Phase Transitions in Logic Networks

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Randomly connected networks of Boolean logic functions of fixed in-degree ("Kauffman Nets") are analyzed using an annealed approximation. While these nets originated as models of genetic regulatory networks, the conclusions and observations obtained by treating them as a complex type of spin system are relevant beyond the purview of genetics and have applications in the construction and control of certain complex dynamical systems. Preliminary results are presented on the properties of nets incorporating bias and redundancy.

Section 1 Introduction to NK Boolean Nets

NK Boolean Nets were first put forth as a model of genetic regulatory systems by Stuart Kauffman in 1969[7, 8, 9, 10], based on the biochemically founded inspiration that genes, through their expression of proteins, can affect other genes by inhibiting or activating their expression. A Nk Boolean Net refers to N nodes and k inputs per node. Each node is characterized by a logical function of its inputs such as $A \,\mathbf{nand}\, (B \,\mathbf{xor}\, C)$. This logical function works dynamically to compute the state of the node at the next time step as a function of the that node's input values of the previous time step. Thus a Boolean net is a discrete dynamical system. A Boolean Net differs from a Boolean expression in that it has N output values instead of one. A random Boolean Net has a randomly chosen topology (usually with duplicated links avoided) and randomly chosen Boolean functions at each node.

The variety of nets which can be constructed in this manner is very large. If there are k inputs per node, the rule table specifying the output for any given combination of binary inputs will be of size 2^k. Each one of these slots can be filled with either a 0 or a 1. Thus each node can have 2^{2^k} possible functions. N raised to this number is therefore the number of possible functional realizations of a Nk net. The number of possible topologies is also large. Since each of the k inputs of each node is linked to some other node, there are $\binom{N}{K}$ ways to distribute the "other ends" of the inputs. There are thus N raised to this power ways of configuring the entire net. Therefore the maximum possible number of ways to construct a Nk net is the product of topological realizations and logical realizations, given by

$$N^{\binom{N}{K}} N^{2^{2^K}}$$

a very large number indeed.

In actuality, the number of unique realizations of a net is smaller than this, as Boolean nets have a number of symmetries (such as the exchange of zeroes and ones) which reduce the size of the space. Another bound on the functional number of nets is given by the maximum number of different dynamics which can be deterministically generated. The state of the net at a given time-slice is given by the values at each of the N nodes. There are 2^N such states, the number of different binary numbers of N bits. Since the dynamics are deterministic, the longest non-repeating path through state space can be at most 2^N steps long. All realizable dynamical trajectories are contained in the power set of the state space, which has 2^{2^N} elements.

The conclusion which can be readily drawn from the above argument is that the number of realizations becomes statistically significant very quickly as a function of increasing N. This invites one to apply the methods of statistical analysis to understand characteristic behaviors of random Boolean nets.

