

Synthesis of Boolean Networks via Semi-tensor Product

Daizhan Cheng

Institute of Systems Science, Academy of Mathematics and Systems Science
Chinese Academy of Sciences

Joint work with
Hongsheng Qi, Zhiqiang Li, Yin Zhao, et al.

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Outline

- 1 **An Introduction to Boolean Network**
- 2 **Two Key Tools of Our Approach**
 - Algebraic Form of Logic
 - State Space Approach
- 3 **Analysis of BN/BCN**
 - Topological Structure of BN/BCN
- 4 **Control of BN/BCN**
 - Controllability, Observability, Realization
 - Disturbance Decoupling Problem
 - Stability and Stabilization
 - Optimal Control of BCN
 - Identification of BN/BCN
- 5 **Concluding Remarks**

I. An Introduction to Boolean Network

👉 Historical Review — Boolean Network

- McCulloch and Pitts (1943): “the **brain could be modeled as a network of logical operations** such as and or not and so forth.”
- Jacob and Monod (Nobel Prize winners) (1961-1963): “Any cell contains a number of **‘regulatory’ genes** that act as switches and **can turn one another on and off**. ...then you can have **genetic circuits**.” (M.M. Waldrop, *Complexity*, 1992)
- Kauffman (1969): “The **Boolean rules describing the activities of different genes** ...” (S. Kauffman, *At Home in the Universe*, 1994)

☞ Boolean Control Network

- Ideker, et al (2001): “**Gene-regulatory networks** are defined by trans and cis logic. . . . Both of these types of regulatory networks **have input and output.**” (*Annu. Rev. Genomics Hum. Genet.*, 2001)
- Akutsu, et al (2007): “**One of the major goals of systems biology is to develop a control theory** for complex biological systems.” (*J. Theoretical Biology*, 2007)

☞ Some Other Applications

- Dynamic Games;
- Logic-based Control;
- Cryptography and Secure Community;
- Circuit Failure Detection, etc.

Boolean Network

👉 Network Graph

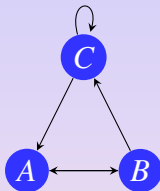


Figure 1: A Boolean network

👉 Network Dynamics

$$\begin{cases} A(t+1) = B(t) \wedge C(t) \\ B(t+1) = \neg A(t) \\ C(t+1) = B(t) \vee C(t) \end{cases} \quad (1)$$

Boolean Control Network

Network Graph

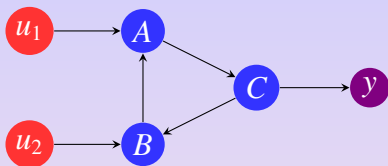


Figure 2: A Boolean control network

Network Dynamics

Its logical equation is

$$\begin{cases} A(t+1) = B(t) \wedge u_1(t) \\ B(t+1) = C(t) \vee u_2(t) \\ C(t+1) = A(t) \\ y(t) = \neg C(t) \end{cases} \quad (2)$$

👉 Dynamics of Boolean Network

$$\begin{cases} x_1(t+1) = f_1(x_1(t), \dots, x_n(t)) \\ \vdots \\ x_n(t+1) = f_n(x_1(t), \dots, x_n(t)), \end{cases} \quad x_i \in \mathcal{D}, \quad (3)$$

where

$$\mathcal{D} := \{0, 1\}.$$

➡ Dynamics of Boolean Control Network

$$\begin{cases} x_1(t+1) = f_1(x_1(t), \dots, x_n(t), u_1(t), \dots, u_m(t)) \\ \vdots \\ x_n(t+1) = f_n(x_1(t), \dots, x_n(t), u_1(t), \dots, u_m(t)), \\ y_j(t) = h_j(x(t)), \quad j = 1, \dots, p, \end{cases} \quad (4)$$

where $x_i, u_k, y_j \in \mathcal{D}$.

