Reconstruction of Boolean networks and optimal control

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Outline of the talk

- Boolean Networks
- Reconstructability of Boolean Networks

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- Finite Horizon Optimal Control problem: solution

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If we represent the Boolean vectors $X(t)$ and $Y(t)$ by means of their “canonical equivalent" $\mathbf{x}(t)$ and $\mathbf{y}(t)$, the BN (1) can be described as

$$\begin{aligned} \mathbf{x}(t+1) &= L\mathbf{x}(t), \\ \mathbf{y}(t) &= H\mathbf{x}(t), \qquad t \in \mathbb{Z}_+, \end{aligned} \tag{2}$$

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where $L \in \mathcal{L}_{2^n \times 2^n}$ and $H \in \mathcal{L}_{2^p \times 2^n}$.

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Definition 1 A BN (2) is reconstructable if there exists $T \in \mathbb{Z}_+$ such that the knowledge of the output trajectory $\mathbf{y}(t), t \in \{0, 1, \ldots, T\}$, allows to uniquely determine $\mathbf{x}(T)$.

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In other words, a BN (2) is reconstructable if $\exists\ T \geq 0$ such that

$$y(0), y(1), \dots, y(T) \quad \underset{\text{uniquely}}{\longrightarrow} \quad x(T).$$

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To each vertex i we associate a output label representing the value of the output associated with the state δ_N^i, namely $y = H\delta_N^i$.

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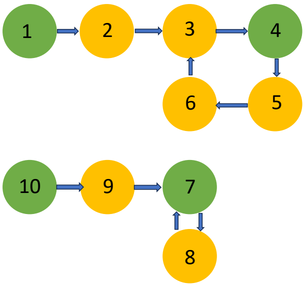
Example:



$$L = \begin{bmatrix} 0&0&0&0&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0&0&0\\ 0&1&0&0&0&1&0&0&0&0\\ 0&0&1&0&0&0&0&0&0&0\\ 0&0&0&1&0&0&0&0&0&0\\ 0&0&0&0&1&0&0&0&0&0\\ 0&0&0&0&0&0&0&1&1&0\\ 0&0&0&0&0&0&1&0&0&0\\ 0&0&0&0&0&0&0&0&0&1\\ 0&0&0&0&0&0&0&0&0&0 \end{bmatrix}$$

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

$$\mathcal{C}_1 = \{(3,4),(4,5),(5,6),(6,3)\}$$
$$\mathcal{C}_2 = \{(7,8),(8,7)\}.$$

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- in the graph associated with the BN, each cycle of length k identifies a periodic output label sequence of minimal period k, and distinct cycles identify distinct periodic output label sequences;
- for every pair of distinct periodic state trajectories of the same minimal period k, described by the two ordered $k$tuples

$$(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k) \neq (\bar{\mathbf{x}}_1, \bar{\mathbf{x}}_2, \ldots, \bar{\mathbf{x}}_k),$$

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the corresponding output trajectories are periodic of minimal period k and described by two different ordered $k$tuples, i.e.

$$(H\mathbf{x}_1, H\mathbf{x}_2, \dots, H\mathbf{x}_k) \neq (H\bar{\mathbf{x}}_1, H\bar{\mathbf{x}}_2, \dots, H\bar{\mathbf{x}}_k)$$

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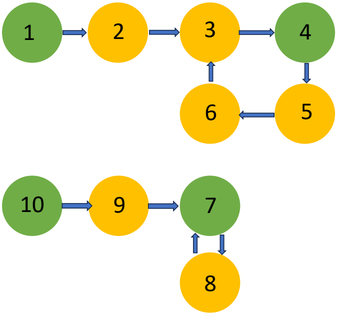

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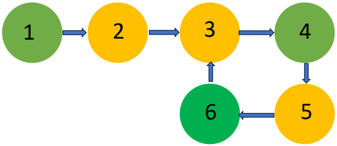

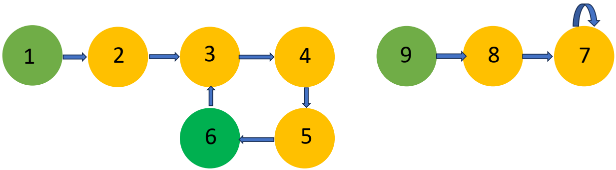

BNs: remarks on reconstructability (1)

Every logical matrix $L \in \mathcal{L}_{2^n \times 2^n}$ can be brought, by means of row-column permutations, to the following form:

$$L = \begin{bmatrix} W & 0 \\ T & C \end{bmatrix},$$

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each C_i being a cyclic permutation matrix.

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The BN described by (L, H) is reconstructable if and only if all columns of the matrix

$$\mathcal{O}_C := \begin{bmatrix} H_C \\ H_C C \\ \vdots \\ H_C C^{N-1} \end{bmatrix}$$

are distinct.

