Lyapunov Exponents in Random Boolean Networks

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\textbf{Abstract}

A new order parameter approximation to Random Boolean Networks (RBN) is introduced, based on the concept of Boolean derivative. A statistical argument involving an annealed approximation is used, allowing to measure the order parameter in terms of the statistical properties of a random matrix. Using the same formalism, a Lyapunov exponent is calculated, allowing to provide the onset of damage spreading through the network and how sensitive it is to minimal perturbations. Finally, the Lyapunov exponents are obtained by means of different approximations: through distance method and a discrete variant of the Wolf’s method for continuous systems.

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1 Introduction

Random Boolean networks (RBN), also called Kauffman nets [1-2], were originally formulated as a model of genetic nets. The computational and mathematical problems arising from continuous dynamical systems with a very high number of coupled non-linear equations lead to the introduction of RBN as an alternative approach. In this way, relevant statistical properties of RBN were derived [18]. This general analysis allowed to test several hypothesis concerning the large-scale organization of biological regulatory networks.

Recent studies in the field try to obtain a natural bridge between discrete and more biologically sensible, continuous networks [3]. In this vein for instance, a characteristic quantitative measure associated to continuous dynamical systems is the Lyapunov exponent $\lambda$ [4]. This parameter measures the degree of instability of continuous dynamical systems, and allows us to characterize the transition to chaos by measuring the pace at which initial conditions tend to diverge as the system evolves. Although Lyapunov exponents have been also derived (or estimated) for discrete systems (as cellular automata [5-8]) there is, as far as we know, no study about this quantity in RBN and related systems. To have a way to estimate Lyapunov exponents for RBN’s would thus establish a natural link between discrete and continuous systems.

The paper is organized as follows. First the RBN formalism and its order-disorder phase transition are introduced. Secondly, using the concept of the Boolean derivative [9] we propose a new order parameter for the RBN phase transition: the percent of 1’s in the Jacobian matrix that represents the Boolean derivative of the system. We then define a Lyapunov exponent for the RBN and compare our results with the distance method [11]. Finally, a second possible order parameter (the self-distance) is introduced. This will allow us, through a discrete analog of Wolf’s method for continuous systems, to reobtain an expression for the Lyapunov exponent consistent with that previously found.

2 Random Boolean Networks

A RBN is a discrete system involving $N$ units/automata with two possible states of a boolean variable $\{0, 1\}$. Each automaton is randomly connected with exactly $K$ neighbors. The state of each unit is updated by means of a Boolean function, also randomly chosen from the set of all the Boolean functions with $K$ binary arguments.
Figure 1: Example of RBN with $N = 3$ and $K = 2$. Left: we show the interaction graph and the corresponding rule-tables (Boolean functions) of each automata. Right: we show explicitly the transitions between global system states as flow diagrams.

Once the neighborhood and functions have been chosen they are fixed in time (i.e., a quenched set is used). The RBN exhibit a second order transition: for $K \leq 2$ a frozen (ordered) phase is observed, while for $K > 2$ a disordered phase sets in. A RBN is by definition a discrete ($N$ cells) deterministic system with a finite number of states ($\{0, 1\}$), and therefore periodic patterns are expected after a maximum of $2^N$ steps. Thus, if we follow strictly the standard definition of low-dimensional deterministic chaos, chaotic behavior is not possible in these systems. Taking this into account, we will define chaotic behavior here through damage spreading [12-14]: a phase will be chaotic if damage spreading takes place, i.e., if changes caused by transient flips of a single unit propagate and grow until they reach a size comparable to that of the system. Thus our disordered phase will be called chaotic phase, analogously to continuous systems.

Let us illustrate the RBN structure and dynamics with a simple example [2] which will be used below. Given a system with $N = 3$ automata with values: $x_1, x_2$ and $x_3$ and connectivity $K = 2$, the net is wired by choosing the input neighbors as indicated in figure 1.
The inputs have been represented in figure 1 as arrows that connect the automata and a simple directed graph is obtained. The state of the system at any time is an ordered array of bits, $X = (x_1, x_2, x_3)$, and the interactions between the automata are described by Boolean functions. In this example the Boolean functions have been randomly sampled from the set of $2^{2^2} = 16$ possible functions with $K = 2$ arguments:

1. For the automaton 1: $f_1(x_2, x_3)$ the function AND.
2. For the automaton 2: $f_2(x_1, x_3)$ the function OR.
3. For the automaton 3: $f_3(x_1, x_2)$ the function AND.

