Single-Experiment Reconstructibility of Boolean Control Networks Revisited

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Abstract: We first demonstrate that, BCNs' single-experiment reconstructibility has three additional forms in addition to its current definition, and briefly introduce the verification algorithms we design for these new definitions. These definitions and algorithms bring the following improvements to BCNs' control theory. First, the solution algorithms of single-experiment reconstruction are enriched to cope with more different scenarios. Second, the verification problem of single-experiment reconstructibility is simplified. Finally, the essential relationship and difference between reconstruction and observation (which focuses on determining the initial state for a BCN), is further clarified.

1 INTRODUCTION

Inspired by the Boolean-type actions in genetic circuits (Jacob and Monod, 1961), Boolean networks (*BNs*) were proposed by Kauffman as a popular and well-established framework for modelling non-linear and complex biological systems (Kauffman, 1968). The main advantage of *BNs* is its simplicity and yet can be used to capture the important dynamic properties of biological systems, thus facilitating the modelling of large systems as a whole. In a *BN*, the nodes are denoted as binary variables, being either 'expressed' or 'not expressed' and activation/inhibition regulations between them are described by Boolean functions.

Boolean control networks (*BCNs*) is a natural extension of *BNs* with external regulations and perturbations (Ideker et al., 2001). A *BCN* has three different types of nodes, namely, *input-nodes*, *state-nodes*, and *output-nodes*. Their value vectors are called the *BCN*'s *input*, *state*, and *output*, respectively. The relationship between these three sets of nodes is described by the *BCN*'s updating rules. *BCNs* have been applied to various problems and typical examples including abduction-based drug target discovery (Biane and Delaplace, 2017), and functional and structural analysis of signalling and regulatory networks (Kaufman et al., 1999; Klamt et al., 2006). The widespread use has led to vast attention on the research of *BCNs*' control theory ((Akutsu et al., 2007; Cheng and Qi, 2009; Zhao et al., 2010; Cheng et al., 2011; Fornasini and Valcher, 2013; Su et al., 2019; Mandon et al., 2019; Zhang et al., 2015a)).

In this paper, we focus on *BCN* reconstruction which plays an important role in state observer design and controller synthesis of *BCNs* (Fornasini and Valcher, 2013). We propose that *BCN*'s single-experiment reconstructibility, which was considered to have only one form (Zhang et al., 2020a), has three other different but equivalent definitions, and design verification algorithms for this new definitions we proposed.

Before introducing *BCN* reconstruction, we discuss observation that is necessary for the quantitative analysis of *BCNs* is of wide interest and remains a topical issue ((Cheng and Qi, 2009; Zhao et al., 2010; Cheng et al., 2011; Fornasini and Valcher, 2013; Zhang et al., 2020b; Zhu et al., 2021; Zhu et al., 2022)). More specifically, observation is about how to determine the initial state of a *BCN* by controlling its inputs and observing its outputs (Zhang et al., 2020b). Observation is further classified into three problems: *multiple-*, *single-*, and *arbitrary*-experiment observation, to investigate how to determine the initial states in three different situations, namely, (1) the *BCN*'s in-

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put can be controlled and initial state can be reset, (2) input can be controlled and initial state cannot be reset, and (3) input cannot be controlled.

To study the solvability of these problems, five types of observability Type-I, II, III, IV & V observability were proposed in the literature (Cheng and Qi, 2009; Zhao et al., 2010; Cheng et al., 2011; Fornasini and Valcher, 2013; Wu et al., 2020). Type-I observability was proposed to formalise the solvability of multiple-experiment observation problem, but was later replaced by Type-II observability because Type-II observability is easier to be satisfied (Zhang et al., 2020b). Therefore, Type-II observability was named as *multiple-experiment observability*. Type-I observability was then named as *strong multiple-experiment observability* because it is stronger than Type-II observability. Type-III observability was considered as *single-experiment observability* (Cheng et al., 2011; Zhang et al., 2020b). More recently, a new notion of Type-V observability, which is easier to be satisfied than Type-III observability, was proposed to replace it in (Wu et al., 2020). Thus, Type-III observability is now named as *strong single-experiment observability*. Type-IV observability was defined to be the *single-experiment observability* of *BCNs* (Fornasini and Valcher, 2013).

Next, we continue to introduce *BCNs*' reconstruction. Reconstruction was divided into two problems: *single-* and *arbitrary*-experiment reconstruction, to investigate how to determine the current states of a *BCN* in two different situations, namely, (1) its input can be controlled and (2) input cannot be controlled. It makes no sense to study *multiple*-experiment reconstruction, because in different experiments, the inputs being fed to the *BCN* may be different, and then the corresponding current states may also be different (Zhang et al., 2020a). As the tasks to be performed in reconstruction and observation are similar, reconstructibility has high similarity in definition with observability. To formalise *BCN*'s reconstructibility in the above mentioned two different situations, Type-I & II reconstructibility that are the counterparts corresponding to Type-IV & III observability, were proposed in (Fornasini and Valcher, 2013; Zhang et al., 2015a).

In this paper, firstly, we propose three new types of reconstructibility for *BCNs*. Since *single-experiment observability* has been redefined as Type-V observability in (Wu et al., 2020), we propose Type-III reconstructibility as the counterpart corresponding to Type-V observability. Moreover, we demonstrate that it makes sense to study the counterparts (Type-IV & V reconstructibility) corresponding to Type-I & II observability, even though these two types of observability were proposed to study multiple-experiment obser-

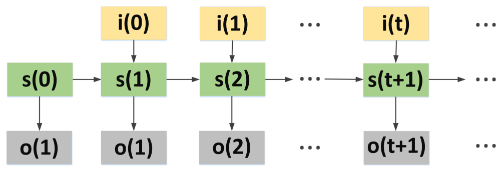

Figure 1: The relationships between inputs, states, and outputs of *BCNs*.

vation. Secondly, we briefly introduce the verification algorithms we design for these new types of reconstructibility, and analyse the computational complexity for them. We claim that with the proposal of Type-V reconstructibility, the verification problem of the *BCNs*' *single-experiment reconstructibility* can be greatly simplified.Finally, we formally prove that Type-II, III, IV& V reconstructibility are equivalent, even if they are the counterparts corresponding to Type-III, V, I& II observability which are not equivalent.

