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Feedback Shaping for Boolean Networks

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Abstract: Boolean networks, as logical dynamical systems where the system states are Boolean variables, arise from applications in biology, computer networks, and social networks etc. In this paper, we present a framework to evaluate whether and how the closed-loop dynamics of a controlled Boolean network can be shaped into any prescribed form by state-feedback control. We refer to this problem as to the feedback shaping for Boolean networks. First of all, based on the linear representation of Boolean networks, we establish a necessary and sufficient rank condition for a controlled Boolean network to be feedback shapable or not. Next, we design an algorithm for the synthesis of closed-loop dynamics for a feedback shapable Boolean network, such that for any given controlled Boolean network and a desired closed-loop dynamics, one can always find a feedback control law so that the closed-loop dynamics is precisely realized.

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1. INTRODUCTION

1.1 Boolean Networks

Boolean networks were proposed by Kauffman in 1960s as a model to characterize the interactions between regulatory genes (Kauffman, 1969). Boolean networks are described by logical dynamics over a network, where each node holds a Boolean (logical) state in the set $\mathcal{B} := \{0, 1\}$ evolving over time. Then $x(t) = (x_1(t) \dots x_n(t))^\top$ is the vector of Boolean states over the network. The evolution of the network dynamics is described as

$$x(t + 1) = f(x(t)), \tag{1}$$

where f maps $\mathcal{B}^n$ to $\mathcal{B}^n$. When there is the presence of control inputs, system (1) becomes

$$x(t + 1) = f(x(t), u(t)), \tag{2}$$

where f maps $\mathcal{B}^{n+d}$ to $\mathcal{B}^n$. Here $u(t) \in \mathcal{B}^d$ is the control input at time t.

Boolean networks have also found applications in describing various system dynamics arising when modelling virus spreading and social opinion dynamics, e.g., van Mieghem et al. (2009); Green et al. (2007); Li et al. (2018). Cheng and Qi (2009, 2010) established a systematic way of representing logical dynamical systems (1) as linear systems based on a novel mathematical concept of semi-tensor product (Cheng et al., 2011). Classical control notions including controllability, observability, limit cycles, stabilizability, steady states, optimal control, etc., can be studied for Boolean networks under this linear-system representation, marking a significant research progress in recent years e.g., Cheng and Qi (2009, 2010); Li et al. (2013); Laschov and Margaliot (2012); Fornasini and Valcher (2013, 2014); Kobayashi and Hiraishi (2017); Zhou et al. (2019); Zhu et al. (2018); Li et al. (2021).

1.2 Linear Representation of Boolean Networks

In Qi et al. (2023), we established a Koopman approach for Boolean networks as a generalized linear system representation. The linear representations from Cheng and Qi (2009) and Qi et al. (2023) can be made consistent with those we propose by the following choice of logical indicator functions.

Definition 1. Let p be any integer. For any $[a] = [a_1 \dots a_p] \in \mathcal{B}^p$, the logical indicator function $\mathsf{g}_{[a]} : \mathcal{B}^p \to \mathcal{B}^p$ is defined as

$$\mathsf{g}_{[a]}([w]) = \begin{cases} 1, & \text{if } [w] = [a]; \\ 0, & \text{if } [w] \in \mathcal{B}^p \setminus \{[a]\}. \end{cases}$$

The key idea of Qi et al. (2023), the set of indicator functions $\mathcal{H}_p^*$ as defined in Definition 1 may be expanded to a linear space $\mathcal{S}(\mathcal{H}_p^*)$ by carefully introducing addition and scalar multiplication operations over the binary field. Such a linear space of logical functions is in fact universally Koopman invariant. As a result, any logical mapping from $\mathcal{B}^a$ to $\mathcal{B}^b$ can be represented as a finite-dimensional Koopman operator, or equivalently, by a $2^b \times 2^a$ matrix.

Definition 2. Let $h(x) : \{0, 1\}^p \to \{0, 1\}^q$ be a logical function. The Koopman operator for $h(\cdot)$, denoted by $\mathcal{K}_h$,

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is a mapping from $\mathcal{H}_q^*$ to $\mathcal{S}(\mathcal{H}_p^*)$, where by definition for any $[a]_q \in \{0,1\}^q \cup \{[\mathbf{0}]_q\}$

$$\mathcal{K}_h(\mathsf{g}_{[a]_q})([w]_p) = \mathsf{g}_{[a]_q}(h([w]_p)) = \begin{cases} 1 & \text{if } h([w]_p) = [a]_q; \\ 0 & \text{otherwise.} \end{cases} \tag{3}$$

Lemma 1. (Qi et al. (2023)) Define for any $[s]_q \in \{0,1\}^q \cup \{[\mathbf{0}]_q\}$ and $[k]_p \in \{0,1\}^p \cup \{[\mathbf{0}]_p\}$

$$\mathsf{H}_{[s]_q,[k]_p} = \begin{cases} 1 & \text{if } h([k]_p) = [s]_q; \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

There holds $\mathcal{K}_h(\mathsf{g}_{[a]_q}) = \sum_{[k]_p \in \{0,1\}^p} \mathsf{H}_{[s]_q,[k]_p} . \mathsf{g}_{[k]_p}$.