These functions are represented in figure 1 (left) by means of rule-tables (all possible inputs with their corresponding outputs). The system is updated synchronously. A possible temporal succession of states will describe a trajectory (orbit) of the system. In figure 1 (right) we represent all possible trajectories of the system as a flow diagram.

In early studies on RBN phase transitions the critical point was estimated through numerical simulations [1,2]. The critical connectivity $K = 2$ gave the transition order-chaos. Later on this transition point was analytically obtained by means of the so-called Derrida’s annealed approximation [6,11], also known as the distance method. Derrida developed a non-correlated (annealed) RBN model by randomizing the inputs and Boolean functions at each time step showing that, in the thermodynamic limit, the transition point is the same in the quenched and the annealed systems. This approach can be extended to a continuous (average) $K$-valued and biased RBN [15,16]. In biased RBN’s the Boolean functions are chosen with a bias $p$, that is: the mean percentage of 1’s in the output is $p$. From two replicas with an initial normalized Hamming distance, $d(t = 0)$, we can derive the equation for the evolution of $d(t)$:

$$d(t + 1) = 2p(1 - p)\left\{1 - [1 - d(t)]^K\right\}$$

(1)

At the frozen phase, the fixed point $d^* = 0$ is stable (i.e. the two initial configurations become identical as they evolve). In the chaotic phase however $d^* = 0$ is unstable, and two initially close configurations diverge to a finite distance. The
critical curve on the parameter space \((p, K)\) is:

\[
K = \frac{1}{2p(1 - p)} \tag{2}
\]

In figure (2) the phase space is shown. On a constant connectivity line (here \(K = 3\)) three different runs of the system have been chosen for a RBN with \(K = 3\) and \(N = 50\). For \(p = 1/2\) equation (2) reduces to the standard RBN problem [2]. Fig. 3 shows with continuous lines the evolution of \(d(t)\) towards the theoretical fixed point \(d^*\) (obtained from iteration of Eq. (1) with \(K = 3\)), \(p\) changing for each line. The values chosen for \(p\) in this figure match the dots on the dashed \(K = 3\) line in Fig 2. The squares represent the average result of 100 runs with two different replicas each. Here we used \(N = 10,000\) automata, and the initial distance is \(d(0) = 0.5\).
Figure 3: Continuous lines: dynamical evolution of the distance between two identical replicas of RBN with initial distance of $= .5$ for $K = 3$ and different values of the bias $p$ through the iteration of equation (1). Squares (points): numerical averages of the distance (auto-distance) for 100 experiments with RBN of size $N = 10,000$, $K = 3$ and the bias showed.

Observe that $d^*$ acts as an order parameter. In fig. 4 the continuous line represents the stationary values obtained by iteration of equation (1) for changing $p$. Again, the squares represent the numerical values obtained by averaging over 100 runs with two different replicas of RBN each, with size $N = 10,000$, and $d(0) = 0.50$.

In [17], Flyvbjerg defined a different order parameter: he defined the stable core at time $t$ as the set of units that have reached stable values at time $t$ (that is, remain unaltered in value for $t' \geq t$ and are independent of the initial conditions). Let us define $s(t)$ as the relative size of the stable core at time $t$, i.e. $s(t)N$ is its absolute value. Then the asymptotic stable core size, $s^* = \lim_{t \to \infty} s(t)$, is an order parameter for the order-chaos transition in RBN’s. Flyvbjerg obtains an iterated equation for the stable core:

$$s(t + 1) = \sum_{i=0}^{K} \binom{K}{i} s(t)^{K-i}(1 - s(t))^i p_i$$

where $p_i$ is the probability that the Boolean function output be independent of a
certain number $i$ of inputs. For the Boolean functions with bias $p$ it yields $p_i = p^{2^i} + (1 - p)^{2^i}$. By analyzing the stability of Eq. (3), he found out an identical transition curve than the one given by Eq. (2). In Fig. 4 (Short-dashed line) we represent this order parameter as $1 - s^*$.  