The remainder of this paper is organised as follows. We introduce necessary notations and the formal definition of *BCNs* in Section 2. In Section 3, we formally define Type-III, IV & V reconstructibility and introduce the new solution algorithm designed for the single-experiment reconstruction problem of *BCNs*. We then present the verification algorithms we have designed for Type-III, IV & V reconstructibility in Section 4. We summarise and compare the results on reconstructibility and observability in Section 5. We conclude the paper by discussing future research directions in Section 6.

2 PRELIMINARIES

We first introduce the following necessary notations:

- $\mathbb{B}$: the set of Boolean values $\{0,1\}$,
- $\mathbb{T}$: the set of discrete time domain which is denoted by the set of natural numbers,
- $v^i_{2^x}$: the x-dimensional Boolean vector whose decimal value is equal to i,
- V_{2^x}: the set $\{v^0_{2^x},\dots,v^{2^x-1}_{2^x}\}$ of Boolean vectors.

A Boolean control network (*BCN*) can be described by the following state equation and output equation (Ideker et al., 2001):

$$\begin{aligned} \mathsf{s}(t+1) &= f(\mathsf{i}(t),\mathsf{s}(t)) \\ \mathsf{o}(t) &= h(\mathsf{s}(t)) \end{aligned} \tag{1}$$

where $t\in\mathbb{T}$; $\mathsf{i}(t)\in\mathbb{B}^\ell$, $\mathsf{s}(t)\in\mathbb{B}^m$, and $\mathsf{o}(t)\in\mathbb{B}^n$ denote the vectors input, state, and output, respectively, at time t; $f:\mathbb{B}^\ell\times\mathbb{B}^m\mapsto\mathbb{B}^m$ and $h:\mathbb{B}^m\mapsto\mathbb{B}^n$ are logical functions. The relation between inputs, states, and outputs of a *BCN* can be illustrated in Fig. 1, where $0, 1, \ldots$ stand for time steps, $\mathsf{i}(0), \mathsf{i}(1), \ldots$ inputs, $\mathsf{s}(0), \mathsf{s}(1), \ldots$ states, $\mathsf{o}(0), \mathsf{o}(1), \ldots$ outputs, and arrows represent dependence. Moreover, as we represent an x-dimensional Boolean vector in the form $v^i_{2^x}$, the input set $\mathbb{B}^\ell$, state set $\mathbb{B}^m$, and output set $\mathbb{B}^n$ can be replaced by V_L, V_M, and V_N, respectively, where $L = 2^\ell$, $M = 2^m$, and $N = 2^n$.

In order to discuss observability and reconstructibility, we define the following classes of functions to represent the relation between the input sequence, output sequence, and state sequence.

$$\begin{aligned} &F^{[t_0,t]} : V_M \times (V_L)^{t-t_0} \mapsto (V_M)^{t-t_0+1}, \\ &F^{[t_0,t]}(\mathsf{s}(t_0), \mathsf{i}(t_0) \ldots \mathsf{i}(t-1)) = \mathsf{s}(t_0) \ldots \mathsf{s}(t), \end{aligned} \tag{2}$$

$$\begin{aligned} &H^{[t_0,t]} : V_M \times (V_L)^{t-t_0} \mapsto (V_N)^{t-t_0+1}, \\ &H^{[t_0,t]}(\mathsf{s}(t_0), \mathsf{i}(t_0) \ldots \mathsf{i}(t-1)) = \mathsf{o}(t_0) \ldots \mathsf{o}(t), \end{aligned} \tag{3}$$

with $t \geq t_0$. For every state $\mathsf{s}(p)$ ($t_0 < p \leq t$) in the state sequence $\mathsf{s}(t_0) \ldots \mathsf{s}(t)$, $\mathsf{s}(p) = f(\mathsf{i}(p-1), \mathsf{s}(p-1))$. For the output sequence $\mathsf{o}(t_0) \ldots \mathsf{o}(t)$, every $\mathsf{o}(p)$ in it satisfies $\mathsf{o}(p) = h(\mathsf{s}(p))$.

Intuitively, these two classes of functions represent the way to calculate the state sequence $\mathsf{s}(t_0) \ldots \mathsf{s}(t)$ and output sequence $\mathsf{o}(t_0) \ldots \mathsf{o}(t)$ of a *BCN*, respectively, in the time interval $[t_0, t]$, by its state $\mathsf{s}(t_0)$ and input sequence $\mathsf{i}(t_0) \ldots \mathsf{i}(t-1)$.

Then, we introduce the way to calculate the possible state set $\mathsf{S}_{ps}(t)$ of a *BCN*, which contains all possible valuations of the *BCN*'s state $\mathsf{s}(t)$ that can be deduced at time step t. Firstly, we define the function $\zeta(\mathsf{S}, \mathsf{i}, \mathsf{o})$ to show how to calculate the state set $\mathsf{S}_{ps}(t)$ for a *BCN* by the state set $\mathsf{S}_{ps}(t-1)$, input $\mathsf{i}(t-1)$, and output $\mathsf{o}(t)$. Before defining the function $\zeta(\mathsf{S}, \mathsf{i}, \mathsf{o})$, we define the following function $\xi(\mathsf{i}, \mathsf{s})$.

$$\begin{aligned} &\xi : (V_L \cup \{\varepsilon\}) \times V_M \mapsto V_M, \\ &\xi(\mathsf{i}, \mathsf{s}) = \begin{cases} f(\mathsf{i}, \mathsf{s}) & \mathsf{i} \neq \varepsilon \\ \mathsf{s} & \mathsf{i} = \varepsilon \end{cases}. \end{aligned} \tag{4}$$

