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Structural controllability of Boolean control networks with an unknown function structure

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Dear editor,

Boolean networks represent one of the most popular models for gene regulatory networks. In a Boolean network, genes are perceived as nodes in a network graph, and the dynamics of each node are determined by a Boolean function of the node's activating and inhibiting neighbors [1, 2]. It is well known that when modeling practical gene regulatory networks, the network graph can be exactly determined, while the function structure is often completely or partially unknown owing to measurement errors [1]. In this case, one should consider the structural properties of Boolean networks. Azuma et al. [1, 3] considered the structural monostability and oscillatority of Boolean networks and presented some new results.

In the last decade, an algebraic state-space representation (ASSR) method has been proposed by Cheng, based on the semi-tensor product (STP) of matrices [2]. The ASSR method has been applied to the study of Boolean networks [4, 5] and other related fields [6–8]. In particular, the controllability of Boolean control networks has been comprehensively studied in [4, 9–11]. However, existing results on the controllability of Boolean control networks only consider function structures that are exactly known. To the best of our knowledge, when the function structure is unknown there are no results available concerning the structural controllability of Boolean control networks. In structured system theory, structural controllability is fundamental for structural controller design [12]. Therefore, it is meaningful to study the structural controllability of Boolean control networks.

In this study, we consider the structural reachability and controllability of Boolean control networks via the ASSR method. The main contributions of this work are as follows. (i) Structurally equivalent Boolean control networks are converted into algebraic forms using the STP, which facilitates the study of structural controllability. (ii) A type of structural controllability matrix is constructed using the Hadamard product, based on which some necessary and sufficient conditions are presented for the structural reachability and controllability of Boolean control networks. Compared with the graph "topological" conditions, the structural controllability matrix is easily calculated via MATLAB.

Some notations are listed as follows. The i-th column of the identity matrix I_n is represented as δ_n^i. $\Delta_n := \{\delta_n^i : i = 1, 2, \ldots, n\}$, and $\mathcal{D} := \{0, 1\}$. An $n \times t$ logical matrix $M = [\delta_n^{i_1}\ \delta_n^{i_2}\ \cdots\ \delta_n^{i_t}]$ is compactly expressed as $M = \delta_n[i_1\ i_2\ \cdots\ i_t]$. The set of $n \times t$ logical matrices is denoted by $\mathcal{L}_{n\times t}$. An $n \times t$ real matrix is called a Boolean matrix if all the elements take values from $\mathcal{D}$. The set of $n \times t$ Boolean matrices is denoted by $\mathcal{B}_{n\times t}$. The symbols "$*$", "$\otimes$", "$\circ$", and "$\ltimes$" represent the Khatri-Rao product, Kronecker product, Hadamard product, and STP of two real matrices, respectively. We often omit the symbol "$\ltimes$" in the following if no confusion arises. The symbols "$\vee$" and "$\wedge$" denote "disjunction" and "conjunction", respectively. Given

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$x \in \mathcal{D}$, "$\bar{x}$" denotes the "negation" of x. The structural matrix of "negation" is $M_n = \delta_2[2\ 1]$. For $P = (p_{i,j}) \in \mathcal{B}_{m\times n}$ and $Q = (q_{i,j}) \in \mathcal{B}_{m\times n}$, define $P +_{\mathcal{B}} Q := (p_{i,j}) \vee (q_{i,j})$. In addition, given $P = (p_{i,j}) \in \mathcal{B}_{m\times n}$ and $Q = (q_{i,j}) \in \mathcal{B}_{n\times p}$, define $R = (r_{i,j}) = P \times_{\mathcal{B}} Q$ as $r_{i,j} = \vee_{k=1}^{n}(p_{i,k} \wedge q_{k,j})$. For $P \in \mathcal{B}_{n\times n}$, define

$$P^{(l)} := \underbrace{P \times_{\mathcal{B}} \cdots \times_{\mathcal{B}} P}_{l}.$$

