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Koopman Representation for Boolean Networks

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Abstract: Boolean networks, as logical dynamical systems whose system states are Boolean variables, arise from applications in biology, computer networks, and social networks etc. The representation and control of Boolean networks have attracted a lot of attention in recent years. On a parallel line of research, Koopman developed an operator view of nonlinear dynamical systems in early 1930s, which shows that using observable functions all nonlinear dynamics can be represented as (infinite dimensional) linear systems. In this paper, we present a framework for representing Boolean networks via Koopman approach. First of all, we construct addition and scalar multiplication operations over the set of logical functions over the binary field, defining a linear Boolean function space. Then associated with any Boolean mapping, the induced Koopman operator is defined as an operator over such Boolean function space. Next, we show that if there exists a set of logical functions that are invariant in the Koopman sense, a Boolean network can be represented by a finite-dimensional linear system. This Koopman perspective for Boolean networks is also extended to controlled Boolean networks.

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1. INTRODUCTION

1.1 Boolean Networks

A Boolean network consists of n nodes, each of which has a logical state taking values in the set $\mathcal{B} := \{0, 1\}$ and evolving over time. The state of node i at time t, $t = 0, 1, 2, \dots$ is represented by $x_i(t) \in \mathcal{B}$. The evolution of the overall system is described by the following equations:

$$\begin{cases} x_1(t+1) = f_1(x_1(t), x_2(t), \cdots, x_n(t)), \\ \quad \vdots \\ x_n(t+1) = f_n(x_1(t), x_2(t), \cdots, x_n(t)), \end{cases} \tag{1}$$

where f_i, $i = 1, \cdots, n$, are logical functions from $\mathcal{B}^n$ to $\mathcal{B}$. Upon setting $x(t) = (x_1(t) \dots x_n(t))^\top$, system (1) can be written as

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

where f is a map from $\mathcal{B}^n$ to $\mathcal{B}^n$. When a logical dynamical system is affected by external control inputs, it becomes

$$x(t+1) = f(x(t), u(t)) \tag{3}$$

where f is a map from $\mathcal{B}^{n+d}$ to $\mathcal{B}^n$, and $u(t) \in \mathcal{B}^d$ is the control input at time t.

Boolean networks as logical dynamical systems described as in (2) were proposed by Kauffman in 1960s in a probabilistic setting for the study of interactions between regulatory genes (Kauffman, 1969). In recent years, logical dynamical systems have become a useful tool in contexts such as virus spreading, gene evolution, and social opinion dynamics, e.g., van Mieghem et al. (2009); Shmulevich et al. (2003); Green et al. (2007); Li et al. (2018). In Cheng and Qi (2009, 2010), a systematic way of representing the logical dynamical system (2) by means of linear systems was developed. Their approach was based on a novel concept of semi-tensor product of matrices (Cheng et al., 2011), which generalizes the conventional matrix (vector) products by allowing for products between matrices (vectors) with arbitrary dimensions. This matrix representation has been proven useful in studying various properties of logical systems such as controllability, observability, limit cycles, stabilizability, steady states, optimal control, etc., e.g., Cheng and Qi (2009, 2010); Li et al. (2013); Laschov and Margaliot (2012); Fornasini and Valcher (2014); Kobayashi and Hiraishi (2017); Zhou et al. (2019); Zhu et al. (2018); Li et al. (2021).

1.2 Koopman Analysis

In the 1930s, Koopman brought out an operator perspective on nonlinear dynamical systems by inspecting the evolution of certain observable functions along the system dynamics, instead of the system dynamics themselves (Koopman, 1931; Koopman and von Neumann, 1932). The

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resulting Koopman analysis has to be performed over an infinite dimensional space of observable functions, while leading to the advantage of having linear dynamics. In recent years, Koopman analysis gained new attention as a powerful way for carrying out nonlinear system analysis, feedback control, and identification, using linear system tools (Brunton et al., 2016; Lan and Mezić, 2013; Korda and Mezić, 2018; Takeishi et al., 2013; Williams et al., 2016). The basic idea behind Koopman operator can be illustrated on the following discrete-time autonomous dynamical system

$$\mathbf{x}(t+1) = \mathbf{f}(\mathbf{x}(t)) \tag{4}$$

where $\mathbf{x}(t) \in \mathbb{R}^m$ is a real-valued dynamical state, and $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ is a nonlinear mapping.