The function $\xi(\mathsf{i}, \mathsf{s})$ is defined to describe how the *BCN*'s state s is affected by its input i. Compared with the updating function $\mathsf{s}(t+1) = f(\mathsf{i}(t), \mathsf{s}(t))$, this function could capture how the state s changes when the input $\mathsf{i} = \varepsilon$. Then we define function $\zeta(\mathsf{S}, \mathsf{i}, \mathsf{o})$.

$$\begin{aligned} &\zeta : 2^{V_M} \times (V_L \cup \{\varepsilon\}) \times (V_N \cup \{\varepsilon\}) \mapsto 2^{V_M} \\ &\zeta(\mathsf{S}, \mathsf{i}, \mathsf{o}) = \begin{cases} \{\xi(\mathsf{i}, \mathsf{s}) \mid \mathsf{s} \in \mathsf{S}, h(\xi(\mathsf{i}, \mathsf{s})) = \mathsf{o}\} & \mathsf{o} \neq \varepsilon \\ \{\xi(\mathsf{i}, \mathsf{s}) \mid \mathsf{s} \in \mathsf{S}\} & \mathsf{o} = \varepsilon \end{cases} \end{aligned} \tag{5}$$

Then, we recursively define the following class of functions $G^{[t]}(\mathsf{i}(0) \ldots \mathsf{i}(t-1), \mathsf{o}(0) \ldots \mathsf{o}(t))$ to present how to determine the set $\mathsf{S}_{ps}(t)$ for a *BCN* by analysing its input sequence $\mathsf{i}(0) \ldots \mathsf{i}(t-1)$ and output sequence $\mathsf{o}(0) \ldots \mathsf{o}(t)$.

$$G^{[t]} : {V_L}^t \times {V_N}^{t+1} \mapsto 2^{V_M} \tag{6}$$

These functions satisfy the following conditions.

- When $t = 0$, $\mathsf{i}(0) \ldots \mathsf{i}(t-1) = \varepsilon$,

  $$G^{[t]}(\mathsf{i}(0) \ldots \mathsf{i}(t-1), \mathsf{o}(0) \ldots \mathsf{o}(t)) = \zeta(V_M, \varepsilon, \mathsf{o}(0)).$$

- When $t > 0$,

  $$\begin{aligned} &G^{[t]}(\mathsf{i}(0) \ldots \mathsf{i}(t-1), \mathsf{o}(0) \ldots \mathsf{o}(t)) \\ &= \zeta(\mathsf{S}_{ps}(t-1), \mathsf{i}(t-1), \mathsf{o}(t)) \\ &\textit{where} \\ &\mathsf{S}_{ps}(t-1) \\ &= G^{[t-1]}(\mathsf{i}(0) \ldots \mathsf{i}(t-2), \mathsf{o}(0) \ldots \mathsf{o}(t-1)). \end{aligned}$$

3 REVISITING RECONSTRUCTIBILITY

In this section, we begin with two existing types of reconstructibility and then introduce three new types of reconstructibility that we propose in this work.

Definition 1 (Type-I reconstructibility (Fornasini and Valcher, 2013)). *A* BCN *satisfies* Type-I reconstructibility *if there exists a finite number $k \in \mathbb{T}$ such that for any input sequence $\mathsf{I} \in (V_L)^p$ where $p \geq k$, $H^{[0,p]}(\mathsf{s}', \mathsf{I}) \neq H^{[0,p]}(\mathsf{s}, \mathsf{I})$ holds for any two distinct states s, $\mathsf{s}' \in V_M$ if their corresponding current states $\mathsf{s}(p)$ and $\mathsf{s}'(p)$ are different.*

The main steps to determine the current state for a *BCN* with this property are as follows:

(1) Input to a *BCN* with an input sequence $\mathsf{I} \in (V_L)^p$ that has sufficient length to distinguish all distinct current states, and run the *BCN* to generate the output sequence $\mathsf{o}(0) \ldots \mathsf{o}(p)$;

(2) Return the current state $\mathsf{s}(p)$ which satisfies $\mathsf{s}(p) \in G^{[p]}(\mathsf{I}, \mathsf{o}(0) \ldots \mathsf{o}(p))$.

Definition 2 (Type-II reconstructibility (Zhang et al., 2015b)). *A* BCN *satisfies* Type-II *reconstructibility if there exists an input sequence $\mathsf{I} \in (V_L)^p$ for some $p \in \mathbb{T}$, such that for any two distinct states s, $\mathsf{s}' \in V_M$, $H^{[0,p]}(\mathsf{s}', \mathsf{I}) \neq H^{[0,p]}(\mathsf{s}, \mathsf{I})$ holds if their corresponding current states $\mathsf{s}(p)$ and $\mathsf{s}'(p)$ are different.*

Similarly, the reconstruction algorithm corresponding to Type-II reconstructibility is shown as follows:

(1) Input to a *BCN* with an input sequence $\mathsf{I} \in (V_L)^p$ which distinguishes all distinct current states, and run the *BCN* to generate the output sequence $\mathsf{o}(0)\ldots\mathsf{o}(p)$;

(2) Return the current state $\mathsf{s}(p)$ which satisfies $\mathsf{s}(p) \in G^{[p]}(\mathsf{I}, \mathsf{o}(0)\ldots\mathsf{o}(p))$.

Next, we introduce the new types of reconstructibility. Firstly, as the *BCNs*' single-experiment observability was redefined as Type-V observability in (Wu et al., 2020), we define Type-III reconstructibility as the counterpart corresponding to Type-V observability. For this purpose, we propose the set of state sets $Set_{\mathsf{S}}(k)$ for *BCNs* which denotes the set that, for every state set $\mathsf{S} \in Set_{\mathsf{S}}(k)$, the set S satisfies that only k time steps are required to determine a *BCN*'s current state $\mathsf{s}(t+k)$ by one experiment when its state set $\mathsf{S}_{ps}(t) = \mathsf{S}$. We recursively define the set $Set_{\mathsf{S}}(k)$ of *BCNs* as the following steps.