Consider the following Boolean control network:

$$z_i(t+1) = f_i\big([z_j(t)]_{j\in U_i}, [\bar{z}_j(t)]_{j\in \overline{U}_i}, [v_j(t)]_{j\in G_i}, [\bar{v}_j(t)]_{j\in \overline{G}_i}\big), \quad i = 1, \ldots, n, \tag{1}$$

where $z_i(t) \in \mathcal{D}$ is the state of node i, $v_j(t) \in \mathcal{D}$ is the control of node i, $U_i \subseteq \{1, \ldots, n\}$ and $G_i \subseteq \{1, \ldots, m\}$ are the index sets of the activating neighbors of node i, $\overline{U}_i \subseteq \{1, \ldots, n\} \setminus U_i$ and $\overline{G}_i \subseteq \{1, \ldots, m\} \setminus G_i$ are the index sets of the inhibiting neighbors of node i, and $f_i : \mathcal{D}^{|U_i|+|\overline{U}_i|+|G_i|+|\overline{G}_i|} \to \mathcal{D}$, $i = 1, \ldots, n$ are Boolean functions composed of the logical operators "$\vee$" and "$\wedge$".

In this study, we assume that the network graph of the system (1) is known, which determines U_i, $\overline{U}_i$, G_i, and $\overline{G}_i$, while the logical operators between nodes in U_i, $\overline{U}_i$, G_i, and $\overline{G}_i$ are unknown, which referred to as an unknown function structure. Therefore, the dynamics of the system (1) are determined by the known network graph and unknown function structure. Two Boolean control networks with the same network graph are called structurally equivalent.

In the following, we convert the structurally equivalent system (1) into an equivalent algebraic form.

For the i-th node of the system (1), $i = 1, \ldots, n$, let

$$U_i = \{a_{i,1}, \ldots, a_{i,|U_i|}\}, \quad a_{i,1} < \cdots < a_{i,|U_i|},$$
$$\overline{U}_i = \{b_{i,1}, \ldots, b_{i,|\overline{U}_i|}\}, \quad b_{i,1} < \cdots < b_{i,|\overline{U}_i|},$$
$$G_i = \{\hat{a}_{i,1}, \ldots, \hat{a}_{i,|G_i|}\}, \quad \hat{a}_{i,1} < \cdots < \hat{a}_{i,|G_i|},$$
$$\overline{G}_i = \big\{\hat{b}_{i,1}, \ldots, \hat{b}_{i,|\overline{G}_i|}\big\}, \quad \hat{b}_{i,1} < \cdots < \hat{b}_{i,|\overline{G}_i|}.$$

Then,

$$\begin{aligned} &z_i(t+1) \\ &= [z_{a_{i,1}}(t)]\sigma_1[z_{a_{i,2}}(t)]\sigma_2 \cdots \sigma_{|U_i|-1}\big[z_{a_{i,|U_i|}}(t)\big] \\ &\quad \sigma_{|U_i|}[\bar{z}_{b_{i,1}}(t)]\sigma_{|U_i|+1}[\bar{z}_{b_{i,2}}(t)]\sigma_{|U_i|+2}\cdots \\ &\quad \sigma_{|U_i|+|\overline{U}_i|-1}\big[\bar{z}_{b_{i,|\overline{U}_i|}}(t)\big]\sigma_{|U_i|+|\overline{U}_i|}[v_{\hat{a}_{i,1}}(t)] \\ &\quad \hat{\sigma}_1[v_{\hat{a}_{i,2}}(t)]\hat{\sigma}_2\cdots\hat{\sigma}_{|G_i|-1}\big[v_{\hat{a}_{i,|G_i|}}(t)\big]\hat{\sigma}_{|G_i|} \\ &\quad \big[\bar{v}_{\hat{b}_{i,1}}(t)\big]\hat{\sigma}_{|G_i|+1}\big[\bar{v}_{\hat{b}_{i,2}}(t)\big]\hat{\sigma}_{|G_i|+2}\cdots \\ &\quad \hat{\sigma}_{|G_i|+|\overline{G}_i|-1}\big[\bar{v}_{\hat{b}_{i,|\overline{G}_i|}}(t)\big], \end{aligned} \tag{2}$$

where $\sigma_j \in \{\vee, \wedge\}$, $j = 1, \ldots, |U_i| + |\overline{U}_i|$, and $\hat{\sigma}_j \in \{\vee, \wedge\}$, $j = 1, \ldots, |G_i| + |\overline{G}_i| - 1$.

