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Abstract

The study of the dynamical behavior of Boolean networks with different update schedules has so far focused primarily on the possible dynamics and equivalent networks that can be obtained. However, few studies have been done about which networks can be obtained from another network with a non-parallel schedule.

In this article, we define the problem of finding a Boolean network that is dynamically equivalent to another network. For the general case, it is shown that the problem is NP-Hard. However, if the problem is restricted to disjunctive Boolean networks, it can be solved in polynomial time.

Keywords: Boolean network, block-sequential update schedule, dynamical behavior, disjunctive network.

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1 Introduction

A Boolean network is defined as a system of n Boolean variables interacting with each other that evolves, in discrete time, according to a predefined update schedule. Applications of Boolean networks include computer science, circuit theory, social systems, among others. In particular, from the initial works of Kauffman and Thomas [9, 10, 14, 15], they are widely used as models of gene networks.

A key aspect in modeling biological systems using Boolean networks is the update schedule used. A widely used type of update schedule is the synchronous or parallel one. However, other schedules have also been investigated, such as block-sequential schedules, which are a generalization of the parallel schedule.

It is well known that the dynamic behavior of a network is very sensitive to changes in the update schedule [3]. Therefore, in the absence of biological information to determine which schedule to use, it is very useful to know if there is any dynamically equivalent network that reproduces the studied phenomenon using a different block-sequential update schedule.

Parallel digraphs, which are preliminary presented by F. Robert [12, 13], calling them Gauss-Seidel operator, are a widely used tool over the years. Thanks to [7, 3], equivalence classes have been defined between different update schedules based on their update digraph, so that elements in the same class have the same dynamic behavior.

In this sense, in [4] the dynamics of discrete neural networks with deterministic update schedules is studied and in [2] we studied how many different dynamics can exist in a Boolean network when the update schedule changes. In the particular case of disjunctive networks, in [1] we studied the complexity of deciding whether there exists a limit cycle of a given length k for some update schedule, and in [6] we classified them according to the robustness of their dynamics concerning changes in the update schedule, all this using parallel digraphs.

However, to our knowledge, the following questions have been little explored: What other networks have the same dynamics as that of a given network? What dynamics are only yielded by a parallel schedule? Research closer to this one is [8], with the difference being that while authors go in one direction, our research goes in the opposite direction, i.e., the authors in [8] study among other things how the network changes when it is updated with a given sequential schedule, while in this article we are interested in studying whether it is possible to obtain a given network from some other network updated with some block-sequential schedule.

This article addresses the above questions. For that, our approach as follows: in Section 1 we define the notations that are used. Then, in Section 3, we formally define the problem and prove that it is NP-hard in the general case. In Section 4, we restrict our problem to disjunctive Boolean networks. Later, in Section 5, we present an algorithm that decides the problem defined in Section 4 in polynomial time for disjunctive (conjunctive) networks. Finally, in the last section, the conclusions reached are presented.

2 Definition and notation

A *Boolean network* with n components is a discrete dynamical system usually defined by a *global transition function*:

$$f : \{0,1\}^n \to \{0,1\}^n\,,\ x \to f(x) = (f_1(x), \dots, f_n(x)),$$

where each function $f_v : \{0,1\}^n \to \{0,1\}$ associated to the component v is called *local activation function.*

Any vector $x = (x_1, \dots, x_n) \in \{0,1\}^n$ is called a *state* of the network f with *local state* x_v on each component v. The *dynamics* of f is given by its application on any state of the network.

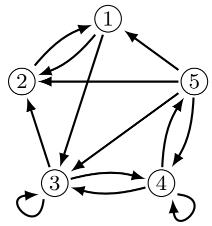
Definition 1. We define the *interaction graph* of a Boolean network $f : \{0,1\}^n \to \{0,1\}^n$, denoted by $G(f) = ([n], A(f))$, as:

$$\begin{aligned} [n] &= \{1, \dots, n\}\,, \\ A(f) &= \{(u,v) \in [n] \times [n] : \exists x \in \{0,1\}^n\,, f_v(x) \neq f_v(x^{\neg u})\} \end{aligned}$$

where $x_v^{\neg u} = x_v \iff u \neq v$.

Also, for each $u \in [n]$ we define the in-neighborhood and the out-neighborhood of u as:

$$\begin{aligned} N_f^-(u) &= \{v \in [n] : (v,u) \in A(f)\} \\ N_f^+(u) &= \{v \in [n] : (u,v) \in A(f)\} \end{aligned}$$



$$
\begin{aligned}
f_1(x) &= \neg x_2 \wedge x_5\\
f_2(x) &= (x_1 \wedge x_3) \vee (x_5 \wedge \neg x_3)\\
f_3(x) &= (\neg x_1 \vee \neg x_5) \wedge x_3 \wedge x_4\\
f_4(x) &= (x_4 \wedge x_3) \vee (x_5 \wedge \neg x_3)\\
f_5(x) &= x_4
\end{aligned}
$$

Figure 1: Example of a Boolean network and its interaction graph.

Example 1. An example of a Boolean network f and its interaction graph $G(f)$ is shown in Figure 1.

Definition 2. Given $f : \{0,1\}^n \to \{0,1\}^n$ a Boolean network, f is called a disjunctive Boolean network if: $\forall u \in [n],\ f_u(x) = 1 \iff (\exists v \in N_f^-(u), x_v = 1)$.

We observe that the global transition function of a disjunctive Boolean network is completely described by its interaction graph.

An *update schedule* is defined by a function $s : [n] \to [n]$ such that $s([n]) = [m]$ for some $m \leq n$, where $s(u)$ indicates the updating order of the component u in a time step. A *block* of an update schedule s is a set $B_i = \{u \in [n] : s(u) = i\}$, with $i \in [m]$. An update schedule s is also denoted by $s = B_1, B_2, \ldots, B_m$. In this case, we say that s has m blocks. If $m = 1$, the update schedule is called *synchronous or parallel* and is denoted by s_p. If $m = n$, the update schedule is called *sequential*. Other kinds of update schedules are named *block-sequential updates*.

Definition 3. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a Boolean network, $x^t = (x_1^t, \ldots, x_n^t) \in \{0,1\}^n$ a state and $s = B_1, B_2, \ldots, B_m$ a block-sequential update schedule. The dynamical behavior of f *updated according to* s is given by:

$$\forall v \in B_1, \qquad x_v^{t+1} = f_v(x^t). \tag{1}$$

$$\forall v \notin B_1, \qquad x_v^{t+1} = f_v(x_u^{t+1} : s(u) < s(v); x_u^t : s(u) \geq s(v)) \tag{2}$$

The expression in (1) is because when updating the elements in B_1, no other elements have been updated. The expression in (2) is because at the time of updating x_v, if its dependency (x_u) belongs to a previous block it has already been updated (x_u^{t+1}) and if its dependency belongs to a later block (or the same block) it takes its value without updating (x_u^t).

This definition is an interpretation of what was introduced by F. Robert in [12], where the origin of this expression is explained in depth.

This is equivalent to applying a function f^s to x:

$$x^{t+1} = f^s(x^t),$$

where f^s is defined by:

$$\forall v \in B_1, \qquad f^s(x)_v = f_v(x). \tag{3}$$

$$\forall v \notin B_1, \qquad f^s(x)_v = f_v(f_u^s(x) : s(u) < s(v); x_u : s(u) \geq s(v)) \tag{4}$$

It is easy to prove that f^s is equivalent to:

$$f^s = f^{B_m} \circ f^{B_{m-1}} \circ \cdots \circ f^{B_2} \circ f^{B_1}$$

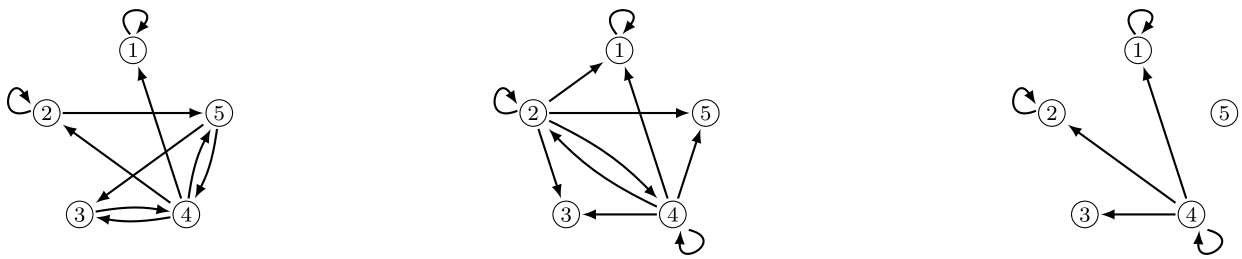
with $f^{B_i} : \{0,1\}^n \to \{0,1\}^n$ given by:

$$\forall x \in \{0,1\}^n, \quad f_v^{B_i}(x) = \begin{cases} x_v & \text{if } v \notin B_i \\ f_v(x) & \text{if } v \in B_i. \end{cases}$$

Note that, under this definition, $f = f^{s_p}$. Moreover, if f is a disjunctive Boolean network, then, by definition, f^s is also a disjunctive Boolean network. This is because the family of disjunctive Boolean networks is closed under composition.

In this way, the dynamical behavior of f updated according to s is equivalent to the dynamical behavior of f^s updated according to the parallel schedule.

An example of a Boolean network f updated according to a block-sequential update schedule s is shown in Figure 2(a) and Figure 2(c).