- When $k = 0$, then $Set_{\mathsf{S}}(k) = \{\mathsf{S} \in 2^{V_M} \,||\mathsf{S}| = 1\}$.
- When $k > 0$, then $Set_{\mathsf{S}}(k) = \{\mathsf{S} \in (2^{V_M} - \bigcup_{p=0}^{k-1} Set_{\mathsf{S}}(p)) | \exists \mathsf{i} \in V_L \cdot \forall \mathsf{o} \in V_N \cdot \exists p \leq (k-1) \cdot \zeta(\mathsf{S}, \mathsf{i}, \mathsf{o}) \in Set_{\mathsf{S}}(p)\}$.

Intuitively, when $|\mathsf{S}| = |\mathsf{S}_{ps}(t)| = 1$, i.e. the *BCN*'s state $\mathsf{s}(t)$ is determined, we need 0 time step to determine its current state. When $k > 0$, we use the sets $Set_{\mathsf{S}}(0)$,..., $Set_{\mathsf{S}}(k-1)$ that have been defined to define the set $Set_{\mathsf{S}}(k)$. Firstly, as the set $Set_{\mathsf{S}}(k)$ should not intersect with the sets $Set_{\mathsf{S}}(0)$,..., $Set_{\mathsf{S}}(k-1)$, we have for every state set $\mathsf{S} \in Set_{\mathsf{S}}(k)$, the condition $\mathsf{S} \in (2^{V_M} - \bigcup_{p=0}^{k-1} Set_{\mathsf{S}}(p))$ should be met. Secondly, as a *BCN* should require more time steps to determine its current state at t than at $t+1$, those following conditions also need to be satisfied.

Then, we can define the function $\Gamma(\mathsf{S})$ to represent the number of time steps needed to determine a *BCN*'s state $\mathsf{s}(t)$ by one experiment, when its possible state set $\mathsf{S}_{ps}(t) = \mathsf{S}$.

$$\Gamma : (2^{V_M} - \{\emptyset\}) \mapsto (\mathbb{T} \cup \{\infty\}) \tag{7}$$

satisfies the following conditions.

- If there exists a finite number k which satisfies that $\mathsf{S} \in Set_{\mathsf{S}}(k)$, then $\Gamma(\mathsf{S}) = k$.
- Otherwise, $\Gamma(\mathsf{S}) = \infty$.

Now, Type-III reconstructibility can be defiend.

Definition 3 (Type-III Reconstructibility)**.** *A* BCN *satisfies* Type-III *reconstructibility if for every* $\mathsf{o} \in V_N$, $\zeta(V_M, \varepsilon, \mathsf{o}) \neq \emptyset$ *implies* $\Gamma(\zeta(V_M, \varepsilon, \mathsf{o})) \neq \infty$.

We provide a reconstruction algorithm corresponding to Type-III reconstructibility as well.

(1) Obtain the state set $\mathsf{S}_{ps}(0)$ of this *BCN* by its initial output $\mathsf{o}(0)$, i.e. $\mathsf{S}_{ps}(0) := \zeta(V_M, \varepsilon, \mathsf{o}(0))$, and set the set variable S by $\mathsf{S}_{ps}(0)$, i.e. $\mathsf{S} := \mathsf{S}_{ps}(0)$.

(2) Feed the *BCN* with an input i which satisfies

$$\max_{\mathsf{o}' \in \{\mathsf{o} | \zeta(\mathsf{S}, \mathsf{i}, \mathsf{o}) \neq \emptyset\}} \Gamma(\zeta(\mathsf{S}, \mathsf{i}, \mathsf{o}')) + 1 = \Gamma(\mathsf{S})$$

and run it to generate the new output $\mathsf{o}(t)$.

(3) Determine the new $\mathsf{S}_{ps}(t)$ by the input i, output $\mathsf{o}(t)$, and set variable S, i.e. $\mathsf{S}_{ps}(t) = \zeta(\mathsf{S}, \mathsf{i}, \mathsf{o}(t))$, and update the set variable S by $\mathsf{S}_{ps}(t)$, i.e. $\mathsf{S} := \mathsf{S}_{ps}(t)$.

(4) If the cardinal number $|\mathsf{S}| = 1$, then return the *BCN*'s current state $\mathsf{s}(t)$ which satisfies $\mathsf{s}(t) \in \mathsf{S}$. Otherwise, update t, i.e. $t = t+1$ and go to step 2.

Finally, we define Type-IV & V reconstructibility as the counterpart corresponding to Type-I & II observability, respectively. We show that, for a *BCN* that satisfies these two properties, the current state of it can also be determined by performing one experiment.

Definition 4 (Type-IV reconstructibility)**.** *A* BCN *satisfies* Type-IV *reconstructibility if for every state* $\mathsf{s} \in V_M$, *there exists an input sequence* $\mathsf{I} \in (V_L)^p$ *for some* $p \in \mathbb{T}$ *such that for any state* $\mathsf{s}' \neq \mathsf{s}$, $H^{[0,p]}(\mathsf{s}', \mathsf{I}) \neq H^{[0,p]}(\mathsf{s}, \mathsf{I})$ *holds if their corresponding current states* $\mathsf{s}(p)$ *and* $\mathsf{s}'(p)$ *are different.*

(1) Obtain the set $\mathsf{S}_{ps}(0)$ of possible valuations of the *BCN*'s initial state $\mathsf{s}(0)$ by its initial output $\mathsf{o}(0)$, i.e. $\mathsf{S}_{ps}(0) = \zeta(V_M, \varepsilon, \mathsf{o}(0))$, and set the set variable $\mathsf{S} := \mathsf{S}_{ps}(0)$, the time variable $\mathsf{T} := 0$, the input sequence variable $\mathsf{I} := []$ and the output sequence variable $\mathsf{O} := []$, where [] denotes an empty sequence.

(2) Assume one state s of the *BCN* under study as a candidate initial state $\mathsf{s}(0)$ from set S.

