On the Relationship between Local Rewiring Rules and Stationary Out-degree Distributions in Adaptive Random Boolean Network Models

Taichi Haruna\textsuperscript{1} and Sayaka Tanaka\textsuperscript{1}

\textsuperscript{1}Department of Earth & Planetary Sciences, Graduate School of Science, Kobe University, 1-1, Rokkodaicho, Nada, Kobe 657-8501, Japan
tharuna@penguin.kobe-u.ac.jp

Abstract

We discuss the relationship between local rewiring rules and stationary out-degree distributions in adaptive random Boolean network models that evolve toward criticality. We derive a theoretical formula for the relationship via a master equation approach. The theoretical result is shown to agree well with numerical simulation in three representative cases.

Introduction

Coupling between structural change of a network and dynamics on it is important to understand functioning of complex systems. Many models have been proposed to capture various types of couplings so far. They are called adaptive networks (Gross and Blasius, 2008; Gross and Sayama, 2009). One interesting type of the adaptive network model is the one in which network topology evolves toward dynamical criticality by a local rewiring rule. Several adaptive network models of this type have been studied numerically so far, for example, extremal dynamics on random networks (Christensen et al., 1998), random threshold networks (Bornholdt and Rohlf, 2000), neural networks (Bornholdt and Röhl, 2003; Meisel and Gross, 2009) and random Boolean networks (Liu and Bassler, 2006).

Random Boolean network (RBN) is a model of gene regulation networks (Kauffman, 1969, 1993). It has been shown that RBN exhibits a continuous phase transition from ordered to chaotic dynamics by a mean-field approximation (Derrida and Pomeau, 1986; Luque and Solé, 1997). In recent years, several approaches to map real-world networks to RBN have been proposed and shown that real-world networks are working close to criticality (Rämö et al., 2006; Balleza et al., 2008; Nykter et al., 2008). Biological significance of criticality has been also discussed: balance between robustness and evolvability (Aldana et al., 2007) and maximum information coordination (Ribeiro et al., 2008).

An RBN consists of a set of nodes connected via regulatory relationships represented as Boolean functions. Let the number of nodes be $N$ and the in-degree of node $i$ $k_i$. Each node can take two values 0 and 1 corresponding to off and on of a gene, respectively. For each node $i$, a random Boolean function $f_i : \{0, 1\}^{k_i} \rightarrow \{0, 1\}$ is chosen. For each input $x \in \{0, 1\}^{k_i}$, the output of $f_i(x)$ is determined to be 1 with probability $p$ and 0 with probability $1 - p$, where $0 \leq p \leq 1$ is a parameter. Here, we consider the standard case $p = 0.5$. The value of each node is updated by a given random Boolean function. For the time evolution of the whole system, we consider the classical synchronous updating scheme. Namely, we assume the existence of a global clock $t$ and all nodes are updated synchronously. Let $x_i(t)$ be the value of node $i$ at time step $t$. The state of the whole system is defined as $x(t) = (x_1(t), \ldots, x_N(t))$. In the limit of large $N$, the dynamics of RBN is ordered if $z < \frac{1}{2p(1-p)}$, critical if $z = \frac{1}{2p(1-p)}$ and chaotic otherwise (Derrida and Pomeau, 1986; Luque and Solé, 1997), where $z$ is the average in-degree of the underlying network of the RBN. When $p = 0.5$, the critical average in-degree is $z_c = 2$.

In this paper, we focus on adaptive random Boolean network models and discuss the relationship between local rewiring rules and the stationary out-degree distributions (Liu and Bassler, 2006). Real-world gene regulation networks have heavy-tailed out-degree distributions (Liu and Bassler, 2006). It is interesting problem whether we can reproduce this feature by an adaptive random Boolean network model that evolves toward criticality. (Liu and Bassler, 2006) reported that the stationary out-degree distribution is wider than the stationary Poisson-like in-degree distribution in their numerical simulation. However, its actual form is unknown. (MacArthur et al., 2010) studied a different type of adaptive network model that evolves toward criticality with a stationary heavy-tailed degree distribution. However, its mechanism is unclear. Here, we extend the model proposed by (Liu and Bassler, 2006) and obtain a theoretical expression for the relationship via a master equation approach. We also consider a new adaptive network model whose local rewiring rule is governed by local information transfer to examine whether our theoretical treatment is sensitive to the detail of local rewiring rules or not. We show that in both adaptive network models our theoretical result agrees well with numerical simulation for three representative cases: Poisson, exponential and truncated power law
stationary out-degree distributions.

