

A Fixed-Parameter Algorithm for Detecting a Singleton Attractor in an AND/OR Boolean Network with Bounded Treewidth

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1 Introduction

The *Boolean network* (BN) is known as a discrete mathematical model of gene regulatory networks [3]. In a BN, each vertex corresponds to a gene and takes one of two values 0 and 1, where 0 (resp., 1) means that the corresponding gene is inactive (resp., active). The value of a vertex at a given time step is determined according to a regulation rule, which is a Boolean function of the values of the predecessors of the vertex at the previous time instant. The values of vertices are updated synchronously, and the (global) *state* of a network at a given time step is the vector of its vertex values. Beginning from any initial state, the system eventually falls into an *attractor*, which is classified into two types: a *singleton attractor* corresponding to a stable state, and a *periodic attractor* corresponding to a sequence of states that repeats periodically.

It is known that the problem of finding an attractor of the shortest period is NP-hard even for BNs with maximum in-degree 2 consisting of AND/OR of literals [5]. Due to this hardness and the fact that there exist 2^n global states for a BN with n vertices, previous theoretical studies focused on the development of $o(2^n)$ time algorithms.

Since it is quite hard to develop such algorithms for general BNs, some restrictions were assumed on types of Boolean functions in all studies. For example, an $O(1.587^n)$ time algorithm and an $O(1.985^n)$ time algorithm were developed for detection of a singleton attractor [4] and an attractor of period 2 [1], respectively, both for *AND/OR BNs* which are BNs consisting of Boolean functions restricted to conjunctions and disjunctions of literals.

An $O(n^{2p(w+1)}poly(n))$ time algorithm was also developed for finding an attractor of period p of a BN having bounded treewidth w and consisting of nested canalizing functions, where p and w are constants, and nested canalizing functions are a super class of AND/OR functions [1]. They also presented a fixed-parameter algorithm (precisely, an algorithm working in $O(g(p, w, d)poly(n))$ time where $g(p, w, d)$ depends only on p, w, d) for a general BN with bounded degree and bounded treewidth [1]. However, it is unknown whether there exists a fixed-parameter algorithm even for an AND/OR BN with bounded treewidth but without degree constraint. In this short report, we present a fixed-parameter algorithm for detection of a singleton attractor in an AND/OR BN with bounded treewidth.

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2 Preliminaries

A BN $N(V, F)$ consists of a set V of n vertices and a corresponding set $F = \{f_v : v \in V\}$ of n Boolean functions. Let $v(t) \in \{0, 1\}$ represent the value of a vertex v at time t , and denote by $\mathbf{v}(t) = \langle v(t) : v \in V \rangle$ the *state of the network* at time t . The values of all vertices are updated simultaneously according to the corresponding Boolean functions, $v(t+1) = f_v(\mathbf{v}(t))$. A directed graph $G(V, E)$ can be associated with the network, with a directed edge $(u, v) \in E$ if and only if f_v depends on u , where edges may be self-loops. The initial assignment of values $\mathbf{v}(1) = \langle v(1) : v \in V \rangle$ uniquely determines the state of the network at all $t > 1$. An initial state is called a *periodic attractor with period p* if $\mathbf{v}(1) = \mathbf{v}(p+1)$ and $\mathbf{v}(1) \neq \mathbf{v}(q)$ holds for all $1 < q < p+1$. An attractor with period $p = 1$ is called a *singleton attractor*.

A *tree decomposition* of a graph $G(V, E)$ is a pair $\langle T(V_T, E_T), (B_t)_{t \in V_T} \rangle$, where $T(V_T, E_T)$ is a rooted tree and $(B_t)_{t \in V_T}$ is a family of subsets of V such that

- for every $v_i \in V$, $B^{-1}(v_i) = \{t \in V_T | v_i \in B_t\}$ is nonempty and connected in T , and
- for every edge $\{v_i, v_j\} \in E$, there exists $t \in V_T$ such that $v_i, v_j \in B_t$.

The *width* of the decomposition is defined as $\max_{t \in V_T} (|B_t| - 1)$ and the *treewidth* of G is the minimum of the widths among all the tree decompositions of G . Graphs with treewidth at most k are also known as *partial k -trees* [2].

3 Algorithm

Let $\langle T(V_T, E_T), (B_t)_{t \in V_T} \rangle$ be a tree decomposition of $G(V, E)$ associated to a given BN $N(V, F)$. Let $des(t)$ denote the set of descendant of $t \in V_T$ with including t . Let $V_t = \bigcup_{t' \in des(t)} B_{t'}$. For each $t \in V_T$, $p(t)$ denotes the parent node of t in V_T .[‡]

For each $t \in V_T$, ϕ_t denotes a function from B_t to $\{0, 1, \omega\}$, where we call such ϕ_t an *assignment*. We define $\hat{\phi}_t$ by

$$\hat{\phi}_t(v) = \begin{cases} \phi_t(v), & \text{if } \phi_t(v) \in \{0, 1\}, \\ 0, & \text{if } \phi_t(v) = \omega \text{ and } f_v \text{ is AND,} \\ 1, & \text{if } \phi_t(v) = \omega \text{ and } f_v \text{ is OR,} \end{cases}$$

It is to be noted that if $\hat{\phi}_t(v) = 1$ and v is an AND vertex (resp., $\hat{\phi}_t(v) = 0$ and v is an OR vertex), Boolean

[‡]We use nodes and vertices for $\langle T(V_T, E_T), (B_t)_{t \in V_T} \rangle$ and $N(V, F)$, respectively.

values of its input vertices are uniquely determined (in a singleton attractor). Therefore, $\phi_t(v) = \omega$ holds only if v is an AND vertex and $\hat{\phi}_t(v) = 0$, or v is an OR vertex and $\hat{\phi}_t(v) = 1$.