(3) Feed the *BCN* with an input sequence $\mathsf{I}' \in (V_L)^p$ that distinguishes the current state $\mathsf{s}(p)$ corresponding to $\mathsf{s}(0)$ from other current states to generate new output sequence $\mathsf{o}(0)\ldots\mathsf{o}(p)$, and set the time variable $\mathsf{T} := \mathsf{T} + p$, the input sequence variable $\mathsf{I} := \mathsf{I} + \mathsf{I}'$ and the output sequence variable $\mathsf{O} := \mathsf{O} + \mathsf{o}(0)\ldots\mathsf{o}(p)$.

(4) Determine the new $\mathsf{S}_{ps}(t)$ by the input sequence I, output sequence O and reset variable $\mathsf{S} := \mathsf{S}_{ps}(t) = G^{[\mathsf{T}]}(\mathsf{I}, \mathsf{O})$.

(5) If the cardinal number $|\mathsf{S}| = 1$, then return the *BCN*'s current state $\mathsf{s}(t)$ which satisfies $\mathsf{s}(t) \in \mathsf{S}$. Otherwise, go to step 2.

Definition 5 (Type-V reconstructibility)**.** *A* BCN *satisfies* Type-V *reconstructibility if for any two distinct states* s, $\mathsf{s}' \in V_M$, *there exists an input sequence*

$\mathsf{I} \in (V_L)^p$ *for some* $p \in \mathbb{T}$ *such that* $H^{[0,p]}(\mathsf{s}',\mathsf{I}) \neq H^{[0,p]}(\mathsf{s},\mathsf{I})$ *holds if their corresponding current states* $\mathsf{s}(p)$ *and* $\mathsf{s}'(p)$ *are different.*

(1) Obtain the set $\mathsf{S}_{ps}(0)$ of possible valuations of the *BCN*'s initial state $\mathsf{s}(0)$ by its initial output $\mathsf{o}(0)$, i.e. $\mathsf{S}_{ps}(0) = \zeta(V_M, \varepsilon, \mathsf{o}(0))$, and set the set variable $\mathsf{S} = \mathsf{S}_{ps}(0)$, the time variable $\mathsf{T} := 0$, the input sequence variable $\mathsf{I} := []$ and the output sequence variable $\mathsf{O} := []$.

(2) Assume two distinct states s and s' of the *BCN* under study as a candidate initial state $\mathsf{s}(0)$ and $\mathsf{s}'(0)$ from the state set S.

(3) Feed the *BCN* with an input sequence $\mathsf{I}' \in (V_L)^p$ that distinguishes the current states $\mathsf{s}(p)$ corresponding to $\mathsf{s}(0)$ from $\mathsf{s}'(0)$ to generate new output sequence $\mathsf{o}(0)\ldots\mathsf{o}(p)$, and set the time variable $\mathsf{T} := \mathsf{T} + p$, the input sequence variable $\mathsf{I} := \mathsf{I} + \mathsf{I}'$ and the output sequence variable $\mathsf{O} := \mathsf{O} + \mathsf{o}(0)\ldots\mathsf{o}(p)$.

(4) Determine the new $\mathsf{S}_{ps}(t)$ by the input sequence I, output sequence O and reset the state set variable $\mathsf{S} := \mathsf{S}_{ps}(t) = G^{[\mathsf{T}]}(\mathsf{I},\mathsf{O})$.

(5) If the cardinal number $|\mathsf{S}| = 1$, then return the *BCN*'s current state $\mathsf{s}(t)$ which satisfies $\mathsf{s}(t) \in \mathsf{S}$. Otherwise, go to step 2.

In the above two algorithms, we perform multiple consecutive experiments without resetting the *BCN*'s initial state. These successive multiple experiments can therefore be considered as single experiment. For this reason, Type-IV reconstructibility and Type-V reconstructibility can be utilised to study the *BCNs*' single-experiment reconstruction. This reflects the difference between the reconstruction and observation, that will further compared in Section 5.

Now we discuss how the above three algorithms enrich the solution of *BCN*'s single-experiment reconstruction. Firstly, by using the reconstruction algorithm corresponding to Type-III reconstructibility, we can determine the current state for a *BCN* in the shortest possible time steps, which reduces the cost of experimentation. Secondly, as the computational cost for verifying Type-V reconstructibility is lower than that for Type-II reconstructibility (will be discussed Section 4), the reconstruction of more and larger *BCNs* can be solved.

4 VERIFICATION OF RECONSTRUCTIBILITY

In this section, we introduce the verification algorithms we design for Type- III, IV & V reconstructibility.

As the reconstructibility and observability of *BCNs* have high similarity in their definitions, the verification algorithm for reconstructibility can be obtained by modifying the corresponding observability's algorithm. As a consequence, the computational complexity of their verification algorithms remains the same. For instance, the verification algorithms that are based on the deterministic finite automata (DFA) for Type-I & II reconstructibility as introduced in (Zhang et al., 2020a) were obtained by modifying the verification algorithms of Type-IV & III observability provided in (Zhang et al., 2020b), and have the same computational complexity as the latter two. Following this common practice, we design the verification algorithm for Type-III reconstructibility based on the verification algorithm of Type-V observability proposed in (Wu et al., 2020), and the verification algorithms for Type-IV & V reconstructibility based on the verification algorithms of Type-I & II observability introduced in (Zhang et al., 2020b). Then, the computational complexity of them can be easily obtained by referring to the results of the papers (Wu et al., 2020; Zhang et al., 2020b).

Given a *BCN* with ℓ input-nodes, m state-nodes, and n output-nodes, the computational complexity of the verification algorithm for Type-III reconstructibility is $O(2^{2^m+\ell-1})$. For Type-IV reconstructibility, the computational complexity of its verification algorithm is $O(2^{2^{2m-1}\ell})$ (Zhang et al., 2020b).

