dominates for $p \rightarrow 0$. The larger K is, the smaller is the fraction of forcing functions⁽²⁾; Fogelman⁽⁷⁾ listed them for $K = 3$. It would be nice if the phase transition between frozen and chaotic behavior would be connected with the percolation threshold of an infinite cluster of neighboring forcing functions. Since the functions are selected randomly apart from the bias connected with the probability p , the phase transition would then

coincide with the random site percolation threshold,⁽⁸⁾ which appears if 59.275% of all sites of the square lattice are forcing functions (69.6% for the honeycomb lattice, $K=3$; 50% for the triangular lattice, $K=6$). We now test this possibility that the concept of forcing functions allows a determination of the phase transition point via a known threshold of random percolation.

Thus we evaluated, similar to series expansions of critical points, how the fraction π of forcing functions, among all functions on the lattice, depends on the fraction p of TRUE functions selected for that lattice randomly. For $K=2$, of the 16 possible functions, only two are not forcing: EQUIVALENCE and its conjugate EXCLUSIVE-OR. The rule EQUIVALENCE appears with probability $p^2(1-p)^2$, since of the $M=2^K=4$ neighbor configurations, two give the result TRUE and the other two give the result FALSE. The same contribution comes from the function EXCLUSIVE-OR; thus,

$$\pi = 1 - 2p^2(1-p)^2 \quad (K=2) \tag{1}$$

For general K , each function gives for the M different neighbor configurations m times the value TRUE and $M-m$ times the value FALSE; it is thus selected with probability $p^m q^{M-m}$, where $q = 1-p$. If there are N_m different functions, among the 2^M possible rules, that give exactly m times TRUE and are forcing, the total probability π for the randomly selected function to be forcing is

$$\pi = \sum_{m=0}^M N_m p^m q^{M-m} \tag{2}$$

Note that the N_m and thus Eq. (2) are independent of any lattice structure or dimensionality and depend only on K .

A simple computer program checked within 4 min on a microcomputer all 16, 256, and 65,536 possible rules for $K=2, 3$, and 4, respectively; determined if they were forcing; if yes, calculated the number m of its TRUE results; and in this way determined the numbers N_m of forcing functions with m out of $M=2^K$ results TRUE. We thus found

$$\pi(K=2) = p^4 + 4p^3q + 4p^2q^2 + 4pq^3 + q^4 \tag{3a}$$

$$\begin{aligned} \pi(K=3) = & p^8 + 8p^7q + 24p^6q^2 + 24p^5q^3 + 6p^4q^4 \\ & + 24p^3q^5 + 24p^2q^6 + 8pq^7 + q^8 \end{aligned} \tag{3b}$$

$$\begin{aligned} \pi(K=4) = & p^{16} + 16p^{15}q + 112p^{14}q^2 + 352p^{13}q^3 + 536p^{12}q^4 + 448p^{11}q^5 \\ & + 224p^{10}q^6 + 64p^9q^7 + 8p^8q^8 + 64p^7q^9 + 224p^6q^{10} + 448p^5q^{11} \\ & + 536p^4q^{12} + 352p^3q^{13} + 112p^2q^{14} + 16pq_{15} + q^{16} \end{aligned} \tag{3c}$$

By definition the polynomials are symmetric about $p=1/2$. The probabilities p^M correspond to TAUTOLOGY, the last terms q^M to CONTRADICTION. Note the bimodal structure for $K > 2$ in the N_m : Forcing functions like to have a high degree of internal homogeneity,⁽⁹⁾ which means usually most of the M function values are TRUE or most of them are FALSE, if the function is forcing. Table I gives numerical results for the reader's convenience.

