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Fixed Point Preserving Model Reduction of Boolean Networks Focusing on Complement and Absorption Laws*

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SUMMARY A Boolean network (BN) is well known as a discrete model for analysis and control of complex networks such as gene regulatory networks. Since complex networks are large-scale in general, it is important to consider model reduction. In this paper, we consider model reduction that the information on fixed points (singleton attractors) is preserved. In model reduction studied here, the interaction graph obtained from a given BN is utilized. In the existing method, the minimum feedback vertex set (FVS) of the interaction graph is focused on. The dimension of the state is reduced to the number of elements of the minimum FVS. In the proposed method, we focus on complement and absorption laws of Boolean functions in substitution operations of a Boolean function into other one. By simplifying Boolean functions, the dimension of the state may be further reduced. Through a numerical example, we present that by the proposed method, the dimension of the state can be reduced for BNs that the dimension of the state cannot be reduced by the existing method.

key words: *Boolean network, complement and absorption laws, interaction graph, model reduction*

1. Introduction

In the last decade, there has been much attention on analysis and control of Boolean networks (BNs). A BN plays an important role in various applications of gene regulatory networks [1], fault diagnosis [2], and many other areas [3], [4]. In a BN, the state takes a binary value, and its time evolution is modeled by a Boolean function. Fundamental results, such as stability [5], stabilization [6]–[8], controllability/observability [9], and optimal control [10]–[12], have been obtained. To model more complex behavior, a probabilistic Boolean network (PBN) [13] and context-sensitive PBN [14] have been proposed as an extended model of BNs.

In analysis and control of large-scale complex networks, it is important to appropriately simplify a mathematical model. For BNs, some results on model reduction have been obtained [15]–[17]. In [15], the model reduction method using l_1-gain analysis has been proposed. In [16], [17], the model reduction methods that the information on fixed points (singleton attractors) is preserved have been proposed. In [16]–[18], a feedback vertex set (FVS), which is a subset of the vertex set of the graph expressing interactions between elements of the state, plays an important role (see Sect. 2.2 for details of an FVS). By applying the methods in [16], [17] to a given BN, the dimension of the state can be reduced to the number of vertices of an FVS. However, the number of vertices of an FVS is in general not a minimal dimension of the state of the reduced model (see, e.g., [19]). The reduced BN obtained by using the methods in [16], [17] may be possible to be further reduced.

In this paper, a new method for model reduction of BNs is proposed. In the proposed method, the interaction graph obtained from a given BN is used. The interaction graph represents interactions between elements of the state in a given BN (logical operations are ignored). The reduced BN obtained by using the methods in [16], [17] may be reduced by substitution operations through paths in the interaction graph. In the proposed method, using the interaction graph, we find substitution operations such that complement and absorption laws of Boolean functions can be applied to a Boolean function. As a result, reduction of states is achieved.

This paper is organized as follows. In Sect. 2, BNs and the model reduction method in [16] are summarized. In Sect. 3, a model reduction method using the interaction graph is proposed. In Sect. 4, a numerical example is presented to demonstrate the proposed method. In Sect. 5, we conclude this paper.

Notation: Let $\{0,1\}^n$ denote the set of n-dimensional vectors, which consists of elements 0 and 1. For the numbers $x_1, x_2, \ldots, x_n$ and the index set $\mathcal{I} = \{i_1, i_2, \ldots, i_m\} \subseteq \{1, 2, \ldots, n\}$, define $[x_i]_{i\in\mathcal{I}} := [x_{i_1}, x_{i_2}, \ldots, x_{i_m}]$.

2. Preliminaries

2.1 Boolean Networks

Consider the following BN:

$$\begin{cases} x_1(k+1) = f_1([x_j(k)]_{j\in\mathcal{N}_1}), \\ x_2(k+1) = f_2([x_j(k)]_{j\in\mathcal{N}_2}), \\ \vdots \\ x_n(k+1) = f_n([x_j(k)]_{j\in\mathcal{N}_n}), \end{cases} \tag{1}$$

where $x = [x_1, x_2, \ldots, x_n]^\top \in \{0,1\}^n$ is the state (e.g., expression level of the genes), and $k = 0, 1, 2, \ldots$ is the discrete time. The function $f_i : \{0,1\}^{|\mathcal{N}_i|} \to \{0,1\}$ is a given Boolean function using logical operators such as logical AND ($\wedge$), logical OR ($\vee$), and logical NOT ($\neg$). The index set $\mathcal{N}_i$ is the set of elements of the state used in the

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function f_i. If the index set $\mathcal{N}_i$ is an empty set, $x_i(k+1)$ is uniquely determined to be 0 or 1. For simplicity, instead of (1), we sometimes use the following notation:

$$\begin{cases} f_1([x_j]_{j\in\mathcal{N}_1}), \\ f_2([x_j]_{j\in\mathcal{N}_2}), \\ \vdots \\ f_n([x_j]_{j\in\mathcal{N}_n}). \end{cases}$$