For Type-V reconstructibility, we actually design two algorithms for verifying it. The first one is based on DFAs, with computational complexity $O(2^{4m+\ell-2})$. For every two distinct current states of the *BCN* with Type-V reconstructibility, the input sequence that distinguishes them can be obtained from the verification result of this algorithm. The computational complexity of this algorithm is smaller than the existing verification algorithm (with the computational complexity of $O(2^{2^{2m-1}l})$ (Zhang et al., 2020a)) for Type-II reconstructibility that provides the input sequence to distinguish all different current states. The second one we design is based on graph theory, and its computational complexity is $O(2^{2m+\ell-1})$ which is equivalent to the computational complexity of the optimised verification algorithm for Type-II reconstructibility as introduced in (Zhang et al., 2020a). However, this algorithm and the optimised verification algorithm for verifying Type-II reconstructibility (Zhang et al., 2020a) can only provide an answer whether the *BCN* to be verified satisfies single-experiment reconstructibility or not. In other words, if and only if the verification result of the second algorithm shows that the *BCN* under study satisfies Type-V reconstructibility, we need the first one to obtain the input sequences that distinguish the pairs of different current states. This also explains why the first one is more complex.

In the following, we mainly focus on the first verification algorithm we design for Type-V reconstructibility and give its details.[1] Our main idea is to construct the weighted pair graph for a *BCN* first, then construct the DFA for the pairs of different states that produce the same output from the weighted pair graph, and finally obtain the input sequences that distinguish the pairs of different current states from the DFA. We need to first introduce the notion of weighted directed graph for *BCNs*.

Definition 6 (Weighted Pair Graph (Zhang et al., 2020a))**.** *Given a* BCN*, a weighted directed graph* $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathcal{W})$*, where* $\mathcal{V}$ *denotes the vertex set,* $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$ *denotes the edge set, and* $\mathcal{W}$ *denotes the weight function, is called the weighted pair graph of the* BCN *if* $\mathcal{V} = \{\{\mathsf{s}, \mathsf{s}'\} | \mathsf{s}, \mathsf{s}' \in V_M, \mathsf{s} \neq \mathsf{s}', h(\mathsf{s}) = h(\mathsf{s}')\}$*, for all* $[\{\mathsf{s}_1, \mathsf{s}_1'\}, \{\mathsf{s}_2, \mathsf{s}_2'\}] \in \mathcal{V} \times \mathcal{V}$*,* $[\{\mathsf{s}_1, \mathsf{s}_1'\}, \{\mathsf{s}_2, \mathsf{s}_2'\}] \in \mathcal{E}$ *iff there exists* $\mathsf{i} \in V_L$ *such that* $f(\mathsf{i}, \mathsf{s}_1) = f(\mathsf{i}, \mathsf{s}_2)$ *and* $f(\mathsf{i}, \mathsf{s}_1') = f(\mathsf{i}, \mathsf{s}_2')$ *or* $f(\mathsf{i}, \mathsf{s}_1) = f(\mathsf{i}, \mathsf{s}_2')$ *and* $f(\mathsf{i}, \mathsf{s}_1') = f(\mathsf{i}, \mathsf{s}_2)$*; for all edges* $e = [\{\mathsf{s}_1, \mathsf{s}_1'\}, \{\mathsf{s}_2, \mathsf{s}_2'\}] \in \mathcal{E}$*,* $\mathcal{W}(e) = \{\mathsf{i} \in V_L | f(\mathsf{i}, \mathsf{s}_1) = f(\mathsf{i}, \mathsf{s}_2)$ *and* $f(\mathsf{i}, \mathsf{s}_1') = f(\mathsf{i}, \mathsf{s}_2')$ *or* $f(\mathsf{i}, \mathsf{s}_1) = f(\mathsf{i}, \mathsf{s}_2')$ *and* $f(\mathsf{i}, \mathsf{s}_1') = f(\mathsf{i}, \mathsf{s}_2)\}$*.*

After introducing the notions of weighted pair graph, we use the *BCN* shown in Table 1 as an example to illustrate how to utilise them to obtain the input sequences that distinguish the pairs of different current states for a *BCN* which satisfies Type-V reconstructibility. For this *BCN*, its weighted pair graph is shown the top part of Fig. 2, and all the DFA constructed from the graph are shown in the lower part of this figure. For every vertex $\{\mathsf{s}_i, \mathsf{s}_i'\}$ (e.g. $\{v_8^1, v_8^3\}$) in the weighted pair graph, we construct a DFA A_i (the second DFA shown in the lower part of Fig. 2) for it. In this DFA, the vertex $\{\mathsf{s}_i, \mathsf{s}_i'\}$ (e.g. $\{v_8^1, v_8^3\}$) is the start state q_0. The other states of the DFA A_i are composed of the vertices ($\{v_8^1, v_8^2\}$ and $\{v_8^4, v_8^5\}$) reachable by $\{\mathsf{s}_i, \mathsf{s}_i'\}$ ($\{v_8^1, v_8^3\}$), in the weighted pair graph. For every two state q (e.g. $\{v_8^1, v_8^2\}$) and q' ($\{v_8^4, v_8^5\}$) in this DFA, $q' = \sigma(q, a)$ holds if their corresponding vertices are connected in the weighted pair graph. Moreover, all states (e.g. $\{v_8^1, v_8^2\}$ and $\{v_8^4, v_8^5\}$) in the DFA A_i are accepting states. Then, for the pair of different *BCN*'s states $\{\mathsf{s}_i, \mathsf{s}_i'\}$ ($\{v_8^1, v_8^2\}$), every word $w \in L(A_i)$ (in this case, $L(A_i) = (v_2^1, v_2^0)^*(\varepsilon \cup v_2^1)$) accepted by this DFA, is the input sequence that could *not* distinguish the corresponding current *BCN*'s states of the states (i.e. v_8^1 and v_8^2), because the accepting state $\sigma^*(q_0, w)$ of this DFA denotes the pair of different *BCN*'s states ($\{v_8^1, v_8^2\}$ or $\{v_8^4, v_8^5\}$) that produce the same output. Thus, the language $L = \Sigma^* - L(A_i)$ contains all input sequences that can distinguish the corresponding current states of s_i and s_i' (e.g. v_8^1 and v_8^3). If the language $L = \Sigma^* - L(A_i) = \emptyset$, which means $L(A_i) = \Sigma^*$, then there is no input sequence can be used to distinguish the corresponding current states of s_i and s_i', this *BCN* thus does not satisfy Type-V reconstructibility. However, if the *BCN* to be verified does not satisfy Type-V reconstructibility, this algorithm would not be used since the second algorithm we design (mentioned in the previous paragraphs) would show the verification result.