For a 0-1 assignment α to $V' \subseteq V$, $\phi_t(v) \in \{0, 1\}$ is called *validated* (by α on V') if the Boolean value v is uniquely determined as $\alpha(v)$ from α regardless of an assignment to $V - V'$. We say that α *violates* a Boolean function f_v (assigned to vertex v) if the value (b_v) of f_v is uniquely determined by α but $b_v \neq \alpha(v)$. It is to be noted that we need not validate if $\hat{\phi}_t(v) = 1$ and v is an AND vertex, or, $\hat{\phi}_t(v) = 0$ and v is an OR vertex since it is enough for such a vertex to examine whether α does not violate f_v . ϕ_t is called *consistent* if the following is satisfied

- (1) $\phi_t(v) \in \{0, 1\}$ holds for all $v \in B_t - B_{p(t)}$, where we let $B_{p(t)} = \emptyset$ if t is the root,
- (2) there exists a 0-1 assignment α to V_t such that $\hat{\phi}_t(v) = \alpha(v)$ holds for all $v \in B_t$, α does not violate any Boolean function assigned to V_t , and $\phi_t(v)$ is validated for all v such that $\phi_t(v) \in \{0, 1\}$ by α on V_t .

Let A_t be the set of consistent assignments to B_t . We describe below how to compute A_t by dynamic programming from leaves to the root in V_T . For each leaf t , A_t is determined by $A_t = \{\phi_t \mid \phi_t \text{ satisfies conditions (1) and (2) for } \alpha = \hat{\phi}_t\}$.

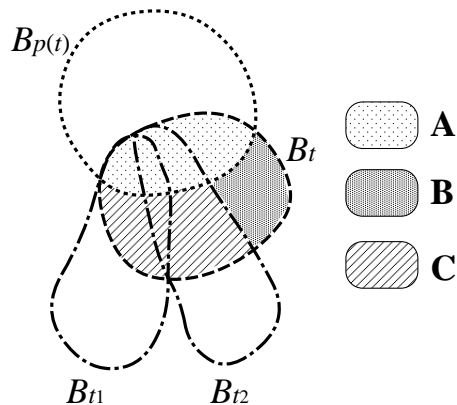


Figure 1: Part A ($B_t \cap B_{p(t)}$) can be validated later, Part B ($B_t - B_{p(t)} - \cup_j B_{t_j}$) must be validated by ϕ_t , and Part C ($(B_t \cap (\cup_j B_{t_j})) - B_{p(t)}$) must be validated by $\phi_t, \phi_{t_1}, \phi_{t_2}$.

Let t_1, \dots, t_d be the children of t . For all possible ϕ_t , we examine whether it is consistent as follows. We call ϕ_t and ϕ_{t_i} are *compatible* if, for each $v \in B_t \cap B_{t_i}$, $\phi_t(v) = \phi_{t_i}(v)$ holds, or $\phi_t(v) \in \{0, 1\}$, $\phi_{t_i}(v) = \omega$ and $\hat{\phi}_t(v) = \hat{\phi}_{t_i}(v)$ hold. We maintain a 0-1 table $X(x_1, \dots, x_h)$ where $\{v_{j_1}, \dots, v_{j_h}\} = B_t$ (i.e., X is a 0-1 table having $2^{|B_t|}$ entries). We say that ϕ_t is a *candidate* assignment if $\phi_t(v) \in \{0, 1\}$ holds for any

vertex in $B_t - B_{t(p)}$, ϕ_t does not violate any function assigned to B_t , and $\phi_t(v)$ is validated by ϕ_t for any vertex $B_t - B_{t(p)} - \cup_{j=1, \dots, d} B_{t_j}$. The following is a pseudocode of the proposed algorithm (see also Fig. 1).

Procedure *FpFindAtt*

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for all leaves in  $V_T$  do compute  $A_t$ ;
for all internal nodes  $t$  in  $V_T$  do
     $A_t \leftarrow \emptyset$ ;
    for all candidate assignments  $\phi_t$  do
        for all  $(x_1, \dots, x_h) \in \{0, 1\}^h$  do
             $X(x_1, \dots, x_h) \leftarrow 0$ ;
             $X(x_1, \dots, x_h) \leftarrow 1$  where  $x_g = 1$  iff  $\phi_t(v_{j_g})$ 
            has already been validated, or  $\phi_t(v_{j_g}) = \omega$ ;
            for  $i = 1$  to  $d$  do
                 $Y \leftarrow X$ ;
                for all  $\phi_{t_i} \in A_{t_i}$  compatible with  $\phi_t$  do
                    let  $z_g = 1$  if  $\phi_{t_i}(v_{j_g}) \in \{0, 1\}$ ,
                    otherwise  $z_g = 0$ ;
                    for all  $(x_1, \dots, x_h)$  with  $X(x_1, \dots, x_h) = 1$ 
                    do
                         $Y(\max(x_1, z_1), \dots, \max(x_h, z_h)) \leftarrow 1$ ;
                 $X \leftarrow Y$ ;
            if  $X(1, 1, \dots, 1) = 1$  then  $A_t \leftarrow A_t \cup \{\phi_t\}$ 
    
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There exists a singleton attractor iff $A_r \neq \emptyset$ for the root r of T . Furthermore, such a singleton attractor can be retrieved by using the standard traceback technique. Since the number of possible ϕ_t is bounded by 3^{k+1} per t and the size of table X is bounded by 2^{k+1} for partial k -trees, we have:

Theorem 1 *The singleton attractor detection problem for an AND/OR BN with bounded treewidth k can be solved in $O(f(k)\text{poly}(n))$ time, where $f(k)$ is a function depending only on k .*

References

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