(a)

$f_1(x) = x_1 \vee x_4$
$f_2(x) = x_2 \wedge x_4$
$f_3(x) = x_4 \wedge \neg x_5$
$f_4(x) = x_3 \wedge \neg x_5$
$f_5(x) = x_2 \wedge \neg x_4$
$s = \{2\}\,\{5\}\,\{3\}\,\{4\}\,\{1\}$

(b)

$f_1^s(x) = x_1 \vee (x_4 \wedge \neg(x_2 \wedge x_4 \wedge \neg x_4))$
$f_2^s(x) = x_2 \wedge x_4$
$f_3^s(x) = x_4 \wedge \neg(x_2 \wedge x_4 \wedge \neg x_4)$
$f_4^s(x) = x_4 \wedge \neg(x_2 \wedge x_4 \wedge \neg x_4)$
$f_5^s(x) = x_2 \wedge x_4 \wedge \neg x_4$

(c)

$f_1^s(x) = x_1 \vee x_4$
$f_2^s(x) = x_2 \wedge x_4$
$f_3^s(x) = x_4 \wedge \neg(0) = x_4$
$f_4^s(x) = x_4 \wedge \neg(0) = x_4$
$f_5^s(x) = (x_2 \wedge x_4) \wedge \neg x_4 = 0$

Figure 2: (a) A Boolean network f and an update schedule s (b) The parallel digraph $G_P(f,s)$ (c) The effective network f^s.

Figure 2 shows that, obtaining $G(f^s)$, that is, the interaction graph that presents the actual dependencies of the local functions of f updated according to s, is not a simple task. In fact, it was proved to be a DP-complete problem [11]. For example, f_5^s is a constant function 0, when the function f_5 depends on x_2 and x_4. Obtaining $G(f^s)$ depends on the local functions of f and how they interact with each other. For this reason, a useful tool to study this is the *potential dependencies digraph of the equivalent parallel network* (in short, *parallel digraph*). This digraph represents the potential effective dependencies of a network if it were to be updated in parallel.

Definition 4. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a Boolean network and s an update schedule, the *parallel digraph*, denoted as $G_P(f,s) = ([n], A)$, where:

$$\forall v \in B_1, (u,v) \in A \iff (u,v) \in A(f) \quad (5)$$
$$\forall v \notin B_1, (u,v) \in A \iff (\exists w \in N_f^-(v), s(w) < s(v) \wedge (u,w) \in A) \vee (s(u) \geq s(v) \wedge (u,v) \in A(f)) \quad (6)$$

which is equivalent to:

$$(u,v) \in A \iff \left[(\exists w \in N_f^-(v), s(w) < s(v) \wedge (u,w) \in A) \vee ((u,v) \in A(f) \wedge s(u) \geq s(v))\right] \quad (7)$$

Note that in the equivalences (6) and (7) the construction of the arc (u, v) depends on the arc (u, w) which was previously constructed (since w is updated before v). Therefore, the set A is well defined.

By calling it a digraph of potential dependencies we mean that transitively these variables may depend on each other. For example, in Figure 2(a), f_3 depends on x_5, and also f_5 depends on x_2, therefore, if x_5 is updated before x_3 (as in the case of update schedule s), it is likely that f_3 depends on x_2. But this is not always the case, since by the nature of the different Boolean functions, some may cancel with others, as is the case of f_3^s in Figure 2(b) and Figure 2(c). Therefore, it is easy to notice that $G(f^s) \subseteq G_P(f, s)$.

In the case of disjunctive networks, from the research conducted in [6], there is a direct relationship between the parallel digraph and the effective network when updated in parallel.

Remark 1. Given $f, h : \{0,1\}^n \to \{0,1\}^n$ two disjunctive Boolean networks and an update schedule s, $h^s = f$ is equivalent to $G_P(h, s) = G(f)$.

Indeed, if we consider the transitivity of dependencies of the parallel digraph, it will produce a composition of functions when defining the effective dependencies of a variable. And considering that the OR function is closed under composition, no potential dependence will be canceled. Therefore, in the case of disjunctive networks, all potential dependencies will be effective dependencies and therefore $h^s = f$ is equivalent to $G_P(h, s) = G(f)$.

Another tool that can provide a better understanding of these concepts is the labeled digraph.

Given a digraph $G = (V, A)$, a *labeling function* is a function $\text{lab} : A \to \{\oplus, \ominus\}$. A pair (G, lab) is called a labeled digraph and is represented by the vertices and arcs from G, but adding the corresponding labels on its arcs (Figure 3). For any arc $(u, v) \in A$:

- if $\text{lab}(u, v) = \oplus$, the arc is called a positive arc,
- if $\text{lab}(u, v) = \ominus$, the arc is called a negative arc.

Let $G = (V, A)$ be a digraph and s an update schedule. We define the labeling function $\text{lab}_s : A \to \{\ominus, \oplus\}$ in the following way:

$$\forall (u, v) \in A, \quad \text{lab}_s(u, v) = \begin{cases} \oplus & \text{if } s(u) \geq s(v) \\ \ominus & \text{if } s(u) < s(v) \end{cases}$$

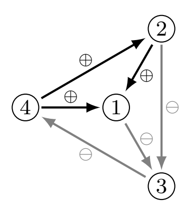


Figure 3: A digraph G labeled by the function lab_s, with $s = \{1\}\{2\}\{3\}\{4\}$

A *labeled digraph* (G, lab) is said to be an *update digraph* if there exists an update schedule s such that $\text{lab} = \text{lab}_s$, that is $\forall a \in A(G), \text{lab}(a) = \text{lab}_s(a)$ (see the example in Figure 4).

Given $f : \{0,1\}^n \to \{0,1\}^n$ a Boolean network, we define the following equivalence relation between updates schedule s and s':

$$s \sim_f s' \iff (G(f), \text{lab}_s) = (G(f), \text{lab}_{s'}).$$

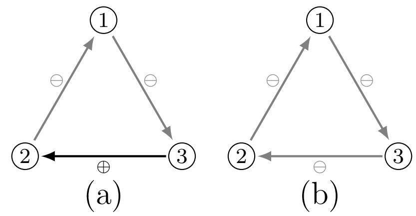


Figure 4: (a) A labeled digraph (G, lab) which is an update digraph. (b) A labeled digraph (G, lab') which is not an update digraph.

We denote $[s]_f$ the equivalence class of s induced by $\sim_f$. In [3] was proved that if two different updates schedules s and s' have the same update digraph, then the Boolean network f updated according to s has the same dynamical behavior that f updated according to s', i.e.

$$s \sim_f s' \implies f^s = f^{s'}. \tag{8}$$

3 Dynamically equivalent networks problem

In this section we focus on the inverse problem, i.e. given a dynamical behavior of a Boolean network, we want to know if there exists a Boolean network with an update schedule different from the parallel that produces the same dynamical behavior.

Definition 5. Let $f, h : \{0,1\}^n \to \{0,1\}^n$ be two Boolean networks and s an update schedule. We say that (h, s) is *dynamically equivalent to* f if $h^s = f$. Moreover, if $h \neq f$, or $h = f$ and $s \nsim_f s_p$, we say that (h, s) and f are *non-trivially dynamically equivalent.*

By Equation (8), remember that if $h = f$, for every s equivalent to s_p, we have $h^s = f$. And there exists $s \neq s_p$ equivalent to s_p if and only if $G(f)$ is not strongly connected. Indeed, if $G(f)$ is not strongly connected, then there is at least one initial (source) strongly connected component. Then, the two-block schedule s wherein the second block are the vertices of the initial component and in the first block, the rest of the vertices, is equivalent to s_p. On the other hand, if $G(f)$ is strongly connected and s is equivalent to s_p, then between any pair of vertices (u, v), there exists a fully positive path from u to v, so by transitivity, $s(u) \geq s(v)$. Therefore, for any pair of vertices u, v, $s(u) = s(v)$, and thus s is the parallel schedule.

Example 2. Let $f : \{0,1\}^2 \to \{0,1\}^2$ be the Boolean network defined by $f(x_1, x_2) = (x_2, x_1)$ (see Figure 5(a)), let us prove that it does not exist another network non-trivially dynamically equivalent to f.

Note that the only update schedules that are not equivalent to s_p are $s = \{1\}\{2\}$ and $s' = \{2\}\{1\}$.

Let us suppose that there exists a Boolean network h such that $h^s = f$, where $s = \{1\}\{2\}$. And let $x \in \{0,1\}^2$ be such that $h_2(x_2, x_2) \neq x_1$. Then,

$$h^s(x_1, x_2) = (h_1^s(x_1, x_2), h_2^s(x_1, x_2)).$$

Since $1 \in B_1$,

$$h_1^s(x_1, x_2) = h_1(x_1, x_2) = f_1(x_1, x_2) = x_2.$$

Thus,

$$h_2^s(x_1, x_2) = h_2(h_1^s(x_1, x_2), x_2) = h_2(x_2, x_2) \neq x_1 = f_2(x_1, x_2).$$

Therefore, there is no network h with update schedule s that are non-trivially dynamically equivalent to f.

Analogously, it is possible to show that there is no network h non-trivially dynamically equivalent to f when $s' = \{2\}\{1\}$.

Example 3. On the other hand, if we consider the function $f'(x) = (f'_1(x), f'_2(x)) = (x_1, x_1)$ (see Figure 5(b)) which only differ with f in the first local activation function, and $s = \{2\}\{1\}$, the Boolean network $h'(x) = (h'_1(x), h'_2(x)) = (x_1 \vee x_2, x_1)$ satisfies $h'^s = f'$.