Table 1: A *BCN* used to illustrate the verification algorithm.

$\mathsf{s}(t)$	v_8^0	v_8^1	v_8^2	v_8^3	v_8^4	v_8^5	v_8^6	v_8^7	$\mathsf{i}(t)$
$\mathsf{s}(t+1)$	v_8^2	v_8^3	v_8^3	v_8^6	v_8^1	v_8^3	v_8^4	v_8^3	v_2^0
	v_8^7	v_8^5	v_8^1	v_8^4	v_8^2	v_8^6	v_8^0	v_8^0	v_2^1
$\mathsf{o}(t)$	v_4^0	v_4^1	v_4^1	v_4^1	v_4^2	v_4^2	v_4^3	v_4^3	·

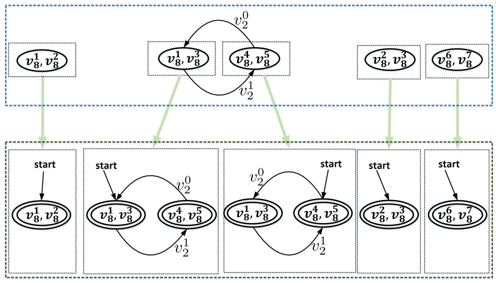

Figure 2: The weighted directed graph and DFAs constructed for the BCN shown in Table 1.

Finally, we analyse the computational complexity of this algorithm. For a *BCN*, for every two different initial states s_i and s_i', the size of the DFA A_i is no greater than that of the weighted pair graph. Since at most $2^m(2^m - 1)/2$ DFA need to be checked and the size of the graph is $O(2^{2m+l-1})$, the computational complexity of this algorithm is $O(2^{4m+l-2})$.

5 COMPARING RECONSTRUCTIBILITY AND OBSERVABILITY

Before comparing the reconstructibility and observability of *BCNs*, we need to present all five existing types of observability. The initial state determining algorithms corresponding to all five types of observ-

[1]Due to the page limit, we will not show the details of other verification algorithms we briefly mentioned in this paper.

ability will be omitted due to the page limit. Type-I & II observability were proposed to study the solvability of the *BCNs*' multiple-experiment observation.

Definition 7 (Type-I observability (Cheng and Qi, 2009))**.** *A* BCN *satisfies* Type-I observability *if for every states* $\mathsf{s} \in V_M$ *there exists an input sequence* $\mathsf{I} \in (V_L)^p$ *for some* $p \in \mathbb{T}$*, such that for any state* $\mathsf{s}' \neq \mathsf{s}$*,* $H^{[0,p]}(\mathsf{s}',\mathsf{I}) \neq H^{[0,p]}(\mathsf{s},\mathsf{I})$.

Type-I observability was later replaced by Type-II observability (Zhang et al., 2020b).

Definition 8 (Type-II observability (Zhao et al., 2010))**.** *A* BCN *satisfies* Type-II observability *if for any two distinct states* s*,* $\mathsf{s}' \in V_M$ *there exists an input sequence* $\mathsf{I} \in (V_L)^p$ *for some* $p \in \mathbb{T}$*, such that* $H^{[0,p]}(\mathsf{s}',\mathsf{I}) \neq H^{[0,p]}(\mathsf{s},\mathsf{I})$.

Type-III & V observability were proposed to research *single-experiment* observation.

Definition 9 (Type-III observability (Cheng et al., 2011))**.** *A* BCN *satisfies* Type-III observability *if there exists an input sequence* $\mathsf{I} \in (V_L)^p$ *for some* $p \in \mathbb{T}$*, such that for any two distinct states* s*,* $\mathsf{s}' \in V_M$*,* $H^{[0,p]}(\mathsf{s}',\mathsf{I}) \neq H^{[0,p]}(\mathsf{s},\mathsf{I})$.

Type-V observability was proposed to redefine single-experiment observability. As the state $\mathsf{s}(t)$ can be guaranteed to be determined in a finite time steps of k, by performing one experiment if and only if

- $|\mathsf{S}_{ps}(t+k)| = 1$, i.e. $\mathsf{s}(t+k)$ is determined.
- For every $t_0 : t+1 \leq t_0 \leq t+k$, for every $\mathsf{s} \in \mathsf{S}_{ps}(t_0)$, there exists only one $\mathsf{s}' \in \mathsf{S}_{ps}(t_0-1)$ that satisfies $\mathsf{s} = f(\mathsf{i}(t_0-1),\mathsf{s}')$, such that $\mathsf{s}(t_0-1)$ can be uniquely determined by $\mathsf{s}(t_0)$ and $\mathsf{i}(t_0-1)$. The state $\mathsf{s}(t)$ then can be uniquely determined step by step by $\mathsf{s}(t+k)$ and $\mathsf{i}(t)\ldots\mathsf{i}(t+k-1)$.

The authors of (Wu et al., 2020) proposed the set of state sets $\dot{Set}_{\mathsf{S}}(k)$ for *BCNs* to denote the set that, for every state set $\mathsf{S} \in \dot{Set}_{\mathsf{S}}(k)$, the set S satisfies that only k time steps are required to determine a *BCN*'s state $\mathsf{s}(t)$ by one experiment when its state set $\mathsf{S}_{ps}(t) = \mathsf{S}$. $\dot{Set}_{\mathsf{S}}(k)$ is recursively determined:

- When $k = 0$, then $\dot{Set}_{\mathsf{S}}(k) = \{\mathsf{S} \in 2^{V_M} \mid |\mathsf{S}| = 1\}$.
- When $k > 0$, then $\dot{Set}_{\mathsf{S}}(k) = \{\mathsf{S} \in (2^{V_M} - \bigcup_{p=0}^{k-1} \dot{Set}_{\mathsf{S}}(p)) \mid \exists \mathsf{i} \in V_L \cdot (|\zeta(\mathsf{S},\mathsf{i},\varepsilon)| = |\mathsf{S}|) \& (\forall \mathsf{o} \in V_N \cdot \exists p \leq (k-1) \cdot \zeta(\mathsf{S},\mathsf{i},\mathsf{o}) \in \dot{Set}_{\mathsf{S}}(p))\}$.

