



Study of the block-sequential operator on Boolean networks. Application to discrete network analysis

Luis Cabrera Crot

Thesis for the PhD degree in Computer Science.¹

Thesis Advisors: Julio Aracena, Adrien Richard, Lilian Salinas

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Boolean networks



Boolean Networks

- A global activation function

$$f = (f_v)_{v \in V} : \{0, 1\}^n \rightarrow \{0, 1\}^n$$

- Composed by local activation functions

$$f_v : \{0, 1\}^n \rightarrow \{0, 1\}$$

$$f_1(x) = x_2 \wedge x_4$$

$$f_2(x) = x_1$$

$$f_3(x) = x_2 \vee x_3$$

$$f_4(x) = x_3 \wedge x_4$$



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- Composed by local activation functions
 $f_v : \{0, 1\}^n \rightarrow \{0, 1\}$
- Schedule $s : V \rightarrow \{1, \dots, n\}$

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Parallel schedule



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Sequential schedule



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Block-sequential schedule



Boolean networks



Interaction Digraph

- A digraph $G(f) = (V, A)$:

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Boolean networks



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(2)

(1)

(3)

(4)



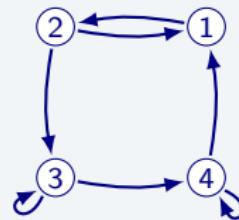
Boolean networks



Interaction Digraph

- A digraph $G(f) = (V, A)$:
- $V = \{1, \dots, n\}$
- $(i, j) \in A \Leftrightarrow f_j \text{ depends on } x_i$

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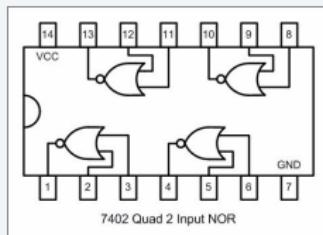




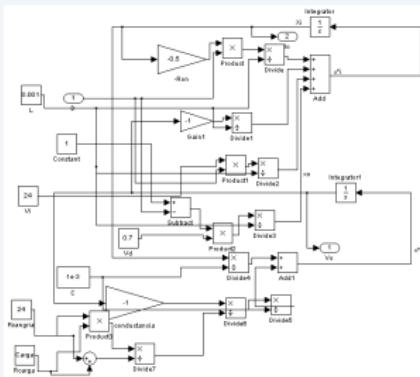
Applications of Boolean networks



Circuit theory



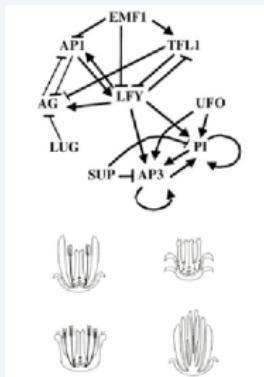
Computer science



Social networks



Biological systems





Dynamic of a Boolean network



The dynamic of a Boolean network (f, s) is given by:

$$x_v(t+1) = f_v(x_u(t'): u \in V), \quad t' = \begin{cases} t & \text{if } s(v) \leq s(u) \\ t+1 & \text{if } s(v) > s(u) \end{cases}$$



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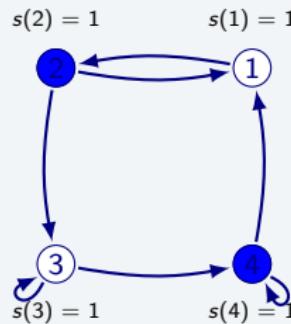
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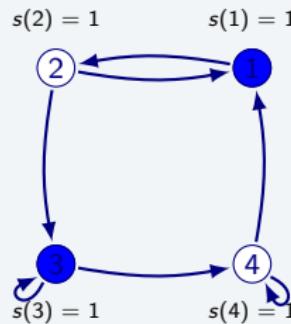
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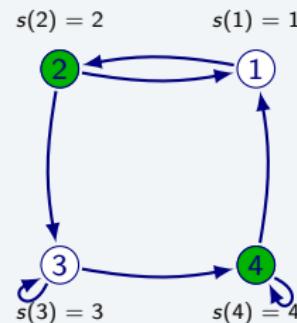
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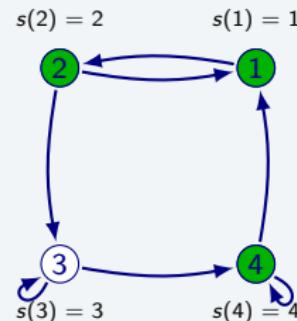
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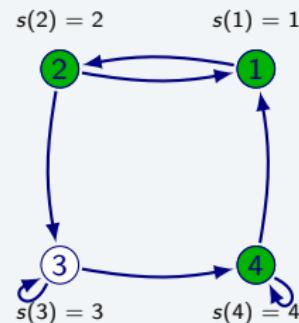
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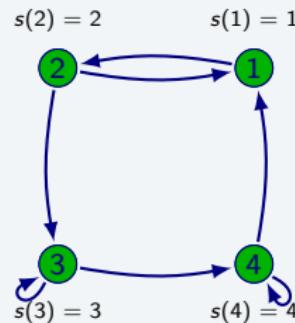
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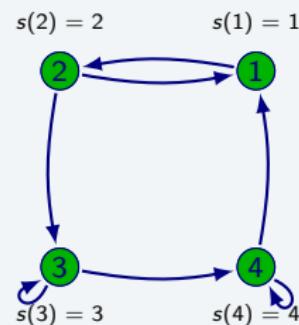
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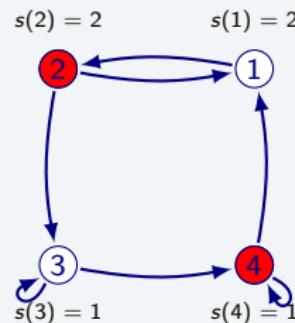
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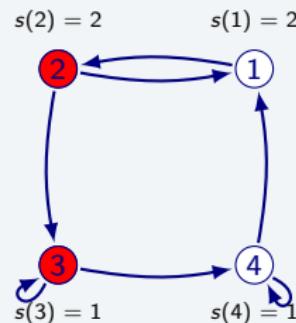
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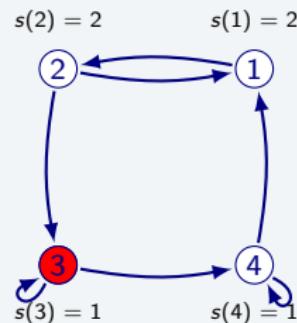
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Dynamical behavior



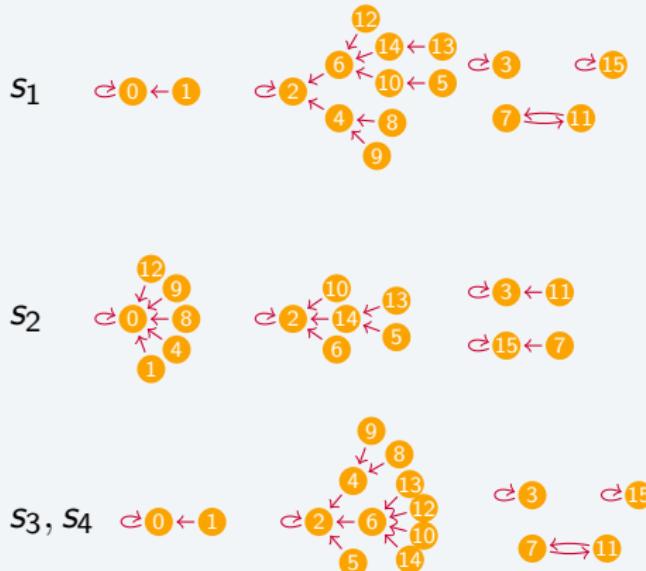
$s_1 = \{1, 2, 3, 4\}$

$s_2 = \{1\} \{2\} \{3\} \{4\}$

$s_3 = \{3, 4\} \{1, 2\}$

$s_4 = \{4\} \{3\} \{1, 2\}$

	State	f^{s_1}	f^{s_2}	$f^{s_3} = f^{s_4}$
0	0000	0000	0000	0000
1	0001	0000	0000	0000
2	0010	0010	0010	0010
3	0011	0011	0011	0011
4	0100	0010	0000	0010
5	0101	1010	1110	0010
6	0110	0010	0010	0010
7	0111	1011	1111	1011
8	1000	0100	0000	0100
9	1001	0100	0000	0100
10	1010	0110	0010	0110
11	1011	0111	0011	0111
12	1100	0110	0000	0110
13	1101	1110	1110	0110
14	1110	0110	0010	0110
15	1111	1111	1111	1111





Initial motivation

The initial motivation was to understand the variations of the interaction digraph of a Boolean network with respect to changes in the update schedule and its relation with some dynamic properties of the network.

- Given a Boolean network, which structural properties of the interaction network are sensitive to the change in the update schedule?
- Given the invariance of fixed points with respect to different update schedules, how can we take advantage of that in an algorithm to find them?
- What are the properties that must be satisfied to find networks that have the same dynamic behavior?



Labeled digraph

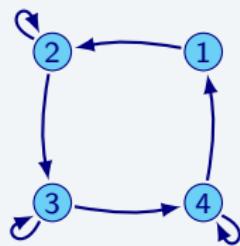


Given an interaction graph $G(f)$ and a block-sequential schedule s , a labeled digraph $(G(f), lab_s)$ is defined, where:

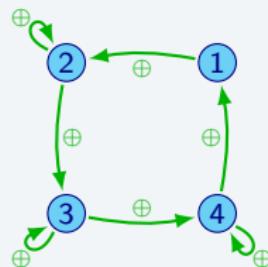
$$lab_s : A(G) \rightarrow \{\oplus, \ominus\}$$

$$lab_s(u, v) = \oplus \iff s(u) \geq s(v)$$

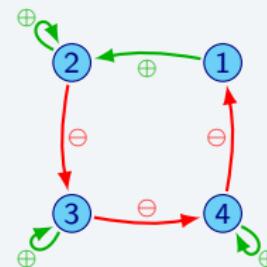
$G(f)$



$$s_1 = \{1, 2, 3, 4\}$$

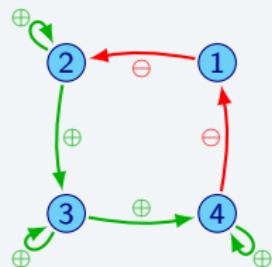


$$s_2 = \{2\} \{3\} \{4\} \{1\}$$



$$s_3 = \{3, 4\} \{1\} \{2\}$$

$$s_4 = \{4\} \{1\} \{3, 2\}$$





Why are we interested in labeled digraphs?



Theorem (Aracena, Goles, Moreira, Salinas (2009))

Given two Boolean networks (f, s) and (f, s') which differ only in the update schedule. If the labeled digraphs associated to them are equal, then both networks have the same dynamical behavior.



