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Dynamics Classification of Boolean Networks and Solutions of Diophantine Equation

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Abstract

An effective scheme for coding Boolean networks is proposed, by which one can uniquely designate a distinguished integer in the range from 0 to $(2^{n\times 2^n}-1)$ for any given n-node Boolean network. More importantly, by analyzing the characteristic polynomial of the linearized matrix of any given Boolean network, the connection between the dynamics of the network and the solution of a linear Diophantine equation can be established. Based on the calculation of the number of nonnegative integer solutions of the Diophantine equation, all n-node Boolean networks can be classified into several classes and the members in the same one have the same limit dynamical behaviors, i.e., same topological structures of invariant sets such as attractors and isles of Eden.

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1 Introduction

Boolean network (or switching net), introduced by Kauffman [1, 2] and then developed in [3] - [12] and many others, has become a powerful tool for modeling cell networks, consisting of behaviors and relationships of cells, proteins, DNA and RNA in biological systems. In a Boolean network, the gene state is quantized to only two levels: True (on) and False (off). The state of each gene is synchronously determined by those of its neighbors. The dynamics of a Boolean network is described in terms of its limit sets as attractors and isles of Eden which may be circles or fixed points, and the corresponding transient states. Since the logic can be arbitrarily specified, in general any state can move to any other state and there can be many different circles in the same network. For any particular Boolean network, most likely defined by n logical tables which can be converted into equations, the main task is to find all limit sets therein. Because of the exponential growth of the number of states, this is the nontrivial task when n is large. It was pointed out in [13] that finding fixed points and circles in a Boolean network is an NP-hard problem.

Several different methods, iterations, scalar and matrix expression forms were developed in [14] - [18] to determine the limit set structures and the transient states, and several useful Boolean networks have also been analyzed and their cyclic structures have been revealed (see, e.g., [14, 15] and references therein). The role of the matrix expression is essentially linearizing a Boolean network, which typically is a discrete-time dynamical system. However, determining the expression matrix associated with a Boolean network is a very complex process when the node number n is large.

In this paper, we propose a scheme for coding n-node Boolean networks, which can uniquely designate a distinguished integer in the range from 0 to $(2^{n\times 2^n} - 1)$ for any given Boolean network. At the same time, we obtain the linearized matrix of the given Boolean network. This matrix actually depends only on the information embed in the logical table of the given network. More importantly, by analyzing the characteristic polynomial of the linearized matrix of a Boolean network, we establish the connection between the dynamics of the network and the nonnegative integer solutions of a linear Diophantine equation. In this way, one can easily deal with the dynamics of the network by using the solutions of the Diophantine equation. Moreover, we successfully derive an innovation recurrence formula for calculating the numbers of the nonnegative integer solutions of the Diophantine equation. Thus, all $2^{n\times 2^n}$ of n-node Boolean networks can be partitioned into several equivalent classes such that the networks in each class possess the same limit sets, such as attracts (contain fixed points or circles) and isles of Eden [19], i.e., same limit dynamical behaviors. For example, all 2-node Boolean networks can be classified into 11 classes, and all 3-node Boolean networks can be classified into 66 classes, and so on.

The rest of the paper is organized as follows. Section 2 describes the code of n-node Boolean network. Section 3 discusses the dynamics of the network via determining the characteristic polynomial, and gives a linear Diophantine equation. Section 4 derives a recurrence formula of the numbers of solutions of the Diophantine equation, and deduces a dynamics classification for all n-node Boolean networks under the viewpoint of the same topological structures of the limit set. Finally, Section 5 briefly concludes the paper.

2 Code of Boolean Network

2.1 Code of Boolean matrix

A $(2^n \times 2^n)$-order matrix B is called a Boolean matrix if there is only one element "1" and the rest are "0" in its each row. i.e., the form of a Boolean matrix is

$$B = (\delta^T_{i_0+1}, \delta^T_{i_1+1}, \delta^T_{i_2+1}, \cdots, \delta^T_{i_{2^n-1}+1})^T, \tag{1}$$

where $i_k \in \{0, 1, 2, \cdots, 2^n - 1\}$, and $\delta^T_{i_k+1}$ denotes the $(k+1)$-th row vector of B, i.e., $\delta^T_{i_k+1} = (\overbrace{0, \cdots, 0}^{i_k}, 1, 0, \cdots, 0)$, in which the $(i_k + 1)$-th element is 1 and the rest are 0, $k = 0, 1, \cdots, 2^n - 1$. For convenience, B may be written for

$$B = \left[\begin{array}{c|ccccc} k & 0 & 1 & \cdots & 2^n-2 & 2^n-1 \\ \hline i_k & i_0 & i_1 & \cdots & i_{2^n-2} & i_{2^n-1} \end{array}\right]. \tag{2}$$

It will be seen that the compact expression formulas are very useful and effective in the code and classification of Boolean networks.