Figure 5: Interaction digraph of the Boolean network from Example 2 and Example 3.

Using the above definition, we introduce the following problem:

Dynamically equivalent networks problem (DEN problem)

Input: A Boolean network f (encoded as a Boolean formula for each f_i).

Question: does there exists a Boolean network h and an update schedule s, such that (h, s) is non-trivially dynamically equivalent to f?

The universe of possible solutions is very large: for n components, there are $O(2^{n^{2^n}})$ possible Boolean networks and $O(n!)$ possible update schedules [5]. The following result shows a relation between different solutions:

Theorem 1. If there exists a solution to DEN problem then there exists a solution to DEN problem with a block-sequential update schedule with two blocks.

To prove the previous theorem, we use the following lemma:

Lemma 2. Let $h, f : \{0,1\}^n \to \{0,1\}^n$ be Boolean networks and $s = B_1, B_2, \ldots, B_m$ with $m > 1$. If $h^s = f$, then there exists $\bar{h}$ and $\bar{s}$ such that $\bar{h}^{\bar{s}} = f$ where $\bar{s} = B_1, B_2, \ldots, B_{m-1} \cup B_m$.

Proof. Without loss of generality, let us suppose that there exists $u \in B_{m-1}$ and $v \in B_m$ such that $(u, v) \in A(h)$. If this condition does not hold, $\bar{s} \sim_{\bar{h}} s$. We define $\bar{h}$ as follows:

$$\bar{h}_v(x) = \begin{cases} h_v(x) & \forall v \notin B_m, \\ h_v(f^{B_{m-1}}(x)) & \forall v \in B_m. \end{cases}$$

Finally:

$$\forall v \in B_j \wedge j < m, \qquad \bar{h}_v^{\bar{s}}(x) = \bar{h}_v(\bar{h}^{B'_{j-1}} \circ \bar{h}^{B'_{j-2}} \circ \cdots \circ \bar{h}^{B'_1}(x)). \tag{9}$$

$$= h_v(h^{B_{j-1}} \circ h^{B_{j-2}} \circ \cdots \circ h^{B_1}(x)). \tag{10}$$

$$= h_v^s(x) = f_v(x). \tag{11}$$

$$\forall v \in B_m, \qquad \bar{h}_v^{\bar{s}}(x) = \bar{h}_v(h^{B'_{m-2}} \circ h^{B'_{m-3}} \circ \cdots \circ h^{B'_1}(x)). \tag{12}$$

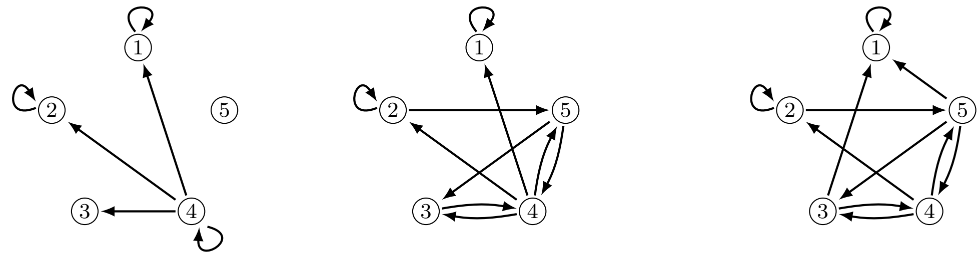
$$= \bar{h}_v(h^{B_{m-2}} \circ h^{B_{m-3}} \circ \cdots \circ h^{B_1}(x)). \tag{13}$$

$$= h_v(h^{B_{m-1}}(h^{B_{m-2}} \circ h^{B_{m-3}} \circ \cdots \circ h^{B_1}(x))). \tag{14}$$

$$= h_v(h^{B_{m-1}} \circ h^{B_{m-2}} \circ h^{B_{m-3}} \circ \cdots \circ h^{B_1}(x)). \tag{15}$$

$$= h_v^s(x) = f_v(x). \tag{16}$$

For this reason, $\bar{h}^{\bar{s}} = f$. □



$f_1(x) = x_1 \vee x_4$
$f_2(x) = x_2 \wedge x_4$
$f_3(x) = x_4$
$f_4(x) = x_4$
$f_5(x) = 0$

(a)

$\tilde{f}_1(x) = x_1 \vee x_4$
$\tilde{f}_2(x) = x_2 \wedge x_4$
$\tilde{f}_3(x) = x_4 \wedge \neg x_5$
$\tilde{f}_4(x) = x_3 \wedge \neg x_5$
$\tilde{f}_5(x) = x_2 \wedge \neg x_4$
$\tilde{s} = \{2\}\{5\}\{3\}\{4\}\{1\}$

(b)

$\bar{f}_1(x) = x_1 \vee (x_3 \wedge \neg x_5)$
$\bar{f}_2(x) = x_2 \wedge x_4$
$\bar{f}_3(x) = x_4 \wedge \neg x_5$
$\bar{f}_4(x) = x_3 \wedge \neg x_5$
$\bar{f}_5(x) = x_2 \wedge \neg x_4$
$\bar{s} = \{2\}\{5\}\{3\}\{4,1\}$

(c)

Figure 6: (a) A Boolean network f (b) A solution with 5 blocks (c) A solution with 4 blocks.

Notice that, $\bar{s}$ is non-equivalent to s if and only if there exists an arc from some vertex in B_{m-1} to a vertex in B_m.

Proof of Theorem 1. If there exists a solution with an update schedule with $k > 2$ blocks, applying the Lemma 2 successively, it is possible to construct a solution with 2 blocks. □

To understand the real complexity of the problem, let us see the following theorem:

Theorem 3. DEN is NP-Hard.

Proof. To prove NP-Hardness we show that 3-SAT $\leq_p$ DEN. Let ϕ be a 3-CNF formula in variables $x_1, \ldots, x_n$. Without loss of generality, let us consider that ϕ has only non-trivial clauses; a non-trivial clause C_i being a clause such that for each variable $x_j \in C_i$, we have $\bar{x_j} \notin C_i$. Note that eliminating trivial clauses from ϕ is a simple task. Now, we consider $f : \{0,1\}^{n+2} \to \{0,1\}^{n+2}$ as follows:

$$\begin{aligned} \forall u \in [n], \qquad f_u(x) &= x_u, \\ f_{n+1}(x) &= \phi(x_1, \ldots, x_n) \vee x_{n+2} \\ f_{n+2}(x) &= x_{n+1}. \end{aligned}$$

See $G(f)$ in Figure 7(a).

($\Rightarrow$) If ϕ is satisfiable, we consider the function $\bar{f} = f$ and the update schedule $s = \{1, \ldots, n\}\{n+1, n+2\}$. Since ϕ is satisfiable and there exists $x \in \{0,1\}^n$ such that $\phi(x) = 0$ (because ϕ has only non-trivial clauses), f_{n+1} depends on x_u for some $u \in [n]$, so s is not equivalent to the parallel update schedule, and $\bar{f}^s = f$.

($\Leftarrow$) If ϕ is not satisfiable $\forall u \in [n]$, $f_u(x) = x_u$, $f_{n+1}(x) = x_{n+2}$ and $f_{n+2}(x) = x_{n+1}$. See $G(f)$ in Figure 7(b). We see that the sub-graph induced by vertices $n+1$ and $n+2$ is isomorphic to the digraph presented in Figure 5(a). And, as in that example, it is shown that there is no Boolean network that is non-trivially dynamically equivalent to the disjunctive Boolean network with this interaction sub-graph. Then there is also no Boolean network that is non-trivially dynamically equivalent to f. In this way, any update schedule that preserves the dynamical behavior is equivalent to the parallel. □

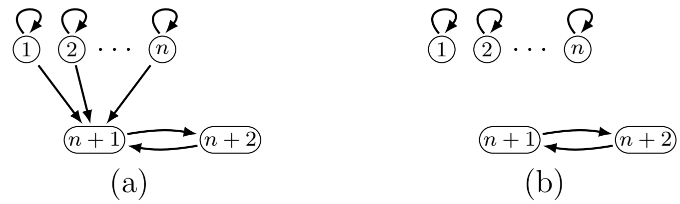


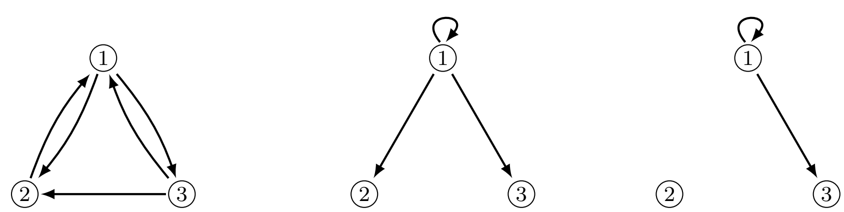
Figure 7: Interaction digraph of the transformation defined in Theorem 3.

4 Dynamically equivalent disjunctive networks problem

As we can see, in the general case, the DEN problem is hard, therefore, we focus on disjunctive networks, defining the following problem:

> Dynamically equivalent disjunctive networks problem (D-DEN problem)
>
> **Input:** A disjunctive Boolean network f (encoded as a Boolean formula for each f_i).
>
> **Question:** does there exists a disjunctive Boolean network h and an update schedule s, such that (h, s) is non-trivially dynamically equivalent to f?

Why only restrict ourselves to disjunctive Boolean networks h? As can be seen in Figure 8, there are non-disjunctive networks (because h_1 and h_2 are linear functions) that can generate disjunctive networks. But in this case, the equality between the parallel digraph and the effective digraph produced by the composition of functions, as analyzed in Remark 1, is lost.