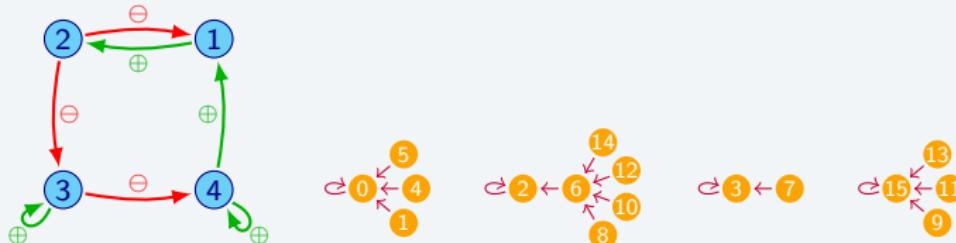
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$$s = \{2\} \{1\} \{3\} \{4\} \text{ and } s' = \{2\} \{3\} \{1\} \{4\}$$





Parallel digraph

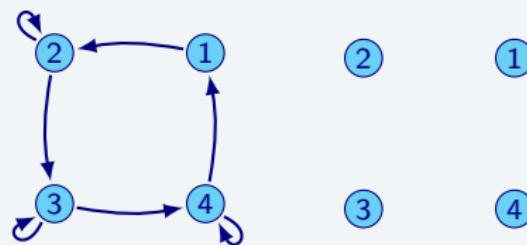


The *parallel digraph* is a digraph that represent the potential dependence of the components of the Boolean network, according with the block-sequential schedule s .

$$s = \{2\} \{3\} \{4\} \{1\}$$

$$G(f)$$

$$G_P(G, s)$$





Parallel digraph



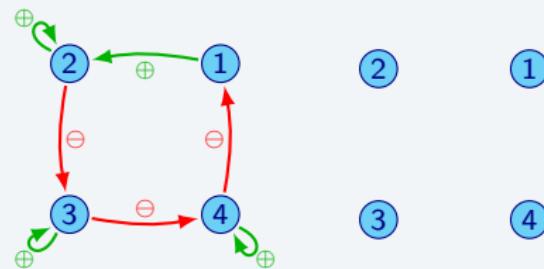
$\forall (u, v) \in V(G) \times V(G), (u, v) \in A(G_P(G, s))$ if and only if:

- (u, v) is labeled \oplus
- $\exists w \in V(G), (u, w)$ is labeled \oplus and exists a path from w to v labeled \ominus

$$s = \{2\} \{3\} \{4\} \{1\}$$

$(G(f), lab_s)$

$G_P(G, s)$





Parallel digraph



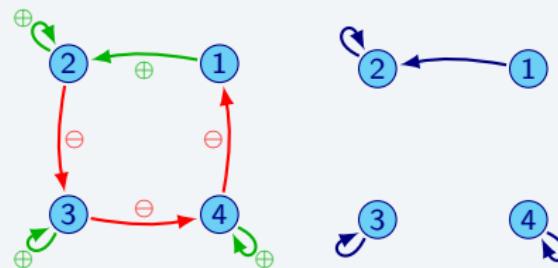
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$G_P(G, s)$





Parallel digraph

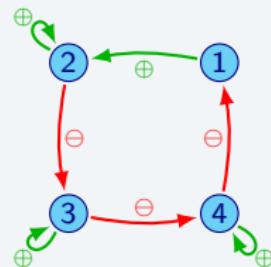


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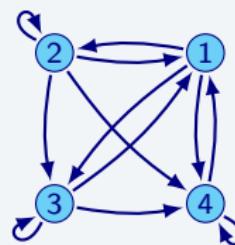
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$(G(f), lab_s)$



$G_P(G, s)$





Parallel digraph



Proposition

$$G(f^s) \subseteq G_P(f, s).$$

Remark

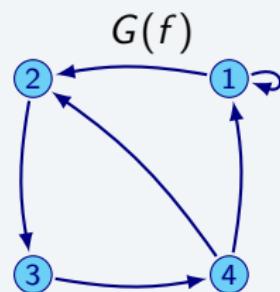
If (f, s) is a conjunctive (or disjunctive) network, then $G(f^s) = G_P(f, s)$.
(Goles and Noual, 2012)



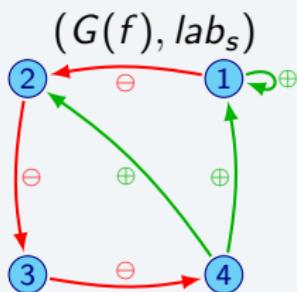
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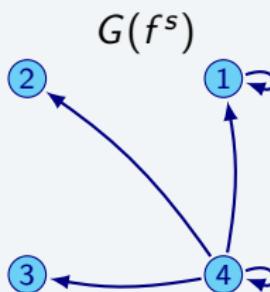
The inclusion could be strict in monotone Boolean networks:



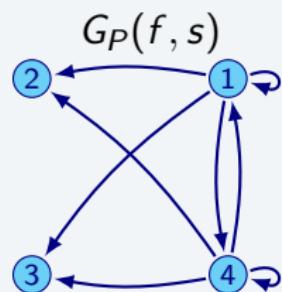
$$\begin{aligned}f_1(x) &= x_1 \wedge x_4 \\f_2(x) &= x_1 \vee x_4 \\f_3(x) &= x_2 \\f_4(x) &= x_3\end{aligned}$$



$$s = \{1\} \{2\} \{3\} \{4\}$$



$$\begin{aligned}f_1^s(x) &= x_1 \wedge x_4 \\f_2^s(x) &= x_4 \\f_3^s(x) &= x_4 \\f_4^s(x) &= x_4\end{aligned}$$





Contents



- 1 Definitions
- 2 Motivation
- 3 Properties of parallel digraph
- 4 Algorithms to find fixed points
- 5 Dynamically equivalent networks
- 6 Subproblems of dynamically equivalent networks
- 7 Final conclusions

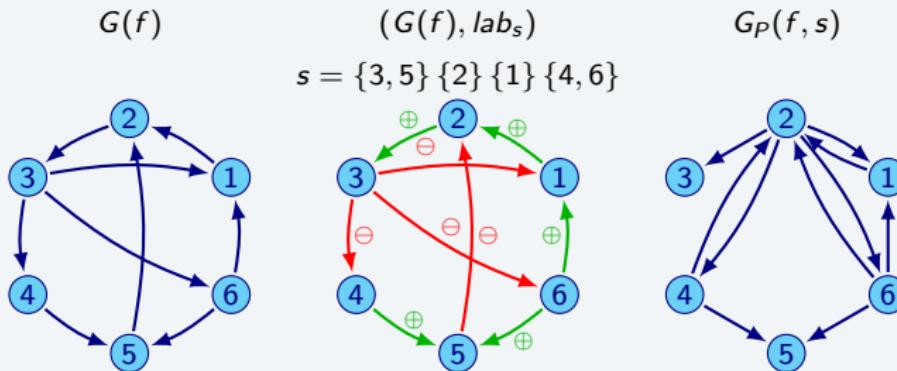


Characterization of the parallel digraph



Proposition

Let (f, s) be a Boolean Network, and $G(f)$ the interaction digraph associated with f . If $G(f)$ is a strongly connected digraph, then $G_P(f, s)$ has one unique strongly connected component composed by the vertices with an arc with \oplus , and the other vertices are pending nodes of $G(f)$.



This is an extension of the result obtained by Goles and Noual (2012).

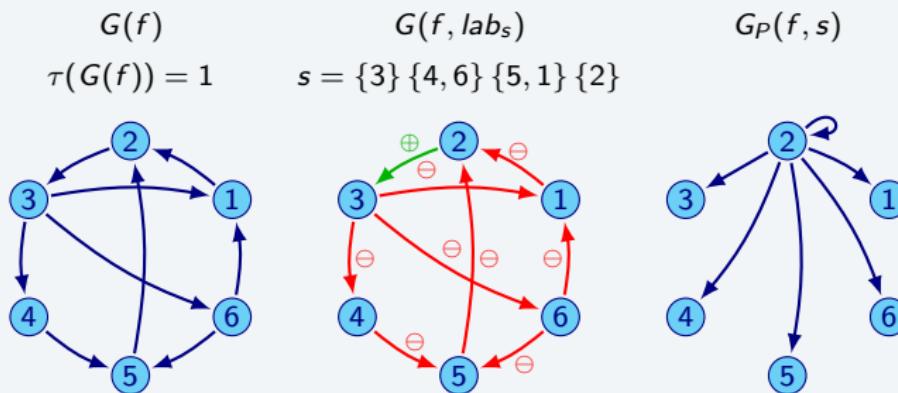


Characterization of the parallel digraph



Proposition

The size of the strongly connected component of $G_P(f, s)$ is greater than or equal to $\tau(G(f))$. Moreover, there exists a schedule s such that the size of the strongly connected component of $G_P(f, s)$ is equal to $\tau(G(f))$.



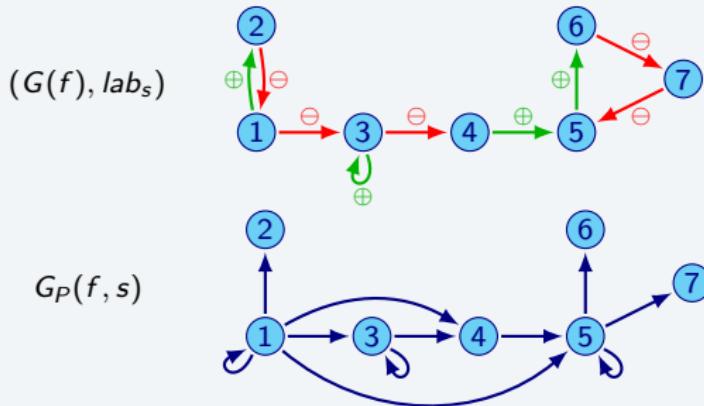


Characterization of the parallel digraph



This result can be extended to not strongly connected digraphs.

$$s = \{2\} \{1, 6\} \{3, 7\} \{4, 5\}$$





Feedback vertex set in parallel digraph



Proposition

Let (f, s) be a Boolean network. Given $U \subseteq V(f)$,

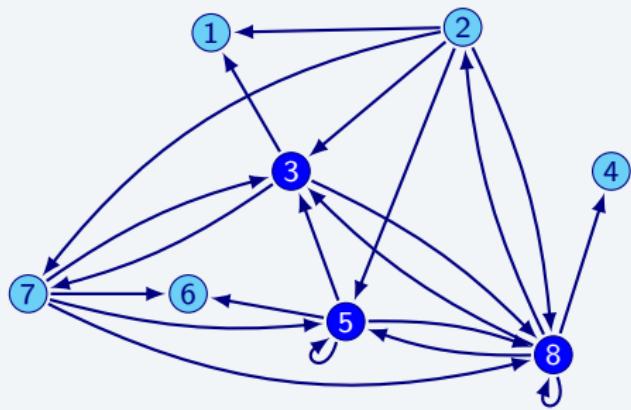
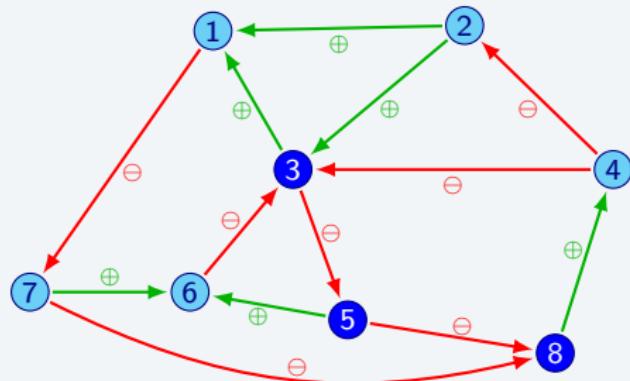
$$U \text{ is a FVS of } G_P(f, s) \implies U \text{ is a FVS of } G(f)$$

Thus,

$$\tau(G_P(f, s)) \geq \tau(G(f)).$$

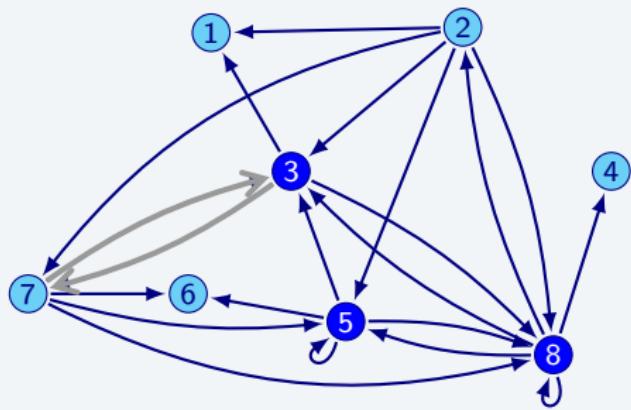
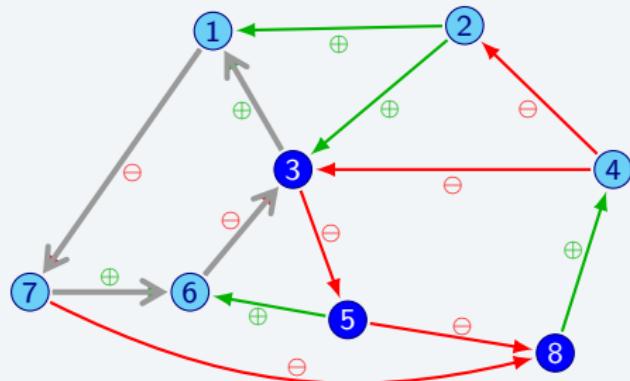