Example 1: Consider the following BN model for a simplified apoptotic network [20]:

$$\begin{cases} x_1(k+1) = x_1(k), \\ x_2(k+1) = x_1(k) \wedge \neg x_3(k), \\ x_3(k+1) = \neg x_2(k) \wedge x_4(k), \\ x_4(k+1) = x_1(k) \vee x_3(k), \end{cases} \tag{2}$$

where x_1 is the concentration level (high or low) of the tumor necrosis factor (TNF, a stimulus), x_2 is the concentration level of the inhibitor of apoptosis proteins (IAP), x_3 is the concentration level of the active caspase 3 (C3a), and x_4 is the concentration level of the active caspase 8 (C8a). See, e.g., [21] for more complicated models of an apoptosis network. In this BN model, $\mathcal{N}_1 = \{1\}$, $\mathcal{N}_2 = \{1,3\}$, $\mathcal{N}_3 = \{2,4\}$, and $\mathcal{N}_4 = \{1,3\}$ hold. □

The interaction between elements of the state in the BN can be represented by an interaction graph defined as follows.

Definition 1: The interaction graph is given by the directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = \{1,2,\ldots,n\}$ is the set of vertices and $\mathcal{E} = \{(j,i) \in \mathcal{V}\times\mathcal{V} \mid j \in \mathcal{N}_i\}$ is the set of arcs.

The adjacency relation of the vertex i of the interaction graph expresses elements of the state used in the Boolean function f_i. When x_j (j-th element of the state) affects the value of the function f_i, the directed edge is connected from the vertex j to the vertex i. The interaction graph of the BN in Example 1 is shown in Fig. 1. The sets $\mathcal{V}$ and $\mathcal{E}$ in this interaction graph are given by

$$\mathcal{V} = \{1,2,3,4\},$$
$$\mathcal{E} = \{(1,1),(1,2),(1,4),(2,3),(3,2),(3,4),(4,3)\},$$

respectively.

Next, we define a fixed point as follows.

Definition 2: The state $x(k)$ is called a *fixed point* if $x(k+1) = x(k)$ holds.

A fixed point is also called a singleton attractor. In this paper, we focus on a fixed point as one of the properties in the steady state.

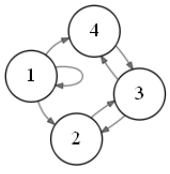

Fig. 1 Interaction graph in Example 1.

2.2 FVS-Based Model Reduction of Boolean Networks

In this section, we explain the FVS-based model reduction method of BNs in which a fixed point is focused on (see Definition 3 for details of an FVS). See [16] for further details. In this method, we regard some of the Boolean functions of a given BN as an algebraic equation. The i-th element of the state $x_i(k)$ is eliminated by substituting $f_i(\cdot)$ into $x_i(k)$. As a result, the dimension of the state can be reduced.

First, we introduce the concept of an FVS. An FVS and a minimum FVS are defined as follows (see, e.g., [22], [23]).

Definition 3: A set of vertices of an interaction graph is called an FVS if removal of vertices results an acyclic graph. In particular, an FVS is called a minimum FVS if the number of its elements is minimum.

The computational complexity of finding a minimum FVS is NP-complete [23]. An approximate algorithm of finding it has been studied (see, e.g., [22]). In [18], a simple greedy algorithm for finding an (not necessarily minimum) FVS has been proposed. When we utilize the model reduction method in [16], the dimension of the state in the reduced BN is characterized by the number of vertices in the minimum FVS of the interaction graph. In addition, each fixed point in the reduced BN is a one-to-one correspondence with that in the original BN. Let $\mathcal{V}_F \subseteq \mathcal{V}$ denote a minimum FVS. To reduce a given BN, we need to eliminate the j-th element of the state, where $j \in \mathcal{V} \setminus \mathcal{V}_F$.

Hereafter, the function f_i and the i-th element x_i of the state corresponding to the minimum FVS of the interaction graph are denoted as $\widehat{f_i}$ and $\widehat{x_i}$, respectively. Under the above preparation, the procedure of the reduction method is given as follows.

Procedure of model reduction of a given BN:

Step 1: Find a minimum FVS $\mathcal{V}_F \subseteq \mathcal{V}$ of the interaction graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$.

Step 2: For $x_j(k+1) = f_j(\cdot)$, $j \in \mathcal{V} \setminus \mathcal{V}_F$, replace $x_j(k+1)$ with $x_j(k)$.

Step 3: Substitute $f_j(\cdot)$ into the variable $x_j(k)$ of the function $\widehat{f_i}(\cdot)$, $i \in \mathcal{V}_F$. This operation is repeated until $x_j(k)$ is no longer in $\widehat{f_i}(\cdot)$.