Set

$$\mathbf{x}(t) = \begin{bmatrix} \mathbf{x}_{[0,\dots,0]_n}(t) \\ \mathbf{x}_{[0,\dots,1]_n}(t) \\ \vdots \\ \mathbf{x}_{[1,\dots,1]_n}(t) \end{bmatrix} := \begin{bmatrix} \mathsf{g}_{[0,\dots,0]_n}(x(t)) \\ \mathsf{g}_{[0,\dots,1]_n}(x(t)) \\ \vdots \\ \mathsf{g}_{[1,\dots,1]_n}(x(t)) \end{bmatrix},$$
$$\mathbf{u}(t) = \begin{bmatrix} \mathbf{u}_{[0,\dots,0]_d}(t) \\ \mathbf{u}_{[0,\dots,1]_d}(t) \\ \vdots \\ \mathbf{u}_{[1,\dots,1]_d}(t) \end{bmatrix} := \begin{bmatrix} \mathsf{g}_{[0,\dots,0]_d}(u(t)) \\ \mathsf{g}_{[0,\dots,1]_d}(u(t)) \\ \vdots \\ \mathsf{g}_{[1,\dots,1]_d}(u(t)) \end{bmatrix}. \tag{5}$$

The following representation of Boolean networks can then be obtained using the notation defined above.

Theorem 1. (Cheng and Qi (2009, 2010); Qi et al. (2023)). (i) The Boolean network (1) can be equivalently represented as

$$\mathbf{x}(t+1) = \mathsf{F}\mathbf{x}(t),$$

where F is a $2^n \times 2^n$ matrix.

(ii) Let $\mathbf{x}(t) \otimes \mathbf{u}(t)$ be the Kronecker product of $\mathbf{x}(t)$ and $\mathbf{u}(t)$. The controlled Boolean network (2) can be equivalently represented as

$$\mathbf{x}(t+1) = \mathsf{F}_{\mathrm{OL}}\big(\mathbf{x}(t) \otimes \mathbf{u}(t)\big), \tag{6}$$

where F_{OL} is a $2^n \times 2^{n+d}$ matrix

1.3 Feedback Linearization and Full Actuation

Feedback linearization is an important concept in nonlinear control theory, where the power of feedback is also utilized to transform a nonlinear system into a linear one. For a dynamical system described by

$$\dot{x} = f(x) + G(x)u, \tag{7}$$

it may be possible to find a state feedback control $u = \alpha(x) + \beta(x)v$ and a change of variable $z = T(x)$, so that the closed-loop dynamics described by state z and input v becomes linear. Formally we have the following definition (Khalil, 2001).

Definition 3. System (7) with $f : D \to \mathbb{R}^n$ and $G : D \to \mathbb{R}^{n\times p}$ being smooth functions on a domain D in $\mathbb{R}^n$, is feedback linearizable if there exists a diffeomorphism $T : D \to \mathbb{R}^n$ such that system (7) is transformed into the form

$$\dot{z} = Az + B\gamma(x)(u - \alpha(x)) \tag{8}$$

with (A, B) controllable and $\gamma(x)$ nonsingular for every $x \in D$.

Fundamental algebraic conditions have been developed to determine when system (7) is feedback linearizable (Khalil, 2001; Duan, 2020, 2021). In particular, if $G(x)$ is right-invertible for every $x \in D$, i.e. $G(x)G^\top(x)$ is nonsingular for every $x \in D$, the system is called fully actuated. In this case, there is a direct solution for the feedback linearization given by $u = G^\top(x)(G(x)G^\top(x))^{-1}(v - f(x))$. The dynamics becomes $\dot{x} = v$, which is a first-order integrator. Then taking $v = h(x)$, the closed-loop dynamics can take any form of the type $\dot{x} = h(x)$ for any function h. In this sense, the plant dynamics has been fully reshaped.

1.4 Main Results

Noticing that full actuation by direct feedback linearization for system (7) represents the power of reshaping the closed-loop dynamics into any form in the context of nonlinear systems, we introduce the following definition.

Definition 4. System (2) is feedback shapable if for any mapping $q : \mathcal{B}^n \to \mathcal{B}^n$, there exist a bijection $T : \mathcal{B}^n \to \mathcal{B}^n$ and a feedback controller $u(t) = k(x(t))$ such that the closed-loop dynamics is transformed through the relation $z(t) = Tx(t)$ into the form

$$z(t+1) = q(z(t)). \tag{9}$$

We provide results on feedback shaping of Boolean networks from both theoretical and computational perspectives. First, based on the above linear representation of Boolean networks, we construct and prove a necessary and sufficient rank condition for a controlled Boolean network to be feedback shapable or not. Second, we show that the method can be extended to the design of a synthesis algorithm, based on which for any given controlled Boolean network and a desired closed-loop dynamics, we may always find a feedback control law such that the closed-loop dynamics is precisely realized. These results have generalized the understandings of feedback control for Boolean networks, and the presented algorithm may be useful in practical settings such as gene regulatory networks.

2. FEEDBACK SHAPING: A RANK CONDITION

In this section, we investigate conditions for the Boolean control system (2) to be feedback shapable.

We note that the bijection $T : \mathcal{B}^n \to \mathcal{B}^n$ in Definition 4 is also a logical mapping. As a result, there is a matrix representation of $T(\cdot)$ as $\mathsf{T} \in \mathbb{R}^{2^n\times 2^n}$. Moreover, a bijection from $\mathcal{B}^n$ to $\mathcal{B}^n$ has to be a permutation, which leads to the fact that T is a permutation matrix. That is, T is a normal matrix, and satisfies $\mathsf{T}\mathsf{T}^{-1} = \mathsf{T}\mathsf{T}^\top = \mathsf{I}_{2^n}$.