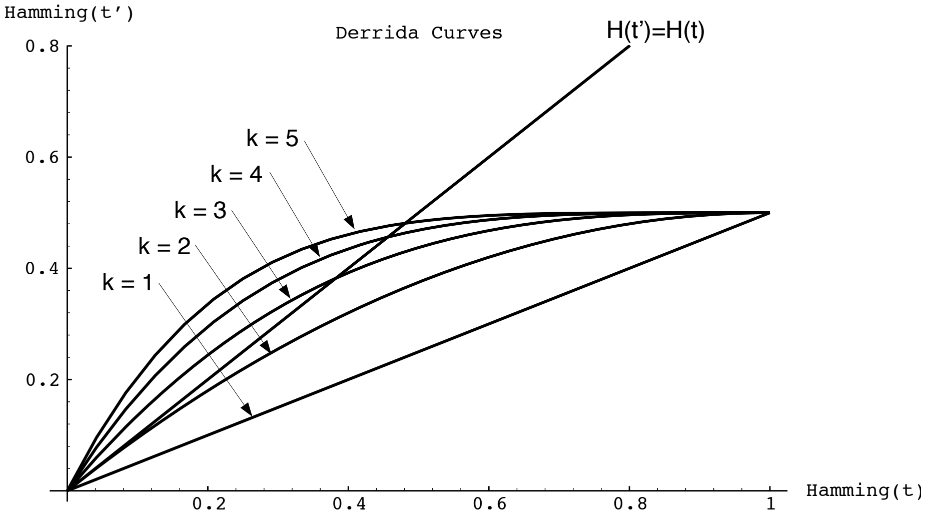
Section 2 Statistics of Boolean Nets

A continuous deterministic dynamical system can be characterized by being in an ordered or chaotic regime by a number of means. With Boolean nets we are dealing with a discrete state space and hence the definition of chaos is different than that of a continuous system. Given enough time, the system *must* return to a state it has visited before, a constraint which continuous systems are not subject to. In addition, we cannot perturb a Boolean net infinitesimally and observe whether this perturbation grows or not, as we have to flip a discrete bit. Given these caveats, it is still possible to ask questions about the stability of Boolean nets. Derrida and Pomeau[4] defined a process in which one takes two nets whose initial conditions differ in $N(1-q)$ bits (the Hamming distance between the nets), where N is the size of the net and $q \in [0,1]$ is the amount of overlap in initial conditions. Each net is then computed forward by one step, and the change in Hamming distance is observed. If differences tend to grow, this is a discrete signature of chaos, and if distances converge, this is a signature of order.[4, 5, 6] This is analogous to the computation of the Lyapunov exponent in continuous systems.

Consider an ensemble of nodes with k inputs per node. Derrida and Pomeau use the annealed approximation in which the connections and node rules are randomly resampled at each time step and are hence uncorrelated and can be treated probabilistically. Each node is therefore statistically identical to every other node. If we prepare two nets of the same topology and rules but different initial values (overlapping on a proportion q of the sites) and then propagate them forwards one time step (redrawing the connections randomly as we do so), we can write down an expression for the iterated overlap

$$q(t+1) = q^K(t) + \frac{1}{2}\Big(1 - q^K(t)\Big)$$

the first term is due to the deterministic contribution to overlap, given by the probability that all k inputs to a node overlap in both cases, hence they all have the same inputs, hence they generate the same output. The second term is from random contributions to overlap, and the prefactor assumes that half of the time the two nets generate the same output value at the node under consideration. The family of curves thus generated for different k is shown below:



The line marked $H(t) = H(t')$ is the dividing line between order and chaos. It is clear that $k = 2$ lies directly on this line, and that higher k is in the chaotic regime and that lower k is in the ordered regime.

Section 3 Biased Nets

It will be essential for the conclusions of this paper to consider the dynamics of biased nets. A biased net is one in which the rule tables have a preponderance of zeroes or ones. Since the dynamics are unchanged under the operation of inversion (swapping zeroes for ones), we are free to call the proportion of ones in the rule table p_1. The overlap calculation follows the calculation above, except that the contribution from the random term is different[4]. If a node has one or more non-overlapping inputs, the contribution to the overlap at the next time step is the sum of the probabilities of both node configurations having a zero and both configurations having a one, giving a prefactor to the random term of

$\Delta q = p_1^2 + (1-p_1)^2$. This reduces to $1/2$ for $p_1 = 1/2$, reproducing our earlier result. We can now calculate the critical value of ρ for which the Derrida curve sits on the order/chaos border. If we write the iterated overlap equation in terms of the Hamming distance $x = 1 - q$ we have

$$x' = -\rho(1-x)^K + \rho$$

where we have defined $\rho = 1 - \left[p^2 + (1-p)^2\right]$ as the 'bias function'. The first and second derivatives yield

$$\frac{\partial x'}{\partial x} = K\rho(1-x)^{K-1}$$

and

$$\frac{\partial^2 x'}{\partial x^2} = -K(K-1)\rho(1-x)^{K-2}$$

If we observe that the second derivative is negative everywhere on the interval $[0,1]$ for $K \geq 1$, we can solve for the order/chaos border by setting the first derivative equal to one at the origin, yielding