Step 4: Simplify $\widehat{f_i}(\cdot)$.

In the case where finding a minimum FVS is difficult, we may replace it with an FVS with as few vertices as possible.

We present a simple biological example to explain this procedure.

Example 2: Consider the following BN with the seven-dimensional state:

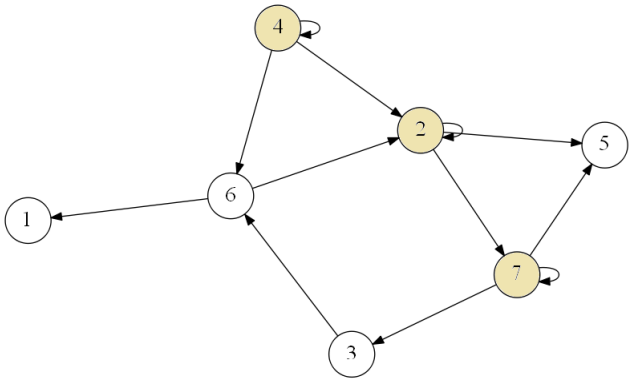

Fig. 2 Interaction graph in Example 2, where the highlighted vertices belong to the minimum FVS.

$$\begin{cases} x_1(k+1) = \neg x_6(k), \\ x_2(k+1) = (\neg x_2(k) \wedge x_4(k) \wedge x_6(k)) \\ \qquad\qquad \vee (x_2(k) \wedge x_4(k)) \vee (x_2(k) \wedge x_6(k)), \\ x_3(k+1) = \neg x_7(k), \\ x_4(k+1) = x_4(k), \\ x_5(k+1) = x_2(k) \vee \neg x_7(k), \\ x_6(k+1) = x_3(k) \vee x_4(k), \\ x_7(k+1) = \neg x_2(k) \vee x_7(k). \end{cases}$$

This BN represents the gene regulatory network with the gene WNT5A, where the concentration level (high or low) of the gene WNT5A is denoted by x_1, the concentration level of the gene pirin by x_2, the concentration level of the gene S100P by x_3, the concentration level of the gene RET1 by x_4, the concentration level of the gene MART1 by x_5, the concentration level of the gene HADHB by x_6, and the concentration level of the gene STC2 by x_7. See [24] for further details. The interaction graph of this BN is shown in Fig. 2.

In Step 1, the minimum FVS of this BN is given by

$$\mathcal{V}_F = \{2, 4, 7\}.$$

In Step 2, $x_j(k+1)$, $j \in \mathcal{V} \setminus \mathcal{V}_F = \{1, 3, 5, 6\}$ is replaced with $x_j(k)$. In the beginning of Step 3, x_i and $f_i(\cdot)$, $i \in \mathcal{V}_F$ are replaced with $\widehat{x}_i$ and $\widehat{f}_i(\cdot)$, respectively. Then, we can obtain

$$\begin{cases} x_1(k) \quad\;\; = \neg x_6(k), \\ \widehat{x}_2(k+1) = (\neg \widehat{x}_2(k) \wedge \widehat{x}_4(k) \wedge x_6(k)) \\ \qquad\qquad \vee (\widehat{x}_2(k) \wedge \widehat{x}_4(k)) \vee (\widehat{x}_2(k) \wedge x_6(k)), \\ x_3(k) \quad\;\; = \neg \widehat{x}_7(k), \\ \widehat{x}_4(k+1) = \widehat{x}_4(k), \\ x_5(k) \quad\;\; = \widehat{x}_2(k) \vee \neg \widehat{x}_7(k), \\ x_6(k) \quad\;\; = x_3(k) \vee \widehat{x}_4(k), \\ \widehat{x}_7(k+1) = \neg \widehat{x}_2(k) \vee \widehat{x}_7(k). \end{cases}$$

In Step 3, the obtained algebraic equations are substituted into the Boolean function of $\widehat{x}_2(k+1)$. Then, we can obtain

$$\begin{aligned} \widehat{x}_2(k+1) &= (\neg \widehat{x}_2(k) \wedge \widehat{x}_4(k) \wedge x_6(k)) \\ &\quad \vee (\widehat{x}_2(k) \wedge \widehat{x}_4(k)) \vee (\widehat{x}_2(k) \wedge x_6(k)) \\ &= (\neg \widehat{x}_2(k) \wedge \widehat{x}_4(k) \wedge (x_3(k) \vee \widehat{x}_4(k))) \\ &\quad \vee (\widehat{x}_2(k) \wedge \widehat{x}_4(k)) \\ &\quad \vee (\widehat{x}_2(k) \wedge (x_3(k) \vee \widehat{x}_4(k))) \\ &= (\neg \widehat{x}_2(k) \wedge \widehat{x}_4(k) \wedge (\neg \widehat{x}_7(k) \vee \widehat{x}_4(k))) \\ &\quad \vee (\widehat{x}_2(k) \wedge \widehat{x}_4(k)) \\ &\quad \vee (\widehat{x}_2(k) \wedge (\neg \widehat{x}_7(k) \vee \widehat{x}_4(k))) \end{aligned}$$