$h_1(x) = x_2 + x_3$	$h_1^s(x) = (x_1 + x_1) + x_1$	$h_1^s(x) = x_1$
$h_2(x) = x_1 + x_3$	$h_2^s(x) = x_1 + x_1$	$h_2^s(x) = 0$
$h_3(x) = x_1$	$h_3^s(x) = x_1$	$h_3^s(x) = x_1$
	$s = \{3\}\{2\}\{1\}$	
(a)	(b)	(c)

Figure 8: (a) A non-disjunctive Boolean network h (b) The parallel digraph $G_P(h, s)$ (a disjunctive network) (c) The effective network f^s (a disjunctive network). [+ represents modulo-two addition]

Remark 2. Based on the last part of Definition 4, it is possible to define the parallel digraph $G_P(f,s) = ([n], A)$ in terms of the labeled digraph as:

$$A = \{(u,v) \in A(f) : \mathrm{lab}_s(u,v) = \oplus\} \cup \{(u,v) : \exists w \in N_f^-(v), (u,w) \in A \wedge \mathrm{lab}_s(w,v) = \ominus\}.$$

where the set $\{(u,v) : \exists w \in N_f^-(v), (u,w) \in A \wedge \mathrm{lab}_s(w,v) = \ominus\}$ represents the arcs generated for the predecessors that were already updated in a previous block.

An example of parallel digraph is shown in Figure 2(b).

In the same way, given a labeled digraph (G, lab) without fully negative cycles, we can define $G_P(G, \mathrm{lab}) = ([n], A)$ as:

$$\begin{aligned} A = &\{(u,v) \in A(G) : \mathrm{lab}(u,v) = \oplus\} \cup \\ &\{(u,v) \in [n] \times [n] : \exists w \in [n], (w,v) \in A(G) \wedge (u,w) \in A \wedge \mathrm{lab}(w,v) = \ominus\}. \end{aligned}$$

In this definition, if f is a disjunctive Boolean network and s is an update schedule, then $G_P(G(f), \mathrm{lab}_s) = G_P(f,s)$.

The following results are consequences of the definition of *parallel digraph*:

Lemma 4. Let $h, f : \{0,1\}^n \to \{0,1\}^n$ be two disjunctive Boolean networks and s an update schedule such that $h^s = f$. Then, for $u, v \in [n]$:

$$[(u,v) \in A(h) \wedge \mathrm{lab}_s(u,v) = \ominus] \Longrightarrow N_f^-(u) \subseteq N_f^-(v).$$

Proof. By Remark 1, we have that $h^s = f$ is equivalent to $G_P(h,s) = G(f)$.

By contradiction, let us suppose that there exists $(u,v) \in A(h)$ such that $\mathrm{lab}_s(u,v) = \ominus$ and $N_f^-(u) \nsubseteq N_f^-(v)$. Since $N_f^-(u) \setminus N_f^-(v) \neq \emptyset$, let $w \in N_f^-(u) \setminus N_f^-(v)$, then, $(w,u) \in A(f)$ and $(u,v) \in A(h)$ with $\mathrm{lab}_s(u,v) = \ominus$, by definition of parallel digraph, there exists a vertex $u \in N_h^-(v)$, such that $(w,u) \in A(f)$ and $\mathrm{lab}_s(u,v) = \ominus$, therefore $(w,v) \in A(f)$, which is a contradiction because $w \notin N_f^-(v)$. □

Remark 3. Based on Lemma 4, for all those disjunctive Boolean networks whose vertex neighborhoods are not comparable there is no network that is non-trivially dynamically equivalent. Some examples are the disjunctive Boolean networks $f : \{0,1\}^n \to \{0,1\}^n$ such that:

- Complete digraphs without loops, for $n \geq 2$, where:

$$\forall v \in [n], \quad N_f^-(v) = [n] \setminus \{v\}$$

- The double chain digraph with loops in the extreme vertices, for $n \geq 3$, where:

$$\forall v \in [n], \quad N_f^-(v) = \begin{cases} \{1,2\} & \text{if } v = 1 \\ \{n-1, n\} & \text{if } v = n \\ \{v-1, v+1\} & \text{otherwise} \end{cases}$$

- The double cycle, for $n \geq 2$ (with exception of $n = 4$), where:

$$\forall v \in [n], \quad N_f^-(v) = \begin{cases} \{n,2\} & \text{if } v = 1 \\ \{n-1, 1\} & \text{if } v = n \\ \{v-1, v+1\} & \text{otherwise} \end{cases}$$

Note that the condition of Lemma 4 is necessary but not sufficient, as shown in the following example.

Example 4. The Figure 9 shows that, given a disjunctive Boolean network f, if there are vertices $u, v \in [n]$ such that $N_f^-(u) \subseteq N_f^-(v)$, then a non-trivially dynamically equivalent network does not necessarily exist. This Boolean network is known because the only equivalent dynamic network is the trivial one, since according to the schedule $\{1\}\{2\}$ there is no way to build the arc $(1, 2)$, and according to the schedule $\{2\}\{1\}$ there is no way to build the arc $(2, 1)$, (the loop in 1 cannot be included for any h, since it is not in $A(f)$). Note also that it is true that $N_f^-(1) = \{2\} \subseteq \{1, 2\} = N_f^-(2)$.

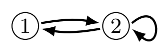


Figure 9: $N_f^-(1) \subseteq N_f^-(2)$ but the only network dynamically equivalent is the trivial one.

However, if we consider the case of equal neighborhoods, we obtain a sufficient condition.

Proposition 5. Let $f : \{0, 1\}^n \to \{0, 1\}^n$ be a disjunctive Boolean network. There exists a disjunctive Boolean network h and an update schedule s, such that (h, s) is non-trivially dynamically equivalent to f and with only one negative arc $(u, v) \in A(h)$ if and only if the following conditions are satisfied:

1. $N_f^-(u) \subseteq N_f^-(v)$,
2. $u \notin N_f^-(v) \setminus N_f^-(u)$,
3. For every vertex $w \in N_f^-(v) \setminus N_f^-(u)$, it does not exist a path from u to w in $G(f) - v$.

Proof. Since f and h are disjunctive Boolean networks, we have that $h^s = f$ is equivalent to $G_P(h, s) = G(f)$.

($\Rightarrow$ 1.) This is true according to Lemma 4.

($\Rightarrow$ 2.) Let us suppose that there exists a Boolean network h and an update schedule s, such that (h, s) is non-trivially dynamically equivalent to f with only one negative arc $(u, v) \in A(h)$ and $u \in N_f^-(v) \setminus N_f^-(u)$. Then $(u, v) \in A(f)$ (because $u \in N_f^-(v)$) and $(u, u) \notin A(f)$ (because $u \notin N_f^-(u)$). Since $(u, u) \notin A(f)$ the only way to create (u, v) in f is that there exists a vertex $w \in [n]$ such that $(u, w) \in A(f)$, $(w, v) \in A(h)$ and $\text{lab}_s(w, v) = \ominus$, but since (u, v) is the only negative arc of $G(h)$, this path does not exist, therefore $(u, v) \notin A(f)$, which is a contradiction.

($\Rightarrow$ 3.) Let us suppose that there exists a Boolean network h and an update schedule s, such that (h, s) is non-trivially dynamically equivalent to f and with only one negative arc $(u, v) \in A(h)$, in this case $s(u) < s(v)$. Also, let us suppose, there exists a vertex $w \in N_f^-(v) \setminus N_f^-(u)$, such that there exists a path from u to w in $G(f) - v$. Since (u, v) is the only negative arc, all arcs in the path from u to w in $G(f) - v$ are in $A(h)$ and their labels are $\oplus$, the same occurs with the arc (w, v) (because $w \in N_f^-(v)$), so $s(u) \geq s(w) \geq s(v)$. Therefore, $s(u) < s(v)$ and $s(u) \geq s(v)$ which is a contradiction.

($\Leftarrow$) Let u^* and v^* be two vertices in $[n]$ such that $N_f^-(u^*) \subseteq N_f^-(v^*)$ and for every vertex $w \in N_f^-(v^*) \setminus N_f^-(u^*), w \neq u^*$ and it does not exists a path from u^* to w in $G(f) - v^*$. We define the Boolean network $h : \{0,1\}^n \to \{0,1\}^n$ such that:

$$A(h) = \big(A(f) \setminus \big\{(w, v^*) : w \in N_f^-(u^*)\big\}\big) \cup \{(u^*, v^*)\}.$$

Notice that:

$$N_h^-(v) = \begin{cases} N_f^-(v) & \text{if } v \neq v^* \\ \{u^*\} \cup N_f^-(v^*) \setminus N_f^-(u^*) & \text{if } v = v^* \end{cases}$$

Let $s = B_1 B_2$ where:

$$B_2 = \{v^*\} \cup \{w \in V(h) : \text{there exists a path from } w \text{ to } v^* \text{ in } G(h) - (u^*, v^*)\}$$

Note that, $B_1 = V(h) \setminus B_2$ is not empty, since condition 3 ensures that the only path from u^* to v^* is the arc (u^*, v^*), so $u^* \in B_1$. Also, the only arc from a vertex in B_1 to a vertex in B_2 is (u^*, v^*), because if there exists a vertex $u \in B_1$ such that u is in the in-neighborhood of a vertex $v \in B_2$ ($v \neq v^*$), then there is a path from u to v^* and, therefore $u \in B_2$ which is a contradiction. In this way, for all $v \in V(h)$ if $v \neq v^*$, $(u, v) \in A(h^s)$ is equivalent to $(u, v) \in A(h)$, therefore $(u, v) \in A(h^s)$ if and only if $(u, v) \in A(f)$. Now, $(u, v^*) \in A(h^s)$ is equivalent to: $u \in N_f^-(v^*) \setminus N_f^-(u^*)$ ($\text{lab}_s(u, v) = \oplus$) or $u \in N_{h^s}^-(u^*) = N_f^-(u^*)$, since $\text{lab}_s(u^*, v^*) = \ominus$. In this way, $(u, v^*) \in A(h^s)$ if and only if $(u, v^*) \in A(f)$.

