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Identification problems for Boolean networks and Boolean control networks

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Abstract: In this paper we address various forms of identification problems for Boolean networks (BNs) and for Boolean control networks (BCNs). For the former, we assume to have a set of infinite or finite support output trajectories and we want to identify a BN compatible with those trajectories. Conditions for the identified BN to coincide (up to a relabeling) with the original BN are provided. For BCNs, the problem of identifying a BCN compatible with a given family of corresponding finite support input/output trajectories is explored.

1. INTRODUCTION

The recent flourishing of papers addressing various aspects of Boolean networks (BNs) and Boolean control networks (BCNs) is mainly credited to the possibility of fruitfully employing these models (as well as probabilistic BNs) in a number of emerging research topics, first of all, genetic regulation networks [15, 24], and consensus problems [14, 22]. However, their success would have not been so remarkable were it not for the algebraic framework, developed by D. Cheng and co-authors [2, 4, 5, 6] to deal with BNs and BCNs. Indeed, by representing these logical networks as linear state-space models (operating on canonical vectors), it has been possible to pose and solve a number of control problems, by making use of a set up very similar to the traditional one employed for linear systems. In addition, for certain control problems, graph-based techniques, similar to the ones typically adopted for positive linear systems, have also proved to be effective. In detail, algebraic representations of BNs and BCNs have provided a very convenient framework to investigate stability and stabilizability problems [3, 9, 10], controllability [17], observability and state observer design [8], and more recently optimal control problems [11, 16, 25].

The interest in identification problems for logical networks was stimulated by biological and genetic applications [1, 21, 23]. Indeed, it is clear that in those contexts a mathematical model of the real logical network in general is not available, and it is necessary to use input/output data to determine a possible logical network that could justify those evolutions. This very interesting application area led D. Cheng and co-workers to investigate the identification problem for BCNs in a recent paper [7] (see also [6]). In [7] the problem of determining under what conditions there exists a pair of finite support corresponding [1] input and output trajectories, such that the smallest BCN compatible with them is just the original BCN generating them. It turns out that such an input/output pair exists if and only if the BCN is endowed with two very strong structural properties (controllability and observability). The goal of our research on this topic is to investigate the general problem of identifying a possible BCN compatible with a given set of corresponding input/output trajectories, without any assumption on the structure of the original BCN, nor on its size, and without assuming that the input/output trajectories we are measuring are the special ones that allow for the BCN identification.

As a preliminary step in this direction, in Section II we investigate a number of different identification problems for BNs, and determine under what conditions a BN can be correctly identified starting from a specific output trajectory, from a family of output trajectories or from any output trajectory it generates. Section III provides some preliminary results, by addressing one specific identification problem for BCNs. Starting from a given family $\mathcal{S}$ of input-output trajectories of length T, we look for a BCN whose input-output behavior on the time interval $[0, T-1]$ exactly fits the family $\mathcal{S}$. Before proceeding, we introduce some preliminary notation and mathematical tools.

Notation. $\mathbb{Z}_+$ denotes the set of nonnegative integers. Given $k, n \in \mathbb{Z}_+$, with $k \le n$, by $[k, n]$ denotes the set of integers $\{k, k+1, \dots, n\}$. We consider Boolean vectors and matrices, taking values in $\mathcal{B} := \{0, 1\}$, with the usual operations (sum $\vee$, product $\wedge$ and negation $\neg$). δ_k^i denotes the ith canonical vector of size k, $\mathcal{L}_k$ the set of all k-dimensional canonical vectors, and $\mathcal{L}_{k\times n} \subset \mathcal{B}^{k\times n}$ the set of $k \times n$ matrices whose columns are canonical vectors. A matrix $L \in \mathcal{L}_{k\times n}$ can be represented as a row vector whose entries are canonical vectors in $\mathcal{L}_k$, namely $L = \left[\, \delta_k^{i_1} \;\; \delta_k^{i_2} \;\; \dots \;\; \delta_k^{i_n} \,\right]$, for suitable $i_1, i_2, \dots, i_n \in [1, k]$. The k-dimensional vector with all entries equal to 1 is denoted by $\mathbf{1}_k$. The (ℓ, j)th entry of a matrix M is denoted by $[M]_{\ell j}$, while the ℓth entry of a vector $\mathbf{v}$ is $[\mathbf{v}]_\ell$. The ith column of a matrix M is $\mathrm{col}_i(M)$. Given a matrix $L \in \mathcal{B}^{k\times k}$ (in particular, $L \in \mathcal{L}_{k\times k}$), we associate with it a *digraph* $\mathcal{D}(L)$, with vertices $1, \dots, k$. There is an arc (j, ℓ) from j to ℓ if and only if the (ℓ, j)th entry of L is unitary. A sequence $j_1 \to j_2 \to \dots \to j_r \to j_{r+1}$ in $\mathcal{D}(L)$ is a *path* of length r from j_1 to j_{r+1} provided that $(j_1, j_2), \dots, (j_r, j_{r+1})$ are arcs of $\mathcal{D}(L)$.

[1] The word "corresponding" is here used to express the concept that the output trajectory is generated by the BCN corresponding to that input trajectory and some unknown initial state.