In Step 4, by simplifying the above state equation, we obtain the following reduced BN:

$$\begin{cases} \widehat{x}_2(k+1) = (\widehat{x}_2(k) \wedge \neg \widehat{x}_7(k)) \vee \widehat{x}_4(k), \\ \widehat{x}_4(k+1) = \widehat{x}_4(k), \\ \widehat{x}_7(k+1) = \neg \widehat{x}_2(k) \vee \widehat{x}_7(k). \end{cases}$$

Finally, we discuss fixed points. The original BN has four fixed points ($[0,1,0,1,1,1,1]$, $[0,1,1,0,1,1,0]$, $[0,1,1,1,1,1,0]$, $[1,0,0,0,0,0,1]$). The reduced BN has also four fixed points ($[1,1,1]$, $[1,0,0]$, $[1,1,0]$, $[0,0,1]$). From these fixed points, we see that each fixed point in the original BN is a one-to-one correspondence with that in the reduced BN. In this example, fixed points can be distinguishable by using three states. □

3. Main Result

Using the FVS-based model reduction method, the dimension of the state is reduced to the number of vertices in the FVS of a given interaction graph. In general, the number of vertices in the minimum FVS is not a minimal number of the reduced states that fixed points are distinguishable. In this section, we propose a method for further reducing states based on a given interaction graph.

Hereafter, for simplicity of notations, $\widehat{\cdot}$ is omitted in $\widehat{f_i}$ and $\widehat{x_i}$.

3.1 Motivating Example

We present a motivating example.

Example 3: Consider the following BN with the three-dimensional state:

$$\begin{cases} f_1 = x_1, \\ f_2 = \neg x_1 \wedge x_2, \\ f_3 = x_1 \wedge x_2 \wedge x_3. \end{cases}$$

All vertices of the interaction graph of this BN have a self-loop. Then, a minimum FVS is given by $\{1, 2, 3\}$. That is, the dimension of the state cannot be reduced by the FVS-based model reduction method. Here, we focus on the Boolean function f_3. Consider substituting $x_2 = f_2$ into f_3. We can obtain

$$f_3' = f_3|_{x_2 = f_2}$$

$$
\begin{aligned}
&= x_1 \wedge x_2 \wedge x_3|_{x_2=f_2} \\
&= x_1 \wedge (\neg x_1 \wedge x_2) \wedge x_3 \\
&= (x_1 \wedge \neg x_1) \wedge x_2 \wedge x_3 \\
&= 0 \wedge x_2 \wedge x_3 \\
&= 0.
\end{aligned}
$$

Hence, we can obtain $x_3(k+1) = 0$, which implies that x_3 can be reduced. Finally, we discuss fixed points. The original BN has three fixed points ([0,0,0], [0,1,0], [1,0,0]). The reduced BN has also three fixed points ([0,0], [0,1], [1,0]). Even if the above substitution operation is performed, each fixed point in the original BN is a one-to-one correspondence with that in the reduced BN. □

From this example, we see that there is a possibility that further reduction can be achieved by substitution operations. Since substitution operations are only continued ignoring the information about FVSs, in a similar to the FVS-based method, each fixed point in the original BN is a one-to-one correspondence with that in the reduced BN. In the proposed method, we focus on the following complement and absorption laws for Boolean functions:

$$A \wedge \bar{A} = 0,\ A \vee \bar{A} = 1, \tag{3}$$

$$A \vee (A \wedge B) = A,\ A \wedge (A \vee B) = A, \tag{4}$$

where $A, B \in \{0,1\}$. We also focus on the property that the i-th element x_i of the state satisfying either $x_i(k+1) = 0$ or $x_i(k+1) = 1$ can be reduced. Moreover, the FVS-based model reduction method may be applied to the BN obtained by performing further substitution operations and deleting constant Boolean functions. This is because the interaction graph is changed by these operations.