The code of the Boolean matrix B thus can be defined as

$$C_B = \sum_{k=0}^{2^n-1} i_k 2^{nk}. \tag{3}$$

Example 1. *Let a* $(2^3 \times 2^3)$*-order Boolean matrix* B *be*

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

then it is easy to see that $i_0 = i_7 = 0,\ i_1 = 2,\ i_2 = 1,\ i_3 = 4,\ i_4 = i_6 = 5,\ i_5 = 3$. *So its compact expression is* $B = \left[\begin{array}{c|cccccccc} k & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline i_k & 0 & 2 & 1 & 4 & 5 & 3 & 5 & 0 \end{array}\right]$, *and its decimal code is* $C_B = 2\times 2^3 + 1\times 2^{3\times 2} + 4\times 2^{3\times 3} + 5\times 2^{3\times 4} + 3\times 2^{3\times 5} + 5\times 2^{3\times 6} = 1431632$.

Conversely, for a given integer n and a number C on the range from 0 to $(2^{n\times 2^n} - 1)$, one can easily derive an $2^n \times 2^n$-order Boolean matrix whose code is C. In particular, the code number C_B of the Boolean matrix $B = (b_{i,j})_{2^n\times 2^n}$ with $b_{i,1} = 1$ $(i = 1, 2, \cdots, 2^n)$ is equal to 0, and the one of the matrix $B = (b_{i,j})_{2^n\times 2^n}$ with $b_{i,2^n} = 1$ $(i = 1, 2, \cdots, 2^n)$ is $(2^{n\times 2^n} - 1)$.

2.2 Code of Boolean network

A Boolean network is a set of n nodes, $A_1, A_2, \cdots, A_n$, which interact with each other in a synchronous manner. At each time $t = 0, 1, 2, \cdots$, a node has only one of two different values: 0 or 1, i.e., the network is a set of equations as follows:

$$\begin{cases} A_1(t+1) = f_1(A_1(t), A_2(t), \cdots, A_n(t)) \\ A_2(t+1) = f_2(A_1(t), A_2(t), \cdots, A_n(t)) \\ \vdots \\ A_n(t+1) = f_n(A_1(t), A_2(t), \cdots, A_n(t)), \end{cases} \tag{4}$$

where f_i $(i = 1, 2, \cdots, n)$ are n-bit Boolean functions.

Equations (4) defines an iteration map $F : \{0,1\}^n \longrightarrow \{0,1\}^n$ starting from the initial value $(A_1(0), A_2(0), \cdots, A_n(0))^T \in \{0,1\}^n$, where $F = (f_1, f_2, \cdots, f_n)^T$. It also can be illustrated as its logical table (Table 1).

Table 1: Logical table of n-node Boolean network

Input Window	f_1	f_2	$\cdots$	f_n
$u^{(0)} = (0, 0, \cdots, 0, 0)^T$	$v_0^{(1)}$	$v_0^{(2)}$	$\cdots$	$v_0^{(n)}$
$u^{(1)} = (0, 0, \cdots, 0, 1)^T$	$v_1^{(1)}$	$v_1^{(2)}$	$\cdots$	$v_1^{(n)}$
$u^{(2)} = (0, 0, \cdots, 1, 0)^T$	$v_2^{(1)}$	$v_2^{(2)}$	$\cdots$	$v_2^{(n)}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$u^{(k)} = (u_1^{(k)}, u_2^{(k)}, \cdots, u_n^{(k)})^T$	$v_k^{(1)}$	$v_k^{(2)}$	$\cdots$	$v_k^{(n)}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$u^{(2^n-2)} = (1, 1, \cdots, 1, 0)^T$	$v_{2^n-2}^{(1)}$	$v_{2^n-2}^{(2)}$	$\cdots$	$v_{2^n-2}^{(n)}$
$u^{(2^n-1)} = (1, 1, \cdots, 1, 1)^T$	$v_{2^n-1}^{(1)}$	$v_{2^n-1}^{(2)}$	$\cdots$	$v_{2^n-1}^{(n)}$

Let the decimal code of a n-dimensional vector $u = (u_i, u_2, \cdots, u_n)$ be $k = \sum_{i=1}^{n} u_i 2^{n-i}$. For a given n-node network (4), let i_k be the decimal code of the vector $(v_k^{(1)}, v_k^{(2)}, \cdots, v_k^{(n)})$ consisting of n elements of the k-th row in Table 1, $k = 0, 1, \cdots, 2^n - 1$, then a $(2^n \times 2^n)$-order Boolean matrix B can be obtained based on formula (1)

The Boolean matrix B derived from the above method is called the linearized matrix or the expression matrix of the Boolean network (4). Obviously, any n-node Boolean network (4) and its linearized matrix B has an one-to-one relationship. Hence, the code of the linearized matrix B of (4) can be considered as the code of the network itself.