2.1 Algebraic Representations

Let $\mathsf{F}_{\mathrm{OL}} \in \mathbb{R}^{2^n\times 2^{n+d}}$, $\mathsf{K} \in \mathbb{R}^{2^d\times 2^n}$, and $\mathsf{Q} \in \mathbb{R}^{2^n\times 2^n}$ be the matrix representations of the logical mappings $f(\cdot), k(\cdot), q(\cdot)$, respectively, under the Koopman analysis in Subsection 4.1 of Qi et al. (2023). More precisely, we suppose system (2) can be represented by

$$\mathbf{x}(t+1) = \mathsf{F}_{\mathrm{OL}}\big(\mathbf{x}(t) \otimes \mathbf{u}(t)\big), \tag{10}$$

with $\mathbf{x}(t) \otimes \mathbf{u}(t)$ defined in (6).

We present the following lemma.

Lemma 2. Let the closed loop dynamics of system (2) under the feedback control $u(t) = k(x(t))$ be represented as $x(t+1) = f_{\rm CL}(x(t))$. Let $\mathsf{F}_{\rm CL}$ be the matrix representation of the logical mapping $f_{\rm CL}(\cdot)$. Then there exists a matrix $\mathsf{M}_{\rm dim} \in \mathbb{R}^{2^{2n} \times 2^n}$ such that

$$\mathsf{F}_{\rm CL} = \mathsf{F}_{\rm OL}(\mathsf{I}_{2^n} \otimes \mathsf{K})\mathsf{M}_{\rm dim}, \tag{11}$$

In fact, $\mathsf{M}_{\rm dim}$ is independent of $\mathsf{F}_{\rm OL}$ and K.

We also need to take care of a technicality arising from the Kronecker product $\mathsf{I}_{2^n} \otimes \mathsf{K}$. The following lemma holds as a special case of the classical theory on commutation matrices (Magnus and Neudecker, 1979).

Lemma 3. (Thm. 3.1 (ix), Magnus and Neudecker (1979)). For all $a \in \mathbb{R}^{2^n}$ and $b \in \mathbb{R}^{2^d}$, there is a permutation matrix $\mathsf{P} \in \mathbb{R}^{2^{n+d} \times 2^{n+d}}$ (with $\mathsf{P} = \mathsf{P}^\top = \mathsf{P}^{-1}$) such that $\mathsf{P}\big(a \otimes b\big) = b \otimes a$.

The permutation matrix P stated in Lemma 3 is termed a commutation matrix, and it can be explicitly computed when the dimensions n and d are given (Magnus and Neudecker, 1979).

2.2 Feedback Shaping Rank Condition

Taking P as the commutation matrix from Lemma 3, let us split $\mathsf{F}_{\rm OL}\mathsf{P}$ into 2^d blocks of size 2^n in the following form:

$$\mathsf{F}_{\rm OL}\mathsf{P} = \Big[\mathsf{F}_1^* \;\; \mathsf{F}_2^* \;\; \dots \;\; \mathsf{F}_{2^d}^*\Big]. \tag{12}$$

Furthermore, for $s = 1, \dots, 2^n$, we define the following sub-matrices of $\mathsf{F}_{\rm OL}\mathsf{P}$:

$$(\mathsf{F}_{\rm OL}\mathsf{P})_s := \big(\mathsf{F}_1^*[s] \;\; \mathsf{F}_2^*[s] \;\; \dots \;\; \mathsf{F}_{2^m}^*[s]\big) \in \mathbb{R}^{2^n \times 2^d}$$

where $\mathsf{F}_l^*[s]$ represents the sth column of F_l^*.

We are ready to present the following main result.

Theorem 2. System (2) is feedback shapable if and only if $\text{rank}((\mathsf{F}_{\rm OL}\mathsf{P})_s) = 2^n$ for all $s = 1, \dots, 2^n$.

It is clear from Theorem 2 that for system (2) to be feedback shapable, the rank condition requires $d \geq n$. This is consistent with classical nonlinear system theory, where the dimension of control input for a fully actuated system must be higher than that of the system state.

3. FEEDBACK DYNAMICS SYNTHESIS

Theorem 2 presents a theoretical guarantee regarding the full actuation of system (2). The problem remains of how to practically synthesize the feedback controller $u = k(x)$. Since from Theorem 2 the coordinate change T is not contributing to the solvability of feedback shaping, we define the following problem.

Problem. (Feedback Shaping Synthesis) Given system (2) and a desired closed-loop dynamics $x(t+1) = q(x(t))$, find a logical mapping $k(\cdot)$ from $\mathcal{B}^n$ to $\mathcal{B}^m$ such that the feedback controller $u(t) = k(x(t))$ applied to system (2) produces the closed-loop dynamics $x(t+1) = q(x(t))$.

3.1 Feedback Shaping Solvability

Under the matrix representations, from Lemma 2, the above feedback shaping synthesis problem is equivalent to the following one. Given fixed logical matrices $\mathsf{F}_{\rm OL} \in \mathbb{R}^{2^n \times 2^{n+m}}$ and $\mathsf{Q} \in \mathbb{R}^{2^n \times 2^n}$, can we compute a logical matrix $\mathsf{K} \in \mathbb{R}^{2^m \times 2^n}$ so that the following equality holds

$$\mathsf{Q} = \mathsf{F}_{\rm OL}(\mathsf{I}_{2^n} \otimes \mathsf{K})\mathsf{M}_{\rm dim}? \tag{13}$$

As a result, the feedback shaping synthesis under the matrix representation amounts to solving the matrix equation (13). Let us denote by $\mathsf{Q}[s] \in (\mathsf{F}_{\rm OL}\mathsf{P})_s$ one of the columns of $(\mathsf{F}_{\rm OL}\mathsf{P})_s$. The solvability of the feedback shaping synthesis problem is described in the following result.