Consider a Hilbert space $\mathcal{H}$, each element of which is a function $\mathbf{g} : \mathbb{R}^m \to \mathbb{R}$. The functions in the space $\mathcal{H}$ are termed observable functions. Then system (4) induces the following operator $\mathcal{K}_{\mathbf{f}}$, termed the Koopman operator w.r.t $\mathbf{f}(\cdot)$, that acts over the space $\mathcal{H}$ as $\mathcal{K}_{\mathbf{f}}(\mathbf{g}) = \mathbf{g} \circ \mathbf{f}$, where $\circ$ is the composition given by

$$\mathbf{g} \circ \mathbf{f}(a) = \mathbf{g}(\mathbf{f}(a)), \quad \forall a \in \mathbb{R}^m. \tag{5}$$

One can verify that the operator $\mathcal{K}_{\mathbf{f}}$ is, as a matter of fact, linear. The space $\mathcal{H}$ is Koopman invariant if it holds $\mathcal{K}_{\mathbf{f}}(\mathbf{g}) \in \mathcal{H}$ for all $\mathbf{g} \in \mathcal{H}$, see e.g., Brunton et al. (2016). In this case we can select a basis of observable functions for $\mathcal{H}$, denoted by $\{\mathbf{g}_k\}_{k=1}^{\infty}$, and then define $\mathbf{y}_k(t) = \mathbf{g}_k(\mathbf{x}(t))$. The dynamics of $\mathbf{y}(t) = (\mathbf{y}_1(t), \mathbf{y}_2(t), \dots), t = 0, 1, \dots$ forms an infinite dimensional linear system.

1.3 Main Results

First of all, we construct a linear structure on logical functions over the binary field, based on which the induced Koopman operator is defined for any logical mapping over such a logical function space. Next, we show that for a Boolean network, the presence of a set of logical functions that are invariant in the Koopman sense will allow the Boolean network to be represented as a finite-dimensional linear system. These results are presented in Section 3. Then Section 4 constructs a set of logical indicator functions which is proven to be universally Koopman invariant. As a result, we manage to show that any Boolean network can be represented as a linear system in the classical sense. This Koopman representation covers the semi-tensor product approach for Boolean network representation as a special case (Cheng and Qi, 2009, 2010). Finally, in Section 5, we extend the Koopman analysis to controlled logical systems by generalizing the Koopman operator definition to general logical functions with different dimensions for domain and co-domain. All the proofs are put in the appendices.

2. PROBLEM DEFINITION

2.1 Matrix Representation of Boolean Networks

A brief and simplified introduction to the matrix representation of Boolean networks by semi-tensor product (Cheng and Qi, 2009, 2010) can be presented as follows.

Logical states as vectors. Let $h(x) : \mathcal{B}^p \to \mathcal{B}^p$ be a logical function, and denote by δ_l^i the i-th column of the identity matrix I_l. Then we can define a one-to-one mapping ϕ_l from $\mathcal{B}^l$ to $\{\delta_{2^l}^i : i = 1, \dots, 2^l\}$ in the following way:

(i) For $l = 1$, we define $\phi_1(0) = \delta_2^1$ and $\phi_1(1) = \delta_2^2$;
(ii) For $l = s$ we define $\phi_s([a_1 a_2 \dots a_s]) = \phi_1(a_1) \otimes \phi_1(a_2) \otimes \cdots \otimes \phi_1(a_s)$, where $a_1, a_2, \dots, a_s \in \mathcal{B}$, and $\otimes$ stands for the Kronecker (tensor) product.

Logical mappings as matrices. Based on the above representation of logical states as vectors, it is easy to verify the commuting diagram in Fig. 1. From the diagram, a logical mapping $y = h(x)$ with $x \in \mathcal{B}^p$ and $y \in \mathcal{B}^p$ has been equivalently represented as $\mathcal{Y} = \mathsf{M}_h \mathcal{X}$, where $\mathcal{X} = \phi_p(x) \in \mathbb{R}^{2^p}$, $\mathcal{Y} = \phi_p(y) \in \mathbb{R}^{2^p}$, and $\mathsf{M}_h \in \mathbb{R}^{2^p \times 2^p}$. The matrix M_h is a sparse matrix with a special structure: each column of M_h contains only one nonzero element which must be unitary.

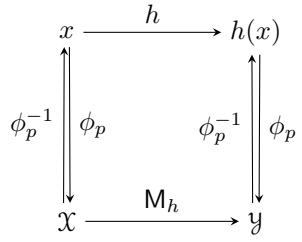

Figure 1. The commutative diagram for mappings over the logical spaces and the vector spaces.