There is a bijection between Boolean variables $X \in \mathcal{B}$ and vectors $\mathbf{x} \in \mathcal{L}_2$, defined by the relationship

$$\mathbf{x} = \begin{bmatrix} X \\ \neg X \end{bmatrix}.$$

We introduce the *(left) semi-tensor product* $\ltimes$ between matrices (and, in particular, vectors) as follows [6, 17, 19]: given $L_1 \in \mathbb{R}^{r_1 \times c_1}$ and $L_2 \in \mathbb{R}^{r_2 \times c_2}$ (in particular, $L_1 \in \mathcal{L}_{r_1 \times c_1}$ and $L_2 \in \mathcal{L}_{r_2 \times c_2}$), we set

$$L_1 \ltimes L_2 := (L_1 \otimes I_{T/c_1})(L_2 \otimes I_{T/r_2}), \quad T := \text{l.c.m.}\{c_1, r_2\},$$

where l.c.m. denotes the least common multiple. The semi-tensor product represents an extension of the standard matrix product, by this meaning that if $c_1 = r_2$, then $L_1 \ltimes L_2 = L_1 L_2$. Note that if $\mathbf{x}_1 \in \mathcal{L}_{r_1}$ and $\mathbf{x}_2 \in \mathcal{L}_{r_2}$, then $\mathbf{x}_1 \ltimes \mathbf{x}_2 \in \mathcal{L}_{r_1 r_2}$. For the properties of the semi-tensor product we refer to [6]. By resorting to the semi-tensor product, we can extend the previous correspondence to a bijective correspondence between $\mathcal{B}^n$ and $\mathcal{L}_{2^n}$. This is possible in the following way: given $X = [\, X_1 \quad X_2 \quad \dots \quad X_n \,]^\top \in \mathcal{B}^n$, set

$$\mathbf{x} := \begin{bmatrix} X_1 \\ \neg X_1 \end{bmatrix} \ltimes \begin{bmatrix} X_2 \\ \neg X_2 \end{bmatrix} \ltimes \dots \ltimes \begin{bmatrix} X_n \\ \neg X_n \end{bmatrix}.$$

2. IDENTIFICATION PROBLEMS FOR BOOLEAN NETWORKS

A *Boolean network* (BN) is given by

$$\begin{aligned} X(t+1) &= f(X(t)), \\ Y(t) &= h(X(t)), \qquad t \in \mathbb{Z}_+, \end{aligned} \tag{1}$$

where $X(t)$ and $Y(t)$ denote the n-dimensional state variable and the p-dimensional output at time t, taking values in $\mathcal{B}^n$ and $\mathcal{B}^p$, respectively. f and h are (logic) functions, i.e. $f : \mathcal{B}^n \to \mathcal{B}^n$ and $h : \mathcal{B}^n \to \mathcal{B}^p$. By resorting to the semi-tensor product $\ltimes$, state and output Boolean variables can be represented as canonical vectors in $\mathcal{L}_N$, $N := 2^n$, and $\mathcal{L}_P$, $P := 2^p$, respectively, and the BN (1) satisfies [6] the following *algebraic description*:

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

where $\mathbf{x}(t) \in \mathcal{L}_N$ and $\mathbf{y}(t) \in \mathcal{L}_P$. $L \in \mathcal{L}_{N \times N}$ and $H \in \mathcal{L}_{P \times N}$ are matrices whose columns are all canonical vectors of size N and P, respectively. For short, we use the pair (L, H) to denote the BN in (2).

Roughly speaking, the identification problem for a BN can be described as follows: given a family $\mathcal{Y}$ of trajectories taking values in $\mathcal{L}_P$, determine an integer $\hat N > 0$, and logic matrices $\hat L \in \mathcal{L}_{\hat N \times \hat N}$ and $\hat H \in \mathcal{L}_{P \times \hat N}$ such that the BN (2) described by those matrices has all the trajectories in $\mathcal{Y}$ as output trajectories. This idea can be formalized in several different ways, depending on whether we assume that $\mathcal{Y}$ consists of a single or of several trajectories, that the trajectories in $\mathcal{Y}$ have infinite or finite duration, that we know a priori that they are generated by a BN or not. In addition, when the problem is solvable, we can search for a BN of minimum size $\hat N$ compatible with the given set of trajectories $\mathcal{Y}$. In this paper we address a number of identification problems for BNs, but we always assume that the trajectories in $\mathcal{Y}$ are output trajectories generated by a BN. So, our task will be that of determining the original BN, say (L, H), that produced those output evolutions or another BN sharing with the original one the given output trajectories.

As a starting point we note that the number of distinct output trajectories of a BN is finite and upper bounded by the size N of the BN. Moreover, every (infinite) output trajectory $\{\mathbf{y}(t)\}_{t \in \mathbb{Z}_+}$ of a BN is *eventually periodic*, meaning that there exist $t_r \in \mathbb{Z}_+$ and $T_p \in \mathbb{Z}_+, T_p > 0$, such that

$$\mathbf{y}(t) = \mathbf{y}(t + T_p), \qquad \forall\, t \geq t_r. \tag{3}$$

Finally, the identification problem from the output trajectories never brings to a unique result: if the pair $(\hat L, \hat H)$ describes a BN compatible with the set of output trajectories $\mathcal{Y}$, then also the pair $(\Pi^\top \hat L \Pi, \hat H \Pi^\top)$ does, for every choice of the permutation matrix Π. So, when we try to identify the original BN generating the set $\mathcal{Y}$, the best we can do is to identify (L, H) up to a relabeling of the BN's states. We are now in a position to solve three identification problems.