Theorem 3. Let Q be the matrix representation of $q : \mathcal{B}^n \to \mathcal{B}^n$. There exists a feedback controller $u(t) = k(x(t))$ for system (2) that leads to the closed-loop dynamics $x(t+1) = q(x(t))$ if and only if $\mathsf{Q}[s] \in (\mathsf{F}_{\rm OL}\mathsf{P})_s$ for all $s = 1, \dots, 2^n$.

When condition $\mathsf{Q}[s] \in (\mathsf{F}_{\rm OL}\mathsf{P})_s$ holds for all $s = 1, \dots, 2^n$, there might be multiple feedback controllers $u(t) = k(x(t))$ such that the closed-loop dynamics of system (2) becomes $x(t+1) = q(x(t))$. Here we say that $u(t) = k_1(x(t))$ and $u(t) = k_2(x(t))$ are two distinct controllers if their matrix representations K_1 and K_2 are not identical. Introduce

$$\chi_s := \#_{\mathsf{Q}[s]}(\mathsf{F}_{\rm OL}\mathsf{P})_s,$$

where $\#_{\mathsf{Q}[s]}(\mathsf{F}_{\rm OL}\mathsf{P})_s$ denotes the number of columns in $(\mathsf{F}_{\rm OL}\mathsf{P})_s$ that are identical to $\mathsf{Q}[s]$. We present the following theorem counting the number of feedback controllers that solves the feedback controller synthesis problem.

Theorem 4. There exist $\Pi_{s=1}^{2^n}\chi_s$ distinct feedback controllers in the form of $u(t) = k(x(t))$ such that the closed-loop dynamics of system (2) becomes $x(t+1) = q(x(t))$.

3.2 Feedback Synthesis Algorithm

We first present the following algorithm that generates the Koopman matrix for a logical mapping $h(\cdot) : \mathcal{B}^p \to \mathcal{B}^q$, by summarizing the procedure in Section 5 of Qi et al. (2023).

Algorithm 1 Koopman Matrix Generation

Require: A Boolean mapping $h(\cdot) : \mathcal{B}^p \to \mathcal{B}^q$;
Ensure: A Koopman matrix $\mathsf{H} \in \mathbb{R}^{2^q \times 2^p}$ for h.
1: Compute $h([x])$ for $[x]_p = [0 \dots 0]_p, \dots, [1 \dots 1]_p$;
2: Compute the Koopman operator $\mathcal{K}_h(\mathsf{g}_{[a]_q})$ for $[a]_q = [0 \dots 0]_q, \dots, [1 \dots 1]_q$;
3: Compute $\mathsf{H}_{[a]_q,[k]_p}$ from $\mathcal{K}_h(\mathsf{g}_{[a]_q}) = \sum_{[k]_p \in \mathcal{B}^p} \mathsf{H}_{[a]_q,[k]_p}.\mathsf{g}_{[k]_p}$;
4: Generate the matrix H;
5: **return** H.

Next, we present Algorithm 2 for the feedback shaping synthesis problem. To this end, we define $\big|[a_1 \dots a_p]\big| = \sum_{s=1}^p 2^{p-s}a_s + 1$ for any logical element $[a_1 \dots a_p] \in \mathcal{B}^p$.

The correctness of Algorithm 2 is guaranteed by Lemma 5 and Lemma 6 (see the appendix).

3.3 Examples

We now provide a few examples illustrating Algorithm 2.

Example 4. Denote by $\bar{\vee}$ the logical XOR operator, and by $\leftrightarrow$ the logical equivalence operator, i.e., $a \leftrightarrow b = 1$ if and only if $a = b$ for $a, b \in \mathcal{B}$. Consider the following logical dynamical system

Algorithm 2 Feedback Dynamics Shaping

Require: A controlled logical system (2), and a target closed-loop dynamics $x(t+1) = q(x(t))$ with $q : \mathcal{B}^n \to \mathcal{B}^n$;

Ensure: A logical mapping $k(\cdot) : \mathcal{B}^d \to \mathcal{B}^n$ satisfying $f(x, u(x)) = q(x)$ for all $x \in \mathcal{B}^n$.

1: Compute the Koopman matrix F_{OL} for f and Q for q with Algorithm 1;
2: Compute the permutation matrix P, and then $(\mathsf{F}_{\mathrm{OL}}\mathsf{P})_s$ for $s = 1, \dots, 2^n$;
3: Verify if $\mathsf{Q}[s] \in (\mathsf{F}_{\mathrm{OL}}\mathsf{P})_s$ for all $s = 1, \dots, 2^n$. If not, **return** *unsolvable*; otherwise go to Step 4;
4: Assign $i_1, \dots, i_{2^n} \in \{1, \dots, 2^d\}$ such that $\mathsf{Q}[s] = (\mathsf{F}_{\mathrm{OL}}\mathsf{P})_s[i_s]$ for $s = 1, \dots, 2^n$, where $(\mathsf{F}_{\mathrm{OL}}\mathsf{P})_s[i_s]$ is the i_s-th column of $(\mathsf{F}_{\mathrm{OL}}\mathsf{P})_s$;
5: Compute the matrix $\mathsf{K} \in \mathbb{R}^{2^d \times 2^n}$ by assuming $\mathsf{K}_{[u]_d, [x]_n} = 1$ if $\big|[u]_d\big| = i_{|[x]_n|}$ for $[u]_d \in \mathcal{B}^d$ and $[x]_n \in \mathcal{B}^n$, and $\mathsf{K}_{[u]_d, [x]_n} = 0$ otherwise;
6: Construct the logical mapping $k(\cdot) : \mathcal{B}^d \to \mathcal{B}^n$ from K by assuming $k([x]_n) = [u]_d$ when $\mathsf{K}_{[y]_n [x]_d} = 1$;
7: **return** $k(\cdot)$.