Feedback vertex set in parallel digraph



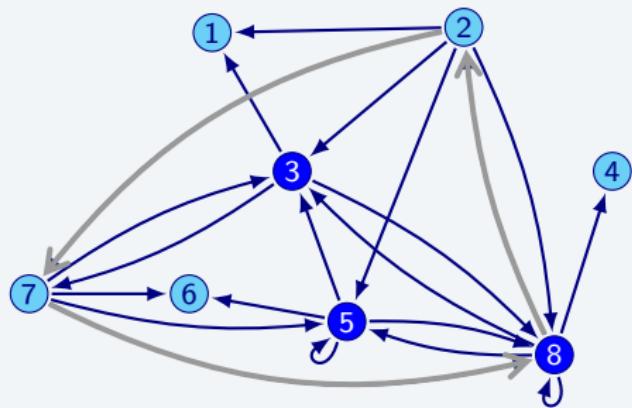
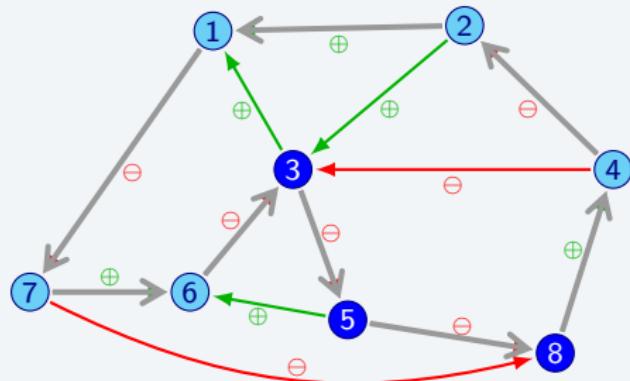


Feedback vertex set in parallel digraph



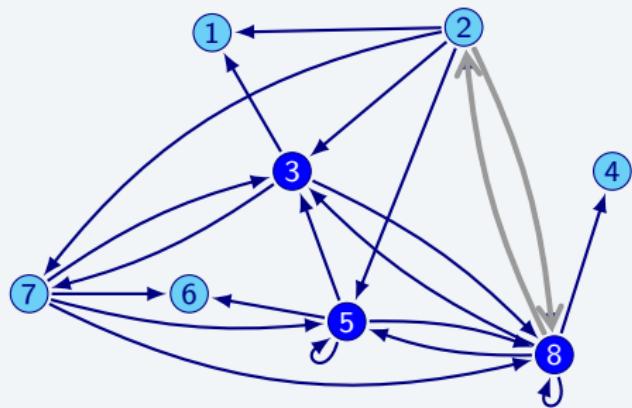
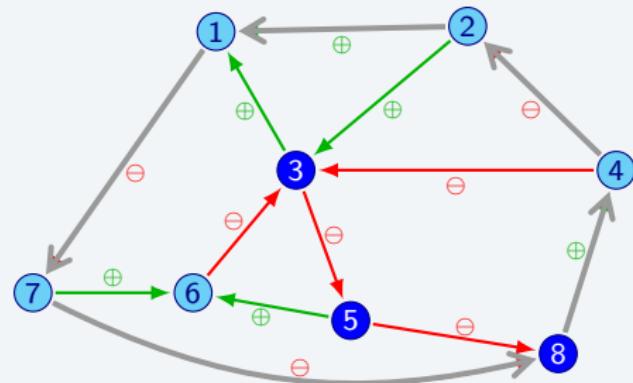


Feedback vertex set in parallel digraph



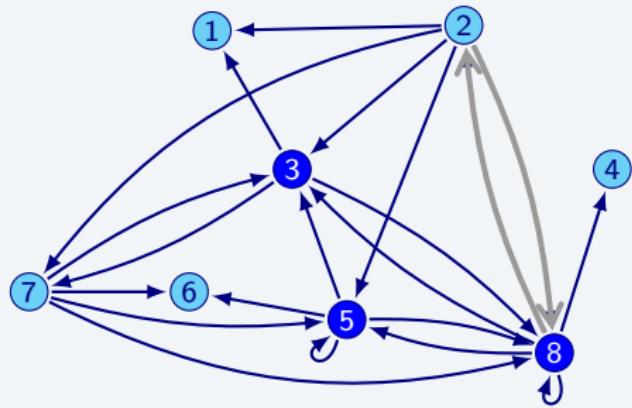
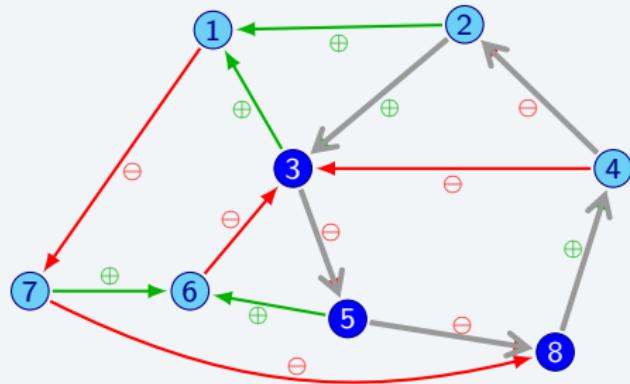


Feedback vertex set in parallel digraph





Feedback vertex set in parallel digraph





Packing number in parallel digraph



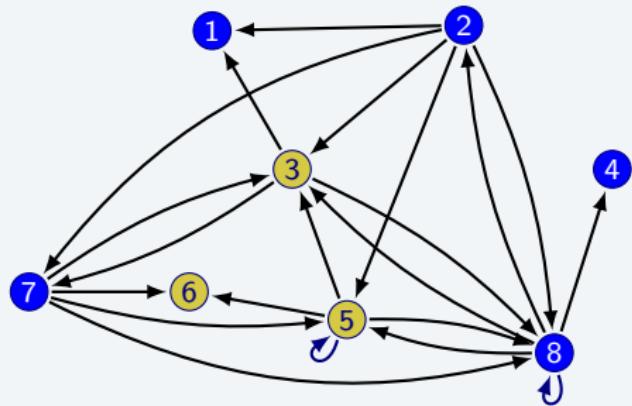
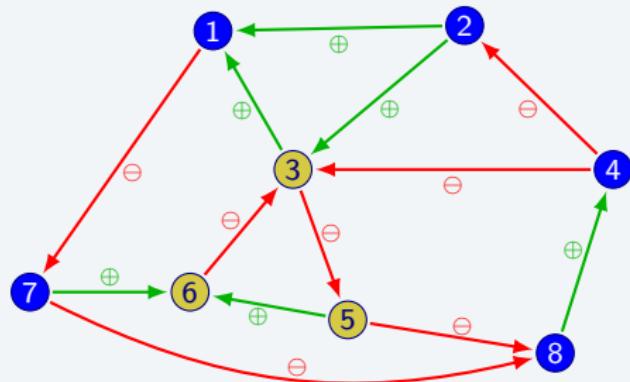
Proposition

Let (f, s) be a Boolean network. Then,

$$\nu(G_P(f, s)) \geq \nu(G(f)).$$

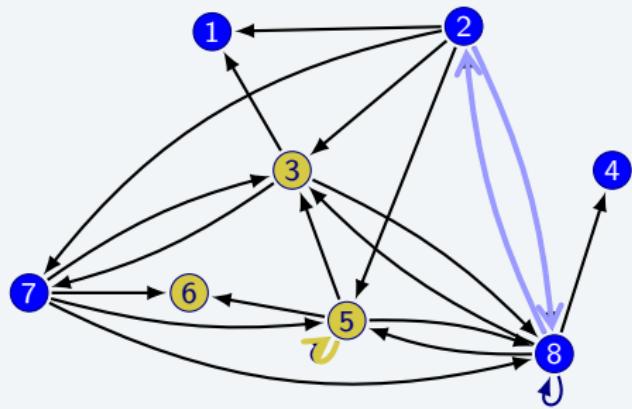
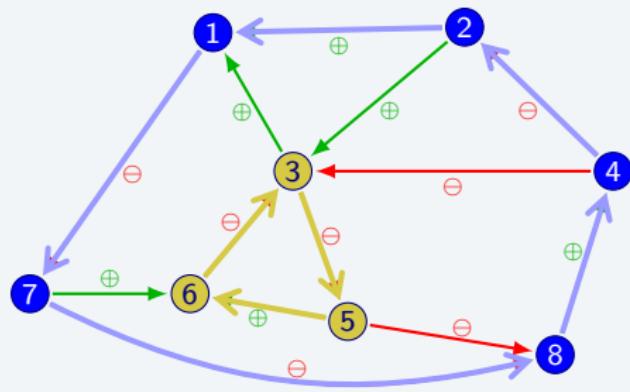


Packing number in parallel digraph



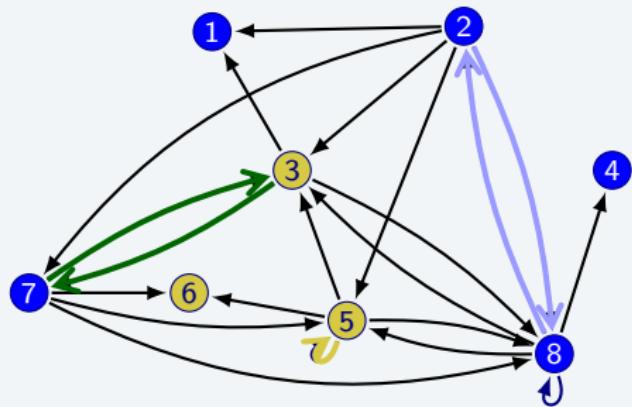
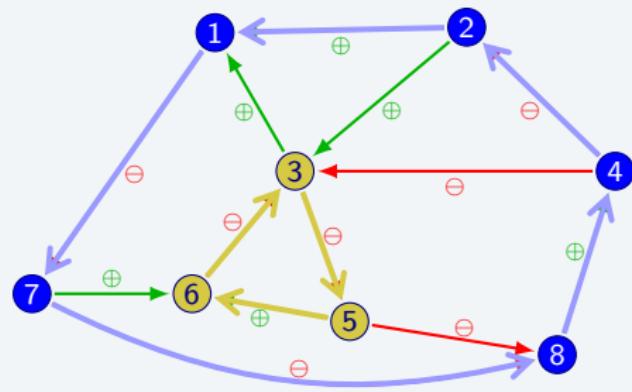


Packing number in parallel digraph





Packing number in parallel digraph





Motivation

Since $\tau(G_P(f, s)) \geq \tau(G(f))$ and $\nu(G_P(f, s)) \geq \nu(G(f))$ and $\tau(G(f)) \geq \nu(G(f))$.