Definition 1. *The code C_B in the formula (3) of the linearized matrix B of the n-node Boolean network (4) is called the code of the network.*

3 Dynamics of n-node Boolean Network and Diophantine Equation

3.1 State transform defined by Boolean network

The network (4) defines a state transform in $\{0,1\}^n$:

$$F(u^{(k)}) = (f_1(u^{(k)}), f_2(u^{(k)}), \cdots, f_n(u^{(k)}))^T = u^{(i_k)}, \tag{5}$$

where $u^{(i_k)} = (v_k^{(1)}, v_k^{(2)}, \cdots, v_k^{(n)})^T \in \{0,1\}^n$ is the state vector consisting of the k-th components of the n Boolean functions f_i $(i = 1, 2, \cdots, n)$, i_k is the decimal code of the vector $(v_k^{(1)}, v_k^{(2)}, \cdots, v_k^{(n)})$.

Supposing $\mathcal{U} = \{u^{(0)}, u^{(1)}, u^{(2)}, \cdots, u^{(2^n-1)}\}$ is the state set, then (5) defines a self-map $B : \mathcal{U} \to \mathcal{U}$ with

$$Bu = u^*, \tag{6}$$

where $u = (u^{(0)}, u^{(1)}, \cdots, u^{(2^n-1)})^T$ and $u^* = (u^{(i_0)}, u^{(i_1)}, \cdots, u^{(i_{2^n-1})})^T$ and B is the linearized matrix of the network (4).

The map (6) also can be considered as a directed graph $\mathcal{G} = \mathcal{G}(\mathcal{U}, \mathcal{E}_\mathcal{B})$, where $\mathcal{U} = \{u^{(0)}, u^{(1)}, u^{(2)}, \cdots, u^{(2^n-1)}\}$ is the vertex set, and $\mathcal{E}_\mathcal{B}$ is the arc set with $\mathcal{E}_\mathcal{B} = \{(i \to j)|\ b_{i,j} = 1,\ i, j = 0, 1, 2, \cdots, 2^n - 1\}$, and b_{ij} is the element of the matrix $B = (b_{ij})_{2^n \times 2^n}$. The graph $\mathcal{G} = \mathcal{G}(\mathcal{U}, \mathcal{E}_\mathcal{B})$ is called the state-transition graph of matrix B containing the dynamics of the network (4). The state-transition graph of the matrix B in Example 1 is shown in Fig.1, where $\{0, 1, 2, \cdots, 7\}$ briefly on behalf of the vertex set $\mathcal{U} = \{u^{(0)}, u^{(1)}, u^{(2)}, \cdots, u^{(7)}\}$.

3.2 Characteristic polynomial of Boolean matrix and Diophantine equation

As mentioned above, there exists only one element "1" and the rest are "0" in its each row in a $(2^n \times 2^n)$-order Boolean matrix B. Thus, according to the basic knowledge of matrix algebra, there exists a non-degenerate matrix W such that $\tilde{B} = WBW^{-1}$ (or say $\tilde{B}$ similar to B), where $\tilde{B}$ is the following

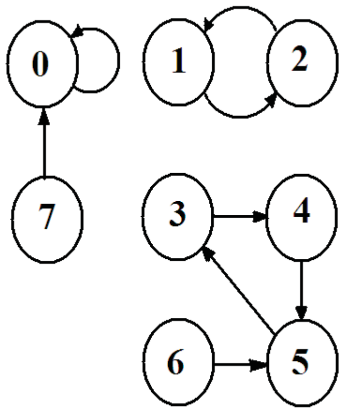

Figure 1: State-transition structures of the network with linearized matrix B in Example 1

form:

$$\tilde{B} = \begin{pmatrix} A_0 & A_1 & A_2 & \cdots & A_r \\ O & B_{i_1} & O & \cdots & O \\ O & O & B_{i_2} & \cdots & O \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O & O & O & \cdots & B_{i_r} \end{pmatrix}_{2^n \times 2^n}, \tag{7}$$