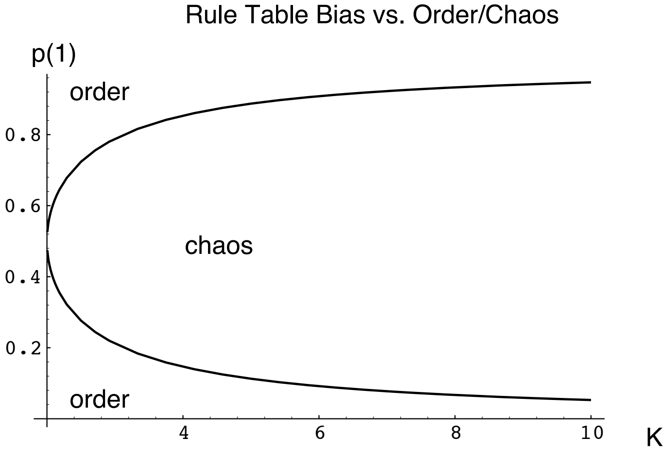
$$\rho = \frac{1}{K}$$

as the condition for the onset of discrete chaos. It is now possible to conclude that we can drive a net into orderly behavior by inducing bias in the rule table. This is intuitively reasonable when one considers the limiting case in which the rule table is all zeroes or all ones. In such a case, any two states converge on the same state in one step regardless of the value of k, driving the net strongly into the ordered regime. The equation for the bias away from $p_1 = p_0 = 1/2$ can be solved, yielding

$$p_{1,0}(K) = \frac{1 \pm \sqrt{1 - 2/K}}{2}$$

This function displays the expected symmetry about $p_1 = 1/2$ and is illustrated below.

1



The above analysis can be extended to mixed nets, nets which have nodes of differing input degree. Consider a weight vector $\vec{l}$, where $\sum_i l_i = 1.$ and the weight associated with in-degree K is l_K. The Derrida curve for such a mixed net is a weighted sum of the Derrida curve for individual K, and is given by

$$D\left(\vec{l}\cdot\vec{K}\right) = \sum_K l_K D(K) = \rho - \rho \sum_K l_K (1-x)^K$$

which is in general a polynomial of degree K_{max} with arbitrarily adjustable coefficients. If we take the first derivative at $x = 0$, however, we obtain

$$\frac{\partial x'}{\partial x}|_{x=0} = \rho \sum l_K K = \rho \langle K \rangle$$

,giving the same order/chaos condition for the expectation value of K as we had for a single value of K. This is a valid condition if the second derivative:

$$\frac{\partial^2 x'}{\partial x^2} = -\rho \sum_K l_K K(K-1)(1-x)^{K-2}$$

is everywhere negative, which is indeed so, as l_K is positive for all K.

Section 4 Perturbative Approach to Stability Analysis

One can also define the order/chaos boundary as the locus of parameter values for which a ‘test’ bit flip causes an expectation value of one more bit flip to occur.

Less than this critical value causes perturbations to die out, greater than this value causes the disturbance to grow to a size on the order of the size of the network. The following derivation closely parallels[11]. If we consider the act of flipping a bit, we must then calculate the expected number of other bits that will flip. If there are k inputs per node and the net is randomly wired, we can expect the probability of the out-degree m to be Poisson distributed when $N \gg K$:

$$p(K,m) = \frac{e^{-K}K}{m!}$$

For a given out-degree m, we can calculate the expectation value of the number of bits flipped as follows

$$\langle flips/m \rangle = \sum_{i=0}^{m} iP_m(i,\rho) = \sum_{i=0}^{m} i\rho^i(1-\rho^i)^{m-i}\binom{m}{i}$$

where ρ is the same as defined above and $P_m(i,\rho)$ is the probability of flipping i out of m spins given bias function ρ. If we convolve the above equation with the Poisson distribution of outputs, we have for the overall expectation value of spin flips

$$\langle flips \rangle = \sum_{i=0}^{\infty} e^{-K}\frac{K}{i!}\sum_{j=0}^{i} j\rho^j(1-\rho)^{i-j}$$

The $j = 0$ term does not contribute, so the second summation can be rewritten as

$$\rho i \sum_{j=1}^{i} \rho^{j-1}(1-\rho)^{i-j}\binom{i-1}{j-1} = \rho i$$

since the sum is equal to one (binomial theorem). The flip expectation value now reduces to

$$\langle flips \rangle = \rho\sum_{i=0}^{\infty} e^{-K}\frac{iK}{i!} = \rho K e^{-K}\sum_{i=1}^{\infty}\frac{K}{(i-1)!} = \rho K$$

Thus we expect the phase transition to occur at $\rho\langle K \rangle = 1$, the same result as before.