Intuitively, when $|\mathsf{S}| = |\mathsf{S}_{ps}(t)| = 1$, i.e. $\mathsf{s}(t)$ is determined, we need 0 time step to determine it. Thus, we set $\dot{Set}_{\mathsf{S}}(k) = \{\mathsf{S} \in 2^{V_M} \mid |\mathsf{S}| = 1\}$ when $k = 0$. When $k > 0$, we use the sets $\dot{Set}_{\mathsf{S}}(0),\ldots, \dot{Set}_{\mathsf{S}}(k-1)$ that have been defined to define the set $\dot{Set}_{\mathsf{S}}(k)$. Firstly, as the set $\dot{Set}_{\mathsf{S}}(k)$ should not intersect with the sets $\dot{Set}_{\mathsf{S}}(0),\ldots, \dot{Set}_{\mathsf{S}}(k-1)$, we have for every state set $\mathsf{S} \in \dot{Set}_{\mathsf{S}}(k)$, the condition $\mathsf{S} \in (2^{V_M} - \bigcup_{p=0}^{k-1} \dot{Set}_{\mathsf{S}}(p))$ should be satisfied. Secondly, as the *BCN*'s state $\mathsf{s}(t)$ should be determined by its state $\mathsf{s}(t+1)$ and input $\mathsf{i}(t)$, those following conditions also need to be satisfied as we discussed in the previous paragraph.

Now, the function $\dot{\Gamma}(\mathsf{S})$ to represent the number of time steps needed to determine a *BCN*'s state $\mathsf{s}(t)$ by one experiment, when its state set $\mathsf{S}_{ps}(t) = \mathsf{S}$, can be defined as follows.

$$\dot{\Gamma} : (2^{V_M} - \{\emptyset\}) \mapsto (\mathbb{T} \cup \{\infty\}) \tag{8}$$

satisfies the following conditions.

- If there exists a finite number k which satisfies that $\mathsf{S} \in \dot{Set}_{\mathsf{S}}(k)$, then $\dot{\Gamma}(\mathsf{S}) = k$.
- Otherwise, $\dot{\Gamma}(\mathsf{S}) = \infty$.

Thus, the *BCNs*' single-experiment observability can be defined as the following Type-V observability.

Definition 10 (Type-V observability (Wu et al., 2020))**.** *A* BCN *satisfies* Type-V *observability if for every possible* $\mathsf{S}_{ps}(0)$ *of this* BCN*,* $\dot{\Gamma}(\mathsf{S}_{ps}(0)) \neq \infty$.

Finally, we introduce Type-IV observability.

Definition 11 (Type-IV observability (Fornasini and Valcher, 2013))**.** *A* BCN *satisfies* Type-IV observability *if there exist a finite number* $k \in \mathbb{T}$ *such that for any input sequence* $\mathsf{I} \in (V_L)^p$ *where* $p \geq k$*,* $H^{[0,p]}(\mathsf{s}',\mathsf{I}) \neq H^{[0,p]}(\mathsf{s},\mathsf{I})$ *holds for any two distinct states* s*,* $\mathsf{s}' \in V_M$.

Now we can compare reconstructibility and observability for *BCNs*. Firstly, for every type of observability and the reconstructibility which as the counterpart of this type of observability, this type of observability implies the counterpart of it. The reason is that once the initial state of a *BCN* can be determined, its current can also be determined by the initial state and inputs of the *BCN*. Secondly, all types of observability are not equivalent. The relationship between them is shown in Fig. 3, where arrows means "implies". Thirdly, the four types of reconstructibility namely Type-II, III, IV & V reconstructibility are equivalent, which is formuated by the following theorem.

Theorem 1. Type-II, III, IV & V reconstructibility *are equivalent.*

Due to space limitation, we omit the detailed proof of this main theorem. Intuitively, it can be proved by showing that Type-V reconstructibility implies Type-II reconstructibility. This proposition can be easily proved by constructing an input sequence that distinguishes all current states for a *BCN* with

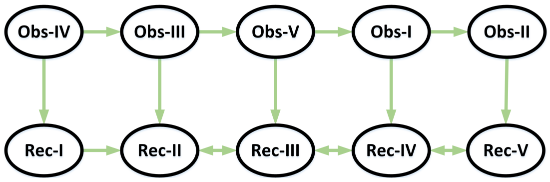

Figure 3: The relationships between all types of the *BCNs*' observability and reconstructibility.

Type-V reconstructibility. The propositions that the reconstructibilities Type-II implies Type-III, Type-III implies Type-IV, and Type-IV implies Type-V are obvious. Therefore, all these properties are equivalent, and the relation between all types of observability and reconstructibility can be illustrated in Fig. 3. It is worth noting that, successive multiple experiments can therefore be considered as single experiment in the reconstruction of a *BCN*, is the main reason for the difference between these two problems.

6 CONCLUSION AND FUTURE WORK

It still requires a significant amount of computational overhead to verify the single-experiment reconstructibility for large scale *BCNs*, due to the computational complexity we have discussed in the paper. Thus, in future, we plan to improve the scalability of the verification algorithm for *BCNs*' single-experiment reconstructibility. We plan to research whether it is possible to determine the current state for a *BCN*, without any information given in advance, about which input should be fed to the *BCN* at every time step. If the answer to this question is positive, the verification of the single-experiment reconstructibility of *BCN* will be further simplified, and the computational complexity of the corresponding algorithm will also be reduced.

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