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A Boolean control network (BCN) is described by the following equations

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If we represent the Boolean vectors by means of their "canonical equivalent", the BCN (3) can be described as

$$\begin{aligned} \mathbf{x}(t+1) &= L \ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t), \qquad t \in \mathbb{Z}_+, \\ \mathbf{y}(t) &= H\mathbf{x}(t) \end{aligned} \tag{4}$$

where $L \in \mathcal{L}_{2^n \times 2^{(n+m)}}$ and $H \in \mathcal{L}_{2^p \times 2^n}$.

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Definition 2 A BCN (4) is reconstructable if if there exists $T \in \mathbb{Z}_+$ such that, for every input sequence and every initial condition $\mathbf{x}(0)$, the knowledge of the input and of the corresponding output trajectory, $\mathbf{u}(t)$ and $\mathbf{y}(t), t \in \{0, 1, \dots, T\}$, allows to uniquely determine $\mathbf{x}(T)$.

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More in detail, a BCN (4) is reconstructable if $\exists\, T \geq 0$ such that

$$\left\{ \begin{array}{c} u(0), u(1), \dots, u(T-1) \\ y(0), y(1), \dots, y(T) \end{array} \right\} \underset{\text{uniquely}}{\longrightarrow} x(T).$$

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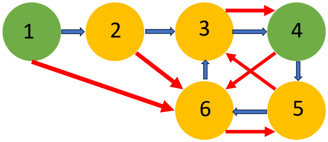

$$L \ltimes \delta_2^2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \end{bmatrix}$$

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$$(i_1, i_2)_{k_1}, (i_2, i_3)_{k_2}, \dots, (i_h, i_1)_{k_h}, \qquad (j_1, j_2)_{k_1}, (j_2, j_3)_{k_2}, \dots, (j_h, j_1)_{k_h},$$

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• for every pair of distinct periodic state-input trajectories of the same minimal period k, described by the $k$tuples

$$((\mathbf{x}_1, \mathbf{u}_1), \dots, (\mathbf{x}_k, \mathbf{u}_k)) \neq ((\bar{\mathbf{x}}_1, \mathbf{u}_1), \dots, (\bar{\mathbf{x}}_k, \mathbf{u}_k)),$$

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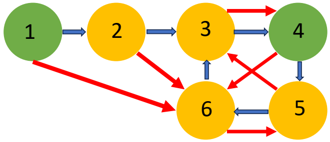

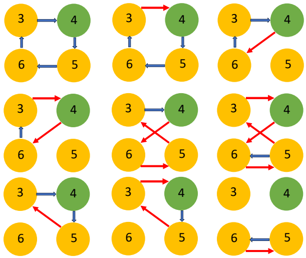

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where $\mathbf{c}_f \in \mathbb{R}^N$ and $\mathbf{c} \in \mathbb{R}^{NM}$.

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By exploiting the fact that the domain of $\mathcal{Q}_f(\cdot)$ and $\mathcal{Q}(\cdot,\cdot)$ is a finite set, we can equivalently rewrite the index $J_T(\mathbf{x}_0, \mathbf{u}(\cdot))$ as:

$$J_T(\mathbf{x}_0, \mathbf{u}(\cdot)) = \mathbf{c}_f^\top \mathbf{x}(T) + \sum_{t=0}^{T-1} \mathbf{c}^\top \ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t), \qquad (6)$$

where $\mathbf{c}_f \in \mathbb{R}^N$ and $\mathbf{c} \in \mathbb{R}^{NM}$.

Also, for every choice of $\alpha, \beta \in \mathbb{R}$, the input sequence that minimizes the cost function (6) (for any given $\mathbf{x}_0$) is the same one that minimizes

$$\tilde{J}_T(\mathbf{x}_0, \mathbf{u}(\cdot)) = [\mathbf{c}_f + \alpha \mathbf{1}_N]^\top \mathbf{x}(T) + \sum_{t=0}^{T-1} [\mathbf{c} + \beta \mathbf{1}_{NM}]^\top \ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t),$$

where $\mathbf{1}_k$ is the k-dimensional vector with all unitary entries.
So, one can assume that in (6)
the weight vectors $\mathbf{c}_f$ and $\mathbf{c}$ are nonnegative.