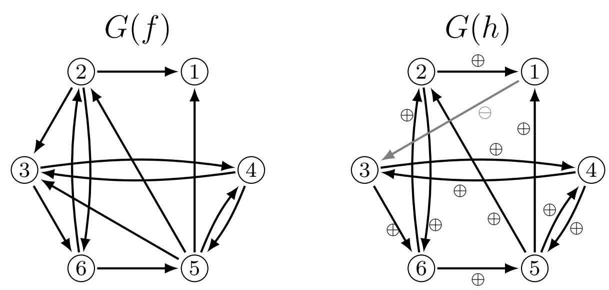


Figure 10: An example of h, f and $(u^*, v^*) = (1, 3)$. Note that $N_f^-(1) = \{2, 5\} \subseteq \{2, 4, 5\} = N_f^-(3)$ and it does not exists a path from 4 to 1 in $G(f) - 3$.

Finally, it has been proven that there exists a disjunctive Boolean network $h \neq f$ and $s \not\sim_h s_p$ such that $G_P(h, s) = G(f)$. $\square$

Corollary 6. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a disjunctive Boolean network. If there exist $u, v \in [n]$ such that $N_f^-(u) = N_f^-(v)$, then there exists a disjunctive Boolean network h and an update schedule s such that (h, s) is non-trivially dynamically equivalent to f.

Proof. If $N_f^-(u^*) = N_f^-(v^*)$ then the conditions of Proposition 5 are satisfied. $\square$

5 Algorithm to decide D-DEN Problem

To design a strategy to recognize all the vertices that meet the necessary condition given by Lemma 4, we introduce the following definitions:

Definition 6. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a disjunctive Boolean network. We define the following set of arcs:

$$A^{\ominus}(f) = \{(u,v) \in [n] \times [n] : u \neq v \wedge N_f^-(u) \subseteq N_f^-(v)\}.$$

This set represents all arcs in $[n]\times[n]$ that can be labeled $\ominus$. Note that the inclusion relationship of these sets is transitive, because if $N_f^-(u) \subseteq N_f^-(w)$ and $N_f^-(w) \subseteq N_f^-(v)$, then $N_f^-(u) \subseteq N_f^-(v)$.

Remark 4. Note that in terms of $A^{\ominus}(f)$ we can reinterpret the previous lemmas as follows:

1. By Lemma 4, if $A^{\ominus}(f) = \emptyset$, then there is no network (h,s) that is non-trivially dynamically equivalent to f.

2. By Corollary 6, if $A^{\ominus}(f)$ induces a digraph with at least one cycle, then there exist at least two vertices with equal in-neighborhoods, for this reason, there exists a network non-trivially dynamically equivalent to f.

3. By Proposition 5, if $|A^{\ominus}(f)| = 1$, there exists a network non-trivially dynamically equivalent to f if and only if for all $w \in N_f^-(v) \setminus N_f^-(u)$, $w \neq u$ and it does not exist a path from u to w in $G(f) - v$.

Definition 7. Given a partially labeled digraph (G, lab) we denoted the sets of arcs $\mathrm{lab}^{\oplus}[G, \mathrm{lab}]$ and $\mathrm{lab}^{\ominus}[G, \mathrm{lab}]$ as follows:

$$\mathrm{lab}^{\oplus}[G, \mathrm{lab}] = \{a \in A(G) : \mathrm{lab}(a) = \oplus\}$$
$$\mathrm{lab}^{\ominus}[G, \mathrm{lab}] = \{a \in A(G) : \mathrm{lab}(a) = \ominus\}$$

Definition 8. Given $n \in \mathbb{N}$ and two sets of arcs $A^-, A^+ \subseteq [n] \times [n]$, such that $A^- \cap A^+ = \emptyset$, we define (G, lab) the *labeled digraph induced by* $[n]$*,* A^- *and* A^+, denoted by $G[A^-, A^+]$, as follows:

- $V(G) = [n]$
- $A(G) = A^- \cup A^+$
- $\forall a \in A(G), \mathrm{lab}(a) = \begin{cases} \ominus & \text{if } a \in A^- \\ \oplus & \text{if } a \in A^+ \end{cases}$

Definition 9. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a disjunctive Boolean network and $A^- \subseteq A^{\ominus}(f)$, we define the operator $\mathcal{G}_{\mathrm{lab}}(f, A^-)$ as the output of the Algorithm 1, where:

$$(A^+)^* = \{(u,v) : \text{ there exists a path from } u \text{ to } v \text{ in } G[A^+]\}.$$

Algorithm 1: $\mathcal{G}_{\mathrm{lab}}(f, A^-)$

Input: A disjunctive Boolean network $f : \{0,1\}^n \to \{0,1\}^n$ and a subset $A^- \subseteq A^{\ominus}(f)$ of $G = G(f)$ such that $G[A^-]$ is acyclic.
Output: A labeled digraph $G[A^-, A^+]$.

$A^+ \leftarrow \{(u,v) \in A(f) : \forall w \in N_f^+(u), (w,v) \notin A^-)\}$;
if $(A^+)^* \cap A^- = \emptyset$ **then return** $G[A^-, A^+]$;
else return $\mathcal{G}_{\mathrm{lab}}(f, A^- \setminus (A^+)^*)$;

Remark 5. It is important to note that, since f is a disjunctive Boolean network, we can encode it by its adjacency matrix, which implies that the size of the input is $O(n^2)$.

If we analyze each operation, we can observe the following: first, constructing the set A^+ takes $O(n^3)$ time; then, obtaining $(A^+)^*$ and intersecting it with A^- also takes $O(n^3)$ and, finally, calculating the difference of sets takes $O(n^2)$.

We must consider that the recursive call will be performed at most $O(n^2)$ times, since at least one arc of A^- is removed in each iteration.

Therefore, the cost of Algorithm 1 is $O(n^5)$.

Note that the result of the $\mathcal{G}_{\text{lab}}(f, A^-)$ operator is a labeled digraph for which its parallel digraph, if update, is equal to $G(f)$. To prove its correctness, we can classify the arcs of $G(f)$ into two classes:

- Directly explained arcs: Those that are in the digraph $G(h)$ and have positive label.
- Indirectly explained arcs: Those arcs (u, v) that need an arc $(u, w) \in A(f)$ and $(w, v) \in A(h)$ with negative label.

Clearly, an indirectly explained arc (u, v) needs that arc (u, w) is directly or indirectly explained.

In the case of Algorithm 1, for each of the arcs $(u, v) \in A(f)$, we have two options:

- either there exists w such that (u, w) is in $A(f)$ and (w, v) is in A^-, so (u, v) is not added to A^+, and clearly (u, v) is an indirectly explained arc, or else
- there is no such w, therefore (u, v) is added to A^+ and thus directly explained.

In this way, to be sure that all the arcs of $A(f)$ can be explained, it is strictly necessary that at least one of the arcs of $A(f)$ is directly explained. This can be guaranteed from the following proposition:

Proposition 7. *Let $h, f : \{0, 1\}^n \to \{0, 1\}^n$ be two disjunctive Boolean networks. If for all arc $(u, v) \in A(f)$, (u, v) is a indirectly explained arc then the set of negative arcs in h has at least one cycle.*

Proof. Let (u, v_0) be an arc indirectly explained, then there exists a vertex v_1 such that $(u, v_1) \in A(f)$ and $(v_1, v_0) \in A(h)$ with negative label. And so on, we can construct a succession of vertices $v_0, v_1, \ldots, v_n$ that fulfill this condition.

Without loss of generality, let us consider $v_n, \ldots, v_0$ the longest path of negative arcs in $A(h)$ that satisfy this condition (Figure 11).

And for the case of (u, v_n), it is necessary that it can be explained indirectly (initial premise), but there does not exist a vertex v_{n+1} such that $(u, v_{n+1}) \in A(f)$ and $(v_{n+1}, v_n) \in A(h)$ with negative label (since, in that case, $v_n, \ldots, v_0$ would not be the longest path). Therefore, that value j such that $(u, v_j) \in A(f)$ and $(v_j, v_n) \in A(h)$ with negative label, must necessarily be in the set $\{0, \ldots, n-1\}$, thus forming a cycle in the set of negative arcs in $G(h)$. □

In addition to each arc of f being explained (directly or indirectly) another interesting condition is that the resulting labeled graph is update. Condition $(A^+)^* \cap A^- = \emptyset$ eliminates several simple cases, but it is not sufficient as can be seen in Figure 12. To find an update solution, based on this one, it is necessary to study some properties previously.