$$\begin{cases} x_1(t+1) = (x_1(t) \vee x_2(t)) \bar{\vee} u_1(t), \\ x_2(t+1) = \neg x_1(t) \leftrightarrow u_2(t), \\ x_3(t+1) = x_2(t) \vee u_3(t). \end{cases} \tag{14}$$

We may compute F_{OL} from Algorithm 1 and then obtain

$$(\mathsf{F}_{\mathrm{OL}}\mathsf{P})_3 = \begin{bmatrix} 0&0&0&0&0&0&0&0 \\ 1&1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&1&1&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&1&1&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&1&1 \end{bmatrix}$$

We can verify that $\mathrm{rank}((\mathsf{F}_{\mathrm{OL}}\mathsf{P})_3) = 4$, and hence it does not fulfill the rank condition in Theorem 2. System (14) is therefore not feedback shapable. In fact, we may conclude that system (14) is not feedback shapable because it is impossible to find any feedback controller $u(t) = k(x(t))$ such that the closed-loop dynamics of the x_3 entry becomes

$$x_3(t+1) = \neg x_2(t).$$

It is also worth mentioning that system (14) is however controllable (Cheng and Qi, 2009) in the sense that for any $\mathsf{x}^0 = (\mathsf{x}_1^0, \mathsf{x}_2^0, \mathsf{x}_3^0) \in \mathcal{B}^3$ and $\mathsf{x}^d = (\mathsf{x}_d^0, \mathsf{x}_2^d, \mathsf{x}_3^d) \in \mathcal{B}^3$, there exist an integer $t_f > 0$ and $u(0), \dots, u(t_f - 1)$ such that system (14) starting from $x(0) = \mathsf{x}^0$ will reach $x(t_f) = \mathsf{x}^d$. □

Example 5. Consider the following logical dynamic system

$$\begin{cases} x_1(t+1) = (x_1(t) \vee x_2(t)) \bar{\vee} u_1(t), \\ x_2(t+1) = \neg x_1(t) \leftrightarrow u_2(t), \end{cases} \tag{15}$$

Again we may compute F_{OL} from Algorithm 1 and then

$$(\mathsf{F}_{\mathrm{OL}}\mathsf{P})_1 = \begin{bmatrix} 0&0&1&0 \\ 0&0&0&1 \\ 1&0&0&0 \\ 0&1&0&0 \end{bmatrix}, \quad (\mathsf{F}_{\mathrm{OL}}\mathsf{P})_2 = \begin{bmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&1&0 \\ 0&0&0&1 \end{bmatrix},$$

$$(\mathsf{F}_{\mathrm{OL}}\mathsf{P})_3 = \begin{bmatrix} 0&1&0&0 \\ 1&0&0&0 \\ 0&0&0&1 \\ 0&0&1&0 \end{bmatrix}, \quad (\mathsf{F}_{\mathrm{OL}}\mathsf{P})_4 = \begin{bmatrix} 0&1&0&0 \\ 1&0&0&0 \\ 0&0&0&1 \\ 0&0&1&0 \end{bmatrix}.$$

The rank condition in Theorem 2 is satisfied. Therefore, system (15) is feedback shapable.

Now, let us propose the closed-loop dynamics $x(t+1) = q(x(t))$ in the following form

$$\begin{cases} x_1(t+1) = x_1(t) \wedge x_2(t), \\ x_2(t+1) = x_1(t) \vee x_2(t). \end{cases} \tag{16}$$

By Algorithm 1 we obtain

$$\mathsf{Q} = \begin{bmatrix} 1&0&0&0 \\ 0&1&1&0 \\ 0&0&0&0 \\ 0&0&0&1 \end{bmatrix}.$$

The goal is then to find a feedback controller $u(t) = k(x(t))$ such that substituting $u(t) = k(x(t))$ into (15) will result in (16). We illustrate the remainder for the procedure of Algorithm 2 in the following.

Step 4: The indices $i_1, \dots, i_4$ can be chosen as $i_1 = 3, i_2 = 2, i_3 = 1, i_4 = 3$.