where $\{i_1, i_2, \cdots, i_r\} \subseteq \{1, 2, \cdots, 2^n\}$, $i_1 < i_2 < \cdots < i_r$, and there exist positive integers s_{i_j} $(j = 1, 2, \cdots, r)$ such that

$$s_0 + i_1 s_{i_1} + i_2 s_{i_2} + \cdots + i_r s_{i_r} = 2^n. \tag{8}$$

In (7), A_0 is a $(s_0 \times s_0)$-order square matrix, A_j $(j = 1, 2, \cdots, r)$ are $(s_0 \times i_j s_{i_j})$-order matrices, and B_{i_j} $(j = 1, 2, \cdots, r)$ are $(i_j s_{i_j} \times i_j s_{i_j})$-order square matrices, where

$$B_{i_j} = \begin{pmatrix} C_j & O & \cdots & O \\ O & C_j & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ O & O & \cdots & C_j \end{pmatrix}_{i_j s_{i_j} \times i_j s_{i_j}}, \tag{9}$$

and C_j $(j = 1, 2, \cdots, r)$ are $(i_j \times i_j)$-order square matrices

$$C_j = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix}_{i_j \times i_j}. \tag{10}$$

When $s_0 = 0$, then $\tilde{B}$ is

$$\tilde{B} = \begin{pmatrix} B_{i_1} & O & \cdots & O \\ O & B_{i_2} & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ O & O & \cdots & B_{i_r} \end{pmatrix}_{2^n \times 2^n}. \tag{11}$$

Moreover, $|E\lambda - A_0| = \lambda^{s_0}$, $|E\lambda - B_{i_j}| = |E\lambda - C_j|^{s_{i_j}} = (\lambda^{i_j} - 1)^{s_{i_j}}$, and

$\Phi(\lambda) = |E\lambda - B| = |E\lambda - \tilde{B}| = |E\lambda - A_0||E\lambda - B_{i_1}||E\lambda - B_{i_2}| \cdots |E\lambda - B_{i_r}|$,

hence, the characteristic polynomial of B is

$$\Phi(\lambda) = \lambda^{s_0}(\lambda^{i_1} - 1)^{s_{i_1}}(\lambda^{i_2} - 1)^{s_{i_2}} \cdots (\lambda^{i_r} - 1)^{s_{i_r}}. \tag{12}$$

Note that $s_0 \neq 2^n$, because otherwise all the eigenvalues are zero.

In formula (8), $\{i_1, i_2, \cdots, i_r\} \subseteq \{1, 2, \cdots, 2^n\}$ and $i_1 < i_2 < \cdots < i_r$, so set $S = \{s_0, s_1, s_2, \cdots, s_{2^n}\}$ can be divided into two parts: one is the set $\{s_{i_1}, s_{i_2}, \cdots, s_{i_r}\}$ that are positive numbers, and the other is the rest elements of S that are zero. Therefore, the characteristic polynomial of $(2^n \times 2^n)$-order Boolean matrix is

$$\Phi(\lambda) = \lambda^{s_0}(\lambda - 1)^{s_1}(\lambda^2 - 1)^{s_2}(\lambda^3 - 1)^{s_3} \cdots (\lambda^{2^n} - 1)^{s_{2^n}}, \tag{13}$$

where s_i $(i = 0, 1, 2, \cdots, 2^n - 1, 2^n)$ are nonnegative integers, $s_0 \neq 2^n$, and satisfy the following equation:

$$s_0 + s_1 + 2s_2 + 3s_3 + \cdots + 2^n s_{2^n} = 2^n. \tag{14}$$

It is quite clear that (14) is a linear Diophantine equation. We thus have established the connection between the characteristic polynomial of a Boolean matrix and the solutions of a Diophantine equation.

3.3 Dynamics of Boolean networks

It is well known that the dynamics of a Boolean Network can be described in terms of the topological structure of the state-transition graph $\mathcal{G}$. In general, there are some circles, which can be fixed points, and the transient states in its state-transition. The cyclic structures may be separated into two kinds: one is the attractor and the other is the so-called isle of Eden [20,21].

A period-p circle $\gamma = \{u^{(k_0)}, F(u^{(k_0)}), F^2(u^{(k_0)}), \cdots, F^{p-1}(u^{(k_0)})\}$ of network (4) with $u^{(k_0)} = F^p(u^{(k_0)})$ is called an attractor if there exist a state $u^{(j_0)} \notin \gamma$ and a positive integer q such that $F^q(u^{(j_0)}) \in \gamma$, and $u^{(j_0)}$ is called a transient state. If period circle γ is not an attractor, it is called an isle of Eden. The special case of $p = 1$, i.e., γ is degraded to be a fixed point which is also contained in these definitions.