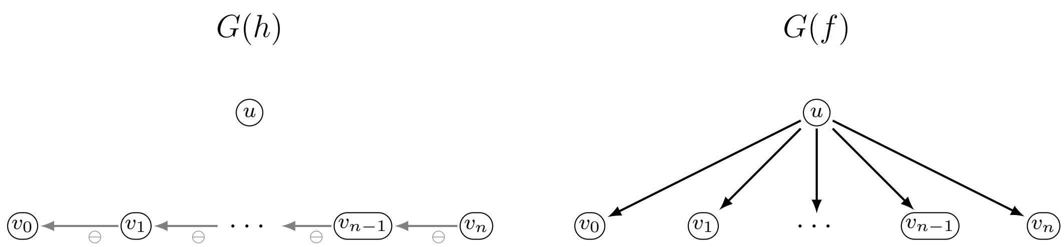


Figure 11: Explanation of Proposition 7.

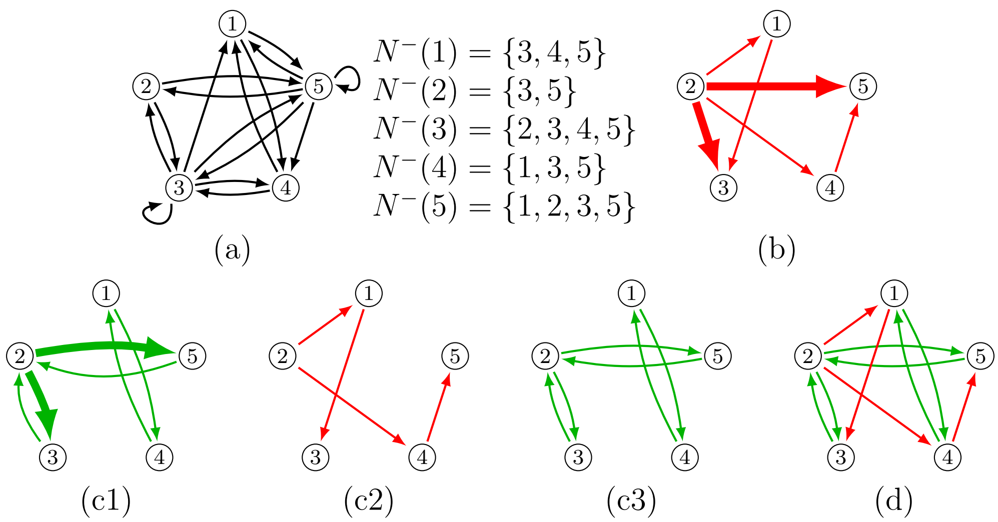


Figure 12: (a) A disjunctive Boolean network f. (b) $A^{\ominus}(f)$. (c) Iterations of $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$. (d) $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$ which is not update, because according to the labeled digraph there should be an update schedule s such that $s(2) < s(1) < s(3) \leq s(2)$, which is a contradiction.

An interesting set to study is the set of positive arcs generated by $\mathcal{G}_{\text{lab}}$, i.e. $\text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f, A^-)]$. An important characteristic of this set is that for all disjunctive Boolean network h and update schedule s such that $h^s = f$, we have $\text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f, A^-)] \subseteq A(h)$.

The following result shows that given two sets of negative arcs (subsets of $A^{\ominus}(f)$), the positive arcs of $\mathcal{G}_{\text{lab}}$ on the larger set are also positive arcs of $\mathcal{G}_{\text{lab}}$ on the smaller set.

Proposition 8. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a disjunctive Boolean network and $A'' \subseteq A' \subseteq A^{\ominus}(f)$, then $\text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f, A')] \subseteq \text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f, A'')]$.

Proof. Let us suppose that $A'' \subseteq A' \subseteq A^{\ominus}(f)$.

Let $(u,v) \in \text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f, A')]$, then $\forall w \in N_f^+(u), (w,v) \notin A'$.

Since $A'' \subseteq A'$, then $\forall w \in N_f^+(u), (w,v) \notin A''$, and therefore, $(u,v) \in \text{lab}^{\oplus}[G(f), A'']$. Hence, $\text{lab}^{\oplus}[G(f), A'] \subseteq \text{lab}^{\oplus}[G(f), A'']$. □

The following result allows us to ensure that if there exists an acyclic set of negative arcs $A^- \subseteq A^{\ominus}(f)$ such that $\mathcal{G}_{\text{lab}}(f, A^-)$ is an update digraph, then $G_P(\mathcal{G}_{\text{lab}}(f, A^-)) = G(f)$.

Proposition 9. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a disjunctive Boolean network and $A^- \subseteq A^{\ominus}(f)$ such that $G[A^-]$ is acyclic. If $\mathcal{G}_{\text{lab}}(f, A^-)$ is an update digraph, then $G_P(\mathcal{G}_{\text{lab}}(f, A^-)) = G(f)$.

Proof. $[G_P(\mathcal{G}_{\text{lab}}(f, A^-)) \subseteq G(f)]$ Let $(u,v) \in A(G_P(\mathcal{G}_{\text{lab}}(f, A^-)))$. We have two cases:

- If $(u,v) \in \text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f,A^-)]$, then $(u,v) \in A(f)$.

- Otherwise, if $(u,v) \notin \text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f,A^-)]$, since $(u,v) \in A(G_P(\mathcal{G}_{\text{lab}}(f,A^-)))$, then, by definition of parallel digraph, there exists a vertex w such that $(u,w) \in A(f)$ and $(w,v) \in A^-$. Since $(w,v) \in A^-$, then $N_f^-(w) \subseteq N_f^-(v)$. For this reason, since $(u,w) \in A(f)$, then $(u,v) \in A(f)$.

$[G(f) \subseteq G_P(\mathcal{G}_{\text{lab}}(f,A^-))]$ Let $(u,v) \in A(f)$. We have two cases:

- If it does not exist $w \in [n]$ such that $(u,w) \in A(f)$ and $(w,v) \in A^-$, then $(u,v) \in \text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f,A^-)]$, therefore, $(u,v) \in A(G_P(\mathcal{G}_{\text{lab}}(f,A^-)))$.

- If there exists $w \in [n]$ such that $(u,w) \in A(f)$ and $(w,v) \in A^-$, then, by definition of parallel digraph, $(u,v) \in A(G_P(\mathcal{G}_{\text{lab}}(f,A^-)))$.

Hence, if $(u,v) \in A(f)$, then $(u,v) \in A(G_P(\mathcal{G}_{\text{lab}}(f,A^-)))$. Therefore, since $G_P(\mathcal{G}_{\text{lab}}(f,A^-)) \subseteq G(f)$ and $G(f) \subseteq G_P(\mathcal{G}_{\text{lab}}(f,A^-))$, we have $G_P(\mathcal{G}_{\text{lab}}(f,A^-)) = G(f)$. □

Remark 6. Note that if $G[A^-]$ has a cycle, it is not possible to calculate $\mathcal{G}_{\text{lab}}(f,A^-)$. Also, it is not necessary, because by Corollary 6 we have a solution for the studied problem.

The following proposition shows that if there is a solution (with negative arcs A^- and positive arcs B), then the set of negative arcs of $\mathcal{G}_{\text{lab}}(f,A^-)$ is exactly A^- and the set of positive arcs of $\mathcal{G}_{\text{lab}}(f,A^-)$ is a subset of B. Therefore, the solution obtained using $\mathcal{G}_{\text{lab}}(f,A^-)$ is minimal in the number of arcs.

Proposition 10. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a disjunctive Boolean network and $A^- \subseteq A^{\ominus}(f)$ such that $G[A^-]$ is acyclic. If there exists $B \subseteq [n]\times[n]$ such that $A^- \cap B = \emptyset$, $G[A^-,B]$ is an update digraph and $G_P(G[A^-,B]) = G(f)$, then $\text{lab}^{\ominus}[(\mathcal{G}_{\text{lab}}(f,A^-)] = A^-$ and $\text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f,A^-)] \subseteq B$.

Proof. Let us suppose that there exists $B \subseteq [n]\times[n]$ such that $A^- \cap B = \emptyset$ and $G_P(G[A^-,B]) = G(f)$.

If the $\mathcal{G}_{\text{lab}}(f,A^-)$ operator is applied, note that $(A^+)^* \cap A^- = \emptyset$, since if there is an arc (or a path) in A^+ that coincides with an arc in A^-, then there is no solution with A^- as negative arcs (because it breaks the update condition, since $s(u) \geq s(w_0) \geq \cdots \geq s(w_n) \geq s(v)$ (according to the positive path), and $s(u) < s(v)$ (according to the negative arc), which is a contradiction). For this reason, the $\mathcal{G}_{\text{lab}}$ operator does not make a new recursive call, hence $\text{lab}^{\ominus}[(\mathcal{G}_{\text{lab}}(f,A^-)] = A^-$. On the other hand, $\text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f,A^-)]$ is not necessarily equal to B, because B, being part of an update solution, may contain arcs that $\mathcal{G}_{\text{lab}}$ omitted (because they are indirectly explained) and that do not affect the rest of the digraph (as can be seen in Figure 13).

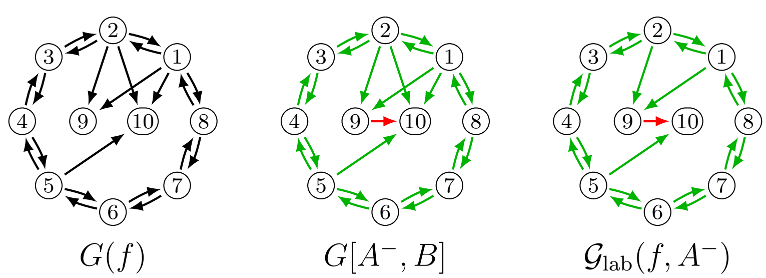


Figure 13: Example of $\text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f,A^-)] \subseteq B$.