This paper is organized as follows. In section 2, we review two adaptive random Boolean network models considered in this paper. In section 3, we present the formula relating local rewiring rules and stationary out-degree distributions and compare it with numerical simulation. We derive it in Appendix. In section 4, we discuss meaning of the result and connection with real-world gene regulation network topology.

Adaptive network models

In this section, we introduce two adaptive random Boolean network models. The first one is an extension of the model proposed and numerically investigated by (Liu and Bassler, 2006). The second one is our own new model.

A model based on activity

The basic idea of the evolutionary rule in this model is active nodes tend to lose links, static nodes tend to get links (Bornholdt and Rohlf, 2000). After the dynamics of an RBN falls onto an attractor, a node is defined to be active if it changes its value on the attractor at least once. Otherwise, the node is static (Bornholdt and Rohlf, 2000). After the dynamics of an RBN falls into a dynamical attractor is reached. In the chaotic phase, it is hard to find an attractor in a realistic number of time steps. To cope with this problem, we follow the procedure adopted in (Liu and Bassler, 2006). We set the maximum attractor period \( T_{\text{max}} \) which we try to find. If no attractor is found in the first \( 2T_{\text{max}} + T' \) time steps, we regard the last \( T_{\text{max}} \) steps as an attractor. Here, we take \( T_{\text{max}} = 1000 \) and \( T' = 100 \) for efficient numerical simulation. It seems that the value of \( T_{\text{max}} \) does not affect the result of numerical simulation as long as it is sufficiently large. Indeed, we checked that \( T_{\text{max}} = 500 \) also reproduces the essentially the same results.

Let \( T' \) be the period of the attractor.

(iii) A node \( i \) is randomly chosen. Calculate its average activity \( A(i) \) over the attractor:

\[
A(i) = \frac{1}{T'} \sum_{t=0}^{T'-1} x_i(t) \tag{1}
\]

where we assume that the attractor is reached at least after \( T' \) time steps. If \( 0 < A(i) < 1 \), then the node is called active. Otherwise, it is called static.

(iv) If chosen node \( i \) is active, then one of its incoming links is removed randomly. If it is static, then it gains a new incoming link. The source node of a new link is chosen by following a probability distribution depending on the out-degree of nodes.

(v) Boolean functions are randomly regenerated. Here, we use the method called annealed model in (Liu and Bassler, 2006): a new Boolean function is generated randomly for every node.

(vi) Go back to step (ii).

The time scale of network topology change (one cycle of step (ii) to step (v)) is called epoch. (Liu and Bassler, 2006) numerically shows that this evolutionary algorithm with the uniform probability distribution in step (iv) drives RBN toward criticality.

A model based on local information transfer

The local rewiring rule of this model depends on information transfer associated with links. To quantify information transfer, we use local transfer entropy (Lizier et al., 2008). Transfer entropy is a measure of the direction and magnitude of information transfer between two stationary stochastic processes (Schreiber, 2000). Let \( X, Y \) be stationary stochastic processes. The transfer entropy from \( Y \) to \( X \) is

\[
T_{Y \rightarrow X} = \sum_{x(t^{(i)}),y(t^{(l)})} p(x(t+1)|x(t^{(k)}),y(t^{(l)}) \times \log_2 \frac{p(x(t+1)|x(t^{(k)})}{p(x(t+1)|x(t^{(l)})}, \tag{2}
\]

where \( x(t^{(i)}) \) and \( y(t^{(l)}) \) are values of \( X \) and \( Y \) at time \( t \), respectively, \( x(t^{(k)}) = (x(t), x(t-1), \ldots, x(t-k+1)) \) and \( y(t^{(l)}) = (y(t), y(t-1), \ldots, y(t-l+1)) \). Namely, the amount of information transfer from \( Y \) to \( X \) is quantified as the reduction of uncertainty to predict the future value of \( X \) from the present and past values of itself when one knows the present and past values of \( Y \). In the following, we only consider the case \( k = l = 1 \).

The local transfer entropy considers the log-ratio at the right hand side of (2). (Lizier et al., 2008) shows that the local transfer entropy works as a filter detecting coherent structures in complex spatiotemporal dynamics. Since the log-ratio can take a negative value, we can define misleading information transfer associated with links. To quantify information transfer for information transfer quantification (Lizier et al., 2008).