Step 5: The matrix K is computed from $i_1 = 3, i_2 = 2, i_3 = 1, i_4 = 3$ as

$$\mathsf{K} = \begin{bmatrix} 0&0&1&0 \\ 0&1&0&0 \\ 1&0&0&1 \\ 0&0&0&0 \end{bmatrix}$$

Step 6: The logical mapping $k(\cdot)$ for the feedback controller is obtained as indicated in the table below:

x_1	x_2	u_1	u_2
0	0	1	1
0	1	0	1
1	0	0	0
1	1	1	0

We can verify that (13) is satisfied, and thus we have illustrated the procedure and verified the correctness of Algorithm 2. □

4. CONCLUSIONS

We have established a theory to check whether the closed-loop dynamics of a controlled Boolean network can be shaped into any prescribed form via state-feedback control. Based on the linear representation of Boolean networks, a necessary and sufficient rank condition was established for a controlled Boolean network to be feedback shapable or not. The approach was also extended to synthesize a feedback controller for a feedback shapable Boolean network, where for any given controlled Boolean network and desired closed-loop dynamics, we may always find a feedback control law such that the closed-loop dynamics is achieved.

APPENDICES

A. Proof of Lemma 2

The closed-loop dynamics of system (2) under the feedback control $u(t) = k(x(t))$ is given by

$$\begin{aligned}\mathbf{x}(t+1) &= \mathsf{F}_{\mathrm{OL}}\big(\mathbf{x}(t)\otimes\mathbf{u}(t)\big)\\ &= \mathsf{F}_{\mathrm{OL}}\big(\mathbf{x}(t)\otimes\mathsf{K}\mathbf{x}(t)\big)\\ &= \mathsf{F}_{\mathrm{OL}}(\mathsf{I}_{2^n}\otimes\mathsf{K})\big(\mathbf{x}(t)\otimes\mathbf{x}(t)\big) \qquad (17)\end{aligned}$$

where the third identity follows from the basic property of Kronecker product: $(\mathsf{AB})\otimes(\mathsf{BD}) = (\mathsf{A}\otimes\mathsf{B})(\mathsf{C}\otimes\mathsf{D})$ for matrices $\mathsf{A},\mathsf{B},\mathsf{C},\mathsf{D}$ with proper dimensions.

Now, as $\mathbf{x}(t)$ is a vector of zeros and ones which contains only one non-zero element, there is a one-to-one mapping between the vectors in form of $\mathbf{x}(t)\otimes\mathbf{x}(t)$ and the vectors $\mathbf{x}(t)$. Moreover, the elements of the form $\mathbf{x}(t)\otimes\mathbf{x}(t)$ can be viewed as the basis of a linear subspace in $\mathbb{R}^{2^{2n}}$, while the elements of the form $\mathbf{x}(t)$ can be viewed as the basis of $\mathbb{R}^{2^n}$. Such a one-to-one mapping can be viewed as a linear mapping between the two subspaces in $\mathbb{R}^{2^n}$ and $\mathbb{R}^{2^{2n}}$, which can be represented by a matrix $\mathsf{M}_{\dim}\in\mathbb{R}^{2^{2n}\times 2^n}$ in

$$\mathsf{M}_{\dim}\mathbf{x}(t) = \mathbf{x}(t)\otimes\mathbf{x}(t). \qquad (18)$$

Substituting (18) into (17) leads to

$$\begin{aligned}\mathbf{x}(t+1) &= \mathsf{F}_{\mathrm{OL}}(\mathsf{I}_{2^n}\otimes\mathsf{K})\big(\mathbf{x}(t)\otimes\mathbf{x}(t)\big)\\ &= \mathsf{F}_{\mathrm{OL}}(\mathsf{I}_{2^n}\otimes\mathsf{K})\mathsf{M}_{\dim}\mathbf{x}(t).\end{aligned} \qquad (19)$$

This proves the desired lemma. Please note that the same matrix $\mathsf{M}_{\dim}$ has been obtained with the semi-tensor product approach in Cheng and Qi (2009, 2010), where it is called the power-reducing matrix. Here we provide a self-contained proof.

B. Proof of Theorem 2

We say that a matrix is a logical matrix if all its elements are either zero or one, and there is exactly one non-zero element in each column. First of all, we understand from Lemma 2 that system (2) being feedback shapable is equivalent to the following algebraic condition:

C*: For any $2^n\times 2^n$ logical matrix Q, there exist logical matrices K (of dimension $2^d\times 2^n$) and T (of dimension $2^n\times 2^n$) such that (i) T is a permutation; (ii) there holds $\mathsf{TQT}^{-1} = \mathsf{F}_{\mathrm{OL}}(\mathsf{I}_{2^n}\otimes\mathsf{K})\mathsf{M}_{\dim}$.

Next, we establish a few structural properties of the matrix $\mathsf{F}_{\mathrm{OL}}(\mathsf{I}_{2^n}\otimes\mathsf{K})$.

Lemma 4. Let P be the commutation matrix introduced in Lemma 3. There holds $\mathsf{F}_{\mathrm{OL}}(\mathsf{I}_{2^n}\otimes\mathsf{K})\mathsf{M}_{\dim} = \mathsf{F}_{\mathrm{OL}}\mathsf{P}(\mathsf{K}\otimes\mathsf{I}_{2^n})\mathsf{M}_{\dim}$.