Given one possible choice of $\sigma_j \in \{\vee, \wedge\}$, $j = 1, \ldots, |U_i|+|\overline{U}_i|$, and $\hat{\sigma}_j \in \{\vee, \wedge\}$, $j = 1, \ldots, |G_i|+|\overline{G}_i| - 1$, by using the vector forms of logical variables we can convert (2) into the following form:

$$\begin{aligned} z_i(t+1) = Q_i \ltimes_{j=1}^{|U_i|} z_{a_{i,j}}(t) \ltimes_{j=1}^{|\overline{U}_i|} (M_n \ltimes z_{b_{i,j}}(t)) \\ \ltimes_{j=1}^{|G_i|} v_{\hat{a}_{i,j}}(t) \ltimes_{j=1}^{|\overline{G}_i|} (M_n \ltimes v_{\hat{b}_{i,j}}(t)), \end{aligned} \tag{3}$$

where Q_i is uniquely determined by the choice of $\sigma_j \in \{\vee, \wedge\}$, $j = 1, \ldots, |U_i|+|\overline{U}_i|$, and $\hat{\sigma}_j \in \{\vee, \wedge\}$, $j = 1, \ldots, |G_i| + |\overline{G}_i| - 1$. Thus, one can obtain $2^{|U_i|+|\overline{U}_i|+|G_i|+|\overline{G}_i|-1}$ different kinds of Q_i. The set of the $2^{|U_i|+|\overline{U}_i|+|G_i|+|\overline{G}_i|-1}$ different kinds of Q_i is denoted by Λ_i.

Using the pseudo-communicative law, swap matrix, power-reducing matrix, and dummy matrix [2], one can obtain a unique matrix P_i such that

$$\begin{aligned} \ltimes_{j=1}^{|U_i|} z_{a_{i,j}}(t) \ltimes_{j=1}^{|\overline{U}_i|} (M_n \ltimes z_{b_{i,j}}(t)) \ltimes_{j=1}^{|G_i|} \\ v_{\hat{a}_{i,j}}(t) \ltimes_{j=1}^{|\overline{G}_i|} (M_n \ltimes v_{\hat{b}_{i,j}}(t)) = P_i v(t) z(t), \end{aligned} \tag{4}$$

where P_i is uniquely determined by the network graph, $z(t) = \ltimes_{j=1}^{n} z_j(t)$, and $v(t) = \ltimes_{j=1}^{m} v_j(t)$.

Using the Khatri-Rao product of matrices, we obtain the following algebraic form of the system (1):

$$z(t+1) = Lv(t)z(t), \tag{5}$$

where

$$L \in \Gamma := \{*_{i=1}^{n}(Q_i \ltimes P_i) : Q_i \in \Lambda_i, i = 1, \ldots, n\}. \tag{6}$$

It is easy to see that

$$|\Gamma| = 2^{\sum_{i=1}^{n}(|U_i|+|\overline{U}_i|+|G_i|+|\overline{G}_i|)-n},$$

where $\Gamma = \{L_1, L_2, \ldots, L_{|\Gamma|}\}$.

We describe the concept of structural controllability for the system (1) as follows.

Definition 1. Consider the system (1). $z_d \in \Delta_{2^n}$ is said to be structurally reachable from $z_0 \in \Delta_{2^n}$, if for any structurally equivalent system $z(t+1) = Lv(t)z(t)$, with $L \in \Gamma$, z_d is reachable from z_0. The system (1) is said to be structurally controllable if for any $z_d \in \Delta_{2^n}$ and $z_0 \in \Delta_{2^n}$, z_d is structurally reachable from z_0.

Split each L_i, $i = 1, 2, \ldots, |\Gamma|$, into 2^m equal blocks as $L_i = [L_{i,1}\ L_{i,2}\ \cdots\ L_{i,2^m}]$, and set

$$\mathcal{C}_i = \underbrace{\sum_{r=1}^{2^{m+n}}}_{\mathcal{B}} (M_i)^{(r)},$$

where $M_i = \underbrace{\Sigma_{j=1}^{2^m}}_{\mathcal{B}} L_{i,j}$. Define

$$\mathcal{C} = \mathcal{C}_1 \circ \mathcal{C}_2 \circ \cdots \circ \mathcal{C}_{|\Gamma|}, \tag{7}$$

where "∘" denotes the Hadamard product of matrices. We call $\mathcal{C}$ the structural controllability matrix of the system (1).

Based on the structural controllability matrix, we present the following results for the structural controllability of system (1).

Theorem 1. $z_d = \delta_{2^n}^{\alpha}$ is structurally reachable from $z_0 = \delta_{2^n}^{\beta}$ if and only if $(\mathcal{C})_{\alpha,\beta} = 1$.