### 3 Boolean Derivatives in RBN

We will now define a RBN in a more formal way. A RBN is a discrete dynamical system whose evolution is given by the iteration of a global mapping:

$$ F_{K,p} : \{0,1\}^N \mapsto \{0,1\}^N $$

(4)

where $F_{K,p} = (f_1, f_2, \ldots, f_N)$, and with each $f_i$ being a Boolean function of $K$ arguments and bias $p$ (mean percentage of ones in the outputs):

$$ f_{K,p} : \{0,1\}^K \mapsto \{0,1\}_p $$

(5)

A given configuration at time $t$, $x(t)$, is updated synchronously, i.e.:

$$ x^{t+1} = F_{K,p}(x^t) $$

(6)

where each automata with $x^t_i \in \{0,1\}$ is updated by mean of its corresponding Boolean function:

$$ x^{t+1}_i = f_i(x^t_1, x^t_2, \ldots, x^t_K) $$

(7)

For a given $F_{K,p}(t)$ we define its $N \times N$ Jacobian matrix, $F'_{K,p}(t)$, as that whose elements are given by the Boolean derivatives at time $t$ [9]:

$$ F'_{i,j}(t) = \frac{\partial f_i(x^t_i, x^t_j, \ldots, x^t_K)}{\partial x^t_j} = \left\{ \begin{array}{ll} f_i(x^t_1, \ldots, x^t_j, \ldots, x^t_K) \oplus f_i(x^t_1, \ldots, x^t_j, \ldots, x^t_K) & \text{if } x_j \text{ inputs } x_i \\ 0 & \text{otherwise} \end{array} \right. $$

(8)

Here $\oplus$ is the exclusive OR (XOR) Boolean operation and $\bar{x}_j = x_j \oplus 1$ (i.e., the binary complement of $x_j$). From the point of view of damage spreading [7], we can see that $F'_{i,j}(t) = 1$ if a flip in the input $x^t_j$ at time $t$ generates a change of $x^{t+1}_i$ to $\bar{x}^{t+1}_i$ in step $t + 1$. In others words, the function spreads the damage. Otherwise, $F'_{i,j}(t) = 0$, and no damage is spread. Note that $F'_{K,p}(t)$ depends on $t$ because its value depends on the concrete configuration at time $t$.

Continuing with our example (see Fig 1), let us suppose that, at $t$, the state of the system is $x(t) = (1, 0, 1)$. If we compute the $3 \times 3$ Jacobian matrix $F'_{2,0,4}(t)$ its components will be:

$$ F'_{1,1} = 0 $$
\[ F'_{1,2} = f_1(0, 1) \oplus f_1(1, 1) = 0 \oplus 1 = 1 \]
\[ F'_{1,3} = f_1(0, 1) \oplus f_1(0, 0) = 0 \oplus 0 = 0 \]
\[ F'_{2,1} = f_2(1, 1) \oplus f_2(0, 1) = 1 \oplus 1 = 0 \]
\[ F'_{2,2} = 0 \]
\[ F'_{2,3} = f_2(1, 1) \oplus f_2(1, 0) = 1 \oplus 1 = 0 \]
\[ F'_{3,1} = f_3(1, 0) \oplus f_3(0, 0) = 1 \oplus 0 = 1 \]
\[ F'_{3,2} = f_3(1, 0) \oplus f_1(1, 1) = 1 \oplus 1 = 0 \]
\[ F'_{3,3} = 0 \]

Thus the Jacobian matrix is:

\[
F'(t) = \begin{pmatrix}
0 & 1 & 0 \\
0 & 0 & 0 \\
1 & 0 & 0
\end{pmatrix}
\]

Analogously to the continuous dynamical systems counterpart we take a configuration state \( x(t) \) and a slight perturbation of it \( y(t) \). A perturbed configuration is a new configuration at a non-zero (but otherwise small) Hamming distance from the original one. In fact, it is possible to define the perturbation \( d(t) \) such that:

\[ y(t) = x(t) \oplus d(t) \quad (9) \]

where the normalized Hamming distance between \( x(t) \) and \( y(t) \) is

\[ |d(t)| = \frac{1}{N} \sum_{i=1}^{N} d_i^t \quad (10) \]