Given an Boolean network f . Is there a schedule s such that:

$$\nu(G_P(f, s)) = \tau(G_P(f, s)) = \tau(G(f))?$$



Labeling function lab_U



lab_U

Let $U \subseteq V(f)$ a feedback vertex set of $G(f)$. We define a labeling function $lab_U : A(f) \rightarrow \{\oplus, \ominus\}$ as:

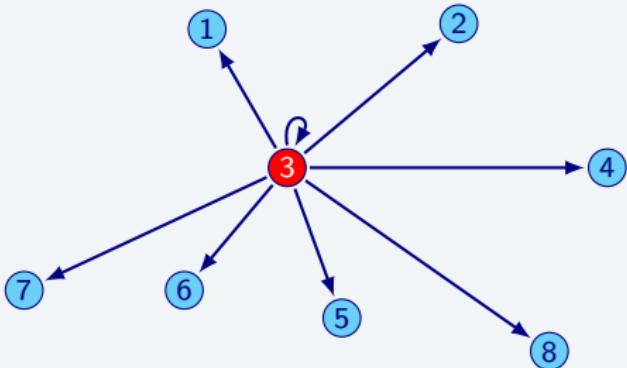
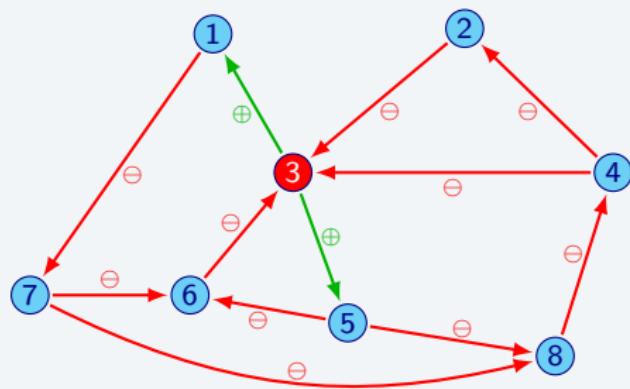
$$\forall (i,j) \in A(G) \quad lab_U(i,j) = \begin{cases} \oplus & \text{if } i \in U \\ \ominus & \text{otherwise.} \end{cases}$$

Proposition

If $|U| = \tau(G(f))$, then $\tau(G_P(f, s)) = \tau(G(f)) = \nu(G_P(f, s))$.



Labeling function lab_U





Contents



- 1 Definitions
- 2 Motivation
- 3 Properties of parallel digraph
- 4 Algorithms to find fixed points
- 5 Dynamically equivalent networks
- 6 Subproblems of dynamically equivalent networks
- 7 Final conclusions



Algorithms to find fixed points



First, it is important to note that the process of finding fixed points in a Boolean network is a difficult task. In 1998, Akutsu et al. show that answering if a network has a fixed point is NP-complete, consequently, counting how many fixed points a Boolean network has is #P-complete.



Algorithms to find fixed points



Strategies used

- Reduction methods - (Veliz-Cuba, 2011; Zañudo and R. Albert, 2013; Veliz-Cuba et al., 2015)
- Representation as polynomial functions - (Hinkelmann et al., 2011; Zou, 2013)
- SAT-based methods - (Devloo et al., 2003; Tamura and Akutsu, 2009; Melkman et al., 2010; Akutsu et al., 2011; Dubrova and Teslenko, 2011)
- Methods based on Integer Programming - (Akutsu et al., 2009)
- Strategic Sampling - (Zhang et al., 2007)
- Methods based on Minimal Feedback Vertex Sets - (Akutsu et al., 1998)



Motivation

$$|FP(f)| \leq 2^{\tau(G(f))}$$

Where:



Motivation



$$|FP(f)| \leq 2^{\tau(G(f))}$$

Where:

- $FP(f)$ is the set of fixed points for a network f .



Motivation



$$|FP(f)| \leq 2^{\tau(G(f))}$$

Where:

- $FP(f)$ is the set of fixed points for a network f .
- $\tau(G(f))$ is the minimum size of a feedback vertex set in $G(f)$.



Motivation



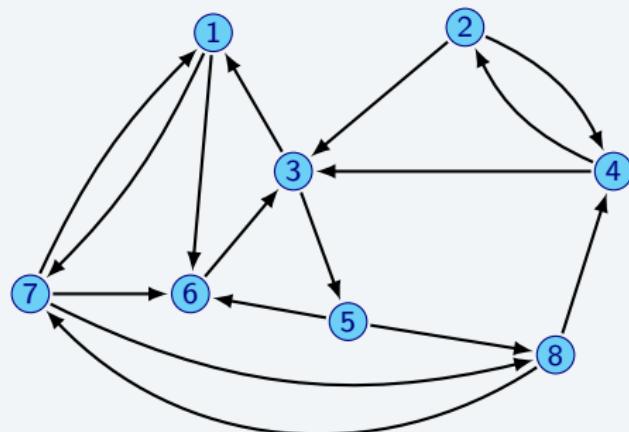
$$|FP(f)| \leq 2^{\tau^+(G(f))} \leq 2^{\tau(G(f))}$$

Where:

- $FP(f)$ is the set of fixed points for a network f .
- $\tau(G(f))$ is the minimum size of a feedback vertex set in $G(f)$.
- $\tau^+(G(f))$ is the minimum size of a positive feedback vertex set in $G(f)$.



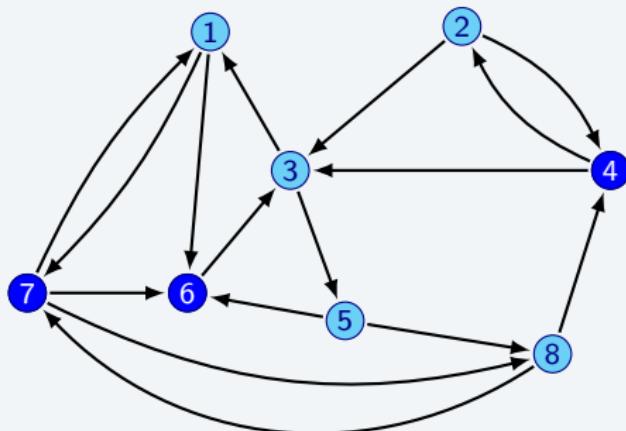
List the fixed points of a Boolean network



Let G be the interaction digraph of a Boolean network



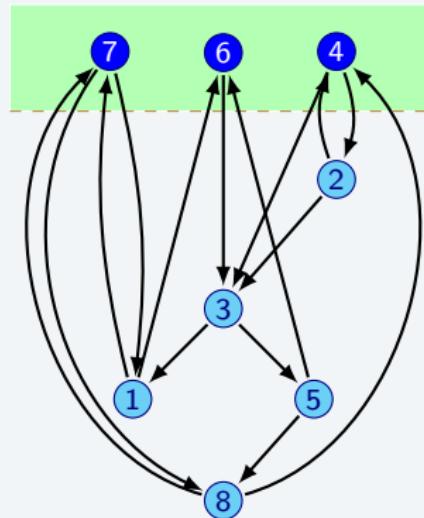
List the fixed points of a Boolean network



And let F be a FVS (not necessarily minimal) of G



List the fixed points of a Boolean network





List the fixed points of a Boolean network



Legend:

- Vertex with True value
- Vertex with False value

$$f_1 = \overline{x}_3 \vee x_7$$

$$f_2 = \overline{x}_4$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

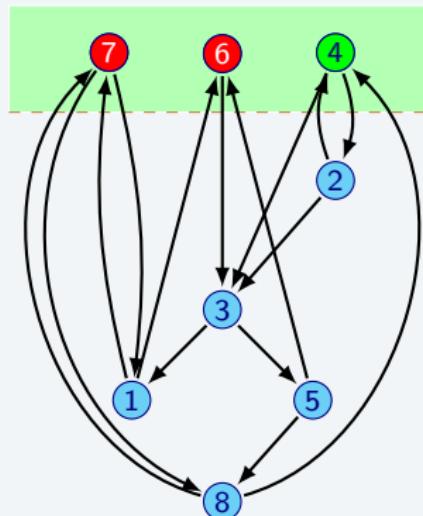
$$f_4 = x_2 \vee \overline{x}_8$$

$$f_5 = x_3$$

$$f_6 = \overline{x}_1 \vee x_5$$

$$f_7 = \overline{x}_1 \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a Boolean network



Legend:

- Vertex with True value
- Vertex with False value

$$f_1 = \overline{x}_3 \vee x_7$$

$$f_2 = \overline{x}_4$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

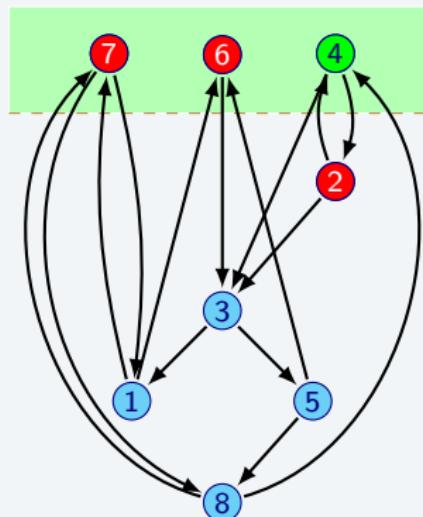
$$f_4 = x_2 \vee \overline{x}_8$$

$$f_5 = x_3$$

$$f_6 = \overline{x}_1 \vee x_5$$

$$f_7 = \overline{x}_1 \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a Boolean network



Legend:

- Vertex with True value
- Vertex with False value

$$f_1 = \overline{x}_3 \vee x_7$$

$$f_2 = \overline{x}_4$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

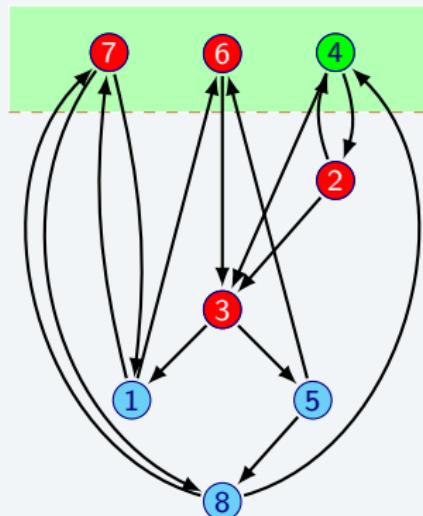
$$f_4 = x_2 \vee \overline{x}_8$$

$$f_5 = x_3$$

$$f_6 = \overline{x}_1 \vee x_5$$

$$f_7 = \overline{x}_1 \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a Boolean network



Legend:

- Vertex with True value
- Vertex with False value

$$f_1 = \overline{x}_3 \vee x_7$$

$$f_2 = \overline{x}_4$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

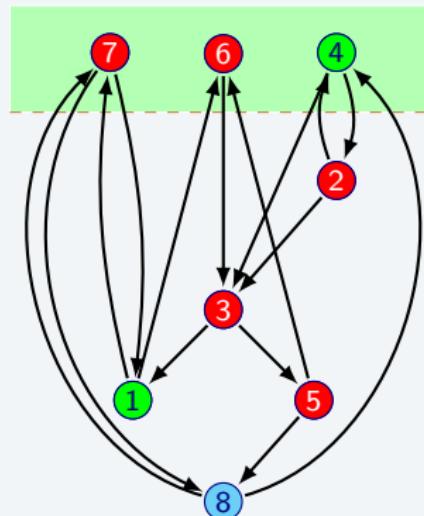
$$f_4 = x_2 \vee \overline{x}_8$$

$$f_5 = x_3$$

$$f_6 = \overline{x}_1 \vee x_5$$

$$f_7 = \overline{x}_1 \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a Boolean network


Legend:

- Vertex with True value
- Vertex with False value

$$f_1 = \overline{x}_3 \vee x_7$$

$$f_2 = \overline{x}_4$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

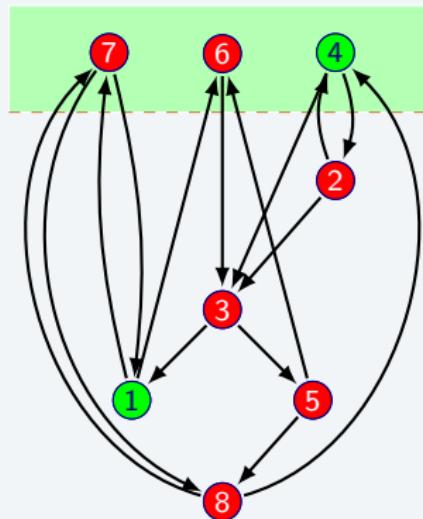
$$f_4 = x_2 \vee \overline{x}_8$$

$$f_5 = x_3$$

$$f_6 = \overline{x}_1 \vee x_5$$

$$f_7 = \overline{x}_1 \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a Boolean network


Legend:


Vertex with True value



Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

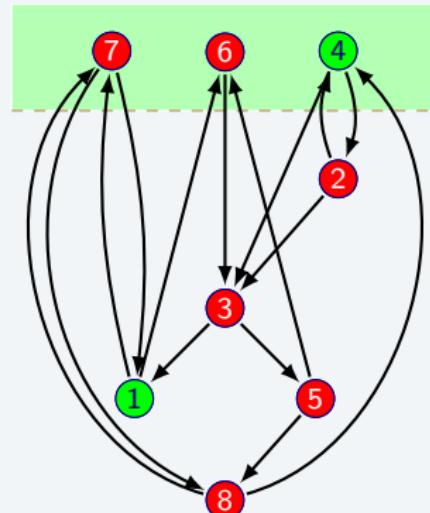
$$f_4 = x_2 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

$$f_8 = x_5 \wedge x_7$$



10010000 is a fixed point of f



List the fixed points of a Boolean network


Legend:


Vertex with True value



Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

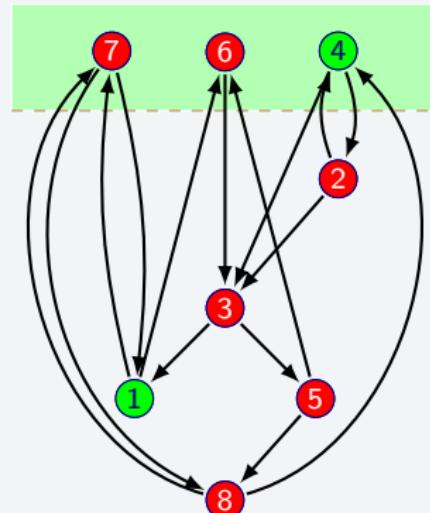
$$f_4 = x_2 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

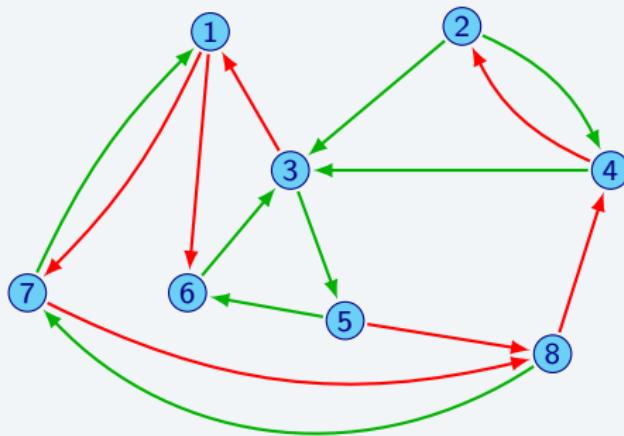
$$f_8 = x_5 \wedge x_7$$



The complexity of this algorithm is $n \cdot 2^{|F|}$



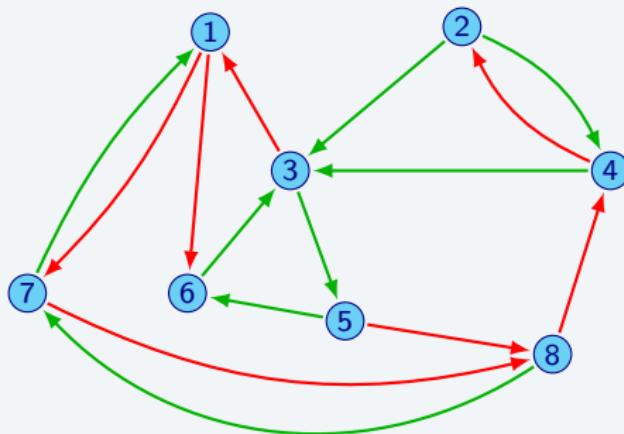
Algorithm for regulatory networks



In the case of regulatory networks, the arcs of the interaction digraph can be weighted positive or negative.



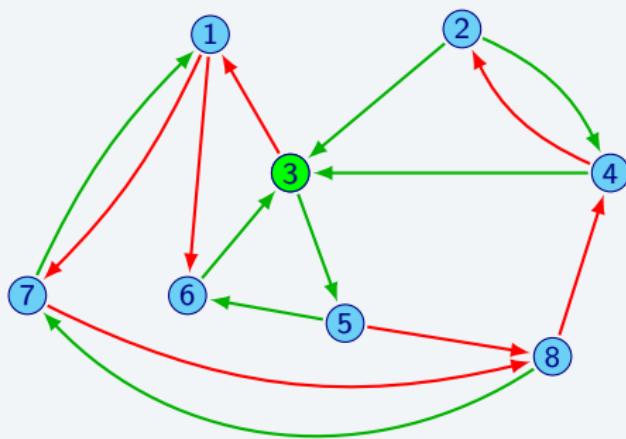
Algorithm for regulatory networks



Let G be the interaction digraph of a Boolean network



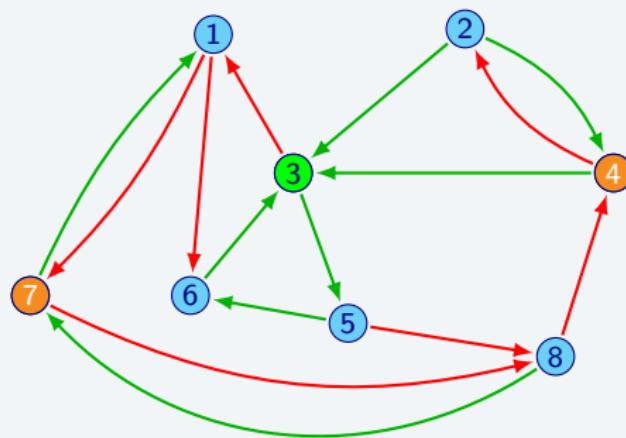
Algorithm for regulatory networks



And let F^+ be a PFVS (not necessarily minimal) of G



Algorithm for regulatory networks



And let $F \setminus F^+$ the complement of F^+ to be a FVS



List the fixed points of a regulatory network

Legend:



Vertex with True value



Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

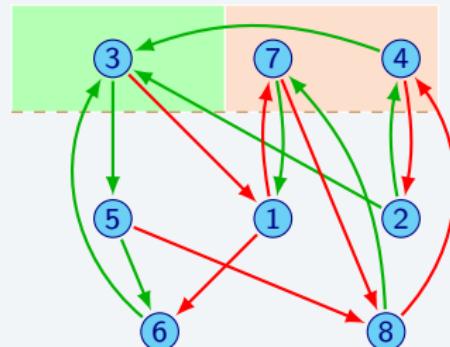
$$f_4 = x_2 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a regulatory network

Legend:



Vertex with True value



Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

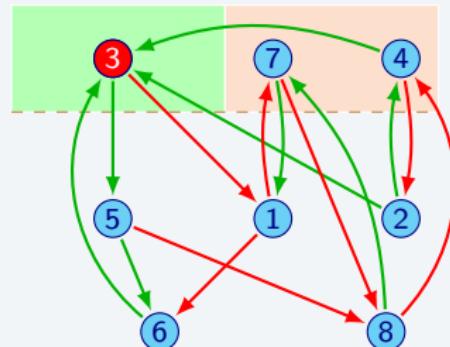
$$f_4 = x_2 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a regulatory network

Legend:



Vertex with True value



Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

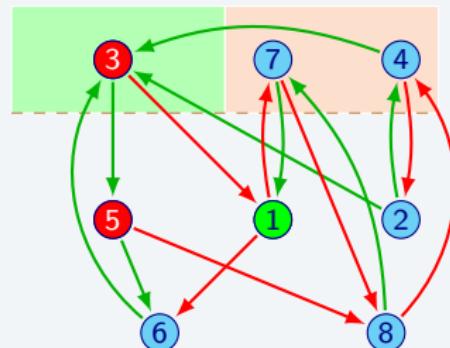
$$f_4 = x_2 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a regulatory network

Legend:



Vertex with True value



Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

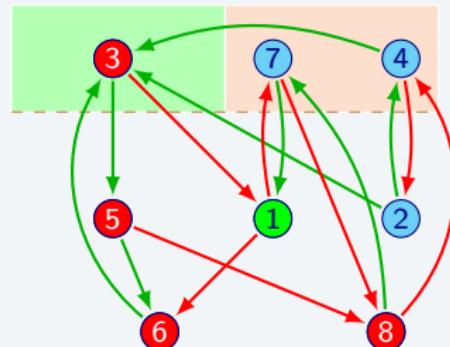
$$f_4 = x_2 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a regulatory network

Legend:

-  Vertex with True value
 -  Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

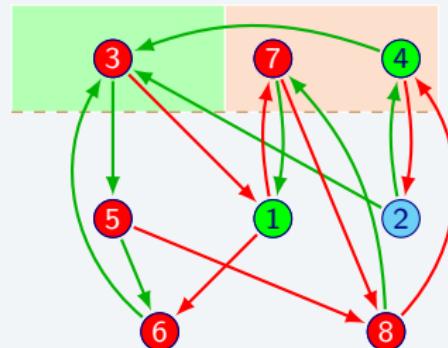
$$f_4 = x_7 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

$$f_9 = x_5 \wedge x_7$$





List the fixed points of a regulatory network

Legend:



Vertex with True value



Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

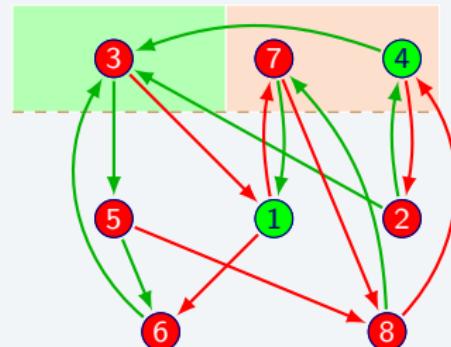
$$f_4 = x_2 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

$$f_8 = x_5 \wedge x_7$$





List the fixed points of a regulatory network



Legend:



Vertex with True value



Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

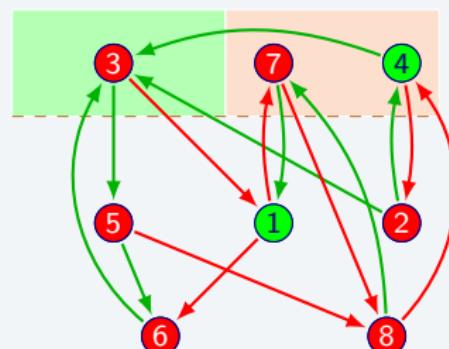
$$f_4 = x_2 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

$$f_8 = x_5 \wedge x_7$$



10010000 is a fixed point of f



List the fixed points of a regulatory network



Legend:



Vertex with True value



Vertex with False value

$$f_1 = \overline{x_3} \vee x_7$$

$$f_2 = \overline{x_4}$$

$$f_3 = (x_2 \wedge x_4) \vee (x_2 \wedge x_6) \vee (x_4 \wedge x_6)$$

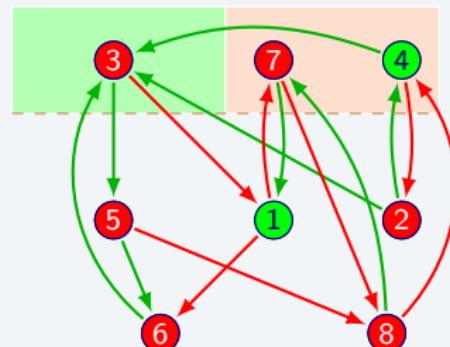
$$f_4 = x_2 \vee \overline{x_8}$$

$$f_5 = x_3$$

$$f_6 = \overline{x_1} \vee x_5$$

$$f_7 = \overline{x_1} \vee x_8$$

$$f_8 = x_5 \wedge x_7$$



The complexity of this algorithm is $((|F| - |F^+|)(n - |F^+|) + n) \cdot 2^{|F^+|}$



Complexity analysis



The complexity of listing fixed points based on a PFVS is



Complexity analysis



The complexity of listing fixed points based on a PFVS is

$$((|F| - |F^+|)(n - |F^+|) + n) \cdot 2^{|F^+|}$$



Complexity analysis



The complexity of listing fixed points based on a PFVS is

$$((|F| - |F^+|)(n - |F^+|) + n) \cdot 2^{|F^+|}$$

If $|F| = |F^+|$:



Complexity analysis



The complexity of listing fixed points based on a PFVS is

$$((|F| - |F^+|)(n - |F^+|) + n) \cdot 2^{|F^+|}$$

If $|F| = |F^+|$:

$$n \cdot 2^{|F|}$$



Complexity analysis



The complexity of listing fixed points based on a PFVS is

$$(|F| - |F^+|)(n - |F^+|) + n \cdot 2^{|F^+|}$$

If $|F| = |F^+|$:

$$n \cdot 2^{|F|}$$

It is equivalent to the execution of FVS-algorithm



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Motivation

State of Art

- (Goles and Salinas, 2008) and (Aracena et al, 2009) define equivalence classes between different update schedules.
- (Eric Goles, 1980) study the dynamics of discrete neural networks with deterministic update schedules.
- (Aracena et al, 2013) study how many different dynamics can exist in a Boolean network when the update schedule changes.
- (Aracena et al, 2023) study the complexity of deciding whether there exists a limit cycle of a given length k for some update schedule.
- (Goles and Noulal, 2012) classify the disjunctive networks according to the robustness of their dynamics concerning changes in the update schedule, all this using parallel digraphs.
- (Goles and Salinas, 2010) study how the network changes when it is updated with a given sequential schedule.