For this reason, we can state that $\text{lab}^{\oplus}[\mathcal{G}_{\text{lab}}(f,A^-)]$ is a minimal set for the positive arcs of $\mathcal{G}_{\text{lab}}(f,A^-)$ and this together with A^- is a minimal set for the arcs of $\mathcal{G}_{\text{lab}}(f,A^-)$. □

Definition 10. Let (G, lab) be a labeled digraph. A partition $\{V_1, V_2\}$ of $[n]$ is said to be *admissible* if satisfies the following conditions:

1. $\exists (u, v) \in A(G), u \in V_1 \wedge v \in V_2$,
2. $\forall (u, v) \in A(G), u \in V_1 \wedge v \in V_2 \implies \text{lab}(u, v) = \ominus$,
3. $\forall (u, v) \in A(G), u, v \in V_2 \implies \text{lab}(u, v) = \oplus$.

Lemma 11. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a disjunctive Boolean network and $\{V_1, V_2\}$ an admissible partition of $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$. If we define $A^- = \{(u, v) \in A(G) : u \in V_1 \wedge v \in V_2\}$, where G is the digraph of the resulting labeled digraph, then $\mathcal{G}_{\text{lab}}(f, A^-)$ is an update digraph and $G_P(\mathcal{G}_{\text{lab}}(f, A^-)) = G(f)$.

Proof. We denoted by (G, lab) the labeled digraph obtained by $\mathcal{G}_{\text{lab}}$ operator.

To show that (G, lab) is an update digraph, we prove that if we define $s = V_1, V_2$, then $\text{lab} = \text{lab}_s$.

Note that for all (u, v) in $A(G)$ such that $u \notin V_1$ or $v \notin V_2$, $\text{lab}(u, v) = \text{lab}_s(u, v) = \oplus$, because all these arcs, if they appear in G (resulting from the $\mathcal{G}_{\text{lab}}$ operator), have a label $\oplus$ since they are not in A^-.

On the other hand, we prove that $\text{lab}^{\ominus}[G, \text{lab}] = A^-$. Note that when choosing the arcs in A^- only the arcs from V_1 to V_1 and from V_2 to V_1 have been removed from $\text{lab}^{\ominus}[G, \text{lab}]$ (those from V_1 to V_2 remain in A^- and there are no negative arcs from V_2 to V_2, since V_1 and V_2 is an admissible partition). For this reason, for every new arc (u, v) in A^+, $v \in V_1$. Therefore, in the first iteration of the $\mathcal{G}_{\text{lab}}$ operator, no edge of A^- will be removed, hence $\text{lab}^{\ominus}[G, \text{lab}] = A^-$.

Thus, since the only negative arcs are from V_1 to V_2, we have $lab = lab_s$, with $s = V_1, V_2$, so (G, lab) is update.

Finally, since $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$ is update, according to Proposition 9, $G_P(\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))) = G(f)$.
□

Theorem 12. Let $f : \{0,1\}^n \to \{0,1\}^n$ be a disjunctive Boolean network. There exists a solution for D-DEN problem if and only if $A^{\ominus}(f)$ has a cycle or $\text{lab}^{\ominus}[\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))] \neq \emptyset$. Besides, if a solution exists, it can be found in polynomial time.

Proof. If $A^{\ominus}(f)$ has a cycle, we have at least 2 vertices with the same input neighborhood. With those vertices with equal neighborhood we have the conditions of Corollary 6 and therefore there is a solution to the D-DEN problem.

On the contrary, if $A^{\ominus}(f)$ is acyclic, the first step is to compute $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$. Next, we use the following algorithm to define the set V_2, where ComponentDigraph(G) is a digraph $(\hat{V}, \hat{A})$ defined as follows:

- $\hat{V} = \{G_1, G_2, \ldots, G_k\}$, where G_i are the strongly connected components of G.
- $(G_i, G_j) \in \hat{A}$ if and only if there exists an arc from a vertex in G_i to a vertex in G_j.

Algorithm 2: AdmPartition(G, lab)

Input: A labeled digraph (G, lab).

Output: A partition $\{V_1, V_2\}$ of $V(G)$.

1 $G^{\oplus} \leftarrow \text{lab}^{\oplus}[(G, \text{lab})]$;

2 $(\hat{V}, \hat{A}) \leftarrow \text{ComponentDigraph}(G^{\oplus})$;

3 $Q \leftarrow \{G_i \in \hat{V} : \nexists G_j \in \hat{V}, (G_j, G_i) \in \hat{A}\}$; `// initial components`

4 $v^* \leftarrow \text{Null}$;

5 **while** $v^* = \textit{Null}$ **do**

6     $G_q \leftarrow$ first element of Q;

7   **if** $\exists u \in G_q \wedge \exists (w, u) \in A(G), \text{lab}(w, u) = \ominus$ **then** $v^* \leftarrow u$;

8   **else** $Q \leftarrow Q \cup \{G_i \in \hat{V} : (G_q, G_i) \in \hat{A}\}$;

9 $V_2 \leftarrow \{v \in V(G)$: $\exists$ a path in $G^{\oplus}$ from v to some vertex in the same component of $v^*\}$;

10 $V_1 \leftarrow V(G) \setminus V_2$;

11 **return** $\{V_1, V_2\}$

Note that the resulting set V_2 will never be empty since $\text{lab}^{\ominus}[\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))] \neq \emptyset$.

Moreover, let us note that the cost of finding this admissible partition is $O(n^2)$, since the while-cycle in lines 5 to 8 can be executed at most $O(n)$ times, and the operation within the while-cycle takes $O(n)$. Therefore, the total cost of the while cycle is $O(n^2)$. In addition, each of the operations in lines 1 to 3 and 9 can be performed in $O(n^2)$ time.

The strategy presented in this algorithm is to do a Breadth First Search in the digraph for strongly connected components of the positive arcs of the labeled digraph. The goal of the search is to find the first strongly connected component that receives a negative arc (which we call the pivot component). Once this component is found, a partition is created: in V_2 are all the vertices that can reach the pivot component by a path of positive arcs and in V_1 the rest of vertices.

Now, we prove that $\{V_1, V_2\}$ is an admissible partition.

- Note that in the arc (w, u) (with label $\ominus$) that activate the line 7 of Algorithm 2, which triggers the construction of V_2, $u \in V_2$ (by how the algorithm is defined) and $w \in V_1$ (because if $w \in V_2$, (w, u) it would have been removed from A^- by applying $\mathcal{G}_{\text{lab}}$ operator). Therefore, $\exists (u, v) \in A(G), u \in V_1 \wedge v \in V_2$,

- By contradiction, let us suppose that there exists an arc $(u, v) \in V_1 \times V_2$, such that $\text{lab}(u, v) = \oplus$. Note that since $v \in V_2$, there exists $k \geq 1$, $(v, p) \in A(\text{lab}^{\oplus}[(G, \text{lab})])^k$ where p is a pivot vertex (found from lines 1 to 7 of Algorithm 2) and since $u \in V_1$, it does not exist $k' \geq 1$, $(u, p) \in A(\text{lab}^{\oplus}[(G, \text{lab})])^{k'}$. Since we suppose that $(u, v) \in A(G)$ and $\text{lab}(u, v) = \oplus$, then there exists $k' = k + 1$, therefore, $u \in V_2$, which is a contradiction. Therefore $\forall (u, v) \in A(G), u \in V_1 \wedge v \in V_2 \implies \text{lab}(u, v) = \ominus$,

- By contradiction, let us suppose that there exists an arc $(u, v) \in V_2 \times V_2$, such that $\text{lab}(u, v) = \ominus$. Note that since $u, v \in V_2$, there exists $k, k' \geq 1$, $(v, p) \in A(\text{lab}^{\oplus}[(G, \text{lab})])^k$ and $(u, p) \in A(\text{lab}^{\oplus}[(G, \text{lab})])^{k'}$ where p is a pivot vertex (found from lines 1 to 7 of Algorithm 2). If $(u, v) \in A(G)$ and $\text{lab}(u, v) = \ominus$, then p would not have been chosen as a pivot (since v appears earlier in the poset), which is a contradiction. Therefore $\forall (u, v) \in A(G), u, v \in V_2 \implies \text{lab}(u, v) = \oplus$.

With what we learned above, we can build the following algorithm:

Algorithm 3: D-DENPSolve(f)

Input: A disjunctive Boolean network $f : \{0,1\}^n \to \{0,1\}^n$.
Output: (G, lab) an update digraph such that $G_P(G, \text{lab}) = G(f)$ if there exists a solution of the D-DEN problem with instance f, or Null otherwise.

1 **if** $A^{\ominus}(f)$ *has a cycle* **then**
2   Let u and v be two vertices such that $N_f^-(u) = N_f^-(v)$;
3   **return** $G[\{(u,v)\}, A(f) \setminus \{(x,v) : x \in N_f^-(v)\}]$
4 **else**
5     $(G, \text{lab}) \leftarrow \mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$;
6   **if** $\text{lab}^{\ominus}[(G, \text{lab})] = \emptyset$ **then return** *Null*;
7   **if** (G, lab) *is update* **then return** (G, lab);
8     $\{V_1, V_2\} \leftarrow \text{AdmPartition}(G, \text{lab})$;
9     $A^- \leftarrow \{(u,v) \in A(G, \text{lab}) : u \in V_1 \wedge v \in V_2\}$;
10   **return** $\mathcal{G}_{\text{lab}}(f, A^-)$;

Given a disjunctive Boolean network $f : \{0,1\}^n \to \{0,1\}^n$, first we obtain the $A^{\ominus}(f)$, in this way, we know which arcs, of a possible digraph G, can be labeled $\ominus$. If $A^{\ominus}(f)$ has a cycle, by Corollary 6, there is a solution (lines 1 to 3).