Problem 1. Given a trajectory $\{\bar{\mathbf{y}}(t)\}_{t \in \mathbb{Z}_+}$, with $\bar{\mathbf{y}}(t) \in \mathcal{L}_P$ for every $t \geq 0$, eventually periodic, determine, if possible, the matrices $\hat L$ and $\hat H$ of a BN (2) having $\{\bar{\mathbf{y}}(t)\}_{t \in \mathbb{Z}_+}$ as an output trajectory.

Introduce the shift operator on the output trajectories

$$\sigma : (\mathcal{L}_P)^{\mathbb{Z}_+} \to (\mathcal{L}_P)^{\mathbb{Z}_+} : (\mathbf{y}(0), \mathbf{y}(1), \dots) \mapsto (\mathbf{y}(1), \mathbf{y}(2), \dots)$$

and let $\mathcal{X}$ be the set of all shifted versions of the trajectory $\{\bar{\mathbf{y}}(t)\}_{t \in \mathbb{Z}_+}$. By the assumption that the given trajectory is eventually periodic, we can find minimal nonnegative integers $t_r \in \mathbb{Z}_+$ and $T_p \in \mathbb{Z}_+, T_p > 0$, such that (3) holds for $\{\bar{\mathbf{y}}(t)\}_{t \in \mathbb{Z}_+}$, and this implies that the number of distinct elements in $\mathcal{X}$ is finite and equal to $\hat N := t_r + T_p$. Set $\mathbf{x}_i := (\mathbf{y}(i-1), \mathbf{y}(i-2), \mathbf{y}(i-3), \dots)$, $\quad i \in [1, \hat N]$. If we represent the state $\mathbf{x}_i$ with the canonical vector $\delta^i_{\hat N}$, a BN (2) of order $\hat N$ that is compatible with the given output trajectory is described by the matrices

$$\begin{aligned} \hat L &= \left[\, \delta^2_{\hat N} \quad \delta^3_{\hat N} \quad \dots \quad \delta^{t_r}_{\hat N} \quad \delta^{t_r+1}_{\hat N} \quad \dots \quad \delta^{\hat N}_{\hat N} \quad \delta^{t_r+1}_{\hat N} \,\right] \\ \hat H &= [\, \mathbf{y}(0) \quad \mathbf{y}(1) \quad \mathbf{y}(2) \quad \dots \quad \mathbf{y}(\hat N - 1) \,]. \end{aligned} \tag{4}$$

To understand under what conditions $\hat L$ and $\hat H$ coincide with the matrices of the original BN, (L, H), generating the given output trajectory, note that the previous algorithm leads to a BN whose associated graph consists of a cycle (the periodic part of the trajectory) together with a chain of transient states leading to the cycle.

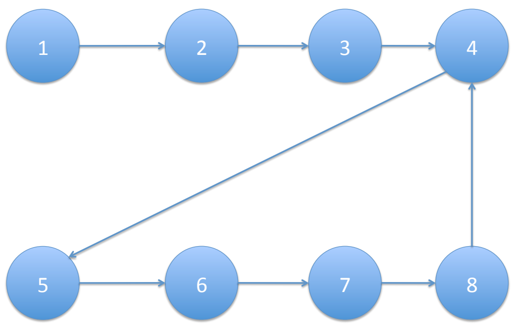

Fig. 1. *Digraph corresponding to the BN identified from a single output trajectory.*

The situation is depicted in Figure 1, where we have omitted the outputs since they are not relevant for this specific discussions. Of course, there may be no transient part, in which case the identified BN consists of a simple cycle (and generates only periodic state and output trajectories). This is intrinsic of the structure of a BN. Indeed, as shown in [8], the following result holds.

Proposition 1. Given a BN (2), there exists $r \in \mathbb{N}$ and a permutation matrix Π such that

$$\Pi^\top L \Pi = \text{blockdiag}\{D_1, D_2, \ldots, D_r\} \in \mathcal{L}_{N\times N}, \quad (5)$$

$$\text{with} \qquad D_\nu = \begin{bmatrix} W_\nu & 0 \\ S_\nu & C_\nu \end{bmatrix} \in \mathcal{L}_{n_\nu \times n_\nu}, \quad (6)$$

where W_ν is a $(n_\nu - k_\nu) \times (n_\nu - k_\nu)$ nilpotent matrix, and C_ν is a $k_\nu \times k_\nu$ cyclic matrix, i.e. $C_\nu = \begin{bmatrix} \delta^2_{k_\nu} & \delta^3_{k_\nu} & \ldots & \delta^{k_\nu}_{k_\nu} & \delta^1_{k_\nu} \end{bmatrix}$.

This proves that the digraph of a BN consists of the union of r independent subgraphs, each of them consisting of a cycle and of a number of chains accessing the cycle. Clearly, each state (and hence each output) trajectory is generated by a specific initial state, and hence it explores only a specific subgraph, and within that subgraph a unique chain and the associated cycle. So, a necessary condition for the pair (L, H) to be identifiable from the output trajectory $\{\bar{\mathbf{y}}(t)\}_{t\in\mathbb{Z}_+}$ is that there exists a permutation matrix Π such that

$$\Pi^\top L \Pi = \begin{bmatrix} W & 0 \\ S & C \end{bmatrix},$$

where

$$W = \begin{bmatrix} 0 & 0 & \ldots & 0 & 0 \\ 1 & 0 & \ldots & 0 & 0 \\ 0 & 1 & \ldots & 0 & 0 \\ & & \ddots & & \\ 0 & 0 & \ldots & 1 & 0 \end{bmatrix} = \begin{bmatrix} \delta^2_{N-k} & \delta^3_{N-k} & \ldots & \delta^{N-k}_{N-k} & 0 \end{bmatrix}$$

$$S = \begin{bmatrix} 0 & 0 & \ldots & 0 & 1 \\ 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & \ldots & 0 & 0 \\ & & \ddots & & \\ 0 & 0 & \ldots & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & \ldots & 0 & \delta^1_k \end{bmatrix},$$

and C is a $k \times k$ cyclic matrix.