Motivation



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?



Dynamically equivalent network



Definition

Let f, h 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 $s \not\sim_f s_p$, we say that (h, s) and f are *non-trivially dynamically equivalent*.



Counter-examples



By reflexivity, any network is dynamically equivalent to itself (considering the parallel schedule). But there are networks that do not have another network that is non-trivial dynamically equivalent, for example:





Dynamically equivalent networks problem



DYNAMICALLY EQUIVALENT NETWORKS PROBLEM (DEN PROBLEM)

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

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

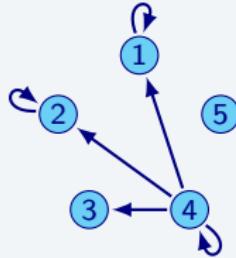


What do we need to solve this problem?

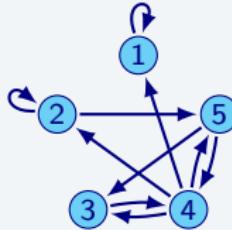


Lemma

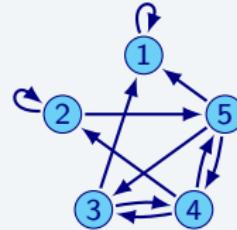
Let h, f be Boolean networks and $s = B_1, B_2, \dots, B_m$ with $m > 1$. If $h^s = f$, then there exists \bar{h} and \bar{s} such that $\bar{h}^{\bar{s}} = f$ where $\bar{s} = B_1, B_2, \dots, B_{m-1} \cup B_m$.



$$\begin{aligned}f_1(x) &= x_1 \vee x_4 \\f_2(x) &= x_2 \wedge x_4 \\f_3(x) &= x_4 \\f_4(x) &= x_4 \\f_5(x) &= 0\end{aligned}$$



$$\begin{aligned}h_1(x) &= x_1 \vee x_4 \\h_2(x) &= x_2 \wedge x_4 \\h_3(x) &= x_4 \wedge \neg x_5 \\h_4(x) &= x_3 \wedge \neg x_5 \\h_5(x) &= x_2 \wedge \neg x_4 \\s &= \{2\} \{5\} \{3\} \{4\} \{1\}\end{aligned}$$



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



How hard is it to solve the problem?



Theorem

DEN is NP-Hard.

Proof

We prove that $3\text{-SAT} \leq_p \text{DEN}$.



Dynamically equivalent disjunctive networks problem



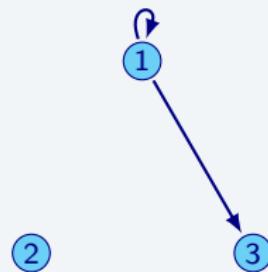
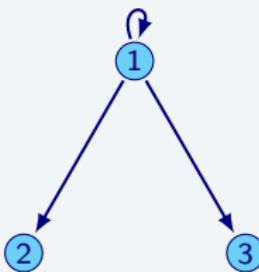
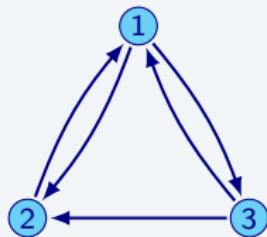
DYNAMICALLY EQUIVALENT DISJUNCTIVE NETWORKS
PROBLEM (D-DEN PROBLEM)

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

Question: does there exist 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 ?



$$\begin{aligned} h_1(x) &= x_2 \vee x_3 \\ h_2(x) &= x_1 \vee x_3 \\ h_3(x) &= x_1 \end{aligned}$$

$$\begin{aligned} h_1^s(x) &= (x_1 \vee x_1) \vee x_1 \\ h_2^s(x) &= x_1 \vee x_1 \\ h_3^s(x) &= x_1 \\ s &= \{3\} \{2\} \{1\} \end{aligned}$$

$$\begin{aligned} h_1^s(x) &= x_1 \\ h_2^s(x) &= 0 \\ h_3^s(x) &= x_1 \end{aligned}$$



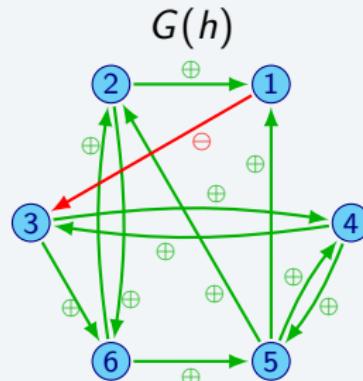
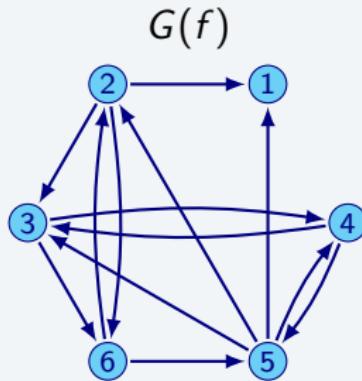
What do we need to solve this problem?



Proposition

Let f 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 $G(f) - v$.





What do we need to solve this problem?



Corollary

Let f 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 .

If $N_f^-(u^*) = N_f^-(v^*)$ then the three 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 $G(f) - v$.

 A^\ominus set

Definition

Let f 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 $N_f^-(u) \subseteq N_f^-(v)$.

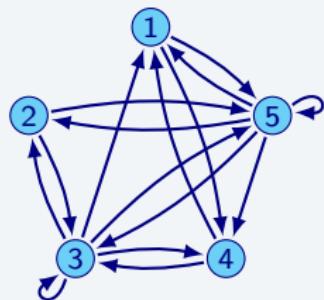
 A^\ominus set

If $A^\ominus(f)$ has a cycle, then D-DEN problem has a solution (since at least two vertices would have the same in-neighborhood).

What occurs if A^\ominus is acyclic?



$\mathcal{G}_{lab}(f, A^-)$ operator



$$N^-(1) = \{3, 4, 5\}$$

$$N^-(2) = \{3, 5\}$$

$$N^-(3) = \{2, 3, 4, 5\}$$

$$N^-(4) = \{1, 3, 5\}$$

$$N^-(5) = \{1, 2, 3, 5\}$$

1

2

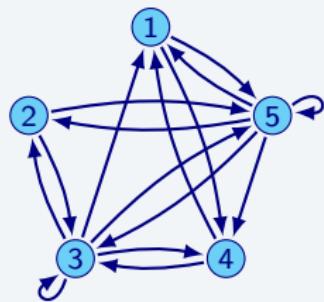
5

3

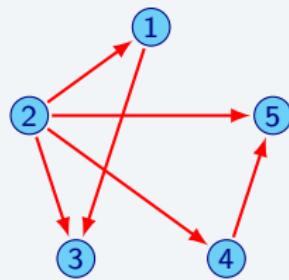
4



$\mathcal{G}_{lab}(f, A^-)$ operator

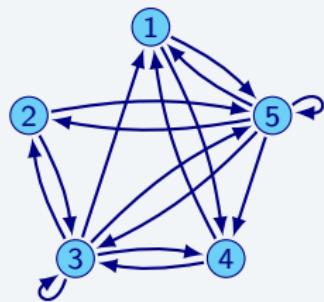


$$\begin{aligned}
 N^-(1) &= \{3, 4, 5\} \\
 N^-(2) &= \{3, 5\} \\
 N^-(3) &= \{2, 3, 4, 5\} \\
 N^-(4) &= \{1, 3, 5\} \\
 N^-(5) &= \{1, 2, 3, 5\}
 \end{aligned}$$

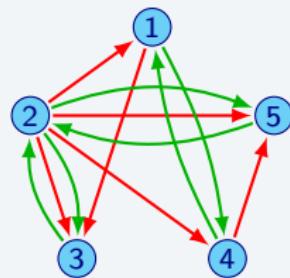




$\mathcal{G}_{lab}(f, A^-)$ operator

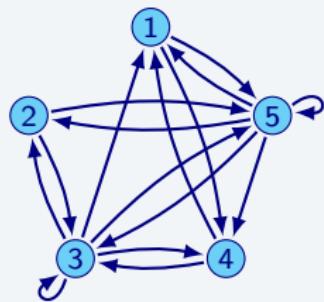


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 \end{aligned}$$

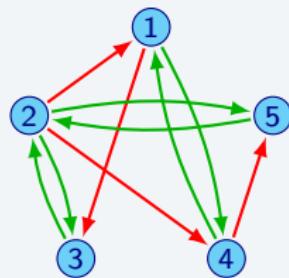




$\mathcal{G}_{lab}(f, A^-)$ operator



$$\begin{aligned}
 N^-(1) &= \{3, 4, 5\} \\
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 \end{aligned}$$





Admissible partition



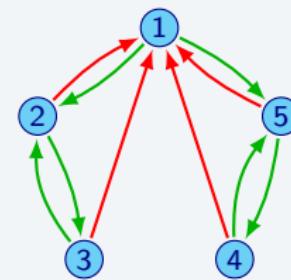
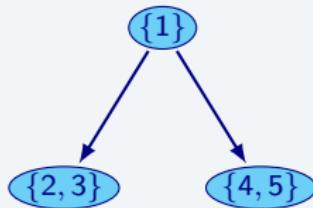
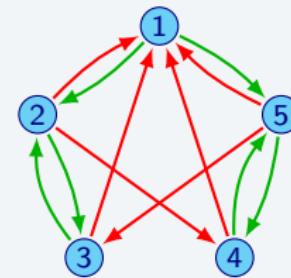
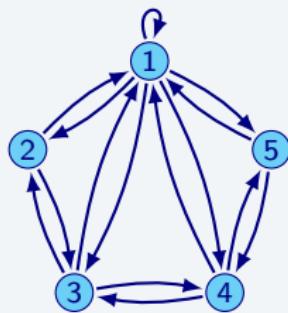
Definition

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 $\forall(u, v) \in A(G), u \in V_1 \wedge v \in V_2 \Rightarrow \text{lab}(u, v) = \ominus,$
- ③ $\forall(u, v) \in A(G), u, v \in V_2 \Rightarrow \text{lab}(u, v) = \oplus.$



Admissible partition





Remarks



- Different approaches to the problem of dynamically equivalent networks are presented.
- Solving the general problem is NP-Hard, since it is as difficult as 3-SAT
- An approach to finding a possible solution is presented: 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.
- The problem restricted to disjunctive networks can be solved in polynomial time.