Some Generalizations

☞ k -valued and Mix-valued Logical Network

- Boolean: $x_i \in \mathcal{D} = \{0, 1\}$;
- k -valued: $x_i \in \mathcal{D}_k = \{0, \frac{1}{k-1}, \dots, 1\}$;
- mix-valued: $x_i \in \mathcal{D}_{k_i}$.

(Example: For a game, player i has k_i strategies.)

☞ Probabilistic Boolean Network

$$f_i = \begin{cases} f_i^1, & P(f_i = f_i^1) = p_i^1; \\ \vdots \\ f_i^{k_i}, & P(f_i = f_i^{k_i}) = p_i^{k_i}, \end{cases} \quad (5)$$

where

$$\sum_{j=1}^{k_i} p_i^j = 1, \quad i = 1, \dots, n.$$

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II.1 Algebraic Form of Logic

☞ Semi-tensor Product of Matrices

$$A \in \mathcal{M}_{m \times n}, \quad B \in \mathcal{M}_{p \times q}, \quad A \times B = ?$$

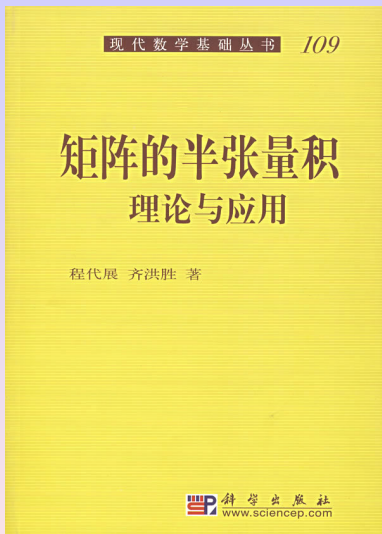
Definition 2.1.1

Let $t = \text{lcm}\{n, p\}$. Then the **semi-tensor product** (STP) of A and B is defined as

$$A \times B := (A \otimes I_{t/n}) (B \otimes I_{t/p}) \quad (6)$$

Remark 2.1.2

- It is a generalization of conventional matrix product (CMP);
- All the properties of the CMP remain true;
- Pseudo-commutativity.



☞ Some Notations:

- δ_k^i : the i -th column of I_k ;
- $\Delta_k: \{\delta_k^1, \delta_k^2, \dots, \delta_k^k\}$; $\Delta := \Delta_2$;
- $\mathcal{L}_{m \times n}$: the set of logical matrices. $A \in \mathcal{L}_{m \times n}$ means $A = [\delta_m^{i_1} \delta_m^{i_2} \dots \delta_m^{i_n}]$. Briefly denote it as

$$A = \delta_m[i_1 \ i_2 \ \dots \ i_n].$$

☞ Vector Form of Boolean Variables (Functions)

Setting Equivalence:

$$1 \sim \delta_2^1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad 0 \sim \delta_2^2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

then $x_i \in \Delta$ and

$$f : \mathcal{D}^n \rightarrow \mathcal{D} \quad \Rightarrow \quad f : \Delta^n \rightarrow \Delta.$$

Algebraic Form of Boolean (Control) Networks

Theorem 2.1.3 (Cheng & Qi, IEEE TAC, 55(10), 2010)

Let $F : \mathcal{D}^n \rightarrow \mathcal{D}^m$ be determined by

$$y_i = f_i(x_1, \dots, x_n), \quad i = 1, \dots, m. \quad (7)$$

Then in **vector form** we have

$$y_i = M_i \times_{j=1}^n x_j := M_i x, \quad i = 1, \dots, m, \quad (8)$$

where $M_i \in \mathcal{L}_{2 \times 2^n}$. Moreover,

$$y := \times_{k=1}^m y_k := M_F x, \quad (9)$$

where $M_F = M_1 * \dots * M_m \in \mathcal{L}_{2^m \times 2^n}$. (*: Khatri-Rao Prod.)

Theorem 2.1.4 (Cheng & Qi, IEEE TAC, 55(10), 2010)

- 1 There exists a unique $L \in \mathcal{L}_{2^n \times 2^n}$ such that (3) can be expressed as

$$x(t+1) = Lx(t), \quad (10)$$

where $x = \times_{i=1}^n x_i$.