Logical dynamics as linear systems. For system (2), we can map $x(t)$ to $\mathcal{X}(t)$ through the mapping ϕ_n, and there will be a matrix $\mathsf{M}_f \in \mathbb{R}^{2^n \times 2^n}$ such that the system dynamics is represented as

$$\mathcal{X}(t+1) = \mathsf{M}_f \mathcal{X}(t). \tag{6}$$

2.2 Koopman Representation of Nonlinear Systems

Let us revisit system (4), and suppose $\mathcal{H}$ is Koopman invariant under the Koopman operator $\mathcal{K}_{\mathbf{f}}$. Take $\{\mathbf{g}_s\}_{s=1}^{\infty}$ as a basis of the observable function space $\mathcal{H}$. Introduce $\mathbf{y}_k(t) = \mathbf{g}_k(\mathbf{x}(t))$ for $k = 1, 2, \dots$, which are the observed values of the observable function $\mathbf{g}_k$ along the evolution of system (4). Then according to the above definitions we have

$$\begin{aligned} \mathbf{y}_k(t+1) &= \mathbf{g}_k(\mathbf{x}(t+1)) = \mathbf{g}_k(\mathbf{f}(\mathbf{x}(t))) = \mathcal{K}_{\mathbf{f}}(\mathbf{g}_k)(\mathbf{x}(t)) \\ &= \sum_{s=1}^{\infty} \mathsf{K}_{ks} \mathbf{g}_s(\mathbf{x}(t)) = \sum_{s=1}^{\infty} \mathsf{K}_{ks} \mathbf{y}_s(t). \end{aligned} \tag{7}$$

Here $\mathsf{K}_{ks} \in \mathbb{R}, s = 1, 2, \dots$ are the coefficients of the linear representation of $\mathcal{K}_{\mathbf{f}}(\mathbf{g}_k)$ with respect to the basis $\{\mathbf{g}_s\}_{s=1}^{\infty}$. Upon setting $\mathbf{y}(t) = (\mathbf{y}_1(t), \mathbf{y}_2(t), \dots)^{\top}$, the dynamics (7) can be written into the following compact form

$$\mathbf{y}(t+1) = \mathsf{K}\mathbf{y}(t), \tag{8}$$

where $\mathsf{K} = [\mathsf{K}]_{ks} : k, s = 1, 2, \dots$, is an infinite matrix. If the mapping from $\mathbf{x}(t)$ to $\mathbf{y}(t)$ is invertible, this means that the infinite dimensional linear system (8) carries all the information on the finite dimensional nonlinear system (4). See the commutative diagram in Fig. 2.

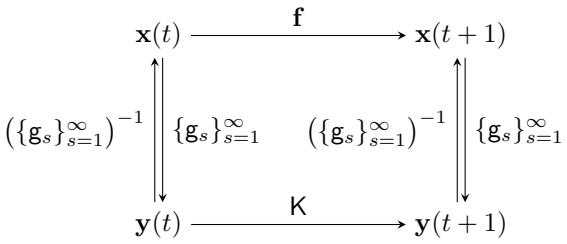

Figure 2. The commutative diagram for Koopman analysis.

3. KOOPMAN REPRESENTATION OF BOOLEAN NETWORKS

In this section, we establish a Koopman interpretation for the Boolean network (2).

3.1 Logical Functions over Binary Field

Let $\mathcal{H}_p$ be the set of all logical functions from $\mathcal{B}^p$ to the binary field $\mathcal{B}$. We introduce the following linear algebra on $\mathcal{H}$, which leads to $\mathcal{H}$ becoming a linear space.

Definition 1. The set $\mathcal{H}_p$ generates a linear space of logical functions over the binary field $\mathcal{B}$ by the prescription of

(i) $\mathsf{g_0}$ is the zero element, i.e., $\mathsf{g_0}([a]) = 0$ for all $[a] = [a_1 \dots a_p] \in \mathcal{B}^p$;
(ii) scalar multiplication is given by $0 \cdot \mathsf{g} = \mathsf{g_0}$ and $1 \cdot \mathsf{g} = \mathsf{g}$ for any $\mathsf{g} \in \mathcal{H}_p$;
(iii) addition between zero and any element is given by $\mathsf{g_0} + \mathsf{g} = \mathsf{g}$ for any $\mathsf{g} \in \mathcal{H}_p$;
(iv) addition between two distinct elements $\mathsf{g} + \mathsf{h}$ for any $\mathsf{g}, \mathsf{h} \in \mathcal{H}_p$ is defined by

$$(\mathsf{g} + \mathsf{h})([w]) = \begin{cases} 1, & \text{if } \mathsf{g}([w]) = 1 \text{ or } \mathsf{h}([w]) = 1; \\ 0, & \text{otherwise.} \end{cases}$$

3.2 Koopman Operators for Logical Functions

Let $h(x) : \mathcal{B}^p \to \mathcal{B}^p$ be a logical mapping. We are ready to introduce the Koopman operator $\mathcal{K}_h$ for the logical function h.