Another necessary condition for identifiability is represented by the observability of the original BN (L, H).

Definition 1. [6, 8] Given a BN (2),

- two states $\mathbf{x}_1 = \delta^i_N$ and $\mathbf{x}_2 = \delta^j_N$ are said to be *indistinguishable*, if the two output evolutions of the BN starting at $t = 0$ from $\mathbf{x}(0) = \mathbf{x}_1$ and from $\mathbf{x}(0) = \mathbf{x}_2$, respectively, coincide at every time instant $t \in \mathbb{Z}_+$; otherwise they are *distinguishable*;
- the BN is said to be *observable* if every two distinct states are distinguishable.

Indeed, suppose that the original BN, of size N, (L, H) is not observable and hence there exist indistinguishable states. If there exist transient states in the BN and the output trajectory $\{\bar{\mathbf{y}}(t)\}_{t\in\mathbb{Z}_+}$ is not generated starting from the first state of the chain (namely the only state with no predecessor), then we will not be able to identify all the states. On the other hand, if the BN consists only of a cycle or the output trajectory is generated starting from the first state of the chain, it will pass through (all the states, and hence through) two indistinguishable states. Accordingly, there will be two time instants $0 \le t_1 < t_2 < N$ such that $\bar{\mathbf{y}}(t_1 + \tau) = \bar{\mathbf{y}}(t_2 + \tau)$ for every $\tau \ge 0$. This ensures that the output trajectory is also compatible with a BN of size $N - (t_2 - t_1)$, thus ruling out identifiability.

Conversely, it is also clear that the two aforementioned necessary conditions are also sufficient for identifiability, since if they are both verified the output trajectory $\{\bar{\mathbf{y}}(t)\}_{t\in\mathbb{Z}_+}$, generated corresponding to the first state of the chain (or any state belonging to the cycle, in case there are no transient states), will generate a set $\mathcal{X}$ of cardinality N. So, we have proved the following result.

Proposition 2. Given a BN (2), a necessary and sufficient condition for the existence of a single output trajectory $\{\bar{\mathbf{y}}(t)\}_{t\in\mathbb{Z}_+}$ that allows to identify the matrices of the BN (up to a permutation) is that the BN is observable and has a graph consisting of a cycle together with a (possibly empty) chain of arcs leading to the cycle (as in Fig.1).

The natural generalization of Problem 1 is the following one:

Problem 2. Given a set $\mathcal{Y}$ of trajectories $\{\bar{\mathbf{y}}_i(t)\}_{t\in\mathbb{Z}_+}$, $i \in [1, k]$, with $\bar{\mathbf{y}}_i(t) \in \mathcal{L}_P$ for every $t \ge 0$, each of them eventually periodic, determine, if possible, the matrices $\hat{L}$ and $\hat{H}$ of a BN (2) having $\mathcal{Y}$ as set of output trajectories.

Clearly, the problem solution is a generalization of the previous one: also in this case we define the set $\mathcal{X}$, consisting of all the distinct shifted versions of the output trajectories, and the elements of $\mathcal{X}$ are the states of a BN compatible with the given set of output trajectories. The first entry of any such $\mathbf{x}_i = \delta^i_{\hat{N}}$, where $\hat{N} := |\mathcal{X}|$, determines the ith column of $\hat{H}$. Moreover, if $\mathbf{x}_i$ corresponds to some shifted output sequence and $\mathbf{x}_j$ corresponds to the one step shifted version of the same sequence, then $L\delta^i_{\hat{N}} = \text{col}_i(L) = \delta^j_{\hat{N}}$.

Proposition 3. Given a BN (2), a necessary and sufficient condition for the existence of a finite set of output trajectories $\mathcal{Y}$ that allows to identify the matrices of the BN (up to a permutation) is that the BN is observable.

Proof. Necessity is obvious. On the other hand, if we choose as $\mathcal{Y}$ the set of all output trajectories generated starting from states that have no predecessors (or any state of a cycle, in case there are no chains accessing it), then the corresponding set $\mathcal{X}$ will have the same cardinality as the original BN and we will be able to reconstruct the original matrices, up to a relabeling, by means of the simple algorithm just illustrated. $\square$

Note that the possibility of identifying (L, H) from the set $\mathcal{Y}$ is strictly related not only to the structural properties of the pair (L, H), but also to the specific choice of $\mathcal{Y}$. Indeed, all the output trajectories generated starting from states that have no predecessors must be in $\mathcal{Y}$, and for every isolated cycle in the digraph there must be at least one output trajectory in $\mathcal{Y}$ generated starting from a state of the cycle. So, the only case when a BN can be identified from *any* set $\mathcal{Y}$ of its output trajectories is when the BN is observable and its digraph is a single cycle. When so, $\mathcal{Y}$ can always consist of a single trajectory.

To conclude the section, we address the identification problem for BNs, by assuming that the output trajectories in $\mathcal{Y}$ have finite support.