Proof. In view of Lemma 3 and (17), the closed-loop dynamics of system (2) under the feedback control $u(t) = k(x(t))$ can be represented as

$$\begin{aligned}\mathbf{x}(t+1) &= \mathsf{F}_{\mathrm{OL}}\big(\mathbf{x}(t)\otimes\mathbf{u}(t)\big)\\ &= \mathsf{F}_{\mathrm{OL}}\mathsf{P}\big(\mathbf{u}(t)\otimes\mathbf{x}(t)\big)\\ &= \mathsf{F}_{\mathrm{OL}}\mathsf{P}\big(\mathsf{K}\mathbf{x}(t)\otimes\mathbf{x}(t)\big)\\ &= \mathsf{F}_{\mathrm{OL}}\mathsf{P}(\mathsf{K}\otimes\mathsf{I}_{2^n})\big(\mathbf{x}(t)\otimes\mathbf{x}(t)\big)\\ &= \mathsf{F}_{\mathrm{OL}}\mathsf{P}(\mathsf{K}\otimes\mathsf{I}_{2^n})\mathsf{M}_{\dim}\mathbf{x}(t). \qquad (20)\end{aligned}$$

Now as (19) and (20) represent the same dynamics, while $\mathbf{x}(t)$ can be any 2^n-dimensional unit vector with only one non-zero element, the desired lemma holds. □

Lemma 5. For any given logical matrix $\mathsf{K}\in\mathbb{R}^{2^d\times 2^n}$, there exist $i_1,\ldots,i_{2^n}\in\{1,\ldots,2^d\}$ such that

$$\mathsf{F}_{\mathrm{OL}}\mathsf{P}(\mathsf{K}\otimes\mathsf{I}_{2^n}) = \Big[\mathsf{F}^*_{i_1}\ \ \mathsf{F}^*_{i_2}\ \ \ldots\ \ \mathsf{F}^*_{i_{2^n}}\Big]. \qquad (21)$$

Conversely, for any $i_1,\ldots,i_{2^n}\in\{1,\ldots,2^d\}$, there exists a logical matrix $\mathsf{K}\in\mathbb{R}^{2^d\times 2^n}$ such that (21) holds.

Proof. There holds

$$\begin{aligned}\mathsf{F}_{\mathrm{OL}}\mathsf{P}(\mathsf{K}\otimes\mathsf{I}_{2^n}) &= \Big(\mathsf{F}^*_1\ \ \mathsf{F}^*_2\ \ \ldots\ \ \mathsf{F}^*_{2^n}\Big)\times\\ &\begin{pmatrix}\mathsf{K}_{11}\mathsf{I}_{2^n} & \mathsf{K}_{12}\mathsf{I}_{2^n} & \ldots & \mathsf{K}_{12^n}\mathsf{I}_{2^n}\\ \mathsf{K}_{21}\mathsf{I}_{2^n} & \mathsf{K}_{22}\mathsf{I}_{2^n} & \ldots & \mathsf{K}_{22^n}\mathsf{I}_{2^n}\\ \vdots & \vdots & \ldots & \vdots\\ \mathsf{K}_{2^d1}\mathsf{I}_{2^n} & \mathsf{K}_{2^d2}\mathsf{I}_{2^n} & \ldots & \mathsf{K}_{2^d2^n}\mathsf{I}_{2^n}\end{pmatrix} \qquad (22)\\ &= \Big[\mathsf{F}^*_{i_1}\ \ \mathsf{F}^*_{i_2}\ \ \ldots\ \ \mathsf{F}^*_{i_{2^n}}\Big],\end{aligned}$$

where $\mathsf{F}^*_{i_k} = \sum_{j=1}^{2^d}\mathsf{F}^*_j\mathsf{K}_{kj}$, $k = 1,\ldots,2^n$. The fact that there must exist $i_k\in\{1,\ldots,2^d\}$ such that $\mathsf{F}^*_{i_k} = \sum_{j=1}^{2^d}\mathsf{F}^*_j\mathsf{K}_{kj}$ is due to the structure of the matrix K, where each column of K contains exactly one non-zero element. The converse statement can be similarly established. This proves the desired lemma. □

Lemma 5 indicates that by multiplying $\mathsf{K}\otimes\mathsf{I}_{2^n}$ from the right to F_{OL}, effectively we are selecting blocks from $\mathsf{F}^*_1,\ldots,\mathsf{F}^*_{2^m}$ in (12). Note that $i_1,\ldots,i_{2^n}$ may take identical values. Then we have the following lemma on the role of the matrix $\mathsf{M}_{\dim}$.

Lemma 6. There exist $i_1,\ldots,i_{2^n}\in\{1,\ldots,2^d\}$ such that

$$\mathsf{F}_{\mathrm{OL}}\mathsf{P}(\mathsf{K}\otimes\mathsf{I}_{2^n})\mathsf{M}_{\dim} = \Big[\mathsf{F}^*_{i_1}[1]\ \ \mathsf{F}^*_{i_2}[2]\ \ \ldots\ \ \mathsf{F}^*_{i_{2^n}}[2^n]\Big], \qquad (23)$$

where $\mathsf{F}^*_{i_s}[s]$ denotes the s-th column of $\mathsf{F}^*_{i_s}$.

Proof. From Lemma 2, we know that $\mathsf{M}_{\dim}$ is the matrix representation of the linear mapping that maps the vectors in the form $\mathbf{x}(t)\otimes\mathbf{x}(t)$ to vectors in the form of $\mathbf{x}(t)$. Now, we write the vectors in the form $\mathbf{x}(t)$ in the standard order from $(1,0,\ldots,0)^\top$ to $(0,0,\ldots,1)^\top$, which implies a corresponding order for vectors in the form $\mathbf{x}(t)\otimes\mathbf{x}(t)$ from $(1,0,\ldots,0)^\top\otimes(1,0,\ldots,0)^\top$ to $(1,0,\ldots,1)^\top\otimes(0,0,\ldots,1)^\top$. As a result, the matrix $\mathsf{M}_{\dim}$ has the special structure

$$\mathsf{M}_{\dim} = \begin{pmatrix}\mathsf{m}_1 & 0 & \ldots & 0\\ 0 & \mathsf{m}_2 & \ldots & 0\\ \vdots & \vdots & \ldots & \vdots\\ 0 & 0 & \ldots & \mathsf{m}_{2^n}\end{pmatrix} \qquad (24)$$

where each m_k is a 2^n dimensional column vector with the kth element being one and all other elements being zero, and each 0 is a 2^n dimensional zero column vector. The desired lemma is then a direct consequence of Lemma 5 and (24). □

We are now ready to prove that C* is equivalent to the condition that $\mathrm{rank}((\mathsf{F}_{\mathrm{OL}}\mathsf{P})_s) = 2^n$ for all $s = 1,\ldots,2^n$, and thus establish Theorem 2.