In our example, we have \( x(t) = (1, 0, 1) \) and we will take as the perturbed configuration \( y(t) = (0, 0, 1) \). Thus:

\[ y(t) = (0, 0, 1) = x(t) \oplus d(t) = (1, 0, 1) \oplus (1, 0, 0) = (0, 0, 1) \]

Note that we have the minimum possible perturbation

\[ |d(t)| = \frac{1}{3}(0 + 0 + 1) = 1 \]

and that we can write the perturbation as

\[ d(t) = x(t) \oplus y(t) \quad (11) \]
Thus, in our example:

\[(1, 0, 1) \oplus (0, 0, 1) = (1 \oplus 0, 0 \oplus 0, 1 \oplus 1) = (1, 0, 0)\]

Now we are ready to find the approximate evolution of the perturbation, as it is done in continuous systems. Using the equations (6), (9), (11), and using the Jacobian matrix to make a linear approximation, we have:

\[
d(t + 1) = y(t + 1) \oplus x(t + 1) = F(y(t)) \oplus F(x(t)) =
\]

\[
= F(x(t) \oplus d(t)) \oplus F(x(t)) \approx F'(x(t)) \oplus d(t)
\]

where we define \(\oplus\) as:

\[
F'(x(t)) \oplus d(t) = \Theta(F'(x(t)) \cdot d(t))
\]

and the vector \(\Theta(x) = (\Theta(x_1), ..., \Theta(x_i), ..., \Theta(x_N))\) having standard Heaviside functions as components:

\[
\Theta(x_i) = \begin{cases} 
0 & \text{if } x_i = 0 \\
1 & \text{otherwise}
\end{cases}
\]

Thus, in our example we have:

\[
d(t + 1) = \begin{pmatrix} 0 & 1 & 0 \\
0 & 0 & 0 \\
1 & 0 & 0 \end{pmatrix} \oplus \begin{pmatrix} 1 \\
0 \\
0 \end{pmatrix} = \Theta \left[ \begin{pmatrix} 0 & 1 & 0 \\
0 & 0 & 0 \\
1 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\
0 \\
0 \end{pmatrix} \right] = \begin{pmatrix} 0 \\
0 \\
1 \end{pmatrix}
\]

4 Jacobi matrix and a new order parameter

Our aim is now to present a new order parameter based on the Jacobian matrix of Boolean derivatives, as previously defined. The dynamical equation (12) can be iterated in \(t\) to determine the evolution of the perturbation with two possible outcomes: as \(t \to \infty\) either the initial perturbation at \(t = 0\) will tend to disappear, \(|d(\infty)| \to 0\), or it will reach a finite value. The behavior of the perturbation will be determined by the successive products of the Jacobian matrix. Thus, we define:

\[
M(t) = F'(x(0)) \oplus F'(x(1)) \oplus \ldots \oplus F'(x(t))
\]

If the number of 1’s in the Jacobian matrix is small the product in (15) will converge to a matrix \(M^*\) formed only by zeros, and any initial perturbation will disappear. We will now attempt to construct an iterated equation for the evolution of the fraction of zeroes in the matrix \(M\) using a mean field approach. If our system has a
connectivity $K$ and bias $p$, we substitute at each time step (mean field approximation) the deterministic matrix $F'(t)$ by a random matrix $\Omega$ of the same form (at most $K$ 1’s at each row). The probability for a randomly generated Boolean function to have a Boolean derivative with value one $F'_{i,j} = 1$ is equal to the probability that a flip in its input $x_{ij}$ generates a change in its output $x_i$ to $\bar{x}_i$. We have two possibilities: the output has a value 1 and changes to 0, with probability $p(1 - p)$ and the symmetric case with probability $(1 - p)p$. Thus the mean number of 1’s per row is $2p(1 - p)K$. At each time step, $t + 1$, we multiply $M(t)$ by a random matrix with a mean number $2p(1 - p)K$ of 1’s per row, i.e. $M(t + 1) = \Omega M(t)$.