3.2 Proposed Model Reduction Method

First, we define a walk and a path for a directed graph. A walk is defined as a sequence of vertices $[v_0, \ldots, v_T]$ that the directed edges (v_i, v_{i+1}), $0 \le i \le T-1$ exist in the directed graph. A path is defined as a walk where all vertices are different. If there exists a path $[v_0, v_1, \ldots, v_{T-1}, v_T]$ on the interaction graph, we can perform the following substitution calculation:

$$
\begin{aligned}
f'_{v_1} &= f_{v_1}, \\
f'_{v_2} &= f_{v_2}\big|_{x_{v_1}=f'_{v_1}}, \\
f'_{v_2} &= f_{v_2}\big|_{x_{v_1}=f'_{v_1},\ x_{v_2}=f'_{v_2}}, \\
&\vdots \\
f'_{v_T} &= f_{v_T}\big|_{x_{v_1}=f'_{v_1},\ x_{v_2}=f'_{v_2},\ldots,\ x_{v_{T-1}}=f'_{v_{T-1}}}.
\end{aligned} \tag{5}
$$

We remark that f'_{v_T} has the variable x_{v_0}.

In the proposed method, we consider performing (3) or (4) by substituting $x_l = f_l(\cdot)$, $l \in \mathcal{N}_i$ into the function $f_i(\cdot)$. A necessary condition for performing (3) or (4) is that $f_i(\cdot)$ and $f_l(\cdot)$ have at least one common variable (i.e., there exists $j \in \mathcal{N}_i \cap \mathcal{N}_l$). This variable corresponds to A in (3) and (4). In the case where there exists no $j \in \mathcal{N}_i \cap \mathcal{N}_l$, if there exists a path $[j, v_0, v_1, \ldots, v_{K-1}, v_K, i]$, and $j \in \mathcal{N}_i$ holds, then it may be possible to perform (3) or (4) by the following substitution operations:

$$
\begin{aligned}
f'_{v_0} &= f_{v_0}, \\
f'_{v_1} &= f_{v_1}\big|_{x_{v_0}=f'_{v_0}}, \\
&\vdots \\
f'_{v_K} &= f_{v_K}\big|_{x_{v_0}=f'_{v_0},\ldots,\ x_{v_{K-1}}=f'_{v_{K-1}}}, \\
f'_i &= f_i|_{x_{v_0}=f'_{v_0},\ldots,\ x_{v_{K-1}}=f'_{v_{K-1}},\ x_{v_K}=f'_{v_K}}.
\end{aligned}
$$

In summary, if there exists a path $p = [v_0, \ldots, v_T]$ that contains the start point in the parent vertices of the end point ($v_0 \in \mathcal{N}_{v_T}$), it may be possible to reduce f_T by the substitution calculation along the path.

Next, we propose a procedure of model reduction using the absorption and complement laws. In the proposed procedure, for each nodes i on the interaction graph, the paths satisfying $[j, \ldots, i]$, $j \in \mathcal{N}_i$ are listed in order from the shortest, and the path that reduce the function f_i can be found from these paths. Let $\mathcal{F}$ denote the set of indexed Boolean functions. Let $\mathcal{I}_{\mathcal{F}}$ denote the index set of $\mathcal{F}$.

Procedure of model reduction using the absorption and complement laws:

Step 1: Apply the FVS-based model reduction method to each Boolean function. Substitute constant functions into other Boolean functions. Set $\mathcal{F} = \emptyset$ (i.e., $\mathcal{I}_{\mathcal{F}} = \emptyset$).

Step 2: Enumerate paths of length 1 in the interaction graph (self-loops are excluded). The set of enumerated paths is defined by $\mathcal{P} := \{p_i \mid i \in \mathcal{A} \subset \{1, 2, \ldots\}\}$.

Step 3: For each $p_i = [v_{i0}, \ldots, v_{iT}]$, find the path set $\{[v_j, v_{i0}, \ldots, v_{iT}] \mid \forall j \in \mathcal{N}_{v_{i0}}\}$. Update the path set $\mathcal{P} := \cup_{i \in \mathcal{A}}\{[v_j, v_{i0}, \ldots, v_{iT}] \mid \forall j \in \mathcal{N}_{v_{i0}}\}$, which is denoted by $\mathcal{P} = \{p_i \mid i \in \mathcal{A}\}$.

Step 4: For each $p_i = [v_{i0}, \ldots, v_{iT}] \in \mathcal{P}$, if $v_{i0} \in \mathcal{N}_{v_{iT}}$ and $\mathcal{I}_{\mathcal{F}} \cap \{v_{i0}, \ldots, v_{iT}\} = \emptyset$ are satisfied, obtain $f'_{v_{iT}}$ by performing the substitution operations according to p_i such as (5). If the number of states in $f'_{v_{iT}}$ is smaller than that in the original $f_{v_{iT}}$, then update $\mathcal{F}$ as $\mathcal{F} := \mathcal{F} \cup \{f'_{v_{iT}}\}$.

Step 5: For each i of $\mathcal{P} = \{p_i \mid i \in \mathcal{A}\}$, delete all p_i that satisfy $\mathcal{I}_{\mathcal{F}} \cap \{v_{i0}, \ldots, v_{iT}\} \neq \emptyset$ from the set $\mathcal{P}$.