Definition 2. *A subset $\mathcal{Y}$ of the state set $\mathcal{U} = \{u^{(0)}, u^{(1)}, u^{(2)}, \cdots, u^{(2^n-1)}\}$ is called the invariant set of the network (4) (or (5)) if $F(\mathcal{Y}) = \mathcal{Y}$. A point (state) $z \in \mathcal{U}$ is called a limit point of (4) if there exist $x \in \mathcal{U}$ and a subsequence $\{n_k\}$ with $n_k \to +\infty$ $(k \to +\infty)$ such that $z = \lim_{k\to+\infty} F^{n_k}(x)$. The set of all limit points of (4), $\mathcal{Q}$, is called the limit set of (4).*

Obviously, all attractors and isles of Eden of any Boolean network are invariant sets. The union of all invariant sets forms the limit set of the network.

Lemma 1. *For two Boolean matrices B and $\tilde{B}$, if $\tilde{B}$ is similar to B, then the dynamics of both the Boolean network with linearized matrix B and the one with linearized matrix $\tilde{B}$ are completely identical.*

Proof. In fact, if $\tilde{B}$ is similar to B, then there exists a non-degenerate W such that $\tilde{B} = WBW^{-1}$, where W is the product of some elementary matrices, and also is a Boolean matrix but $|W| \neq 0$. Thus, let $\bar{u} = Wu$, then $\bar{u}^* = Wu^*$, and based on (6), one has $u^* = Bu = BW^{-1}\bar{u}$, and $\bar{u}^* = WBW^{-1}\bar{u}$, i.e.,

$$\bar{u}^* = \tilde{B}\bar{u}, \tag{15}$$

where u and u^* are two vectors defined in (6). Hence the state-transition graph $\mathcal{G}(\bar{\mathcal{U}}, \mathcal{E}_{\tilde{\mathcal{B}}})$ is same as $\mathcal{G}(\mathcal{U}, \mathcal{E}_{\mathcal{B}})$, i.e., the dynamics of the both two networks are completely identical.

Theorem 1. *For a Boolean network (4), which associated with linearized matrix B, the characteristic polynomial of B is denoted in (12), then:*

(i) if $s_0 = 0$ *in (12), then there exist* $(s_{i_1} + s_{i_2} + \cdots + s_{i_r})$ *circles. They are all isles of Eden and their periods respectively are* i_j $(j = 1, 2, \cdots, r)$ *and further satisfy* $i_1 s_{i_1} + i_2 s_{i_2} + \cdots + i_r s_{i_r} = 2^n$*, where* s_{i_j} *is the number of the period-*i_j *circle* $(j = 1, 2, \cdots, r)$*;*
(ii) if $s_0 \neq 0$ *in (12), then there exist* s_0 *transient states and* $(s_{i_1} + s_{i_2} + \cdots + s_{i_r})$ *circles, and the periods of these circles respectively are* i_j $(j = 1, 2, \cdots, r)$ *and further satisfy* $s_0 + i_1 s_{i_1} + i_2 s_{i_2} + \cdots + i_r s_{i_r} = 2^n$*, where* s_{i_j} *is the number of the period-*i_j *circle* $(j = 1, 2, \cdots, r)$*. Further, if there exists* q $(1 \leq q \leq r)$ *such that the matrix* A_q *in (7) is a null matrix, the period-*i_q *circle associated with the matrix block* B_{i_q} *is an isle of Eden.*