This approach is clearly analogous to the distance method [11], where the Boolean functions and inputs of the system vary at random at each time step. So, if we assume that at a time step $t$ the matrix $M(t)$ has a percentage $q_t$ of zeros, in the
Figure 5: Open circles: values of Lyapunov exponent define from equation (27) with 

\[ K = 3 \]  and different \( p \) varying. Filled circles: numerical estimation of the Lyapunov exponent by avering the expansion rate (18) calculate through the distance equation (1) with \( T = 10 \) in equation (19).

In the thermodynamic limit, the \( q_{t+1} \) will be:

\[
q_{t+1} = \lim_{N \to \infty} \left[ 1 - \frac{2p(1-p)K}{N} (1 - q_t) \right]^N = e^{-(1-q^*)2p(1-p)K}
\]  

(16)

Where \( 2p(1-p)K/N \) is the probability that \( \Omega_{ij} = 1 \) and \( 1 - q_t \) is the probability that \( M_{jk} = 1 \). By analyzing the stability of (16) around \( q^* = 1 \) (i.e. all the elements of \( \mathbf{M}^* \) are zero), we find out the critical transition curve, given again by

\[
\left. \frac{\partial q_{t+1}}{\partial q_t} \right|_{q^* = 1} = K^2 p(1-p) < 1
\]  

(17)

in agreement with previous results [7,11,17]. In Fig. 4 we indicate (long-dashed line) this order parameter as \( 1 - q^* \) (the percentage of 1’s in the infinite product of Jacobians) for \( K = 3 \).
5 Lyapunov exponents and RBN

In the previous section, we have introduced the Boolean derivative $F'(x(t))$, in analogy with the standard continuous counterpart. This operator was then used in order to define the discrete map (12) which gives us the time evolution of the perturbation $d(t)$. Using this definition, an expansion rate of perturbations for RBN can be easily defined. The damage expansion rate will be [6]:

$$\eta(t) = \frac{|d(t + 1)|}{|d(t)|}$$

(18)

This allows us to define a Lyapunov exponent:

$$\lambda(T) = \frac{1}{T} \sum_{t=1}^{T} \log \eta(t)$$

(19)

Under the previous approach we can determine the mean damage expansion rate $\bar{\eta}$ which will be given by (here $\langle ... \rangle$ are time averages):

$$\bar{\eta} = \langle \eta(t) \rangle$$

(20)

$$= \langle \frac{|d(t + 1)|}{|d(t)|} \rangle$$

(21)

$$= \langle \frac{|F'(x(t)) \circ d(t)|}{|d(t)|} \rangle$$

(22)

such quantity can be easily computed by analyzing the statistical behavior of $|F'(x(t)) \circ d(t)|$. This can be done by assuming that, on mean field grounds, $F'(x(t))$ can be replaced by a random matrix $\Omega$. The previous average (19) can then be estimated by considering the percent of 1’s in $d(t)$ (i.e. $|d(t)|/N$) and the same quantity for $t+1$ (i.e. $|d(t+1)|/N$). We have:

$$\frac{|d(t + 1)|}{N} = 1 - \left[ 1 - \frac{2p(1-p)K |d(t)|}{N} \right] N$$

(23)

Now, in the thermodynamic limit ($N \to \infty$) we get:

$$\bar{\eta} = 1 - \exp \left[ \frac{-2p(1-p)K |d(t)|}{|d(t)|} \right] N \approx 2p(1-p)K$$

(24)
This result could be derived in another way. By defining the normalized Hamming distance of a Boolean matrix $\Omega$ as:

$$|\Omega| = \frac{1}{N^2} \sum_{i,j}^{N} \Omega_{ij}$$

where $\Omega_{ij} \in \{0, 1\}$. We have:

$$\bar{\eta}(t) = \frac{|\Omega \odot d(t)|}{|d(t)|} = \frac{|\Omega|}{|d(t)|} = |\Omega| = 2p(1 - p)K$$

From (19) and (24), the Lyapunov exponent will be:

$$\lambda = \log[2p(1 - p)K]$$

which determine the two classical regimes: $\lambda < 0$ (order) and $\lambda > 0$ (chaos) with the marginal case $\lambda = 0$. In agreement with the boundary phase transition (2).