Consider a node \( i \) in an RBN and neighboring nodes \( j_1, j_2, \ldots, j_k \), that have a link to \( i \). The local transfer entropy from node \( j_m \) to \( i \) at time \( t \) is defined by

\[
lte(j_m \rightarrow i, t) = \log_2 \frac{p(x_i(t+1)|x_i(t),x_{j_m}(t))}{p(x_i(t+1)|x_{j_m}(t))}, \tag{3}
\]

where the conditional probabilities at the right hand side are calculated from the frequency of each tuple of values from the all pairs \((i, j_n), n = 1, 2, \ldots, k\) over the attractor to which the RBN dynamics reaches.

The idea for the evolutionary algorithm based on local information transfer is links with misleading information transfer should be deleted. Here, we implement this idea by
replacing steps (iii) and (iv) in the model based on activity by the following (iii') and (iv').

(iii') Choose a node \(i\) and a time \(T \leq t < T + 1\) randomly. Calculate the local transfer entropy \(l(t) \to i, t\) for all \(m = 1, 2, \cdots, k_i\).

(iv') If there is at least one link such that \(l(t) \to i, t\) \(< 0\), then the link with the smallest value of the local transfer entropy is deleted. If there are multiple such links, then one of them is chosen randomly and is deleted. If \(l(t) \to i, t\) \(\geq 0\) for all \(m = 1, 2, \cdots, k_i\), then node \(i\) gets a new incoming link. The source node of a new link is chosen by following a probability distribution depending on the out-degree of nodes.

We numerically check that the model based on the local transfer entropy evolves toward criticality. Fig. 1 shows that time evolution of average in-degree for different \(k_0\) values converges to a common value slightly above 3. Here, we adopt the uniform random choice of the source node of a newly added link at step (iv'). The deviation from the critical value 2 is rather large because of the finite size effect \((N = 30)\). Fig. 2 shows that the converged value of average in-degree approaches to the critical value 2 as \(N\) becomes larger. Indeed, it approaches algebraically to the criticality as we will see in next section (See Fig. 5).

Average in-degree evolves toward criticality in both adaptive RBN models. However, they have different stationary in-degree distributions as one can see in Fig. 3. On one hand, the stationary in-degree distribution for the model based on activity can be fitted by the Poisson distribution for all three link addition rules considered in next section. On the other hand, the width of that for the model based on local information transfer is strictly narrower than the Poisson distribution with the same average in-degree due to different local rewiring rules from those in the activity-based model.

**Main result**

In this section, we present the formula relating local rewiring rules and stationary out-degree distributions. The theoretical result is tested against numerical simulation. The formula is derived in Appendix.

In the link addition part of the evolutionary algorithms described in section 2, the source node of a newly added link is chosen by following a probability distribution depending on the out-degree of nodes. Let \(\sigma_{+, l}(e)\) be the probability that a particular node with out-degree \(l\) is chosen as the source of a new link given that the number of link increases at epoch \(e\). In Appendix, we derive the following equation by analyzing the master equation describing time evolution of the out-degree distribution under the assumption that we can ignore the structure of networks except their degree distributions in the limit of large \(N\):

\[
\sigma_{+, l}^* = \frac{l + 1}{N z_s} \frac{P_{out}^\sigma(l + 1)}{P_{out}^\sigma(l)},
\]

where \(\sigma_{+, l}^* = \lim_{e \to \infty} \sigma_{+, l}(e)\), \(z_s\) is the stationary average in-degree and \(P_{out}^\sigma(l)\) is the stationary out-degree distribution. By (4), we can predict the link addition algorithm which produces the stationary out-degree distribution satisfying \(P_{out}^\sigma(l) = P(l)\) for any given probability distribution \(P(l)\) with \(\sum_{l=0}^{\infty} l P(l) = z_s\). Here, we study three representative cases.

**Example 1 (Poisson distribution)** If \(P(l) = \frac{e^{-z_s}}{z_s^l l!}\), then \(\frac{P(l + 1)}{P(l)} = \frac{z_s}{l + 1}\). It follows that \(\sigma_{+, l}^* = \frac{1}{N}\) by (4). Thus, we expect the stationary Poisson out-degree distribution when we choose the source node of a newly added link uniformly at random.