Problem 3. Given a time $T > 0$ and a set $\mathcal{Y}$ of finite support trajectories $\{\bar{\mathbf{y}}_i(t)\}_{t\in[0,T-1]}$, $i \in [1,k]$, with $\bar{\mathbf{y}}_i(t) \in \mathcal{L}_P$ for every $t \in [0, T-1]$, determine, if possible, matrices $\hat{L}$ and $\hat{H}$ of minimal size $\hat{N}$ of a BN (2) having $\mathcal{Y}$ as set of output trajectories.

In this case the problem is always solvable, since one can trivially choose a BN of size equal to kT, whose matrix $\hat{L}$ is described as in (5) and (6), for $r = k$ and diagonal blocks

$$D_\nu = [\,\delta_T^2 \quad \delta_T^3 \quad \dots \quad \delta_T^T \quad \delta_T^1\,], \qquad \nu \in [1,k],$$

while

$$\hat{H} = [\,\bar{\mathbf{y}}_1(0) \quad \dots \quad \bar{\mathbf{y}}_1(T-1) \quad | \quad \bar{\mathbf{y}}_2(0) \quad \dots \\ \dots \quad \bar{\mathbf{y}}_{k-1}(T-1) \quad | \quad \bar{\mathbf{y}}_k(0) \quad \dots \quad \bar{\mathbf{y}}_k(T-1)\,].$$

So, the only nontrivial question is the minimization issue.

For the sake of simplicity, we consider the case when $k = 1$, namely $\mathcal{Y} = \left\{\{\bar{\mathbf{y}}(t)\}_{t\in[0,T-1]}\right\}$. Two cases possibly arise:
(1) $\bar{\mathbf{y}}(T-1) \neq \bar{\mathbf{y}}(t)$ for every $t \in [0, T-2]$;
(2) there exists $t \in [0, T-2]$ such that $\bar{\mathbf{y}}(t) = \bar{\mathbf{y}}(T-1)$.

Case (1) corresponds to the situation when the output trajectory has not entered the periodic phase yet, and hence necessarily $T \leq N$, namely the number of output samples is not bigger than the size of the generating BN. Then the trivial solution previously provided (for $k = 1$) is also the smallest one compatible with the given $\mathcal{Y}$.

In Case (2), define the following sets (of finite cardinality):

$$\mathcal{S} := \{\tau \in [0, T-2] : \bar{\mathbf{y}}(\tau) = \bar{\mathbf{y}}(T-1)\}$$
$$\mathcal{P} := \{T - \tau : \tau \in \mathcal{S}\}.$$

Set $d := |\mathcal{P}|$. For every $p_i \in \mathcal{P}, i \in [1,d]$, define also

$$t_{ri} := \min\{t \in [0, T-1-p_i] : \\ \bar{\mathbf{y}}(t) = \bar{\mathbf{y}}(t+p_i), \forall\, t \in [t_{ri}, T-1-p_i]\}.$$

So, the idea is to be able to regard the finite sequence $\bar{\mathbf{y}}(t), t \in [0, T-1]$, as the initial portion of an infinite output trajectory having transient phase of length t_{ri} and period p_i. A minimal realization compatible with $\mathcal{Y}$ has size $\hat{N} := \min\{t_{ri} + p_i, i \in [1,d]\}$.
If $(t_r, T_p) := \operatorname{argmin}\{t_{ri} + p_i, i \in [1,d]\}$, namely $t_r = t_{ri}$ and $T_p = p_i$ for some $i \in [1,d]$ and $t_r + T_p = \min\{t_{ri} + p_i, i \in [1,d]\}$, such a minimal BN is described as in (4).

Note that, by similar reasonings to the ones adopted for the identification of a BN from a single infinite support output trajectory (see Proposition 2), we can deduce the following result.

Proposition 4. Given a BN (L,H), a necessary and sufficient condition for the existence of a positive integer T and an output trajectory $\{\bar{\mathbf{y}}(t)\}_{t\in[0,T-1]}$ such that the BN can be identified from such a trajectory is that the BN is observable and its digraph consists of a cycle together with a (possibly empty) chain of arcs leading to the cycle.

The case when $\mathcal{Y}$ consists of several trajectories follows the same lines but it is more involved, since the minimization is achieved by also verifying whether different trajectories in $\mathcal{Y}$ can be regarded as generated by the same portion of the BN digraph. Due to page constraint we omit this analysis here and we refer the interested reader to [12].

3. IDENTIFICATION PROBLEMS FOR BCNS

A *Boolean Control Network* (BCN) is described by the following equations

$$\begin{aligned} X(t+1) &= f(X(t), U(t)), \\ Y(t) &= h(X(t)), \qquad t \in \mathbb{Z}_+, \end{aligned} \tag{7}$$

where $X(t)$, $U(t)$ and $Y(t)$ denote the n-dimensional state variable, the m-dimensional input and the p-dimensional output at time t, taking values in $\mathcal{B}^n, \mathcal{B}^m$ and $\mathcal{B}^p$, respectively. f and h are logic functions, i.e. $f : \mathcal{B}^n \times \mathcal{B}^m \to \mathcal{B}^n$ and $h : \mathcal{B}^n \to \mathcal{B}^p$. By resorting to the semi-tensor product $\ltimes$, the BCN (7) can be described [6] as

$$\begin{aligned} \mathbf{x}(t+1) &= L \ltimes \mathbf{u}(t) \ltimes \mathbf{x}(t), \\ \mathbf{y}(t) &= H \ltimes \mathbf{x}(t) = H\mathbf{x}(t), \qquad t \in \mathbb{Z}_+, \end{aligned} \tag{8}$$