Otherwise, if $A^{\ominus}(f)$ is acyclic, the operator $\mathcal{G}_{\text{lab}}$ can be applied. If the resulting labeled digraph (G, lab) has no negative arcs, then no neighborhood is contained in another one and, according to Lemma 4, there is no non-trivial solution, therefore the algorithm ends (line 6).

If $\text{lab}^{\ominus}[(G, \text{lab})]$ is not empty and (G, lab) is update, then we found a solution (line 7).

Finally, if (G, lab) is not update, since we know that $\text{lab}^{\ominus}[(G, \text{lab})] \neq \emptyset$, we can find an admissible partition of $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$ and with that partition build a solution (lines 8 to 10).

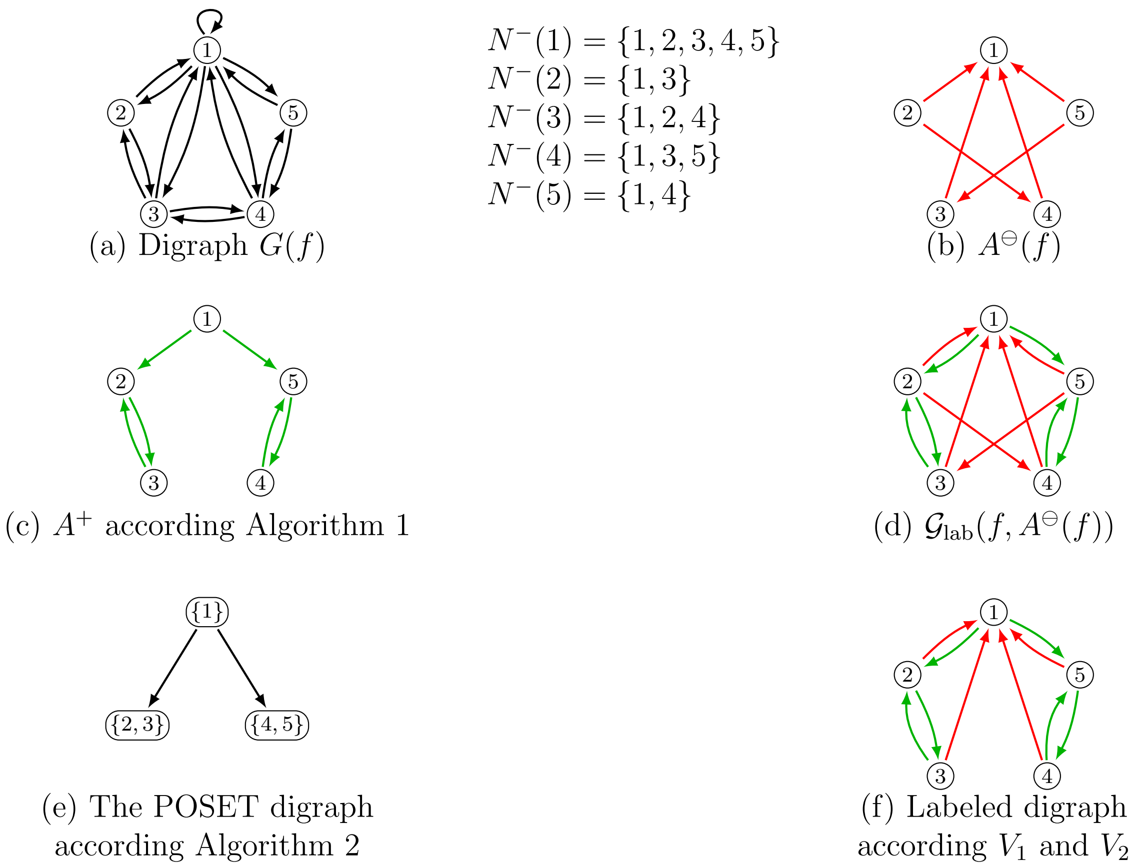
Let us analyze that Algorithm 3 is a polynomial algorithm, since constructing $A^{\ominus}(f)$ takes $O(n^3)$ and checking whether it has a cycle requires $O(n^2)$. Therefore, the cost of the if-section is $O(n^3)$. In the else-section, we must construct $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$, which takes $O(n^5)$ (Remark 5), and then the operations in lines 6 to 9 require $O(n^2)$. Therefore, the total cost of the else-section and the whole Algorithm 3 is $O(n^5)$. □

Example 5. Given f a disjunctive Boolean network (Figure 14(a)), the first step is to create the digraph $A^{\ominus}(f)$ (Figure 14(b)).

Since $A^{\ominus}(f)$ has no cycles, the algorithm continues. The next step is to get $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$. First, A^+ is calculated (Figure 14(c)). Then, since no edge (or path) of A^+ coincides with the arcs of $A^{\ominus}(f)$, the operator $\mathcal{G}_{\text{lab}}$ ends and the result is Figure 14(d) and its negative arcs are Figure 14(b). Since $\text{lab}^{\ominus}[\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))] \neq \emptyset$, the algorithm continues.

The labeled digraph of the operator $\mathcal{G}_{\text{lab}}$ (Figure 14(d)) is not update. For this reason, we look for an admissible partition. First, $G^{\oplus}$ (Figure 14(c)) is obtained. Then, the POSET digraph (Figure 14(e)) is generated, where we have three strongly connected components: $\{1\}, \{2,3\}, \{4,5\}$. We find negative arcs from the component $\{2,3\}$ to $\{1\}$. With this, we can define $V_2 = \{1\}$ and $V_1 = \{2,3,4,5\}$. With this set, we define the labeling in Figure 14(f). Finally, the parallel digraph of the labeling digraph in Figure 14(f) is exactly Figure 14(a).

Corollary 13. D-DEN can be decided in polynomial time.



(a) Digraph $G(f)$

(b) $A^{\ominus}(f)$

(c) A^+ according Algorithm 1

(d) $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$

(e) The POSET digraph according Algorithm 2

(f) Labeled digraph according V_1 and V_2

Figure 14: Figures of Example 5.

Proof. With what we learned above, we can build the following algorithm:

Algorithm 4: D-DENDecider(f)

Input: A disjunctive Boolean network $f : \{0,1\}^n \to \{0,1\}^n$.
Output: **True** if there exists a solution of the D-DEN problem with instance f, or **False** otherwise.

1 **if** $A^{\ominus}(f)$ *has a cycle* **then return** ***True***;
2 **if** $\text{lab}^{\ominus}[\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))] \neq \emptyset$ **then return** ***True***;
3 **return** ***False***;

Note that the simplicity of this algorithm lies in answering two questions:

- Does $A^{\ominus}(f)$ have a cycle?: If the answer is yes, we have at least two vertices with the same input neighborhood, therefore, according to Corollary 6, there is a solution.
- $\text{lab}^{\ominus}[\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))] \neq \emptyset$?: If the answer is yes, according to Theorem 12, there is a solution.

If the answer to both questions is no, then there is no solution, because all the candidates to be negative arcs in some solution have been discarded.

In the first line, constructing $A^{\ominus}(f)$ takes $O(n^3)$ and checking if it has a cycle requires $O(n^2)$. In the second, constructing $\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))$ takes $O(n^5)$ and then getting $\text{lab}^{\ominus}[\mathcal{G}_{\text{lab}}(f, A^{\ominus}(f))]$ requires $O(n^2)$. Therefore, the total cost of Algorithm 4 is $O(n^5)$. □

6 Conclusions and future work

In this paper, we present different approaches to the problem of dynamically equivalent networks.

As could be seen in this paper, solving the general problem, i.e., given a Boolean network f, finding another Boolean network $\bar{f}$ and an update schedule $\bar{s}$ such that $\bar{f}^{\bar{s}} = f$ is NP-Hard, since it is as difficult as 3-SAT, but it does present an approach to finding a possible solution: if there exists a solution with an update schedule with more than two blocks, then there exists a solution with an update schedule of only two blocks.

Now, if we restrict the problem to disjunctive networks, finding a disjunctive Boolean network h and an update schedule s such that $h^s = f$, this problem can be solved in polynomial time.

It is worth noting that the fact that in the labeled digraph contains an arc (u, v) whose label is negative only if $N_f^-(u) \subseteq N_f^-(v)$ in the parallel digraph is a very important result since it implies that any digraph whose neighborhoods are not comparable, has no other dynamically equivalent network different to the trivial one.

With all these results, there remain several ideas to explore, such as finding an algorithm that can solve the general problem, and explore enumeration algorithms, in the case we fix some element of the triplet (h, s, f). Another idea would be to analyze if for a Boolean network f, there exists a Boolean network h and an update schedule s such that s has some particularity (e.g.: s is a sequential update schedule) and that $h^s = f$.

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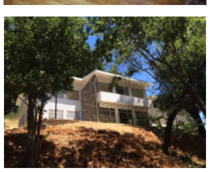

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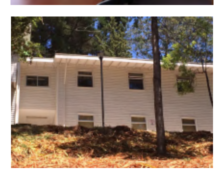

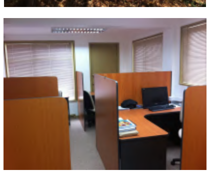

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