Definition 2. Let $h(x) : \mathcal{B}^p \to \mathcal{B}^p$ be a logical function. The Koopman operator associated with $h(\cdot)$, denoted by $\mathcal{K}_h$, is a mapping from $\mathcal{H}$ to $\mathcal{H}$ defined by

$$\mathcal{K}_h(\mathsf{g})([w]) = \mathsf{g}(h([w])) \tag{9}$$

for all $[w] \in \mathcal{B}^p$, and $\mathsf{g} \in \mathcal{H}$.

3.3 Koopman Representation for Boolean Networks

Now, let $\mathsf{h}_1, \dots, \mathsf{h}_l$ be l logical functions that map $\mathcal{B}^p$ to $\mathcal{B}$. We introduce the following definition.

Definition 3. Let $h(x) : \mathcal{B}^p \to \mathcal{B}^p$ be a logical mapping. The set of logical functions $\mathsf{h}_1, \dots, \mathsf{h}_l$ is $\mathcal{K}_h$-Koopman invariant if $\mathcal{K}_h(\mathsf{h}_k)$ can be represented as a linear combination of the $\mathsf{h}_1, \dots, \mathsf{h}_l$ over the binary field in the sense of Definition 1.

Now, consider system (2) where f is a logical function mapping from $\mathcal{B}^n$ to $\mathcal{B}^n$. Let $\mathsf{g}_1, \dots, \mathsf{g}_k$ be k logical functions that map $\mathcal{B}^n$ to $\mathcal{B}$. We further define

$$\mathbf{y}(t) := \begin{bmatrix} \mathsf{g}_1(x(t)) \\ \mathsf{g}_2(x(t)) \\ \vdots \\ \mathsf{g}_k(x(t)) \end{bmatrix}, \tag{10}$$

where $x(t)$ is the system state in (2). We are ready to present the following result.

Theorem 1. Consider the Boolean network (2) and let $\mathbf{y}(t)$ be defined as in (10). Suppose the set $\{\mathsf{g}_1, \dots, \mathsf{g}_k\}$ is $\mathcal{K}_f$-Koopman invariant. Then there exists a $k \times k$ matrix $\mathsf{G}_{\text{Koopman}}$ such that there holds

$$\mathbf{y}(t+1) = \mathsf{G}_{\text{Koopman}} \mathbf{y}(t). \tag{11}$$

In the following, we present a geometric condition for such Koopman invariance. To this end, we define

$$\Gamma_{\mathsf{g}_s} := \{x : \mathsf{g}_s(x) = 1\} \tag{12}$$

$$\Gamma^f_{\mathsf{g}_s} := \{x : \mathsf{g}_s(f(x)) = 1\} \tag{13}$$

for $s = 1, \dots, k$. We can present the following result.

Proposition 1. Consider a logical mapping $f : \mathcal{B}^n \to \mathcal{B}^n$. Let $\mathsf{g}_1, \dots, \mathsf{g}_k$ be k logical functions that map $\mathcal{B}^n$ to $\mathcal{B}$.

The following two statements are equivalent.

(i) $\{\mathsf{g}_1, \dots, \mathsf{g}_k\}$ is $\mathcal{K}_f$-Koopman invariant;

(ii) For any fixed $j = 1, \dots, k$, if $\Gamma^f_{\mathsf{g}_j} \neq \emptyset$, then the set $\Gamma^f_{\mathsf{g}_j}$ is the union of certain selected sets in $\Gamma_{\mathsf{g}_s}, s = 1, \dots, k$.

4. UNIVERSAL KOOPMAN REPRESENTATION

In this section, we present a special construction of the observables $\{\mathsf{g}_1, \dots, \mathsf{g}_k\}$ so that we may establish a universal Koopman representation for the Boolean network (2).

4.1 Logical Indication Functions

We introduce the following definition.

Definition 4. 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 by

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

The set $\mathcal{H}^* := \{\mathsf{g}_{[a]} : [a] \in \mathcal{B}^p\}$ contains 2^p elements, where the zero function, denoted by $\mathsf{g_0}$, satisfies by definition

$$\mathsf{g_0}([w]) = 0, \ \forall [w] \in \mathcal{B}^p.$$

The following algebraic structure is introduced. We define for any $[a], [b] \in \mathcal{B}^p$ a scalar $\mathsf{H}_{[a],[b]}$ by

$$\mathsf{H}_{[a],[b]} = \begin{cases} 1, & \text{if } h([b]) = [a]; \\ 0, & \text{otherwise.} \end{cases} \tag{14}$$

Then according to Definition 1, the following lemma can be immediately verified.