### 6 Distance and Wolf’s method

This result has been consistent with the equation of distance evolution (1). If we interpret one of the replicas in the distance method as a perturbation of the another replica, the expansion in the time $t$ of the perturbation will be:

$$\eta(t) = \frac{|d_{12}(t + 1)|}{|d_{12}(t)|} = \frac{2p(1 - p)\{1 - [1 - d(t)]^K\}}{d(t)}$$

and approximating for small $d(t)$:

$$(1 - d(t))^K \approx 1 - Kd(t)$$

we have:

$$\eta(t) \approx 2p(1 - p)K$$

i.e an expansion rate identically to (24).

This approximation is prove sufficiently good as we show in fig. 5. The values of Lyapunov exponents through equation (27) with $K = 3$ and $p$ varying and there equivalents values calculated through the distance equation (1) coincides.

There are different methods to compute Lyapunov exponents in continuous systems [4]. In order to show consistence we will demonstrate that it is possible compute Lyapunov exponents from self-distance in consonance with the previous result.
The Wolf’s method is used to numerically estimate Lyapunov exponents from time series. In short, the method is as follow: get two points of the time series, let us say $X(t_1)$ and $X(t_2)$ and compute their relative distance: $|X(t_2) - X(t_1)|$. Assume that $|X(t_2) - X(t_1)| < \epsilon$, being $\epsilon > 0$ very small. Next, compute the distance after $T$ steps, i.e: $|X(t_2 + T) - X(t_1 + T)|$. This time $T$ is a fraction of the characteristic period or is defined in terms of the autocorrelation function. Repeating for $n$ pairs of points and averaging, we obtain an estimation of the Lyapunov exponent:

$$\lambda = \frac{1}{nT} \sum_{t_2 \neq t_1}^{n} \log \frac{|X(t_2 + T) - X(t_1 + T)|}{|X(t_2) - X(t_1)|} \quad (31)$$

For RBN, we can write an equation for the normalized Hamming distance between successive time steps in our system, i.e. the self-distance: $d_{t,t-1}$. It easy to see that the self-distance is a new order parameter. This is a consequence of the combination of the distance method and the stable core.

The iterated equation for the self-distance is:

$$d_{t+1,t} = 2p(1-p)[1 - (1 - d_{t,t-1})^K] \quad (32)$$

Wich formally is equivalent to equation (1) but different conceptually. The self-distance, as the stable core, does not require annealed replicas (as the distance method), and is computationally more easily to determine. In fig. 3-4 the numerical values of self-distance (points) are calculated in similar way that the distance (squares) with a very good agreement.

If we approximate linearly close to the fixed point $d^* = 0$, the function becomes:

$$d_{t+1,t} = 2p(1-p)Kd_{t,t-1} \quad (33)$$

The iterated equation now is resoluble:

$$d_{t+T,t} = [2p(1-p)K]^Td_{t,t-1} \quad (34)$$

Thus, we have:

$$\frac{d_{t_2+T} - d_{t_1+T}}{d_{t_2} - d_{t_1}} = [K2p(1-p)]^T$$

i. e. a constant value that, after introduced in the sum of (31), gives the Lyapunov exponents (27).
7 Summary

In this paper we have analyzed a new order parameter for RBN in terms of a $\Omega$-random matrix approach. Our order parameter deals with the percent of non-zero elements that is obtained from the limit $\lim_{t \to \infty} \Omega^t$. It is shown that the order parameter describes a (second order) phase transition at a critical point consistent with other previous analyses.

An immediate extension of the Boolean derivative approach is the construction of a measure for the damage expansion rate, $\eta(t)$ that gives a quantitative characterization of how small perturbations propagate through the network. It has been shown that $\eta(t)$ provides a consistent measure of such sensitivity to spin flips. The time average over the Boolean products of the Jacobi matrix on the distance vectors can be successfully translated to a simple annealed method where only the statistical properties of the random matrix $\Omega$ matter.

We also have calculated the Lyapunov exponents through the distance method. And we propose a new order parameter: the self-distance. This quantity opens the possibility of defining the Lyapunov exponent in a discrete system in analogy with the Wolf’s method for continuous systems and the result is in agreement with the previously obtained.

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