- 2 There exist unique $L \in \mathcal{L}_{2^n \times 2^{n+m}}$ and unique $H \in \mathcal{L}_{2^p \times 2^n}$, such that (4) can be expressed as

$$\begin{cases} x(t+1) = Lx(t)u(t) \\ y(t) = Hx(t), \end{cases} \quad (11)$$

where $u = \times_{i=1}^m u_i$, $y = \times_{i=1}^p y_i$.

Example

Example 2.1.4

- Consider Boolean network (1) for Fig. 1. We have

$$L = \delta_8[3 \ 7 \ 7 \ 8 \ 1 \ 5 \ 5 \ 6].$$

- Consider Boolean control network (2) for Fig. 2. We have

$$\begin{aligned} L &= \delta_8[1 \ 1 \ 5 \ 5 \ 2 \ 2 \ 6 \ 6 \ 1 \ 3 \ 5 \ 7 \ 2 \ 4 \ 6 \ 8 \\ &\quad 5 \ 5 \ 5 \ 5 \ 6 \ 6 \ 6 \ 6 \ 5 \ 7 \ 5 \ 7 \ 6 \ 8 \ 6 \ 8]; \\ H &= \delta_2[2 \ 1 \ 2 \ 1 \ 2 \ 1 \ 2 \ 1]. \end{aligned}$$

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II.2 State Space Approach

State Space and Subspace

Definition 2.2.1

Consider Boolean network (3)

(1) State space:

$$\mathcal{X} = F_\ell(x_1, \dots, x_n). \quad (12)$$

(2) Subspace: Let $y_1, \dots, y_k \in \mathcal{X}$.

$$\mathcal{Y} = F_\ell(y_1, \dots, y_k) \subset \mathcal{X}. \quad (13)$$

(3) Regular Subspace: Let $\{x_{i_1}, \dots, x_{i_k}\} \subset \{x_1, \dots, x_n\}$.

$$\mathcal{Z} = F_\ell(x_{i_1}, \dots, x_{i_k}). \quad (14)$$

👉 Physical Meaning: Dual Space

In \mathbb{R}^n , let $\{x_1, x_2, \dots, x_n\}$ be the coordinate frame.

To describe the state subspace generalized by $\{x_{i_1}, \dots, x_{i_k}\}$, we may use the linear functions over this subspace as

$$V^* = \{c_1x_{i_1} + \dots + c_kx_{i_k} \mid c_1, \dots, c_k \in \mathbb{R}\}.$$

Coordinate Transformation

Definition 2.2.2

Let $\mathcal{X} = F_\ell(x_1, \dots, x_n)$ be the state space of (3). Assume there exist $z_1, \dots, z_n \in \mathcal{X}$, such that

$$\mathcal{X} = F_\ell(z_1, \dots, z_n),$$

then the logical mapping $T : (x_1, \dots, x_n) \mapsto (z_1, \dots, z_n)$ is a **coordinate transformation**.

Proposition 2.2.3

A mapping $T : \mathcal{D}^n \rightarrow \mathcal{D}^n$ is a coordinate transformation, **if and only if**, T is bijective.

👉 Algebraic Form of Coordinate Transformation

Theorem 2.2.4 (Cheng & Qi, IEEE TNN, 21(4), 2010)

Assume $z_1, \dots, z_n \in \mathcal{X}$, with

$$\begin{cases} z_1 = f_1(x_1, \dots, x_n) \\ \vdots \\ z_n = f_n(x_1, \dots, x_n). \end{cases} \quad (15)$$

Moreover, the algebraic form of (15) is

$$z = Tx, \quad (16)$$

where $z = \times_{i=1}^n z_i$, and $x = \times_{i=1}^n x_i$, $T \in \mathcal{L}_{2^n \times 2^n}$. Then $\pi : (x_1, \dots, x_n) \mapsto (z_1, \dots, z_n)$ is a coordinate transformation, **if and only if**, T is nonsingular.