where $\mathbf{x}(t) \in \mathcal{L}_N, \mathbf{u}(t) \in \mathcal{L}_M$ and $\mathbf{y}(t) \in \mathcal{L}_P$, with $N := 2^n, M := 2^m$ and $P := 2^p$. $L \in \mathcal{L}_{N\times NM}$ and $H \in \mathcal{L}_{P\times N}$ are matrices whose columns are canonical vectors of size N and P, respectively. We will refer to a BCN described as in (8) by means of the pair (L,H). Note however, that in this case L is a rectangular matrix and not a square one. For every choice of the input variable at t, namely for every $\mathbf{u}(t) = \delta_M^j$, $L \ltimes \mathbf{u}(t) =: L_j$ is a matrix in $\mathcal{L}_{N\times N}$. So, we can think of the state equation of the BCN (8) as a Boolean switched system (see [18, 20]),

$$\mathbf{x}(t+1) = L_{\sigma(t)}\mathbf{x}(t), \qquad t \in \mathbb{Z}_+, \tag{9}$$

where $\sigma(t), t \in \mathbb{Z}_+$, is a switching sequence taking values in $[1,M]$. For every $j \in [1,M]$, the BN

$$\mathbf{x}(t+1) = L_j\mathbf{x}(t), \qquad t \in \mathbb{Z}_+, \tag{10}$$

represents the jth subsystem of (9).

The identification problem for BCNs has been recently posed in [6, 7] in the following terms:

Problem 4. Given a BCN (L,H), under what conditions there exist a positive integer T and a pair of input/output trajectories $\{(\bar{\mathbf{u}}(t), \bar{\mathbf{y}}(t))\}_{t\in[0,T-1]}$, generated by the BCN corresponding to some unknown initial state, such that the BCN can be identified from such a pair of trajectories?

The problem solution provided in [6, 7] is as follows.

Proposition 5. Given a BCN (L,H), there exist a positive integer T and a pair of input/output trajectories $\{(\bar{\mathbf{u}}(t), \bar{\mathbf{y}}(t))\}_{t\in[0,T-1]}$, generated by the BCN corresponding to some unknown initial state, such that the BCN can be identified (up to a relabeling of the states) from such a pair of trajectories if and only if the following two conditions hold:

i) the BCN is controllable, namely [6] for every $\mathbf{x}_0$ and $\mathbf{x}_f \in \mathcal{L}_N$ there exist $d \in \mathbb{Z}_+$ and an input sequence

$\mathbf{u}(t), t \in [0, d-1]$, that leads the state trajectory from $\mathbf{x}(0) = \mathbf{x}_0$ to $\mathbf{x}(d) = \mathbf{x}_f$;

ii) the BCN is observable, in the sense that [6] there exists an input sequence $\mathbf{u}(t), t \in \mathbb{Z}_+$, such that the initial state $\mathbf{x}(0)$ can be uniquely determined from the knowledge of the pair of corresponding input/output trajectories $\{(\mathbf{u}(t), \mathbf{y}(t))\}_{t\in\mathbb{Z}_+}$.

This characterization is useful from a theoretical point of view, as it tells us under what conditions we may hope to identify a BCN from the measurement of a corresponding pair of (finite support) input/output trajectories. However, in general, we have no guarantee to be so lucky to be able to measure a pair of trajectories endowed with these features. In addition, the algorithms illustrated in [6, 7] to identify the BCN presume that the size N of the BCN is a priori known, and either consider all pairs $(\hat{L}, \hat{H})$ of appropriate size, by moving from one to another according to some distance function to be minimized (see Algorithm 17.1 in [6]), or suppose to have some information about the underlying digraph of the BCN.

The identification problem we investigate in this section is slightly different. On the one hand, we do not impose controllability or observability properties on the BCN originating the input/output trajectories, and hence weaken our requirements on the system. On the other hand, we strengthen our requirements on the data, and assume to have all the possible input/output trajectories of a given duration T, $\left\{\{(\mathbf{u}(t), \mathbf{y}(t))\}_{t\in[0,T-1]}\right\}$, generated by the BCN corresponding to the various initial states. To explore this case, we provide an algorithm inspired by the work of Gill [13]. For the sake of brevity we omit here all the proofs that can be derived, mutatis mutandis, by suitably adjusting those provided in [13]. A detailed derivation of the following algorithm can be found in [12].

Denote by $\mathcal{S}$ the set of all possible corresponding input/output trajectories generated by the BCN in $[0, T-1]$. Note that the last input sample, $\mathbf{u}(T-1)$, is useless from an identification point of view, and hence we set

$$\mathcal{S} := \{\mathbf{z}_{[0,T-1]} := (\mathbf{y}(0), \mathbf{u}(0), \mathbf{y}(1), \mathbf{u}(1), \dots, \mathbf{u}(T-2), \mathbf{y}(T-1))\}.$$

$\mathcal{S}$ is called *the input/output set of length T of the BCN.* We now define the set of all possible corresponding input/output trajectories generated by the BCN in $[0, k-1], 1 \le k \le T$:

$$\mathcal{S}^{(k-1)} := \{\mathbf{z}_{[0,k-1]} := (\mathbf{y}(0), \mathbf{u}(0), \mathbf{y}(1), \mathbf{u}(1), \dots, \mathbf{u}(k-2), \mathbf{y}(k-1))\}.$$

Clearly, $\mathcal{S} = \mathcal{S}^{(T-1)}$. The I/O set $\mathcal{S}$ is *compatible*, namely

(1) $\mathcal{S}^{(0)}$ has at least one element;