Section 5 Redundancy and Canalization

It has been widely observed in experimentally studied genetic networks that the Boolean nets which most closely approximate them have a property called *canalization*. This is the property that constrains the rule table such that one value of one input is sufficient to uniquely determine the output value of the entire node, regardless of the values of the other inputs. It is possible to have canalization on more than one input, a simple example of this being the *or* function. If so, this can be perceived as a kind of 'fail-safe' design in which redundancies exist to ensure that the desired output of the regulated node can be generated by more than a single combination of inputs. Canalization would be a natural way to design in robustness against noise and uncertainty. As such it is of general interest to the study of the reliability of large switching networks.

To develop some intuition regarding the behavior of statistical ensembles of canalizing nodes, consider the reduction of degrees of freedom caused by introducing redundancies into the system. This reduces the space of possible behaviors of the Boolean net, and therefore should drive nets into the ordered regime. We can study this effect analytically through the following means: Calculate the effect that introducing canalization has on the statistical structure of rule tables, and then observe the effect that this has on the bias function ρ. The change in ρ induced by the introduction of canalization can then be correlated to a change in position relative to the order/chaos axis on the Derrida plot. Since the Derrida plot is only a measure of "differential" (single-step) dynamics, certain global properties of the network unique to canalizing networks might be missed, but it serves as a useful first approximation.

To understand the effect of canalization on rule-table bias, consider the example of a node which canalyzes on two of its three inputs. Its rule table might look like the following (a number of permutations are possible) The output

Input 1	Input 2	Input 3	Output
0	0	0	A
0	0	1	A
0	1	0	A
0	1	1	A
1	0	0	*

Input 1	Input 2	Input 3	Output
1	0	1	*
1	1	0	A
1	1	1	A

'A' signifies either a zero or a one. A '*' signifies 'don't care', although this is somewhat constrained because we might accidentally canalyze on more than two inputs if we choose these values injudiciously. As the function is written, it canalyzes on the first input when that input has value zero and the second input when it has value one. As can be seen, a minimum of six out of eight output values have to be the same to canalyze on two inputs out of three. The rule table is now biased away from $\rho = 1/2$. In general, if we wish to canalyze on c inputs,

$$p_{(0\ or\ 1)} > 1 - 1/2^c$$

where the subscript of p is chosen such that it is the output value of the canalyzing inputs. If we assume that the entries marked by '*' are filled out with $p_{0,1} = 0.5$ (not exactly correct, but close), we can approximate the expected bias as

$$p_{0,1} \approx 1 - 1/2^{c+1}$$

This gives a bias function $\rho(c) = 1/2^c - 1/2^{2c+1}$. Since c appears in the exponent of the bias function and the condition for the order/chaos boundary is $\rho = 1/k$, we can conclude that there is a nonlinear dependence of the order/chaos boundary condition on the amount of canalization. If we are dealing with a net with mixed canalization, we replace ρ with

$$\langle \rho \rangle = \sum_{c=0}^{k} p(c)\rho(c)$$

where $\sum p(c) = 1$. In order to know where we are in the order/chaos plane, it is therefore necessary to know the *distribution* of canalization, not just the proportion of inputs which are canalizing. This implies that there exist more and less economical ways to build robustness into a highly connected switching network.

Section 6 Simulation Results

In order to understand the characteristics of Boolean nets more thoroughly, we have simulated their behavior computationally. The question arises as to what is simulating what, as digital computers are essentially large configurable Boolean circuits. Boolean nets can be characterized by many different parameters in addition to the Derrida curve and bit—flip perturbation dynamics discussed above. Since they are discrete dynamical systems, they must eventually revisit a state they've encountered before, thus engendering a loop or *attractor*, which can very in length from one (a fixed point) to 2^N. These attractors can be characterized by their size (what proportion of initial states create dynamics which terminate on this attractor), by their multiplicity per net, and by the length of the transients which occur before arriving at the attractors.