Definition 2.2.5

Let $\mathcal{Z}_0 = F_\ell(z_1, \dots, z_k) \subset \mathcal{X}$. If there exist $\{z_{k+1}, \dots, z_n\}$ such that

$$\mathcal{X} = F_\ell(z_1, \dots, z_n),$$

then \mathcal{Z}_0 is a **regular subspace**.

Theorem 2.2.6 (Cheng & Qi, IEEE TNN, 21(4), 2010)

Let the algebraic form of \mathcal{Z}_0 be

$$z^0 = Gx,$$

where $G = [g_{i,j}] \in \mathcal{L}_{2^k \times 2^n}$. Then \mathcal{Z}_0 is a regular subspace, **if and only if**,

$$\sum_{j=1}^{2^n} g_{i,j} = 2^{n-k}, \quad i = 1, \dots, 2^k. \quad (17)$$

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III. Topological Structure of BN/BCN

👉 Fix Points and Cycles

Theorem 3.1 (Cheng & Qi, IEEE TAC, 55(10), 2010)

Let the algebraic form of a Boolean network be

$$x(t + 1) = Lx(t). \quad (18)$$

Then the number of cycles of length s (denoted by N_s) are

$$\begin{cases} N_1 = \text{tr}(L), \\ N_s = \frac{\text{tr}(L^s) - \sum_{t \in \mathcal{P}(s)} tN_t}{s}, \quad 2 \leq s \leq 2^n. \end{cases} \quad (19)$$

- There are similar formulas for BCN (**Zhao & Cheng, IEEE TAC, to appear.**)

Rolling Gear Structure

Theorem 3.2 (Cheng, IEEE TNN, 20(3), 2009)

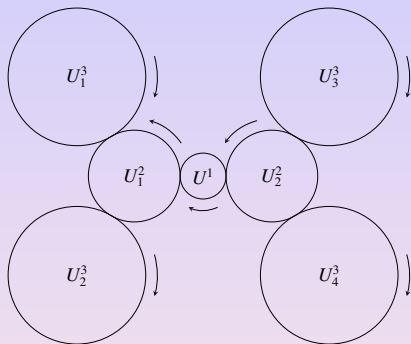
If the network has cascading form as

$$\begin{cases} z^1(t+1) = F^1(z^1(t)) \\ z^2(t+1) = F^2(z^1(t), z^2(t)), \end{cases} \quad (20)$$

then

$$C_Z = C_{Z^1} \circ C_{Z^2}. \quad (21)$$

☞ Rolling Gear Structure ($V_1 \subset V_2 \subset V_3 = \mathcal{X}$)



- RGS explains why “**tiny cycles decide vast order**”(Kaufman, *At Home in the Universe*)

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IV.1 Controllability, Observability, Realization

☞ Controllability Matrix

Assume a Boolean control network has its algebraic form as

$$\begin{cases} x(t+1) = Lu(t)x(t) \\ y(t) = Hx(t). \end{cases} \quad (22)$$

Let

$$M = \sum_{i=1}^{2^m} \text{Blk}_i(L).$$

Controllability Matrix

$$\mathcal{M}_C := \sum_{s=1}^{2^{m+n}} M^{(s)} := (c_{ij}) \in \mathcal{B}_{2^n \times 2^n}. \quad (23)$$

☞ Controllability

Theorem 4.1.1 (Zhao & Cheng, SCL, 59(12), 2010)

Consider Boolean control network (22).

- (i) $x^0 = \delta_{2^n}^j \Rightarrow x^d = \delta_{2^n}^i$ is reachable, iff, $c_{ij} > 0$;
- (ii) (22) is controllable at $x^0 = \delta_{2^n}^j$, iff, $\text{Col}_j(\mathcal{M}_c) > 0$;
- (iii) (22) is controllable, iff, $\mathcal{M}_c > 0$.