We see that for $K=3$ the probability π reaches the site percolation threshold 0.6962 of the honeycomb lattice at $p=0.278$, consistent with a preliminary Monte Carlo simulation of the Kauffman model on that lattice (p_c about 0.3). However, for $K=4$ the concept of forcing functions works less well: π reaches the square site percolation threshold 0.59275 already at $p=0.192$, far below the numerical^(3,5) estimates $p_c=0.26 \pm 0.02$ and 0.26 ± 0.01 for the transition to chaos in the Kauffman model on square lattices. Thus, for p between 19 and 26% we still have frozen behavior and no chaos, even though the forcing functions no longer form a connected network of neighboring lattice sites. (For the square lattice the transition to chaos agrees well with the percolation threshold for the nonforcing functions, i.e., $1-\pi=0.59275$; but such an identification fails to work in the honeycomb lattice, where the nonforcing functions never percolate,

Table I. Probability π , Eq. (3), of a Randomly Selected Boolean Function to Be Forcing If These Boolean Functions Give TRUE with Probability p and FALSE with Probability $1-p$ ^a

p	$K=2$	$K=3$	$K=4$
0	1	1	1
0.05	0.9955	0.9892	0.9718
0.10	0.9838	0.9554	0.8770
0.15	0.9675	0.8997	0.7313
0.20	0.9488	0.8268	0.5655
0.25	0.9297	0.7440	0.4072
0.30	0.9118	0.6599	0.2739
0.35	0.8965	0.5832	0.1730
0.40	0.8848	0.5219	0.1048
0.45	0.8775	0.4824	0.0661
0.50	0.8750	0.46875	0.0536

^a In total we have 14, 120, and 3514 forcing functions among the 16, 256, and 65,536 possible rules for $K=2, 3$, and 4, respectively. For $p > 1/2$, π is the same as for $1-p$.

since $1 - \pi$ is never larger than $0.53125 = 17/32$, far below the percolation threshold of 0.69.) Thus, the old definition⁽²⁾ of forcing functions has to be generalized if their percolation threshold is to coincide with the transition to chaos on the nearest neighbor square lattice.

Hartman and Vichniac⁽⁶⁾ took a different approach to the connection of forcing functions, percolation, and chaos in the Kauffman model on a square lattice ($K=4$). Instead of working with all possible 2^M rules, they selected one forcing and one nonforcing function, and mixed these two randomly. They find agreement between the percolation threshold 0.59275 and the phase transition limiting the growth of damage, and thus support Kauffman's concept of the importance of forcing functions.

However, one can also find a counterexample with two nonforcing functions that nevertheless still give a transition from frozen to chaotic behavior. We take with probability p the rule that gives TRUE iff an even number of neighbors is TRUE on the nearest neighbor square lattice. For the other lattice sites, i.e., with probability $1 - p$, we take the rule that is TRUE iff at most two of the four neighbors are TRUE. The earlier symmetry of p and $1 - p$ now is no longer valid. For both functions the knowledge of one neighbor spin does not yet determine the outcome, since we need to know the total number of TRUE neighbors; thus, not a single site carries a forcing function. Nevertheless, for $p = 0$, i.e., using the second function only, one has a checkerboard distribution of spin orientations as a time-independent solution of this rule, and the flipping of one spin only causes this spin to fall back to its original checkerboard orientation in the next time step. Thus, we are in the frozen phase. With the first function only, i.e., for $p = 1$, a time-independent solution is reached if all sites are TRUE. Turning one of the spins in this configuration causes numerous neighbors to be flipped later, with the distance between the spins flipped later and the originally flipped spin increasing linearly with time. Thus, the damage can spread over the whole lattice, which corresponds to chaotic behavior. Thus, we have a frozen situation at $p = 0$ and chaos at $p = 1$; a simple Monte Carlo simulation (with a random initial spin distribution) suggested a phase transition near $p = 1/4$. This transition cannot be connected with forcing functions, since there are none in this example.

In summary, the definition of forcing functions needs to be generalized if their percolation threshold is supposed to coincide with the dynamical transition to chaos in the Kauffman model. The more complicated forcing domains of Fogelman⁽⁷⁾ might be a possibility, but seem no longer equivalent to a random percolation process.

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NOTE ADDED IN PROOF

Better simulations (D. Stauffer, Bar Ilan Conference, *Phil. Mag.*, to be published) of the Kauffman model gave chaos above $p = 0.28$ (instead of $p = 0.26$) on the square lattice but no chaos on the honeycomb lattice. Thus the agreement between the onset of chaos and the percolation of nonforcing functions seems worse on the square lattice; on the honeycomb lattice, where nonforcing functions never percolate, we now have always a frozen phase.

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