Lemma 1. For any $[a] \in \mathcal{B}^p$, the following holds.

$$\mathcal{K}_h(\mathsf{g}_{[a]}) = \sum_{[b] \in \mathcal{B}^p} \mathsf{H}_{[a],[b]} \mathsf{g}_{[b]}. \tag{15}$$

From Lemma 1, the logical function subspace generated by $\mathcal{H}^*$ is Koopman invariant.

Example 1. Let "$\wedge$", "$\vee$", and "$\neg$" be the logical "AND", "OR", "NOT" operations, respectively. Consider the following Boolean mapping $f : \mathcal{B}^3 \to \mathcal{B}^3$ with $f(x) = (f_1(x), f_2(x), f_3(x))$ given by

$$\begin{aligned} f_1(x) &= x_1 \vee x_2 \vee \neg x_3, \\ f_2(x) &= x_1 \vee x_2, \\ f_3(x) &= x_2 \wedge x_3. \end{aligned}$$

(i) The set of observable functions $\mathcal{H}^* := \{\mathsf{g}_{[a]} : [a] \in \mathcal{B}^3\}$ consists of 8 elements. Taking $[a] = [001]$, the corresponding elementary logical indicator function is

$$\mathsf{g}_{[001]}(x) = \begin{cases} 1, & \text{if } x = [001]; \\ 0, & \text{otherwise.} \end{cases}$$

(ii) Let us present two instances of the images of Koopman operator $\mathcal{K}_f$.

a) For $[a] = [111]$, we have $f([011]) = f([111]) = [111]$. Then from (9), we have
$$\mathcal{K}_f(\mathsf{g}_{[111]}) = \mathsf{g}_{[011]} + \mathsf{g}_{[111]}.$$
b) Take $[a] = [001]$. We can verify there is no $x \in \mathcal{B}^3$ satisfying $f(x) = [001]$. Consequently, we have $\mathcal{K}_f(\mathsf{g}_{[001]}) = \mathsf{g}_{\mathbf{0}}$.

We have now illustrated the procedure for establishing the Koopman operator for a logical function. □

4.2 Universal Koopman Representation for Boolean Networks

Consider again system (2), and introduce

$$\mathbf{y}^{\mathrm{u}}(t) := \Phi(x(t)) = \begin{bmatrix} \mathsf{g}_{[0,\dots,0]}(x(t)) \\ \mathsf{g}_{[0,\dots,1]}(x(t)) \\ \vdots \\ \mathsf{g}_{[1,\dots,1]}(x(t)) \end{bmatrix}, \tag{16}$$

which is a vector of dimension 2^n. Then from Lemma 1 it holds that

$$\mathbf{y}^{\mathrm{u}}(t+1) = \mathsf{H}_f \mathbf{y}^{\mathrm{u}}(t), \tag{17}$$

where H_f is a $2^n \times 2^n$-dimensional matrix, with rows indexed by $[a]$ and columns indexed by $[b]$ for $[a], [b] \in \mathcal{B}^n$, and $\left[\mathsf{H}_f\right]_{[a],[b]}$ defined in (14). The vector $\mathbf{y}^{\mathrm{u}}(t)$ and the matrix H_f have rich structures, as shown in the following result.

Theorem 2. (i) For any t, the vector $\mathbf{y}^{\mathrm{u}}(t)$ is a 2^n-dimensional unit vector containing only one nonzero element whose value is 1.

(ii) Every element of the matrix H_f is either zero or one. Moreover, there exists one and only one nonzero element in each column of H_f.

System (17) is indeed a linear system. In the following result, we show that system (17) is a minimal lossless representation of the logical system (2).

Theorem 3. System (17) carries the full information of system (2), i.e., knowing the state $\mathbf{y}^{\mathrm{u}}(t)$ of (17) is equivalent to knowing $x(t)$ of (2). Moreover, the Koopman representation (17) is a minimal lossless representation in the sense that the minimal number of basis functions $\mathcal{H}^*$ encoding the full information of Boolean networks in the form of (2) for all choices of f is 2^n.

Example 2. Consider the following logical dynamical system

$$\begin{aligned} x_1(t+1) &= x_1(t) \vee x_2(t) \vee \neg x_3(t), \\ x_2(t+1) &= x_1(t) \vee x_2(t), \\ x_3(t+1) &= x_2(t) \wedge x_3(t). \end{aligned}$$

Then we have

$$\begin{aligned} \mathbf{y}^{\mathrm{u}}_1(t) &= \mathsf{g}_{[000]}(x(t)), \\ \mathbf{y}^{\mathrm{u}}_2(t) &= \mathsf{g}_{[001]}(x(t)), \\ &\vdots \\ \mathbf{y}^{\mathrm{u}}_8(t) &= \mathsf{g}_{[111]}(x(t)). \end{aligned}$$