Related Works:

- Controllability and Observability (**Cheng & Qi, Automatica, 45(7), 2009**)
- Realization (**Cheng, Li & Qi, Automatica, 46(1), 2010**)

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IV.2 Disturbance Decoupling Problem (DDP)

Network Model

$$\left\{ \begin{array}{l} x_1(t+1) = f_1(x_1(t), \dots, x_n(t), u_1(t), \dots, u_m(t), \\ \quad \xi_1(t), \dots, \xi_q(t)) \\ \quad \vdots \\ x_n(t+1) = f_n(x_1(t), \dots, x_n(t), u_1(t), \dots, u_m(t), \\ \quad \xi_1(t), \dots, \xi_q(t)), \end{array} \right. \quad (24)$$
$$y_j(t) = h_j(x(t)), \quad j = 1, \dots, p,$$

where $\xi_i(t)$, $i = 1, \dots, q$ are disturbances.

Definition 4.2.1

The DDP is: Finding, if possible, state feedback controls

$$u_i(t) = g_i(x_1(t), \dots, x_n(t)), \quad i = 1, \dots, m, \quad (25)$$

such that for the closed-loop system the outputs are not affected by the disturbances.

☞ \mathcal{Y} -friendly Subspace

Definition 4.2.2

Let $\mathcal{Y} = F_\ell\{y_1, \dots, y_p\}$. $\mathcal{S} \subset \mathcal{X}$ is called the \mathcal{Y} -friendly subspace, if \mathcal{S} is a regular subspace and

$$y_i \in \mathcal{S}, \quad i = 1, \dots, p.$$

☞ \mathcal{Y} -friendly Form

Proposition 4.2.3 (Cheng, IEEE TAC, 56(1), 2011)

Let $\mathcal{S} = F_\ell\{z^2\}$ be an \mathcal{Y} -friendly subspace. Then we have the follow \mathcal{Y} -friendly Form:

$$\begin{cases} z^1(t+1) = F_1(z_1(t), \dots, z_n(t), u_1(t), \dots, u_m(t), \\ \quad \xi_1(t), \dots, \xi_q(t)) \\ z^2(t+1) = F_2(z_1(t), \dots, z_n(t), u_1(t), \dots, u_m(t), \\ \quad \xi_1(t), \dots, \xi_q(t)), \\ y_j(t) = h_j(z^2(t)), \quad j = 1, \dots, p. \end{cases} \quad (26)$$

Theorem 4.2.4 (Cheng, IEEE TAC, 56(1), 2011)

Consider Boolean control network (24) with disturbances. The disturbance decoupling problem is solvable, **if and only if**,

- (i) there exists a \mathcal{Y} -friendly subspace with \mathcal{Y} -friendly form (26);
- (ii) there exist state-feedback controls

$$u_i(t) = \phi_i(z(t)), \quad i = 1, \dots, m,$$

such that

$$F_2(z_1(t), \dots, z_n(t), \phi_1(z(t)), \dots, \phi_m(z(t)), \xi_1(t), \dots, \xi_q(t)) = \tilde{F}_2(z^2(t)).$$

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IV.3 Stability and Stabilization

Definition 4.3.1

- 1 The Boolean network (3) is stable, if there exists an $N > 0$ such that $x_i(t) = \text{const.}$, $t \geq N$, $i = 1, \dots, n$.
- 2 The Boolean control network (4) is stabilizable, if there exists controls $\{u_i\}$ such that the closed-loop network is stable. Particularly, if

$$u_i = \text{const.}, \quad i = 1, \dots, m, \quad (27)$$

it is said to be stabilized by constant control; if

$$u_i(t) = g_i(x_1(t), \dots, x_n(t)), \quad i = 1, \dots, m, \quad (28)$$

it is said to be stabilized by state feedback control.

☞ Constant Mapping

Definition 4.3.2

① Let $F : \mathcal{D}^n \rightarrow \mathcal{D}^k$ be

$$z_i = f_i(x_1, \dots, x_n), \quad i = 1, \dots, k.$$

F is called a **constant mapping**, if $f_i = \text{const.}$,
 $i = 1, \dots, k$.