Step 6: Follow the following conditional branch.
- **Case 1:** If $\mathcal{P} \neq \emptyset$, then go to Step 3.
- **Case 2:** If $\mathcal{P} = \emptyset$ and $\mathcal{F} \neq \emptyset$, then update f_i, $i \in \mathcal{I}_{\mathcal{F}}$ in a given BN as $f_i := f'_i \in \mathcal{F}$. Go to Step 1.
- **Case 3:** If $\mathcal{P} = \emptyset$ and $\mathcal{F} = \emptyset$, then terminate the procedure.

We explain each step.

In Step 1, the FVS-based model reduction method is applied to a given BN. Substitution operations with constant functions are also performed.

In Step 2, paths of length 1 are enumerated for each vertex.

In Step 3, the length of each path is extended by one.

In Step 4, substitution operations using each path are performed. A Boolean function may be simplified by the complement law (3) and the absorption law (4), because substitution operations such that these laws occur are included. When a Boolean function is simplified by substitution operations, this Boolean function is added to the set $\mathcal{F}$.

In Step 5, paths related to paths used in simplification of Boolean functions are deleted.

In Case 1 of Step 6, the length of each path is extended by one. Because substitution operations using paths of a longer length are required. In Case 2 of Step 6, a given BN is reduced. Since the graph structure is changed, we perform Step 1 again. In Case 3 of Step 6, the procedure is terminated.

We present a simple example to demonstrate the proposed procedure.

Example 4: Consider the following 5-node BN:

$$\begin{cases} f_1 = x_1 \vee \neg x_4, \\ f_2 = (x_1 \wedge \neg x_5) \vee x_2 \vee (\neg x_3 \wedge \neg x_4), \\ f_3 = x_3 \vee x_4, \\ f_4 = x_1 \vee x_2 \vee x_4 \vee x_5, \\ f_5 = x_4 \vee x_5. \end{cases} \tag{6}$$

The interaction graph of this BN is shown in the Fig. 3. Since all vertices have a self-loop, that is, a minimum FVS is given by all vertices, this BN cannot be reduced by the FVS-based model reduction method.

In Step 1 of the proposed procedure, only the action $\mathcal{F} := \emptyset$ is required.

In Step 2, we enumerate all the paths of length 1 in the interaction graph as follows:

$$\begin{aligned} \mathcal{P} = \{ &[4,1],\ [1,2],\ [3,2],\ [4,2],\ [5,2],\ [4,3], \\ &[1,4],\ [2,4],\ [5,4],\ [4,5] \} \end{aligned}$$

(i.e., $\mathcal{A} = \{1, 2, \ldots, 10\}$).

In Step 3, we extend the paths by one on the start point side. Then, we can obtain the following set $\mathcal{P}$:

$$\begin{aligned} \mathcal{P} = \{ &[2,4,1],\ [5,4,1],\ [4,1,2],\ [4,3,2],\ [1,4,2], \\ &[5,4,2],\ [4,5,2],\ [1,4,3],\ [2,4,3],\ [5,4,3], \\ &[1,2,4],\ [3,2,4],[5,2,4],\ [1,4,5],\ [2,4,5] \}. \end{aligned}$$

In Step 4, the paths whose parent vertices of the end point contain the start point are given as follows:

$$\begin{aligned} &[4,1,2],\ [4,3,2],\ [1,4,2],\ [5,4,2],\ [4,5,2], \\ &[1,2,4],\ [5,2,4]. \end{aligned}$$

Substitution calculations according to these paths are performed, but there are no Boolean functions that can be reduced.

In Step 5, since $\mathcal{F} = \emptyset$ holds, any path is not deleted.

In Step 6, since the condition of Case 1 holds, go to Step 3.

In Step 3, we extend the paths by one on the start point side again.

$$\begin{aligned} P = \{ &[3,2,4,1],\ [5,2,4,1],\ [5,4,1,2],\ [1,4,3,2], \\ &[5,4,3,2],\ [1,4,5,2],\ [1,2,4,3],\ [5,2,4,3], \\ &[1,2,4,5],\ [3,2,4,5] \} \end{aligned}$$

In Step 4, the paths whose parent vertices of the end point contains the start point are given as follows:

$$[5,4,1,2],\ [1,4,3,2],\ [5,4,3,2],\ [1,4,5,2].$$

We perform substitution calculations according to these paths. Then, by substitution operations using the $[5,4,1,2]$, the Boolean function f_2 with five states can be reduced to f_2' with four states as follows.