We can compute

$$\begin{aligned} &\mathcal{K}_f(\mathsf{g}_{[000]}) = \mathsf{g}_{[001]}, \\ &\mathcal{K}_f(\mathsf{g}_{[001]}) = \mathcal{K}_f(\mathsf{g}_{[010]}) = \mathcal{K}_f(\mathsf{g}_{[011]}) = \mathcal{K}_f(\mathsf{g}_{[101]}) = \mathsf{g}_{\mathbf{0}}, \\ &\mathcal{K}_f(\mathsf{g}_{[100]}) = \mathsf{g}_{[000]}, \\ &\mathcal{K}_f(\mathsf{g}_{[110]}) = \mathsf{g}_{[010]} + \mathsf{g}_{[100]} + \mathsf{g}_{[101]} + \mathsf{g}_{[110]}, \\ &\mathcal{K}_f(\mathsf{g}_{[111]}) = \mathsf{g}_{[011]} + \mathsf{g}_{[111]}. \end{aligned}$$

The matrix H_f is then

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

We can readily verify Theorem 1. Furthermore, letting $\mathbf{y}^{\mathrm{u}}(t) = [00100000]$, we can immediately obtain $x(t) = [010]$, and this illustrates Theorem 2. □

5. KOOPMAN REPRESENTATION OF CONTROLLED BOOLEAN NETWORKS

In this section, we develop a constructive extension of the Koopman operator for general logical functions, and then establish the corresponding Koopman analysis for system (3).

5.1 Koopman Operator for General Logical Functions

Let $h(x) : \mathcal{B}^p \to \mathcal{B}^q$ be a general logical function whose domain and codomain may have different dimensions. In order to distinguish between the two logical state spaces, we use $[a]_p$ and $[a]_q$ to indicate points $[a] \in \mathcal{B}^p$ and $[a] \in \mathcal{B}^q$, respectively. Following Definition 4, we obtain the corresponding observable function spaces for $\mathcal{B}^p$ and $\mathcal{B}^q$:

$$\mathcal{H}^*_p := \{\mathsf{g}_{[a]_p} : [a]_p \in \mathcal{B}^p\}, \quad \mathcal{H}^*_q := \{\mathsf{g}_{[a]_q} : [a]_q \in \mathcal{B}^q\}. \tag{18}$$

Similarly, there will be two zero functions, respectively, associated with the two function spaces. We denote them by $\mathsf{g}_{[\mathbf{0}]_p}$ and $\mathsf{g}_{[\mathbf{0}]_q}$. Further more, let $\mathcal{S}(\mathcal{H}^*_p)$ be the subspace of functions generated by $\mathcal{H}^*_p$ under the linear structure introduced in Definition 1. The Koopman operator for $h(\cdot)$ can be introduced as follows.

Definition 5. Let $h(x) : \mathcal{B}^p \to \mathcal{B}^q$ be a logical function. The Koopman operator for $h(\cdot)$, denoted by $\mathcal{K}_h$, is a

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

$$\mathcal{K}_h(\mathsf{g}_{[a]_q})([w]_p) = \mathsf{g}_{[a]_q}(h([w]_p)) = \begin{cases} 1, & \text{if } h([w]_p) = [a]_q; \\ 0, & \text{otherwise.} \end{cases} \tag{19}$$

Similarly, each $\mathcal{K}_h(\mathsf{g}_{[a]}) \in \mathcal{S}(\mathcal{H}_p^*)$ can be written as a linear combination of the elements in $\mathcal{H}_p^*$, as summarized in the following lemma.

Lemma 2. Define for any $[s]_q \in \mathcal{B}^q \cup \{[\mathbf{0}]_q\}$ and $[k]_p \in \mathcal{B}^p \cup \{[\mathbf{0}]_p\}$

$$\mathsf{H}_{[s]_q,[k]_p} = \begin{cases} 1, & \text{if } h([k]_p) = [s]_q; \\ 0, & \text{otherwise.} \end{cases} \tag{20}$$

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

5.2 Koopman Picture of Controlled Logical Systems

Now let us apply the above Koopman operator for general logical functions to build a Koopman analysis for the controlled logical system (3). To this end, we introduce