In his book, *The Origins of Order*[10], Stuart Kauffman discusses early simulation work on the dynamics of Boolean nets. Kauffman observed a sharply-defined qualitative and quantitative change in behavior between nets in the ordered and chaotic regimes. 'Chaotic' nets were characterized by an exponential increase in the number and length of attractors as a function of the size of the net, whereas 'ordered' nets had a weak (logarithmic) or nonexistent dependence of numbers and lengths of attractors on net size. . Chaotic behavior was observed for $k > 2$, and ordered behavior was observed for $k < 2$. Nets of $k = 2$ showed power-law behavior, with both lengths and numbers of attractors scaling as $\sqrt{N}$. This work was taken up again much more recently by Bhattacharjya and Liang[3], who studied the behavior of biased nets along the order/chaos boundary for a variety of k values utilizing much greater computational resources, seeking to characterize this boundary as a well-defined phase transition in the physics sense. This was inspired by theoretical and computational work of Bastolla and Parisi [1, 2] who showed that the entire order/chaos boundary was, modulo certain assumptions, a member of a single universaility class characterized by scaling laws.

Canalizing networks display power-law (square-root) behavior of attractor numbers and less than square-root power-law behavior of attractor lengths across a spectrum of canalization values, not just at the canalization values which cause the bias variable ρ to take on a value which puts the net at the phase transition in the Derrida sense. It has not yet been shown if this can be described in terms of a phase transition displaying analytically derivable scaling exponents, though work is in progress on this point. Even though a given choice of canalization implies a certain ρ, the reverse is not the case. Canalizing rules are a very particular subset of rules, and form an exponentially decaying fraction of all possible rules as a function of increasing k. Thus we cannot expect that all of the conclusions which apply to biased networks should necessarily apply to canalizing networks.

Section 7 Discussion

Even though logical networks have been a subject of study in electrical engineering for many decades, very little emphasis has been placed on characterizing their behaviors statistically. This is because the primary interest in constructing networks has been that of reverse engineering—given a desired output, construct the minimal circuit network which will give one that output. Interest in the statistics of networks has come more recently and from a biological direction. Modeling genetic regulatory networks with Boolean nets has been a fruitful approach to understanding genetic function. As soon as one begins to discuss genetics, issues of evolution, selection, and randomness come to the fore. Genetics deals with the evolution of populations and is thus inherently statistical. One is then led to ask questions about the characteristics of genetic regulatory networks which would be evolved by natural selection. This is also relevant to adaptive programming and control theory, as one wishes to "evolve" a computer program or, more specifically, a logical circuit which produces the desired output. Many problems are too complex to arrive at by deterministic means the minimal circuit which produces the desired result, hence the question becomes "Are there many more non-minimal circuits which will give the desired result?" If one does not require the minimal circuit, but instead wishes to select for higher robustness or some other characteristic, there are many instances in which the computational complexity required to construct the circuit becomes much less, since one is attempting to arrive at a *family* of logical realizations rather than a unique solution.

The implications of universal behavior near the Derrida boundary and the observation that canalizing networks cause this characteristic behavior to appear for a large spectrum of $\rho(c)$ implies that canalizing networks are robust. This means that a canalizing network will display 'phase-transition' type behavior even if the amount of canalization varies across a substantial spectrum, hence individual nodes can be modified without changing the length or number of attractors. This makes canalizing networks a good candidate for control networks in the presence of noise or misinformation. This is not surprising, given early indications that nature uses these networks in the architecture of genetic regulatory networks which control the development and maintenance of the most complex systems we know, namely living things. Genes must accomplish their tasks reliably in the presence of a noisy, complex environment. Boolean nets are an attempt at a digital realization of genetic control circuitry, and have many properties which would make them useful for complex control of man-made systems. They are parallel, networked, and display higher-order emergent organization, namely the structure due to attractors.

Section 8 Acknowledgments

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