Finite Horizon Optimal Control: Problem solution

For every choice of a family of real vectors $\mathbf{m}(t), t \in [0, T]$, and every state trajectory of the BCN $\mathbf{x}(t), t \in [0, T]$, one has

$$\begin{aligned} 0 &= \sum_{t=0}^{T-1} [\mathbf{m}(t+1)^\top \mathbf{x}(t+1) - \mathbf{m}(t)^\top \mathbf{x}(t)] \\ &+ \mathbf{m}(0)^\top \mathbf{x}(0) - \mathbf{m}(T)^\top \mathbf{x}(T). \end{aligned}$$

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Consequently, the cost function can be equivalently rewritten

$$\begin{aligned} J(\mathbf{x}_0, \mathbf{u}(\cdot)) &= \mathbf{m}(0)^\top \mathbf{x}(0) + [\mathbf{c}_f - \mathbf{m}(T)]^\top \mathbf{x}(T) \\ &+ \sum_{t=0}^{T-1} \mathbf{c}^\top \ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t) + \sum_{t=0}^{T-1} [\mathbf{m}(t+1)^\top \mathbf{x}(t+1) - \mathbf{m}(t)^\top \mathbf{x}(t)]. \end{aligned}$$

By making use of the state update equation of the BCN (4) and of the fact that, for every choice of $\mathbf{u}(t) \in \mathcal{L}_M$, one has

$$\mathbf{m}(t)^\top \mathbf{x}(t) = \begin{bmatrix} \mathbf{m}(t)^\top & \mathbf{m}(t)^\top & \dots & \mathbf{m}(t)^\top \end{bmatrix} \ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t),$$

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we get this final version of the cost function:

$$J(\mathbf{x}_0, \mathbf{u}(\cdot)) = \mathbf{m}(0)^\top \mathbf{x}(0) + [\mathbf{c}_f - \mathbf{m}(T)]^\top \mathbf{x}(T)$$

$$+ \sum_{t=0}^{T-1} \left(\mathbf{c}^\top + \mathbf{m}(t+1)^\top L - \begin{bmatrix} \mathbf{m}(t)^\top & \dots & \mathbf{m}(t)^\top \end{bmatrix} \right) \ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t).$$

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Then, the term in the summation becomes:

$$\left(\mathbf{c}^\top + \mathbf{m}(t+1)^\top L - \begin{bmatrix} \mathbf{m}(t)^\top & \dots & \mathbf{m}(t)^\top \end{bmatrix} \right) \ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t) =$$

$$\begin{bmatrix} \mathbf{c}_1^\top + \mathbf{m}(t+1)^\top L_1 - \mathbf{m}(t)^\top & \dots & \mathbf{c}_M^\top + \mathbf{m}(t+1)^\top L_M - \mathbf{m}(t)^\top \end{bmatrix}$$

$$\ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t).$$

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Now, since the vectors $\mathbf{m}(t), t \in [0, T]$, can be freely chosen without affecting the value of the index, we choose them according to the following ALGORITHM:

- [Initialization] Set $\mathbf{m}(T) := \mathbf{c}_f$;
- [Recursion] For $t = T-1, T-2, \dots, 1, 0$, the jth entry of the vector $\mathbf{m}(t)$ is chosen according to the recursive rule:

$$[\mathbf{m}(t)]_j := \min_{i \in [1,M]} \Big([\mathbf{c}_i^\top + \mathbf{m}(t+1)^\top L_i]_j \Big), \ \forall\, j \in [1, N].$$

As a result, the index takes the form

$$J(\mathbf{x}_0, \mathbf{u}(\cdot)) = \mathbf{m}(0)^\top \mathbf{x}(0)$$

$$+ \sum_{t=0}^{T-1} \begin{bmatrix} \mathbf{w}_1(t)^\top & \mathbf{w}_2(t)^\top & \dots & \mathbf{w}_M(t)^\top \end{bmatrix} \ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t)$$

and for each $j \in [1, N]$, there is some row vector $\mathbf{w}_i(t)$ whose jth entry is zero, while the jth entry of all the other row vectors $\mathbf{w}_k(t)$ is nonnegative.

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Therefore the cost function is minimized by any input sequence $\mathbf{u}(t), t \in [0, T-1]$, that is obtained according to this rule:

$$\mathbf{x}(t) = \delta_N^j \qquad \longrightarrow \qquad \mathbf{u}(t) = \delta_M^{i^*(j,t)},$$

where

$$i^*(j,t) = \arg \min_{i \in [1,M]} [\mathbf{w}_i(t)]_j = \arg \min_{i \in [1,M]} \Big([\mathbf{c}_i + \mathbf{m}(t+1)^\top L_i]_j \Big).$$

In this way,

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- The optimal control input can be implemented by means of a time-varying feedback law:

$$\mathbf{u}(t) = K(t)\mathbf{x}(t),$$

  where the (not necessarily unique) feedback matrix is expressed as

$$K(t) = \begin{bmatrix} \delta_M^{i^*(1,t)} & \delta_M^{i^*(2,t)} & \dots & \delta_M^{i^*(N,t)} \end{bmatrix}.$$

Thanks for your attention!

Questions?