Contents

- 1 Definitions
- 2 Motivation
- 3 Properties of parallel digraph
- 4 Algorithms to find fixed points
- 5 Dynamically equivalent networks
- 6 Subproblems of dynamically equivalent networks
- 7 Final conclusions



D-DEN problem with fixed update schedule



DYNAMICALLY EQUIVALENT DISJUNCTIVE BOOLEAN
NETWORK WITH FIXED SCHEDULE PROBLEM

Input: f is a disjunctive Boolean network and s is an update schedule.

Question: Does there exist h a disjunctive Boolean network such that $h^s = f$?



Scenarios of D-DEN problem with fixed update schedule

$$s = \{1\} \{2\}$$

$$G(f)$$



$$\text{DENs}$$



Unique solution



Multiple solutions



No solution



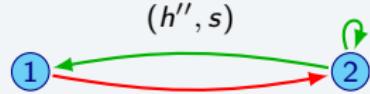
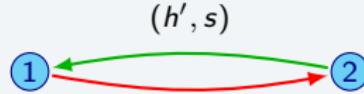
Results

Theorem

Let s be a block-sequential schedule and h and h' two Boolean networks such that $G_P(h, s) = G_P(h', s)$. Then $G_P(h \cup h', s) = G_P(h)$.



There are three preimages:





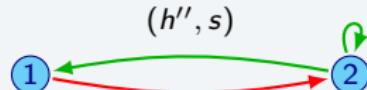
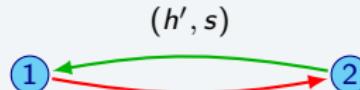
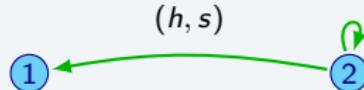
Results

Theorem

For this reason, if for a Boolean network f and a block-sequential schedule s there exists at least one DEN h , then there exists a maximum DEN.



There are three preimages:

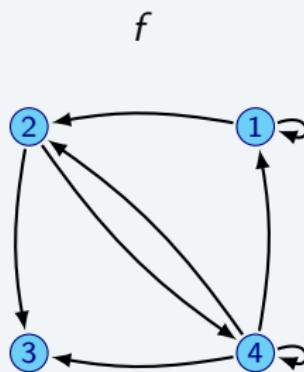




Algorithm MaximumDEDBN

Input

Given the following Boolean network f and a block-sequential schedule $s = \{3\} \{1\} \{2, 4\}$.



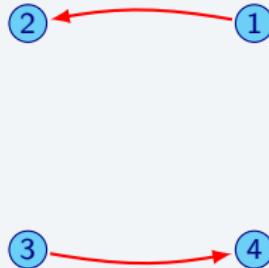


Algorithm MaximumDEDBN: Step 1 - Defining negative arcs

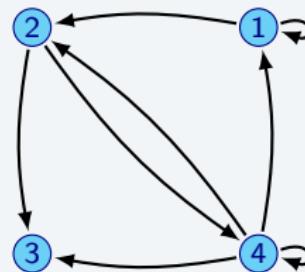
Rule

If there exists $(u, v) \in A^\ominus$, $s(u) < s(v)$, then (u, v) is a negative arc in $G(h, lab_s)$.

$G(h, lab_s)$



f





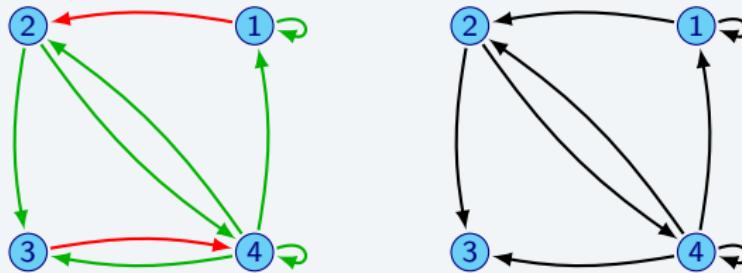
Algorithm MaximumDEDBN: Step 2 - Defining positive arcs

Rule

If there exists $(u, v) \in A(f)$, $s(u) \geq s(v)$, then (u, v) is a positive arc in $G(h, lab_s)$.

$$G(h, lab_s)$$

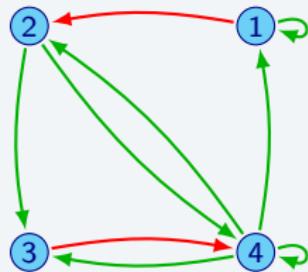
$$f$$



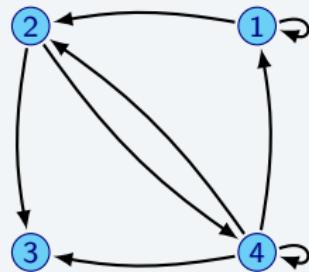


Algorithm MaximumDEBN: Step 3 - Validation

$G(h, lab_s)$

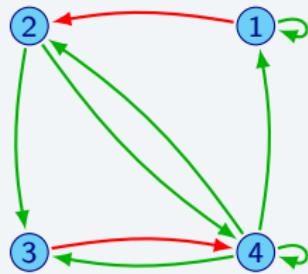
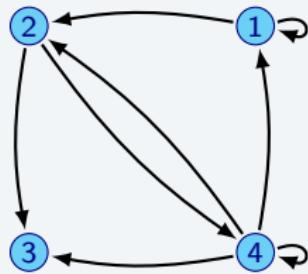
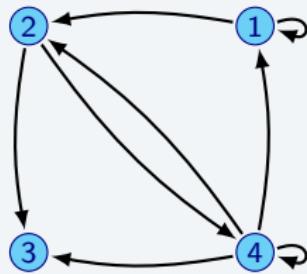


f



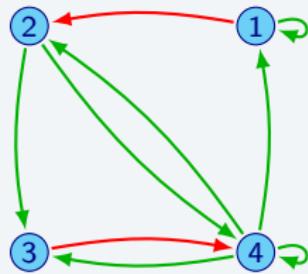
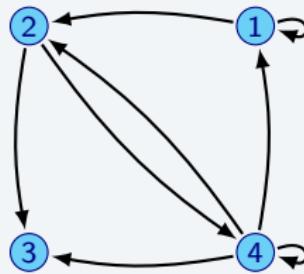
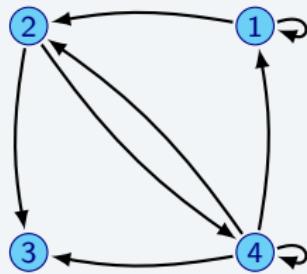


Algorithm MaximumDEBN: Step 3 - Validation

 $G(h, lab_s)$  $G_P(h, s)$  f 



Algorithm MaximumDEBN: Step 3 - Validation

 $G(h, lab_s)$  $G_P(h, s)$  f 

Output

Since $G_P(h, s) = f$, the algorithm return $G(h, lab_s)$ as maximum DEN of f with the update schedule s .



Enumeration of solutions with fixed schedule



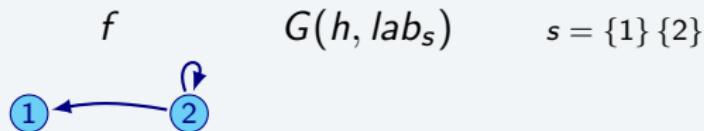
ENUMERATION OF DYNAMICALLY EQUIVALENT DISJUNCTIVE
BOOLEAN NETWORKS WITH FIXED UPDATE SCHEDULE

Input: f is a disjunctive Boolean network and s is an update schedule.

Question: Is it possible to find the complete set of disjunctive Boolean networks h such that $h^s = f$?