$$\begin{aligned} \mathbf{x}(t) &= \begin{bmatrix} \mathbf{x}_{[0,\dots,0]_n}(t) \\ \mathbf{x}_{[0,\dots,1]_n}(t) \\ \vdots \\ \mathbf{x}_{[1,\dots,1]_n}(t) \end{bmatrix} := \begin{bmatrix} \mathsf{g}_{[0,\dots,0]_n}(x(t)) \\ \mathsf{g}_{[0,\dots,1]_n}(x(t)) \\ \vdots \\ \mathsf{g}_{[1,\dots,1]_n}(x(t)) \end{bmatrix}, \\ \mathbf{u}(t) &= \begin{bmatrix} \mathbf{u}_{[0,\dots,0]_d}(t) \\ \mathbf{u}_{[0,\dots,1]_d}(t) \\ \vdots \\ \mathbf{u}_{[1,\dots,1]_d}(t) \end{bmatrix} := \begin{bmatrix} \mathsf{g}_{[0,\dots,0]_d}(u(t)) \\ \mathsf{g}_{[0,\dots,1]_d}(u(t)) \\ \vdots \\ \mathsf{g}_{[1,\dots,1]_d}(u(t)) \end{bmatrix}. \end{aligned} \tag{21}$$

We also define

$$\begin{aligned} \mathbf{x}(t) \otimes \mathbf{u}(t) &:= \begin{bmatrix} \mathsf{g}_{[0,\dots,0]_n[0,\dots,0]_d}(x(t),u(t)) \\ \mathsf{g}_{[0,\dots,0]_n[0,\dots,1]_d}(x(t),u(t)) \\ \vdots \\ \mathsf{g}_{[0,\dots,0]_n[1,\dots,1]_d}(x(t),u(t)) \\ \mathsf{g}_{[0,\dots,1]_n[0,\dots,0]_d}(x(t),u(t)) \\ \vdots \\ \mathsf{g}_{[1,\dots,1]_n[1,\dots,1]_d}(x(t),u(t)) \end{bmatrix} \\ &= \begin{bmatrix} \mathsf{g}_{[0,\dots,0]_{n+d}}(x(t),u(t)) \\ \mathsf{g}_{[0,\dots,1]_{n+d}}(x(t),u(t)) \\ \vdots \\ \mathsf{g}_{[1,\dots,1]_{n+d}}(x(t),u(t)) \end{bmatrix}. \end{aligned} \tag{22}$$

Then we can extend the analysis in (7) and establish from Lemma 2

$$\begin{aligned} \mathbf{x}_{[a]_n}(t+1) &= \mathsf{g}_{[a]_n}(x(t+1)) \\ &= \mathsf{g}_{[a]_n}(f(x(t),u(t))) \\ &= \mathcal{K}_f(\mathsf{g}_{[a]_n})(x(t),u(t)) \\ &= \sum_{[k]_{n+d} \in \mathcal{B}^{n+d}} \mathsf{F}_{[a]_n,[k]_{n+d}} \mathsf{g}_{[k]_{n+d}}(x(t),u(t)) \end{aligned} \tag{23}$$

Here $\mathsf{F}_{[a]_n,[k]_{n+d}}$ is defined based on (20) by

$$\mathsf{F}_{[a]_n,[k]_{n+d}} = \begin{cases} 1, & \text{if } f([k]_{n+d}) = [a]_n; \\ 0, & \text{otherwise.} \end{cases} \tag{24}$$

Let F be the $2^n \times 2^{n+d}$ matrix with rows indexed by $[a]_n \in \mathcal{B}^n$ and columns indexed by $[k]_{n+d} \in \mathcal{B}^{n+d}$, where $\mathsf{F}_{[a]_n,[k]_{n+d}}$ obeys (24). The entry-wise representation (23) can further be written in a compact form as

$$\mathbf{x}(t+1) = \mathsf{F}\big(\mathbf{x}(t) \otimes \mathbf{u}(t)\big), \tag{25}$$

and this has established a Koopman picture for the logical dynamical system (3). Similar to Theorem 2 and Theorem 3, we have the following result, whose proof is omitted.

Theorem 4. (i) The matrix F contains only zero or one values, and there exists one and only one nonzero element in each column of F.

(ii) System (25) carries the full information of the system (3), i.e., knowing any state $\mathbf{x}(t), \mathbf{u}(t)$ of (25) is equivalent to knowing $x(t), u(t)$ of (3).

6. CONCLUSIONS

We established a framework to derive Boolean network dynamics from classical Koopman analysis (Koopman, 1931; Koopman and von Neumann, 1932). The key step was the construction of a set of observable logical functions as elementary indicator functions. With properly defined linear structure, such set of logical indicator functions was shown to be Koopman invariant. In view of this, logical dynamical systems were rewritten as standard linear systems in the space of observable functions. By creating this link between the semi-tensor product approach and the Koopman analysis, the rich tools in Koopman operator theories may shed light on data-driven approach for logical dynamical systems.