Proof. Suppose that $(\mathcal{C})_{\alpha,\beta} = 1$; that is, $(\mathcal{C}_i)_{\alpha,\beta} = 1$, $i = 1, 2, \ldots, |\Gamma|$. For any structurally equivalent system $z(t+1) = L_i v(t) z(t)$, $i = 1, 2, \ldots, |\Gamma|$, according to [4] $z_d = \delta_{2^n}^{\alpha}$ is reachable from $z_0 = \delta_{2^n}^{\beta}$ if and only if $(\mathcal{C}_i)_{\alpha,\beta} = 1$. Thus, by Definition 1 $z_d = \delta_{2^n}^{\alpha}$ is structurally reachable from $z_0 = \delta_{2^n}^{\beta}$.

Theorem 2. The system (1) is structurally controllable if and only if $\mathcal{C} = \mathbf{1}_{2^n \times 2^n}$.

Proof. The proof of Theorem 2 follows from Definition 1 and Theorem 1.

Finally, we study the structural controllability of a protein regulation network for apoptosis, the network graph of which is shown in Figure 1.

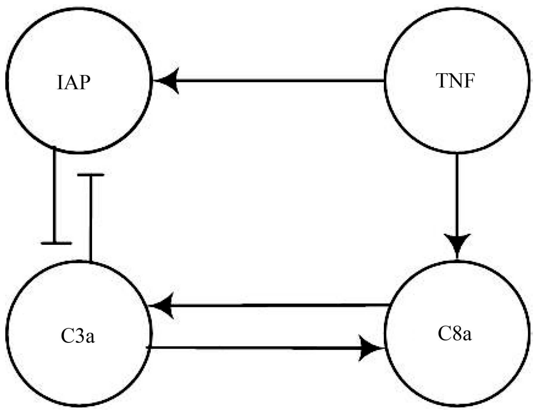

Figure 1 Protein regulation network for apoptosis.

Example 1. Consider the following protein regulation network for apoptosis:

$$\begin{cases} z_1(t+1) = f_1(\overline{z}_2(t), v(t)), \\ z_2(t+1) = f_2(\overline{z}_1(t), z_3(t)), \\ z_3(t+1) = f_3(z_2(t), v(t)), \end{cases} \tag{8}$$

where z_1, z_2, z_3, and v denote IAP, C3a, C8a, and TNF, respectively. The biological meanings of each node are given in [1].

Based on (3)–(6), we obtain the following algebraic form of system (8):

$$z(t+1) = Lv(t)z(t),$$

where $L \in \Gamma$, $\Gamma = \{L_1, L_2, L_3, L_4, L_5, L_6, L_7, L_8\}$, and

$$L_1 = \delta_8[7\ 7\ 4\ 4\ 5\ 7\ 2\ 4\ 8\ 8\ 8\ 8\ 6\ 8\ 6\ 8],$$
$$L_2 = \delta_8[7\ 7\ 3\ 3\ 5\ 7\ 1\ 3\ 7\ 7\ 8\ 8\ 5\ 7\ 6\ 8],$$
$$L_3 = \delta_8[5\ 7\ 2\ 4\ 5\ 5\ 2\ 2\ 6\ 8\ 6\ 8\ 6\ 6\ 6\ 6],$$
$$L_4 = \delta_8[5\ 7\ 1\ 3\ 5\ 5\ 1\ 1\ 5\ 7\ 6\ 8\ 5\ 5\ 6\ 6],$$
$$L_5 = \delta_8[3\ 3\ 4\ 4\ 1\ 3\ 2\ 4\ 8\ 8\ 4\ 4\ 6\ 8\ 2\ 4],$$
$$L_6 = \delta_8[3\ 3\ 3\ 3\ 1\ 3\ 1\ 3\ 7\ 7\ 4\ 4\ 5\ 7\ 2\ 4],$$
$$L_7 = \delta_8[1\ 3\ 2\ 4\ 1\ 1\ 2\ 2\ 6\ 8\ 2\ 4\ 6\ 6\ 2\ 2],$$
$$L_8 = \delta_8[1\ 3\ 1\ 3\ 1\ 1\ 1\ 1\ 5\ 7\ 2\ 4\ 5\ 5\ 2\ 2].$$

A straightforward calculation shows that

$$\mathcal{C} = \mathbf{0}_{8\times 8}.$$

By Theorem 2, the system (8) is not structurally controllable.

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