(*Sufficiency*). Let Q be any logical function with dimension $2^n\times 2^n$. Suppose that $\mathrm{rank}((\mathsf{F}_{\mathrm{OL}}\mathsf{P})_s) = 2^n$ for all $s =$

$1, \ldots, 2^n$. Take $\mathsf{T} = \mathsf{I}_{2^n}$. As a result, for any column $\mathsf{Q}[j]$ of Q, there holds

$$\mathsf{Q}[j] \in (\mathsf{F}_{\rm OL}\mathsf{P})_s$$

for all $s = 1, \ldots, 2^n$. In other words, there exist $i_1, \ldots, i_{2^n} \in \{1, \ldots, 2^d\}$ such that

$$\mathsf{Q}[1] = \mathsf{F}^*_{i_1}[1], \quad \mathsf{Q}[2] = \mathsf{F}^*_{i_2}[2], \quad \ldots, \mathsf{Q}[2^n] = \mathsf{F}^*_{i_{2^n}}[2^n].$$

Now we apply Lemma 5 to construct the logical matrix K such that (21) holds. In turn, from Lemma 4 and Lemma 6 we know that

$$\begin{aligned} &\mathsf{F}_{\rm OL}(\mathsf{I}_{2^n} \otimes \mathsf{K})\mathsf{M}_{\rm dim} = \mathsf{F}_{\rm OL}\mathsf{P}(\mathsf{K} \otimes \mathsf{I}_{2^n})\mathsf{M}_{\rm dim} \\ &= \begin{bmatrix} \mathsf{F}^*_{i_1}[1] & \mathsf{F}^*_{i_2}[2] & \ldots & \mathsf{F}^*_{i_{2^n}}[2^n] \end{bmatrix} = \mathsf{Q}. \end{aligned} \tag{25}$$

The sufficiency of the theorem has been established.

(*Necessity*). We prove the necessity statement by a contradiction argument. Suppose there exists $\tau \in \{1, \ldots, 2^n\}$ such that $\mathrm{rank}((\mathsf{F}_{\rm OL}\mathsf{P})_\tau) < 2^n$. This means that there must exist a unit vector β, which contains only one nonzero element as one, such that β is not one of the columns of $(\mathsf{F}_{\rm OL}\mathsf{P})_\tau$. We construct Q^* by assuming

$$\mathsf{Q}^*[1] = \mathsf{Q}^*[2] = \cdots = \mathsf{Q}^*[2^n] = \beta.$$

As a result, no matter how we select the permutation matrix T, there holds $\mathsf{T}\mathsf{Q}^*\mathsf{T}^{-1} = \mathsf{Q}^*$, ie., the τth column of $\mathsf{T}\mathsf{Q}^*\mathsf{T}^{-1}$ will remain equal to β, which will not be one of the columns of $\mathsf{F}_{\rm OL}[\tau]$. Thus, it is impossible to have

$$\mathsf{Q}^* = \mathsf{T}\mathsf{Q}^*\mathsf{T}^{-1} = \begin{bmatrix} \mathsf{F}^*_{i_1}[1] & \mathsf{F}^*_{i_2}[2] & \ldots & \mathsf{F}^*_{i_{2^n}}[2^n] \end{bmatrix}.$$

for certain $i_1, \ldots, i_{2^n} \in \{1, \ldots, 2^d\}$ and T. Based on Lemma 6, it is impossible to have K and T such that

$$\mathsf{T}\mathsf{Q}^*\mathsf{T}^{-1} = \mathsf{F}_{\rm OL}(\mathsf{I}_{2^n} \otimes \mathsf{K})\mathsf{M}_{\rm dim}.$$

Recalling condition C*, we have established the proof of the necessity statement of Theorem 1.

C. Proof of Theorem 3

We only need to verify the conditions under which the identity (13) can be satisfied for a selected K, given $\mathsf{F}_{\rm OL}$ and Q. There exists K such that (13) holds if and only if there exist $i_1, \ldots, i_{2^n}$ such that

$$\begin{bmatrix} \mathsf{F}^*_{i_1}[1] & \mathsf{F}^*_{i_2}[2] & \ldots & \mathsf{F}^*_{i_{2^n}}[2^n] \end{bmatrix} = \mathsf{Q}. \tag{26}$$

The desired theorem immediately holds.

D. Proof of Theorem 4

The number of feedback controllers $u(t) = k(x(t))$ guaranteeing that the closed-loop dynamics of system (2) becomes $x(t+1) = q(x(t))$ is equal to the number of choices for $(i_1, \ldots, i_{2^n})$, $i_k \in \{1, \ldots, 2^d\}$ under which (26) holds. The desired theorem is straightforward to verify.

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