Proof. In fact, matrix B is similar to matrix $\tilde{B}$ denoted in (11) (when $s_0 = 0$), or in (7) (when $s_0 \neq 0$), thus:
(i) when $s_0 = 0$, each matrix block C_j in B_{i_j} determines a state-transition graph $\mathcal{G}(\mathcal{U}_j, \mathcal{E}_{C_j})$, where $\mathcal{U}_j \subset \mathcal{U}$ is the state set consisting of i_j states, and $\mathcal{E}_{C_j}$ is the arc set determined by C_j. Obviously, the graph $\mathcal{G}(\mathcal{U}_j, \mathcal{E}_{C_j})$ generates a period-i_j circle, so each B_{i_j} has s_{i_j} period-i_j circles $(j = 1, 2, \cdots, r)$, and $i_1 s_{i_1} + i_2 s_{i_2} + \cdots + i_r s_{i_r} = 2^n$. Moreover, any state in a circle will not be transferred to any another circle, so these period-i_j $(j = 1, 2, \cdots, r)$ circles are isles of Eden;
(ii) when $s_0 \neq 0$, same as (i), it holds s_{i_j} period-i_j circles $(j = 1, 2, \cdots, r)$, but at the time, $i_1 s_{i_1} + i_2 s_{i_2} + \cdots + i_r s_{i_r} = 2^n - s_0$, and the first s_0 rows of the matrix $\tilde{B}$ consist of a $(s_0 \times 2^n)$-order matrix $(A_0\ A_1\ A_2\ \cdots\ A_r)$. On one hand, a state-transition graph determined by A_0 can not generate a circle because its eigenvalues are zeros, so the states except all circles are transient ones, and their number is s_0. On the other hand, if a matrix block A_{q_0} $(1 \leq q_0 \leq r)$ in (7) is a null matrix, then there exists not a state which transfers to any circle, thus, the period-i_{q_0} circle associated with the matrix block $B_{i_{q_0}}$ is an isle of Eden. Note that $s_0 \neq 2^n$, otherwise all 2^n states will become transient states, and this is not possible.

Corollary 1. *The limit set of the Boolean network (4) consists of the* $(2^n - s_0)$ *points that form* s_{i_j} *period-*i_j *circles* $(j = 1, 2, \cdots, r)$*, where* $i_1 s_{i_1} + i_2 s_{i_2} + \cdots + i_r s_{i_r} = 2^n - s_0$.

Example 2. *For the matrix* B *in Example 1, it is easy to know that there* *exists a non-degenerate matrix* W *such that* $\tilde{B} = WBW^{-1}$, *where*

$$\tilde{B} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} A_0 & A_1 & A_2 & A_3 \\ O & B_{i_1} & O & O \\ O & O & B_{i_2} & O \\ O & O & O & B_{i_3} \end{pmatrix},$$

where

$$A_0 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix},\ A_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix},\ A_2 = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix},\ A_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$

$$B_{i_1} = \begin{pmatrix} 1 \end{pmatrix},\ B_{i_2} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ B_{i_3} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},$$

and $i_1 = 1,\ i_2 = 2,\ i_3 = 3,\ s_0 = 2,\ s_{i_1} = s_{i_2} = s_{i_3} = 1$. *Clearly that there exist two transient states* $\{u^{*(0)}, u^{*(1)}\}$, *a fixed point* $\{u^{*(2)}\}$, *a period-*2 *circle* $\{u^{*(3)}, u^{*(4)}\}$, *a period-*3 *circle* $\{u^{*(5)}, u^{*(6)}, u^{*(7)}\}$. *The fixed point and period-*3 *circle are attractors, and the period-*2 *circle is an isle of Eden. They constitute the invariant sets. The union of these invariant sets forms the limit set* $\mathcal{Y} = \{u^{*(2)}, u^{*(3)}, u^{*(4)}, u^{*(5)}, u^{*(6)}, u^{*(7)}\}$. *Its state-transition graph is the same with Fig. 1, with* $u^{*(0)} = u^{(6)}, u^{*(1)} = u^{(7)}, u^{*(2)} = u^{(0)}, u^{*(3)} = u^{(1)}, u^{*(4)} = u^{(2)}, u^{*(5)} = u^{(3)}, u^{*(6)} = u^{(4)}, u^{*(7)} = u^{(5)}$.

4 Solutions of Diophantine Equation and Dynamics Classification of Boolean Networks

In the previous section, the relationship between the characteristic polynomial of Boolean matrix and the solutions of a linear Diophantine equation is established. Now, one can derive a recurrence formula for calculating the numbers of nonnegative integer solutions of the Diophantine equation (14), and discuss the dynamics classification of n-node Boolean networks from the viewpoint of the same topological structures of the limit set.

4.1 Numbers of solutions of Diophantine equation

A Diophantine equation is an equation in which only integer solutions are allowed. The linear diophantine equations and their solutions are among the well-known results in number theory. The study of these equations can be found in many works such as [20].

For Diophantine equation (14), $s_0 + s_1 + 2s_2 + 3s_3 + \cdots + 2^n s_{2^n} = 2^n$, the existence of solution is obvious, since its coefficient set is $\{1, 1, 2, \cdots, 2^n\}$. The difficult problem is how to find the number of its solutions.