**Example 2 (Exponential distribution)** If \(P(l) = (1 - e^{-1/\kappa}) e^{-l/\kappa}\), where \(\kappa = 1/\ln(1 + 1/z_s)\), then
Figure 3: Stationary in-degree distributions for the two adaptive network models with different link addition rules introduced in section 2. (a) Results for the model based on activity. (b) Results for the model based on local information transfer. For every case, $N = 200$, $k_0 = 4$ and the numerical stationary in-degree distribution is obtained by averaging in-degree distributions over 10000 epochs after 10000 initial transient epochs for a single trial. For reference, Poisson distribution with the same average degree is plotted for each case. Legends indicate different link addition algorithms described in section 3.

We compare the numerical stationary out-degree distributions with the theoretical ones for both models of adaptive RBN in Fig. 4. In every case, the theoretical line agrees well with the numerical result. Fig. 5 shows that the stationary average in-degree approaches algebraically to the critical value 2 as the system size $N$ increases irrespective of models and link addition rules though the speed of convergence is case-by-case. These results suggest that we can control the stationary out-degree distribution by (4) while keeping evolution toward criticality.

**Discussion**

In this paper, we have shown that we can control the stationary out-degree distribution of two adaptive RBN models that evolve toward criticality by modifying the link addition part of the local rewiring rule. Only the information of neighboring nodes that have a link to a node to be removed is used for the link deletion part of the rule. In this sense, the link deletion part is informationally local. On the oth-
er hand, the link addition part is informationally global: it inevitably needs global information because the source node of a newly added link is chosen from the set of all nodes in the whole system although the resulting structural change of network topology is local. Thus, there is asymmetry between the link deletion part and the link addition part in terms of information used. Our result indicates that evolution toward criticality can be achieved irrespective of the form of informationally global link addition part.

It has been suggested that real-world gene regulation networks have heavy-tailed out-degree distributions (Aldana et al., 2007). Assuming that the local rewiring rule studied in this paper is a good approximation to realistic network evolutionary process, the emergence of heavy-tailed out-degree distributions in real-world gene regulation networks cannot be directly associated with evolution toward dynamical criticality. Rather, it could be a consequence of an unknown macroscopic constraint. Some models that evolve toward criticality and also generate a heavy-tailed degree distribution have been proposed so far (MacArthur et al., 2010; Torres-Sosa et al., 2012). In these models, mechanism to generate a heavy-tailed degree distribution would be involved implicitly in a whole evolutionary rule that takes into account global properties of the system. In contrast, the mechanism related to evolution toward criticality and that generates a given out-degree distribution can be separated explicitly in the adaptive network models studied in this paper.

If a macroscopic constraint forces a specific form of stationary out-degree distribution, then the underlying local rewiring rule is uniquely selected via (4). What macroscopic constraints can give rise to heavy-tailed out-degree distributions found in real-world gene regulation networks? Answering this question is out of the scope of the present paper and we leave it for future work.

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Appendix

In this Appendix, we derive equation (4).

Let $p_k$ be the probability that a chosen node with in-degree $k$ gets a new incoming link. The time evolution of in-degree distribution $P_{\text{in}}(k,e)$ is described by the master equation $P_{\text{in}}(k,e+1) = (1 - \frac{1}{N}) P_{\text{in}}(k,e) + \frac{1}{N} \left( p_{k-1} P_{\text{in}}(k-1,e) + (1 - p_{k+1}) P_{\text{in}}(k+1,e) \right)$ for $k \geq 1$ and $P_{\text{in}}(0,e+1) = (1 - \frac{1}{N}) P_{\text{in}}(0,e) + \frac{1}{N} (1 - p_1) P_{\text{in}}(1,e)$.

By equating $P_{\text{in}}(k,e+1)$ to $P_{\text{in}}(k,e)$, we obtain the condition for the stationary in-degree distribution $P_{\text{in}}^s(k)$:

$$(1 - p_{k+1}) P_{\text{in}}^s(k+1) = p_k P_{\text{in}}^s(k)$$

for all $k \geq 0$. Here, we only assume that the existence of $p_k$ and we leave the problem how to calculate $p_k$ for a future work. It could be obtained under a certain mean-field approximation of the models. In the following, we concentrate on the analysis of the stationary out-degree distribution.

The time evolution of out-degree distribution $P_{\text{out}}(l,e)$ follows the following master equation: $P_{\text{out}}(l,e+1) = (1 - q_{+,l}(e) - q_{-,l}(e)) P_{\text{out}}(l,e) + q_{+,l-1}(e) P_{\text{out}}(l-1,e) + q_{-,l+1}(e) P_{\text{out}}(l+1,e)$ for $l \geq 1$ and $P_{\text{out}}(0,e+1) = (1 - q_{+,0}(e)) P_{\text{out}}(0,e) + q_{-,0}(e) P_{\text{out}}(1,e)$, where $q_{+,l}(e)$ is the probability that a node with out-degree $l$ gets a new outgoing link at epoch $e$ and $q_{-,l}(e)$ is the probability that a node with out-degree $l$ loses an outgoing link at epoch $e$.