$$\begin{aligned} f_4' &= x_1 \vee x_2 \vee x_4 \vee x_5, \\ f_1' &= x_1 \vee \neg x_4|_{x_4 = f_4'} \\ &= x_1 \vee \neg(x_1 \vee x_2 \vee x_4 \vee x_5) \\ &= x_1 \vee (\neg x_2 \wedge \neg x_4 \wedge \neg x_5), \\ f_2' &= (x_1 \wedge \neg x_5) \vee x_2 \vee (\neg x_3 \wedge \neg x_4)|_{x_1 = f_1',\ x_4 = f_4'} \\ &= ((x_1 \vee (\neg x_2 \wedge \neg x_4 \wedge \neg x_5)) \wedge \neg x_5) \vee x_2 \\ &\quad \vee (\neg x_3 \wedge \neg(x_1 \vee x_2 \vee x_4 \vee x_5)) \\ &= x_2 \vee (x_1 \wedge \neg x_5) \vee ((\neg x_2 \wedge \neg x_4 \wedge \neg x_5) \\ &\quad \vee ((\neg x_2 \wedge \neg x_4 \wedge \neg x_5) \wedge (\neg x_1 \wedge \neg x_3))) \\ &= x_2 \vee (x_1 \wedge \neg x_5) \vee (\neg x_2 \wedge \neg x_4 \wedge \neg x_5) \\ &= x_2 \vee (x_1 \wedge \neg x_5) \vee (\neg x_4 \wedge \neg x_5), \end{aligned}$$

where the absorption law (4) is used in calculation of f_2'. The obtained Boolean function f_2' is added to the $\mathcal{F}$.

In Step 5, we delete the paths through the vertex of the function of $\mathcal{F} = \{f_2'\}$ from the set $\mathcal{P}$, and we obtain $\mathcal{P} = \emptyset$.

In Step 6, since the condition of Case 2 holds, f_2 in a given BN (6) is replaced with $f_2' \in \mathcal{F}$ as follows:

$$\begin{cases} f_1 = x_1 \vee \neg x_4, \\ f_2 = x_2 \vee (x_1 \wedge \neg x_5) \vee (\neg x_4 \wedge \neg x_5), \\ f_3 = x_3 \vee x_4, \\ f_4 = x_1 \vee x_2 \vee x_4 \vee x_5, \\ f_5 = x_4 \vee x_5. \end{cases} \tag{7}$$

In Step 1, since all the nodes of the interaction graph of the modified BN (7) have a self-loop, only the action $\mathcal{F} := \emptyset$

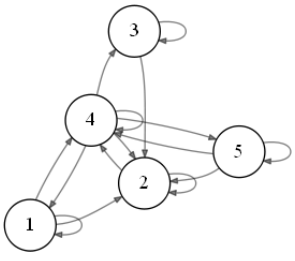

Fig. 3 Interaction graph of the BN (6).

is required.

In Step 2, we enumerate all the paths of length 1 in the interaction graph as follows:

$$\mathcal{P} = \{\ [4,1],\ [1,2],\ [4,2],\ [5,2],\ [4,3],\ [1,4],\ [2,4],\ [5,4],\ [4,5]\ \}.$$

In Step 3, we extend the path of P by one on the start point side as follows:

$$\mathcal{P} = \{\ [2,4,1],\ [5,4,1],\ [4,1,2],\ [1,4,2],\ [5,4,2],\ [4,5,2],\ [1,4,3],\ [2,4,3],\ [5,4,3],\ [1,2,4],\ [5,2,4],\ [1,4,5],\ [2,4,5]\ \}.$$

In Step 4, the paths whose parent vertices of the end point contains the start point are given by

$$[4,1,2],\ [1,4,2],\ [5,4,2],\ [4,5,2],\ [1,2,4],\ [5,2,4].$$

We perform substitution calculations according to these paths. Then, by substitution operations using two paths $[4,5,2]$ and $[5,2,4]$, the Boolean functions f_2 and f_4 can be reduced as follows:

$$\begin{aligned} f_5' &= x_4 \vee x_5, \\ f_2' &= x_2 \vee (x_1 \wedge \neg x_5) \vee (\neg x_4 \wedge \neg x_5)|_{x_5=f_5'} \\ &= x_2 \vee (x_1 \wedge \neg(x_4 \vee x_5)) \vee (\neg x_4 \wedge \neg(x_4 \vee x_5)) \\ &= x_2 \vee (\neg x_4 \wedge \neg x_5) \vee ((\neg x_4 \wedge \neg x_5) \wedge x_1) \\ &= x_2 \vee (\neg x_4 \wedge \neg x_5) \end{aligned}$$

(the absorption law (4) is used) and

$$\begin{aligned} f_2' &= x_2 \vee (x_1 \wedge \neg x_5) \vee (\neg x_4 \wedge \neg x_5), \\ f_4' &= x_1 \vee x_2 \vee x_4 \vee x_5|_{x_2=f_2'} \\ &= x_1 \vee (x_2 \vee (x_1 \wedge \neg x_5) \vee (\neg x_4 \wedge \neg x_5)) \vee x_4 \vee x_5 \\ &= x_1 \vee x_2 \vee (x_1 \wedge \neg x_5) \vee \neg(x_4 \vee x_5) \vee (x_4 \vee x_5) \\ &= 1 \end{aligned}$$

(the complement law (3) is used). Two Boolean functions f_2' and f_4' are added to the set $\mathcal{F}$.