Theorem 2. *Let $\varphi_m(M)$ denote the number of the nonnegative integer solutions of the following equation*

$$s_0 + s_1 + 2s_2 + 3s_3 + \cdots + ms_m = M, \tag{16}$$

where m and M are positive integers. Then,
(i) $\varphi_1(M) = M + 1$;
(ii) when $m > M$, $\varphi_m(M) = \varphi_M(M)$;
(iii) when $m \leq M$, it satisfies the recursive formula:

$$\varphi_m(M) = \begin{cases} \sum_{j=0}^{[\frac{M}{m}]} \varphi_{m-1}(M - j \cdot m) & if\ \frac{M}{m} \neq [\frac{M}{m}] \\ \sum_{j=0}^{[\frac{M}{m}]-1} \varphi_{m-1}(M - j \cdot m) + 1 & if\ \frac{M}{m} = [\frac{M}{m}], \end{cases} \tag{17}$$

where $[\frac{M}{m}]$ is a positive integer no than $\frac{M}{m}$.

Proof. (i) it is clear that the number of the nonnegative integer solutions of the equation $s_0 + s_1 = M$ is $\varphi_1(M) = M + 1$;
(ii) when $m > M$, (16) is

$$s_0 + s_1 + 2s_2 + 3s_3 + \cdots + Ms_M + (M + 1)s_{M+1} + \cdots + ms_m = M,$$

then all s_i $(i = M + 1, \cdots, m)$ will be zeros, this implies $\varphi_m(M) = \varphi_M(M)$;
(iii) when $m \leq M$, the equation (16) can be turned into another form:

$$s_0 + s_1 + 2s_2 + 3s_3 + \cdots + (m - 1)s_{m-1} = M - ms_m, \tag{18}$$

if s_m to be determined, then the number of the nonnegative integer solutions of (18) is $\varphi_{m-1}(M - ms_m)$. Because s_m can only be allowed to be nonnegative integer, so if $M - ms_m > 0$, i.e., $\frac{M}{m} \neq [\frac{M}{m}]$, then for $m = 2, 3, \cdots$,

$$\varphi_m(M) = \sum_{j=0}^{[\frac{M}{m}]} \varphi_{m-1}(M - j \cdot m),$$

if $M - ms_m = 0$, i.e., $s_m = \frac{M}{m} = [\frac{M}{m}]$, then $\{s_0, s_1, \cdots, s_{m-1}, s_m\} = \{0, 0, \cdots, 0, \frac{M}{m}\}$ is an nonnegative integer solution of (16), so for $m = 2, 3, \cdots$,

$$\varphi_m(M) = \sum_{j=0}^{[\frac{M}{m}]-1} \varphi_{m-1}(M - j \cdot m) + 1.$$

Note that Diophantine equation (14) is a special case of equation (16) when $m = M = 2^n$, thus we know that the number of the nonnegative integer solutions of Diophantine equation (14) is $\varphi_{2^n}(2^n)$. These values of $\varphi_{2^n}(2^n)$ for $n = 1, 2, \cdots, 8$ are listed in the second column in Table 2.

4.2 Dynamics classification of Boolean networks

Note that the number of all n-node Boolean networks and the decimal coding number of all $(2^n \times 2^n)$-order Boolean matrices are exactly identical, both equalling to $2^{n \times 2^n}$, and the relationship between the Boolean network (4) and its linearized matrix B is an one-to-one bijection. Thus, one can classify Boolean networks by using the characteristic of B, especially the numbers of nonnegative integer solutions of the Diophantine equation (14).

Two n-node Boolean networks are said to be equivalent if the topological structures of their state-transition graphs are identical. For example, in Fig. 2, the networks (a) and (b) are equivalent, because they have the same state-transition structure. But (c) and (a) (or (c) and (b)) are not equivalent. Obviously, two topologically equivalent Boolean networks have the same dynamical behaviors. Thus, one of the most important objectives in studying Boolean networks is the topological equivalence classification of all n-node Boolean networks. Unfortunately, with the increase of n, the number of all n-node Boolean networks will increase rapidly, and therefore, the topological equivalence classification of Boolean networks becomes more and more difficult. But from another point of view, since $F^n(\mathcal{U}) \to \mathcal{Q}$ $(n \to +\infty)$, where $\mathcal{U}$ is the state set and $\mathcal{Q}$ is the limit set of the Boolean network. The limit set $\mathcal{Q}$ reflects the asymptotic behavior of the network.