(2) for every $\bar{\mathbf{z}}_{[0,k-1]} \in \mathcal{S}^{(k-1)}$ and every $\bar{\mathbf{u}}(k-1) \in \mathcal{L}_M$ there exists $\bar{\mathbf{y}}(k) \in \mathcal{L}_P$ such that
$$\bar{\mathbf{z}}_{[0,k]} = (\bar{\mathbf{z}}_{[0,k-1]}, \bar{\mathbf{u}}(k-1), \bar{\mathbf{y}}(k)) \in \mathcal{S}^{(k)};$$

(3) $\bar{\mathbf{z}}_{[0,k]} = (\bar{\mathbf{y}}(0), \bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(k-1), \bar{\mathbf{y}}(k)) \in \mathcal{S}^{(k)}$ if and only if $\bar{\mathbf{z}}_{[0,k-1]}$ and $\bar{\mathbf{z}}_{[1,k]} = (\bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \bar{\mathbf{y}}(2), \bar{\mathbf{u}}(2), \dots, \bar{\mathbf{u}}(k-1), \bar{\mathbf{y}}(k))$ belong to $\mathcal{S}^{(k-1)}$.

Two cases possibly arise: **A)** there exists some index $k \in [1, T-1]$ such that $|\mathcal{S}^{(k)}| = M \cdot |\mathcal{S}^{(k-1)}|$ (in this case we say that the I/O set $\mathcal{S}$ is *bounded*); **B)** no such k exists.

In Case **A)**, we set $b := \min\{k \in [1, T-1] : |\mathcal{S}^{(k)}| = M \cdot |\mathcal{S}^{(k-1)}|\}$ and denote by d the cardinality of $\mathcal{S}^{(b-1)}$. Also we distinguish two subcases:

A1) for every $\bar{\mathbf{z}}_{[0,b-1]} \in \mathcal{S}^{(b-1)}$ there exists $\hat{\mathbf{z}}_{[0,b]} \in \mathcal{S}^{(b)}$ such that $\hat{\mathbf{z}}_{[1,b]} = \bar{\mathbf{z}}_{[0,b-1]}$. If we regard the elements of $\mathcal{S}^{(b-1)}$ as states, this amounts to saying that every state in $\mathcal{S}^{(b-1)}$ has a predecessor;

A2) not every element in $\mathcal{S}^{(b-1)}$ has a predecessor.

In Case **A1)** a solution of size $\hat{N} := d$ can be obtained in the following way: represent the d distinct elements of $\mathcal{S}^{(b-1)}$ with the d canonical vectors $\delta_d^i, i \in [1, d]$. If δ_d^i is the representation of the string $(\bar{\mathbf{y}}(0), \bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(b-2), \bar{\mathbf{y}}(b-1))$ then
$$\mathrm{col}_i(\hat{H}) = \hat{H}\delta_d^i = \bar{\mathbf{y}}(b-1).$$
On the other hand, for every $\bar{\mathbf{u}}(b-1) \in \mathcal{L}_M$, the boundedness property ensures that there exists a unique $\bar{\mathbf{y}}(b) \in \mathcal{L}_P$ such that $(\bar{\mathbf{y}}(0), \bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(b-1), \bar{\mathbf{y}}(b)) \in \mathcal{S}^{(b)}$. If the string $(\bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(b-1), \bar{\mathbf{y}}(b)) \in \mathcal{S}^{(b-1)}$ is represented by the canonical vector δ_d^j, then
$$\mathrm{col}_i(\hat{L} \ltimes \bar{\mathbf{u}}(b-1)) = \hat{L} \ltimes \bar{\mathbf{u}}(b-1) \ltimes \delta_d^i = \delta_d^j.$$
In this way, we can obtain all the columns of the matrices $\hat{L}$ and $\hat{H}$ of a BCN compatible with the given set of input/output trajectories $\mathcal{S}$. Note that, by the assumption that every state has a predecessor, each row of $\hat{L}$ has at least one unitary entry.

It is worthwhile noticing that is we assume that the set of input/output trajectories $\mathcal{S}$ is generated by a controllable BCN, then every state in $\mathcal{S}^{(b-1)}$ has a predecessor.

Proposition 6. If the BCN (L, H), of size N, generating the set of input/output trajectories $\mathcal{S}$ is controllable, then every state in $\mathcal{S}^{(b-1)}$ has a predecessor.

Proof. Let
$$\bar{\mathbf{z}}_{[0,b-1]} = (\bar{\mathbf{y}}(0), \bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(b-2), \bar{\mathbf{y}}(b-1))$$
be an element of $\mathcal{S}^{(b-1)}$. This means that there exists $\bar{\mathbf{x}}_0 \in \mathcal{L}_N$ such that $\bar{\mathbf{z}}_{[0,b-1]}$ is the input/output trajectory generated by the BCN (L, H) corresponding to $\mathbf{x}(0) = \bar{\mathbf{x}}_0$ and $\mathbf{u}(t) = \bar{\mathbf{u}}(t), t \in [0, b-2]$. As the BCN is controllable, there exists $\bar{x}_{-1} \in \mathcal{L}_N$ and $\bar{\mathbf{u}}_{-1} \in \mathcal{L}_M$ such that $\mathbf{x}_0 = L \ltimes \bar{\mathbf{u}}_{-1} \ltimes \bar{\mathbf{x}}_{-1}$. Then the input/output trajectory $(H\bar{\mathbf{x}}_{-1}, \bar{\mathbf{u}}_{-1}, \bar{\mathbf{y}}(0), \bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(b-2), \bar{\mathbf{y}}(b-1))$ is in $\mathcal{S}^{(b)}$ and the state
$$(H\bar{\mathbf{x}}_{-1}, \bar{\mathbf{u}}_{-1}, \bar{\mathbf{y}}(0), \bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(b-3), \bar{\mathbf{y}}(b-2))$$
is a predecessor of $\bar{\mathbf{z}}_{[0,b-1]}$. □