In Step 5, we delete the paths through the vertex of the function of $F = \{f_2',\ f_4'\}$ from $\mathcal{P}$, and we obtain $P = \emptyset$.

In Step 6, since the condition of Case 2 holds, f_2 and f_4 in the modified BN (7) are replaced with f_2' and f_4' as follows:

$$\begin{cases} f_1 = x_1 \vee \neg x_4, \\ f_2 = x_2 \vee (\neg x_4 \wedge \neg x_5), \\ f_3 = x_3 \vee x_4, \\ f_4 = 1, \\ f_5 = x_4 \vee x_5, \end{cases}$$

and return to Step 1.

In Step 1, we substitute the constant function $x_4 = f_4 = 1$. As a result, we can obtain

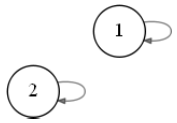

Fig. 4 Interaction graph of the BN (8).

$$\begin{cases} f_1 = x_1, \\ f_2 = x_2. \end{cases} \tag{8}$$

The interaction graph is shown in Fig. 4. In Step 2, any path cannot be generated (i.e., $\mathcal{P} = \emptyset$). Then, in Step 6, the condition of Case 3 holds, and the procedure is terminated. Therefore, we can obtain (8) as a reduced BN.

Finally, the original BN has four fixed points ($[0,0,1,1,1]$, $[0,1,1,1,1]$, $[1,0,1,1,1]$, $[1,1,1,1,1]$). The reduced BN has also four fixed points ($[0,0]$, $[0,1]$, $[1,0]$, $[1,1]$). Thus, fixed points are distinguishable by x_1 and x_2. □

From this example, we see that a given BN can be reduced while the interaction graph is changed.

4. Numerical Example

In this section, we present a numerical example to validate the proposed method.

Consider 100 BNs with 20 states. Interaction graphs are randomly generated such that the scale-free property is satisfied for the in-degrees of the vertices. If there is a vertex that has no self-loop, then a self-loop is added. Logical operations are randomly assigned. In implementation, we use BDDs (binary decision diagrams). When the FVS-based model reduction method is applied to these BNs, the dimension of the state cannot be reduced. This is because the vertex sets of the interaction graphs for these BNs are an FVS.

We present the computation result using the proposed procedure. In 100 reduced BNs, the dimension of the states is derived as follows:

- The mean dimension: 18.35,
- The maximum dimension: 20,
- The minimum dimension: 7.

From these values, we see that the dimension of the state can be reduced using the proposed procedure. In addition, we present the information about $|\mathcal{N}_i|$ (the in-degree, that is, the number of elements of the state used in the Boolean function f_i). In 100 BNs, the max and mean of the maximum in-degree are as follows:

- Max: 18 (original), 11 (reduced),
- Mean: 3.13 (original), 1.99 (reduced).

From these values, we see that Boolean functions are simplified using the proposed procedure. In some methods of analysis and control of BNs, the computational complexity exponentially grows with the dimension of the state in each Boolean function (see, e.g. [25]). Hence, simplification of Boolean functions is important.

Finally, we comment on the computation time of the proposed procedure. For 100 BNs, the computation time of the proposed procedure is derived as follows:

- The mean computation time: 205 sec,
- The worst computation time: 11445 sec,

where we use Python 3.8.5 on the computer (CPU: Intel Core i7-4770K 3.50 GHz, Memory: 8 GB, OS: Windows 10). In 75 BNs of 100 BNs, the proposed method can be solved within 10 sec. In only a part of BNs, the long computation time is required. To derive the reduced model faster, it is future work to improve the proposed procedure.

5. Conclusion

In this paper, we proposed a new method for model reduction of BNs. Focusing on the complement and absorption laws of Boolean functions, the dimension of the state is reduced based on the structure of the interaction graph of a given BN. The proposed method was demonstrated by a numerical example.

In future work, it is important to discuss the minimality of the reduced BN. In general, the dimension of the state in the reduced BN obtained by the proposed method is not minimal. Hence, it is important to find the structure of the interaction graph such that the reduced BN obtained by the proposed method is minimal. In the proposed method, the FVS-based model reduction method is utilized. It is also future work to develop a simpler procedure that the FVS-based model reduction method is not utilized.

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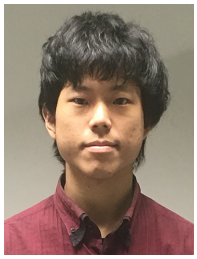

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