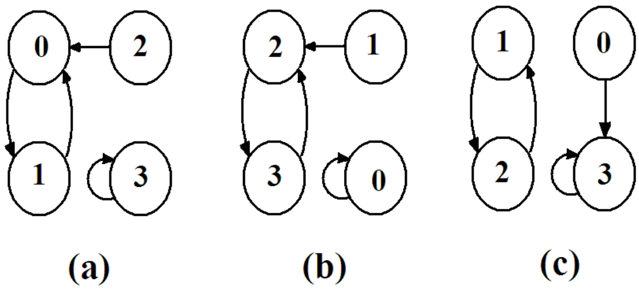

Figure 2: State-transition structures of Boolean networks (a), (b) and (c)

Fortunately, the nonnegative integer solution of Diophantine equation (14) contains the information of the limit set of a Boolean network.

Theorem 3. *A group of solutions* $\{s_0, s_1, \cdots, s_{2^n}\}$ *of Diophantine equation (14) except of* $s_0 = 2^n$ *corresponds to a class of n-node Boolean networks, the networks in the class have the same limit set, i.e., they have exactly the same limit dynamical behaviors.*

Proof. In fact, for a given n-node Boolean network, its dynamics was completely characterized by the characteristic polynomial (13) or the nonnegative integer solutions of Diophantine equation (14) of the Boolean matrix associated with the network. In brief, it has s_0 $(s_0 \neq 2^n)$ transient states and the limit set which is the union of all attractors and isles of Eden consisting of $(2^n - s_0)$ states. Thus, two n-node Boolean networks that have same nonnegative integer solutions of Diophantine equation (14) have the same limit set.

Based on this theorem, and taking note of $s_0 \neq 2^n$, we finally get the following dynamics classification result of Boolean networks:

Theorem 4. *All n-node Boolean networks can be divided into* $(\varphi_{2^n}(2^n) - 1)$ *classes, the networks in each class have the same limit set, where* $\varphi_{2^n}(2^n)$ *is the number of the nonnegative integer solutions of Diophantine equation (14).*

Table 2: Number of nonnegative integer solutions of Diophantine equation (14) $\varphi_{2^n}(2^n)$ and proportion $\frac{\varphi_{2^n}(2^n)-1}{2^{n\times 2^n}}$ for $n = 1, 2, \cdots, 8$.

n	$\varphi_{2^n}(2^n)$	$(\varphi_{2^n}(2^n) - 1)/2^{n\times 2^n}$
1	4	0.75
2	12	$\approx 4.296875 \times 10^{-2}$
3	67	$\approx 3.933907 \times 10^{-6}$
4	915	$\approx 4.96739130 \times 10^{-17}$
5	43820	$\approx 3.00130136 \times 10^{-44}$
6	12308139	$\approx 3.12389289 \times 10^{-109}$
7	41959382090	$\approx 7.946852668 \times 10^{-260}$
8	4861560552351727	$\approx 1.593954279 \times 10^{-601}$
$\vdots$	$\cdots$	$\cdots$

For example, the topological structures of the limit sets of the state-transition graphs (a), (b) and (c) in Fig. 2 are completely the same, i.e., these networks associated with (a), (b) and (c) have the same asymptotic behaviors, and thus are in the same class.

The proportion, $\frac{\varphi_{2^n}(2^n)-1}{2^{n\times 2^n}}$, of the number of dynamics classification of n-node Boolean networks in all $2^{n\times 2^n}$ Boolean networks is listed in the third column in Table 2 for $n = 1, 2, \cdots, 8$. As for the larger n, the classification number are also readily available, but more computer capacity and longer calculation time are need. It is particularly important that the proportion of number of dynamics classification in all $2^{n\times 2^n}$ n-node Boolean networks is becoming smaller and smaller with the increase of n. For $n = 3$, the proportion of number of dynamics classification can be approximated at zero. This implies a substantial and considerable saving of otherwise wasted man hours in the sense that the limit dynamics of any one of the remaining 3-node Boolean networks can be derived exactly from one of the 66 equivalent networks.

5 Conclusion

The simplest possible conceptual model that mimics signal transduction might be Boolean network, due to the only alternative values 0 and 1 of each node at any time. In this paper, an effective scheme for coding n-node Boolean networks has been proposed via coding its linearized matrix. Meanwhile, the connection between the dynamics of the networks and a linear Diophantine equation is established, and a recurrence formula for calculating the number of nonnegative integer solution of the Diophantine equation is derived. Moreover, a dynamics classification for all n-node Boolean networks is obtained under the viewpoint of the same topological structures of the limit set.

Indeed, Boolean networks are useful for modeling cell networks such as genetic regulation in biological systems. The results presented in this work maybe provide a new basis for the elucidation of the function of complexity in the living cells, and therefore are significant and meaningful for systems biology and mathematical biosciences research.

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