② A logical matrix, M , is called a **constant mapping matrix (CMM)**, if

$$\text{Col}_i(M) = M_0, \quad \forall i.$$

☞ Constant Mapping \Leftrightarrow Constant Matrix

Proposition 4.3.3

Let $F : \mathcal{D}^n \rightarrow \mathcal{D}^k$ be a constant mapping and its algebraic form is

$$z = M_F X, \quad M_F \in \mathcal{L}_{2^k \times 2^n}.$$

Then M_F is a CMM.

☞ Power-reducing Matrix

$$\Phi_k := \prod_{i=1}^k I_{2^{k-1}} \otimes [(I_2 \otimes W_{[2,2^{k-i}]} \delta_4[1,4]),$$

where $W_{[m,n]}$ is a swap matrix.

☞ Stability

Theorem 4.3.4 (Cheng, Qi, Li & Liu, IJRNC, 21(2), 2011)

- The network (3) is stable if there exists a $k \leq n$, such that ($\mathcal{I}(F)$: incidence matrix)

$$[\mathcal{I}(F)]^{(k)} = 0. \quad (29)$$

- The network (3) is stable if there exists a $k \leq 2^n$, such that the system structure matrix satisfies that L^k is a CMM. That is,

$$\text{Col}_i(L^k) = M_0, \quad \forall i. \quad (30)$$

👉 Stabilization

Theorem 4.3.5 (Cheng, Qi, Li & Liu, IJRNC, 21(2), 2011)

1 Define

$$L [I_{2^m} \otimes L) \Phi_m]^{k-1} := [L_1^k \ L_2^k \ \dots \ L_{2^m}^k] .$$

The network (4) is stabilizable by constant controls, **if and only if**, there exists at least a L_j^k , $1 \leq k \leq 2^n$, $1 \leq j \leq 2^m$, which is a CMM.

2 The network (4) is stabilizable by state feedback controls $u = Gx$, **if and only if**, there exists a $1 \leq k \leq 2^n$, such that $(LG\Phi_n)^k$ is a CMM.

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IV.4 Optimal Control of BCN

👉 Problem Formulation

Definition 4.4.1

Consider the Boolean control network (4). The payoff function is assumed to be

$$p(t) = P(x(t), u(t)), \quad t = 1, 2, \dots .$$

The optimization problem is: Finding, if possible, an optimal control sequence, which maximize the average payoff

$$J(u) = \overline{\lim}_{T \rightarrow \infty} \frac{1}{T} \sum_{t=1}^T P(x(t), u(t)). \quad (31)$$

Theorem 4.4.2 (Zhao & Cheng, IEEE TAC, to appear)

Consider Boolean control network (4). There exists an optimal control $u^*(t)$ of the form

$$\begin{cases} u_1^*(t+1) = g_1(x_1(t), \dots, x_n(t), u_1^*(t), \dots, u_n^*(t)) \\ \vdots \\ u_m^*(t+1) = g_m(x_1(t), \dots, x_n(t), u_1^*(t), \dots, u_n^*(t)), \end{cases} \quad (32)$$

which maximize (31). Moreover, the corresponding optimal trajectory $w^*(t) = u^*(t)x^*(t)$ becomes periodic after finite steps.

- The key issue is to calculate the cycles for BCN (refer to: **Zhao & Cheng, IEEE TAC, to appear**)

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IV.5 Identification of BN/BCN

👉 Identification of BN

- Observed data:

$$\{X(0), X(1), \dots, X(N)\}.$$

- Network:

$$x_i(t+1) = f_i(x_1(t), \dots, x_n(t)), \quad i = 1, \dots, n. \quad (33)$$

- Component-wise algebraic form:

$$x_i(t+1) = M_i x(t), \quad i = 1, \dots, n, \quad (34)$$

where $M_i \in \mathcal{L}_{2 \times 2^n}$.

- Purpose: Identify $M_i, i = 1, \dots, n$.