In Case **A2)** the set of states defined by means of the sequences in $\mathcal{S}^{(b-1)}$ is not sufficient to account for the given set of trajectories. So, we have to add to all the states defined in $\mathcal{S}^{(b-1)}$ the states obtained as follows: for every $\bar{\mathbf{z}}_{[0,b-1]} = (\bar{\mathbf{y}}(0), \bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(b-2), \bar{\mathbf{y}}(b-1))$ in $\mathcal{S}^{(b-1)}$ having no predecessor, define as states the following b strings:
$$(\bar{\mathbf{y}}(0)),\ (\bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1)),\ (\bar{\mathbf{u}}(1), \bar{\mathbf{y}}(2)),\ \dots,\ (\bar{\mathbf{u}}(b-3), \bar{\mathbf{y}}(b-2)).$$

If we let $\mathcal{X}$ denote the set of all states (either belonging to $\mathcal{S}^{(b-1)}$ or defined as just shown) and we let $\hat{N}$ denote its cardinality, then all such states can be represented by canonical vectors $\delta_{\hat{N}}^i$. (It can be proved that $\hat{N} \le (b +$

$1)(MP)^b)$. For those $i \in [1, \hat{N}]$ such that $\delta^i_{\hat{N}}$ corresponds to a sequence in $\mathcal{S}^{(b-1)}$, the ith column of H and of the various matrices $L \ltimes \bar{\mathbf{u}}(b-1)$ are obtained as in point **A1)**. For those indices $i \in [1, \hat{N}]$ such that $\delta^i_{\hat{N}}$ corresponds to one of the new strings, if $\delta^i_{\hat{N}} = (\bar{\mathbf{u}}(k), \bar{\mathbf{y}}(k+1)), 0 \le k < b-1$ then $\mathrm{col}_i(\hat{H}) = \hat{H}\delta^i_{\hat{N}} = \bar{\mathbf{y}}(k+1)$; if $\delta^i_{\hat{N}} = (\bar{\mathbf{u}}(k), \bar{\mathbf{y}}(k+1))$, and $\delta^j_{\hat{N}} = (\bar{\mathbf{u}}(k+1), \bar{\mathbf{y}}(k+2))$, then $\mathrm{col}_i(\hat{L} \ltimes \bar{\mathbf{u}}(k+1)) = \hat{L} \ltimes \bar{\mathbf{u}}(k+1) \ltimes \delta^i_{\hat{N}} = \delta^j_{\hat{N}}$; if $\delta^i_{\hat{N}} = (\bar{\mathbf{u}}(b-3), \bar{\mathbf{y}}(b-2))$, and $\delta^j_{\hat{N}} = \bar{\mathbf{z}}_{[0,b-1]} = (\bar{\mathbf{y}}(0), \bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(b-2), \bar{\mathbf{y}}(b-1))$, then $\mathrm{col}_i(\hat{L} \ltimes \bar{\mathbf{u}}(b-2)) = \hat{L} \ltimes \bar{\mathbf{u}}(b-2) \ltimes \delta^i_{\hat{N}} = \delta^j_{\hat{N}}$.

In this way the BCN is not completely determined, as some columns of L are undefined. Indeed, for the new states we do not know the transitions corresponding to all possible inputs. However, it is possible to complete L in such a way to not create additional input/output trajectories in $[0, T-1]$ with respect to the ones belonging to $\mathcal{S}$.

So, we are now remained with case **B)**, when no index $k \in [1, T-1]$ can be found such that $|\mathcal{S}^{(k)}| = M \cdot |\mathcal{S}^{(k-1)}|$. In this case we want to construct $\mathcal{S}^{(T)}$ from $\mathcal{S} = \mathcal{S}^{(T-1)}$ in such a way that the previous relationship holds for $k = T$. For every $\bar{\mathbf{z}}_{[0,T-1]} = (\bar{\mathbf{y}}(0), \bar{\mathbf{u}}(0), \bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(T-2), \bar{\mathbf{y}}(T-1))$ in $\mathcal{S}$ and every input value $\bar{\mathbf{u}}(T-1)$ choose an arbitrary output value $\bar{\mathbf{y}}(T)$ such that $(\bar{\mathbf{y}}(1), \bar{\mathbf{u}}(1), \dots, \bar{\mathbf{u}}(T-1), \bar{\mathbf{y}}(T))$ is in $\mathcal{S}$. As $\mathcal{S}$ is unbounded, this choice is not unique and hence one can construct in this way several different sets $\mathcal{S}^{(T)}$. However, the set $\hat{\mathcal{S}} := \mathcal{S}^{(T)}$ is now bounded, since, by construction, $|\mathcal{S}^{(T)}| = M \cdot |\mathcal{S}^{(T-1)}|$. So, we can apply the reasonings adopted in the bounded case **A)**, and obtain a BCN that has all the trajectories of $\hat{\mathcal{S}}$ as input/output trajectories in $[0, T]$, and hence all the trajectories in $\mathcal{S}$ as input/output trajectories in $[0, T-1]$.

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