APPENDICES

A. Proof of Proposition 1

Suppose that for any $j = 1, \dots, k$, $\Gamma_{\mathsf{g}_j}^f$ (if nonempty) can be represented as a union of certain selected sets in $\Gamma_{\mathsf{g}_s}, s = 1, \dots, k$. Then $\mathcal{K}_f(\mathsf{g}_j)$ can be represented as a linear combination of $\mathsf{g}_1, \dots, \mathsf{g}_k$ over the binary field. As a result, $\{\mathsf{g}_1, \dots, \mathsf{g}_k\}$ is $\mathcal{K}_f$-Koopman invariant, and hence the desired result holds.

B. Proof of Theorem 2

(i) From Definition 4 we have $\mathsf{g}_{[x(t)]}(x(t)) = 1$ and $\mathsf{g}_{[a]}(x(t)) = 0$ for all $[a] \in \mathcal{B}^n \setminus \{x(t)\}$. The desired statement holds.

(ii) It is clear from the definition (14) that the elements in the matrix H_f are either zero or one.

Next, let us take an arbitrary $[b] \in \mathcal{B}^n$. The $[b]$-th column of H_f contains 2^n elements: $\big[\mathsf{H}_f\big]_{[0,\dots,0],[b]}$, $\big[\mathsf{H}_f\big]_{[0,\dots,1],[b]}$, $\dots$, $\big[\mathsf{H}_f\big]_{[1,\dots,1],[b]}$. Let $f([b]) = [z]$. Then from (14) we have $\big[\mathsf{H}_f\big]_{[z],[b]} = 1$, and $\big[\mathsf{H}_f\big]_{[w],[b]} = 0$ for all $[w] \in \mathcal{B}^n \setminus \{[z]\}$. Therefore, there exists only one nonzero element in the $[b]$-th column of H_f. Since $[b]$ is arbitrarily chosen, we have established the desired result.

B. Proof of Theorem 3

First, we need to show that Φ defined in (16) is invertible. We have from (16) that

$$\begin{aligned}\mathbf{y}_1^{\mathrm{u}}(t) &= \mathbf{g}_{[0,\dots,0]}(x(t)),\\ \mathbf{y}_2^{\mathrm{u}}(t) &= \mathbf{g}_{[0,\dots,1]}(x(t)),\\ &\vdots\\ \mathbf{y}_{2^n}^{\mathrm{u}}(t) &= \mathbf{g}_{[1,\dots,1]}(x(t)).\end{aligned}$$

Again from Definition 4 we have $\mathbf{g}_{[x(t)]}(x(t)) = 1$ and $\mathbf{g}_{[a]}(x(t)) = 0$ for all $[a] \in \mathcal{B}^n \setminus \{x(t)\}$. As a result, taking $s \in \{1, \dots, 2^n\}$ satisfying $\mathbf{y}_s(t) = 1$, the inverse mapping of Φ can be obtained as

$$x(t) = \Phi^{-1}(\mathbf{y}^{\mathrm{u}}(t)) = [x_1(t) \dots x_n(t)] \tag{26}$$

where $[x_1(t) \dots x_n(t)]$ is the unique element in $\mathcal{B}^n$ satisfying $\sum_{k=1}^{n} 2^{k-1} x_k(t) = s - 1$. We have established the fact that system (17) carries the full information of system (2).

Second, let us suppose there exists another choice of $\mathcal{H}^*$, with m elements indexed by $\mathbf{g}_1^*, \dots, \mathbf{g}_m^*$, that generates a Koopman invariant subspace. Then we can still obtain a linear system representation in the form of (17). In order for the representation to be lossless, we need to make sure that it is possible to uniquely recover $x(t)$ from

$$\begin{aligned}\mathbf{y}_1^*(t) &= \mathbf{g}_1^*(x(t)),\\ \mathbf{y}_2^*(t) &= \mathbf{g}_2^*(x(t)),\\ &\vdots\\ \mathbf{y}_m^*(t) &= \mathbf{g}_m^*(x(t)).\end{aligned} \tag{27}$$

No matter how we choose $\mathbf{g}_1^*, \dots, \mathbf{g}_m^*$, (27) is a system of equations with 2^n unknown variables in $x(t)$ and m equations. As a result, if $m < 2^n$, there will have to exist certain $x(t) \in \mathcal{B}^n$ that can not be recovered [1] from $\mathbf{y}_1^*(t), \dots, \mathbf{y}_m^*(t)$. The desired theorem holds.

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[1] Suppose all $x(t) \in \mathcal{B}^n$ can be recovered from $\mathbf{y}_1^*(t), \dots, \mathbf{y}_m^*(t)$. Combined with (27), we can construct a 1-to-1 mapping between $\mathcal{B}^n$ and a subset of $\mathbf{y}_1^*(t), \dots, \mathbf{y}_m^*(t)$. Thus $m \geq 2^n$, providing an alternative argument.