👉 Identifying Column

Theorem 4.5.1 (Cheng, Qi & Li, IEEE TNN, 22(4), 2011)

Let $x(t) = \delta_{2^n}^j$ and $x_i(t+1) = \delta_2^k$. Then

$$\text{Col}_j(M_i) = \delta_2^k. \quad (35)$$

Assume we have partly identified structure matrices M_i ,
 $i = 1, \dots, n$.

Define

$$M_{i,j} := M_i W_{[2,2^{j-1}]}, \quad j = 1, 2, \dots, n. \quad (36)$$

Then split it into two equal-size blocks as

$$M_{i,j} = \begin{bmatrix} M_{i,j}^1 & M_{i,j}^2 \end{bmatrix}. \quad (37)$$

☞ Least In-degree Model

Theorem 4.5.2 (Cheng, Qi & Li, IEEE TNN, 22(4), 2011)

f_i has a realization which is independent of x_j , **if and only if**

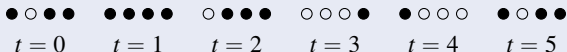
$$M_{i,j}^1 = M_{i,j}^2 \quad (38)$$

has solution for unidentified columns.

- Using (38), we can find a least in-degree realization.
- Identification of BCN: Refer to **Cheng & Zhao, Automatica, 47(4), 2011**.

Example 9.3

Observed Data:

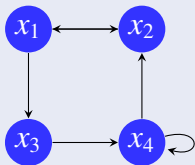


Partly identified structure matrix:

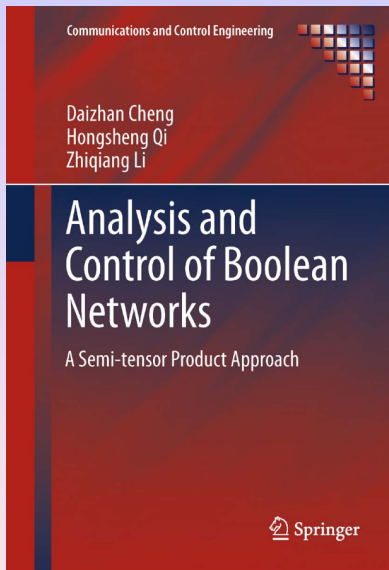
$$\begin{aligned}M_1 &= \delta_2[* 2 * * * * * 1 * 2 * 2 * * * 1] \\M_2 &= \delta_2[* 1 * * * * * 1 * 1 * 2 * * * 2] \\M_3 &= \delta_2[* 1 * * * * * 1 * 2 * 2 * * * 2] \\M_4 &= \delta_2[* 1 * * * * * 2 * 2 * 2 * * * 2].\end{aligned}$$

Example 9.3 (Cont'd)

Least In-degree Realization:



$$\begin{cases} x_1(t+1) = \neg x_2(t), \\ x_2(t+1) = x_4(t) \vee x_1(t), \\ x_3(t+1) = x_1(t), x_4(t+1) = x_3(t) \bar{\vee} x_4(t). \end{cases} \quad (39)$$



V. Concluding Remarks

👉 Conclusion

- Boolean network is a proper model for cellular networks;
- **Semi-tensor Product:**
Logical Dynamics \Rightarrow Discrete-time Dynamics;
- **State space/subspaces:**
Control Theory(applicable) \Rightarrow Systems Biology.
- Control Problems Considered: Controllability, Observability, Realization, DDP, Stabilization, Optimal control, Identification, etc.
- There are many open problems, and several follow up papers (IEEE TAC, Automatica, IEEE TNN ..., CCC Invited Session)

👉 Topics for Further Study

- Properties and control of probabilistic Boolean networks;
- Application to general biological systems (size problem);
 - Multi-agent Boolean network (Metabolic network: module + network motif)
 - Protein network (self similar, scale-free network)
- Dynamic games with finite strategies and finite memories;
- Fuzzy control (Fuzzy relational equations);
- Logic-based control;
- Cryptography, Coding by Boolean function, Secure community;
- Circuit Design, Failure Detection, etc.
- ...

Thank you!

Question?