Put $\rho_+(e) := \sum_{k=0}^{\infty} P_{\text{in}}(k,e) p_k$ and $\rho_-(e) := \sum_{k=0}^{\infty} P_{\text{in}}(k,e) (1 - p_k)$. Let $\sigma_{+,l}(e)$ be the probability that a particular node with out-degree $l$ is chosen as the source of

Figure 5: System size dependence of deviation from criticality $\Delta z = z_s - 2$. (a) Results for the model based on activity. The slopes of the lines are $-0.230$ (real, Poisson), $-0.236$ (dashed, Exponential) and $-0.269$ (dotted, Truncated power law). (b) Results for the model based on local information transfer. The slopes of the lines are $-0.253$ (real, Poisson), $-0.257$ (dashed, Exponential) and $-0.281$ (dotted, Truncated power law). For every case, the stationary average in-degrees cannot be directly associated with evolution toward out-degree distributions in real-world gene regulation network evolutionary process, the emergence of heavy-tailed distributions have heavy-tailed out-degree distributions (Aldana et al., 2007). In this Appendix, we derive equation (4).
a new link given that the number of link increases at epoch \(e\) and \(\sigma_{-1}(e)\) the probability that an outgoing link of a particular node with out-degree \(l\) is deleted given that the number of link decreases at epoch \(e\). By definitions of \(\rho\) and \(\sigma\), we have

\[
q_{+,l}(e) = \rho_{+,l}(e)\sigma_{+,l}(e)
\]

(6)

and

\[
q_{-,l}(e) = \rho_{-,l}(e)\sigma_{-,l}(e).
\]

(7)

We now introduce the configuration model (random networks with a specified degree distribution (Newman et al., 2001)) approximation: links are randomly shuffled while keeping the degree of each node at the end of each epoch. Then, we have

\[
\sigma_{-,l}(e) = \frac{l}{Nz(e)}
\]

(8)
in the limit of large \(N\), where \(z(e)\) is the average in-degree at epoch \(e\) (which is equal to the average out-degree). Indeed, suppose that the chosen node at epoch \(e\) has in-degree \(k\) and it loses one of its incoming link. Noting that \(Nz(e)\) is the number of arcs, we find that the probability that there is a link from a node with out-degree \(l\) to a node with in-degree \(k\)

\[
1 - \left(1 - \frac{l}{Nz(e)}\right)^k \approx 1 - \left(1 - \frac{kl}{Nz(e)}\right)
\]

in the limit of large \(N\). The probability of deletion of this link is \(1/k\) under the approximation. Thus, we obtain

\[
\sigma_{-,l}(e) = \frac{l}{Nz(e)}
\]

As in the case with the stationary in-degree distribution, the stationary out-degree distribution \(P^s_{out}(l)\) should satisfy

\[
q^{s}_{-,l+1}P^s_{out}(l+1) = q^{s}_{+,l}P^s_{out}(l),
\]

(9)

for all \(l \geq 0\), where

\[
q^{s}_{+,l} = \rho^{s}_{+,l}\sigma^{s}_{+,l},
\]

\[
q^{s}_{-,l} = \rho^{s}_{-,l}\sigma^{s}_{-,l},
\]

\[
\rho^{s}_{+,l} = \sum_{k=0}^{\infty} P^s_{in}(k)p_k,
\]

\[
\rho^{s}_{-,l} = \sum_{k=0}^{\infty} P^s_{in}(k)(1-p_k)
\]

and \(\sigma^{s}_{+,l}\) and \(\sigma^{s}_{-,l}\) are stationary values for corresponding epoch-dependent quantities, respectively. Since \(p_0 = 1\), we have

\[
\rho^{s}_{+,l} = \rho^{s}_{-,l}
\]

(10)

by (5). Substituting the stationary analogue of (8) and (10) into (9), we obtain equation (4)

\[
\sigma^{s}_{+,l} = \frac{l+1}{Nzs} \frac{P^s_{out}(l+1)}{P^s_{out}(l)},
\]

where \(zs\) is the stationary average in-degree.

References