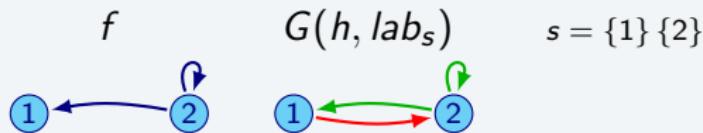


Enumeration of solutions with fixed schedule



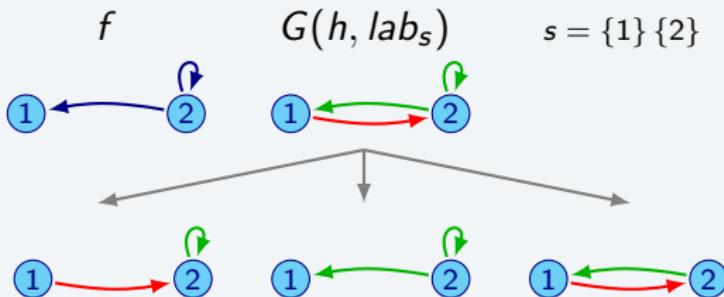


Enumeration of solutions with fixed schedule



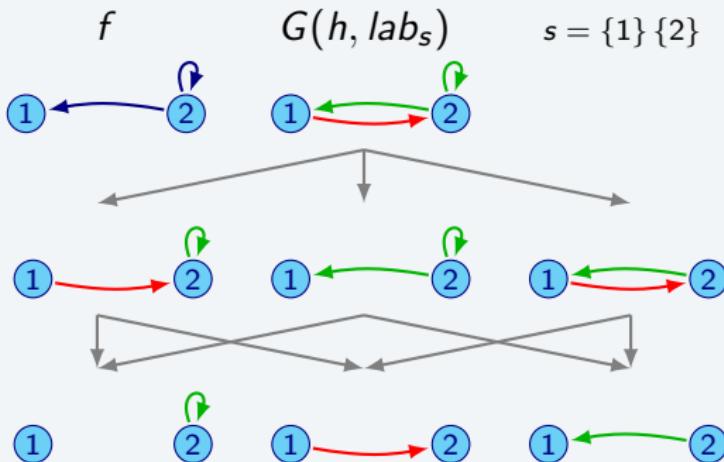


Enumeration of solutions with fixed schedule



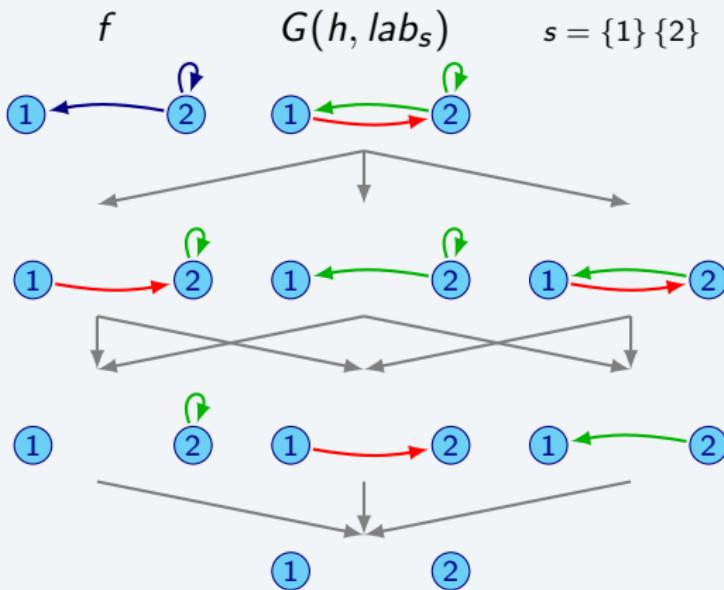


Enumeration of solutions with fixed schedule



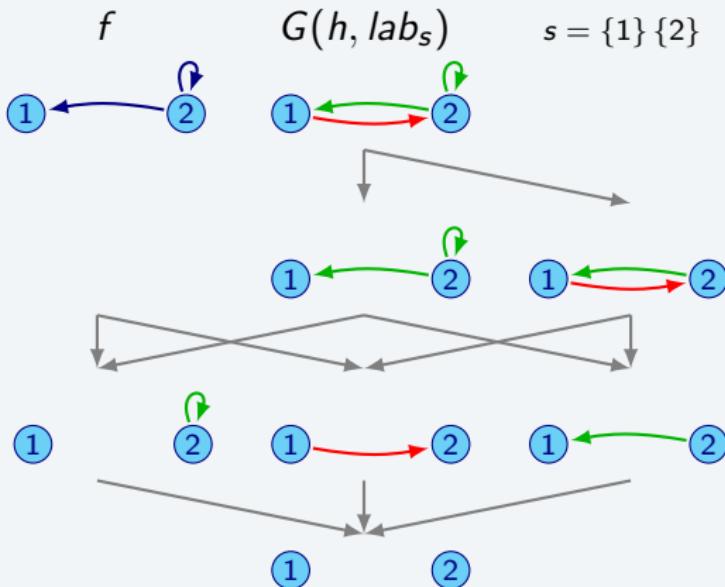


Enumeration of solutions with fixed schedule



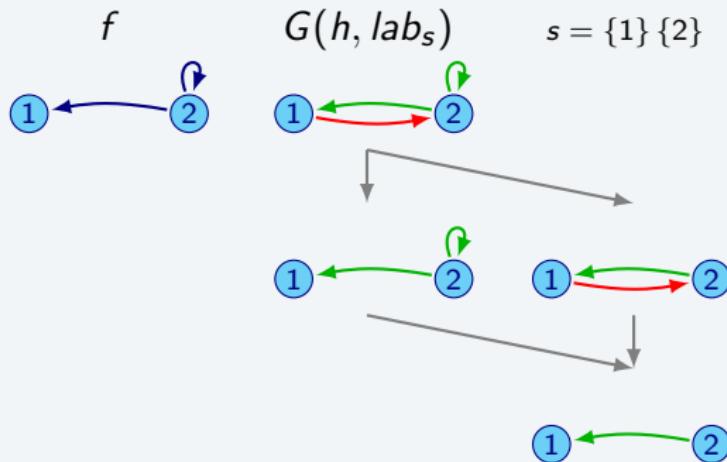


Enumeration of solutions with fixed schedule



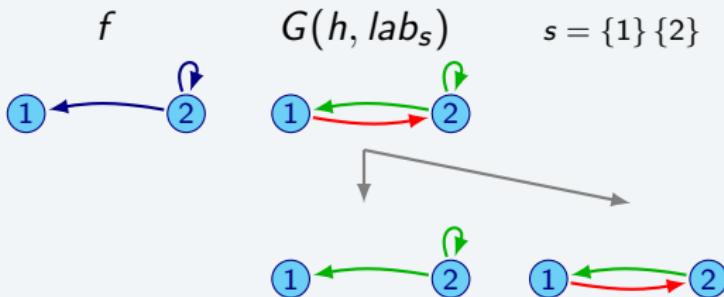


Enumeration of solutions with fixed schedule





Enumeration of solutions with fixed schedule





Enumeration of solutions with fixed schedule



Complexity

The complexity of this algorithm have a **polynomial delay**.



Enumeration of solutions with fixed schedule



Complexity

The complexity of this algorithm have a **polynomial delay**.

Since there are cases with an exponential number of DENs, listing all the DENs has an **exponential cost**



Enumeration of solutions with fixed schedule



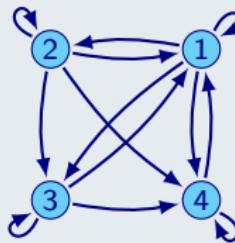
Complexity

The complexity of this algorithm have a **polynomial delay**.

Since there are cases with an exponential number of DENs, listing all the DENs has an **exponential cost**

For example, this digraph with the block-sequential schedule

$\{2\} \{3\} \{4\} \{1\}$ has 8 different DENs, corresponding to $2^{\frac{(n-2)(n-1)}{2}}$.





Dynamically equivalent disjunctive Boolean networks with fixed Boolean network problem

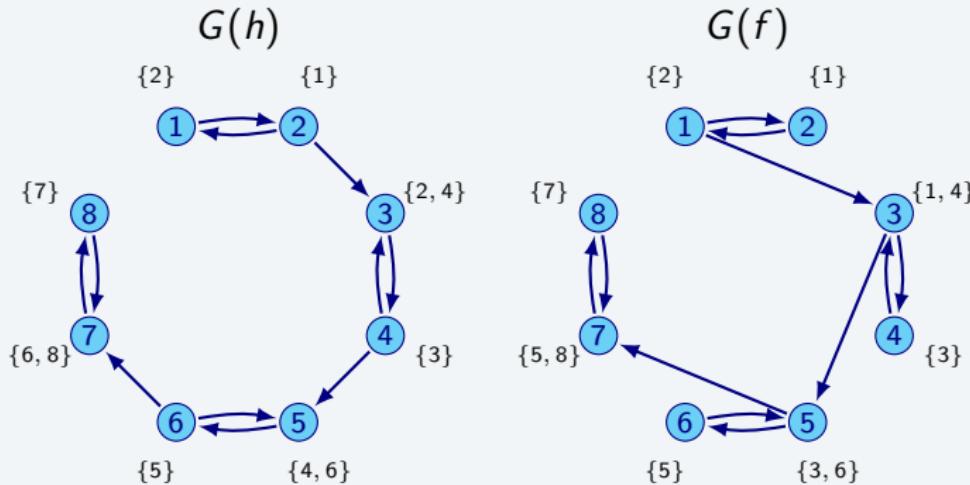
DYNAMICALLY EQUIVALENT DISJUNCTIVE BOOLEAN NETWORKS WITH FIXED BOOLEAN NETWORK PROBLEM

Input: h and f be two disjunctive Boolean networks.

Question: Does there exist an update schedule $s \asymp s_p$ such that $h^s = f$?



Preprocessing

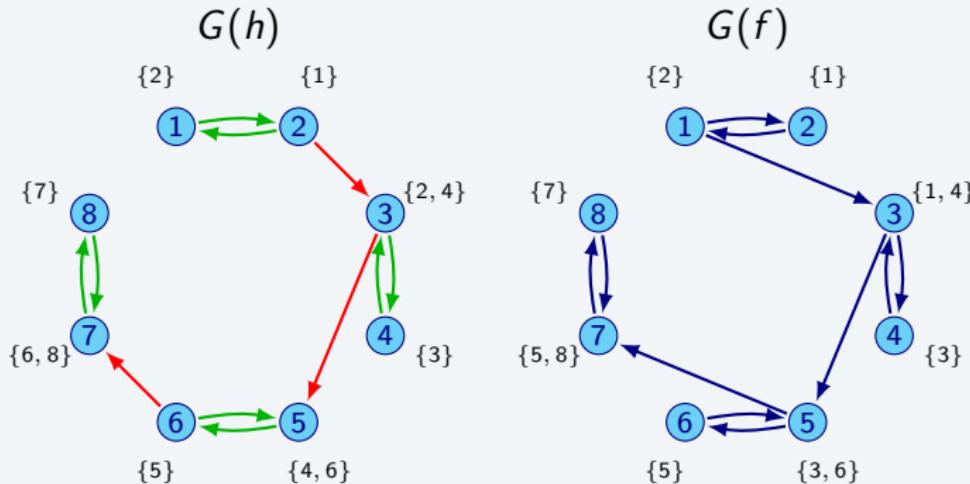


Key concept

K-valid update schedule.



Preprocessing



Key concept

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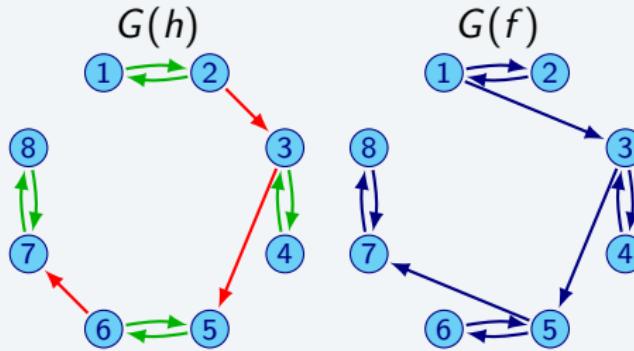


s-divider procedure



Given a k -valid update schedule:

- ① Select candidate vertices to belong to a block $k + 1$.
- ② It discards elements of this new block according to three criteria:
 - Negative criteria — Positive criteria — Potential criteria.
- ③ Finally, returns a $k + 1$ -valid update schedule (if it exists).



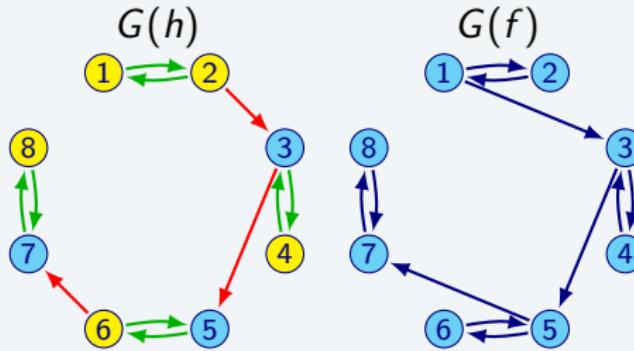


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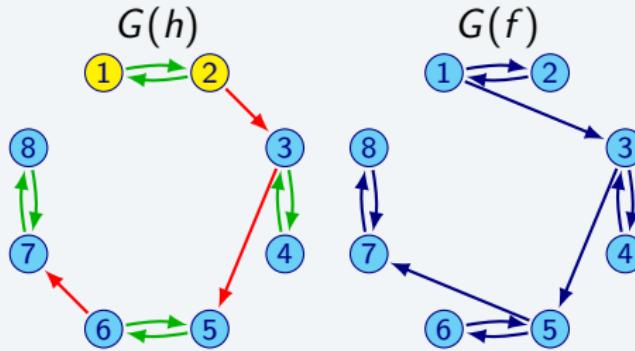


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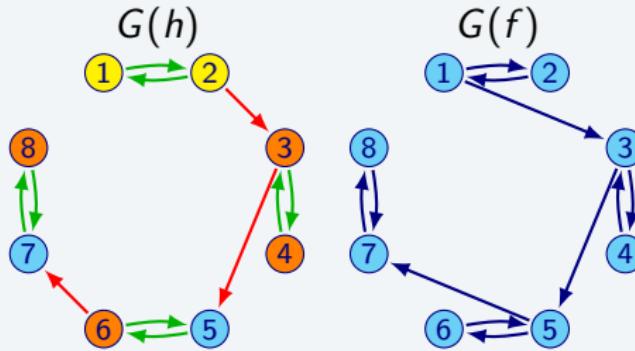


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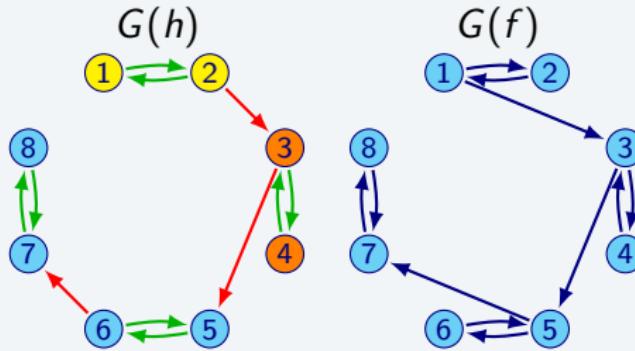


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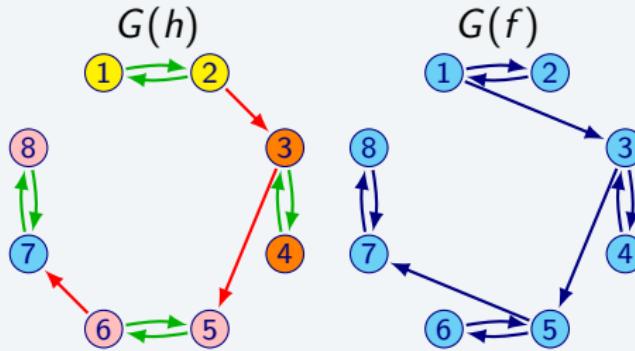


s-divider procedure



Given a k -valid update schedule:

- ① Select candidate vertices to belong to a block $k + 1$.
- ② It discards elements of this new block according to three criteria:
 - Negative criteria — Positive criteria — Potential criteria.
- ③ Finally, returns a $k + 1$ -valid update schedule (if it exists).



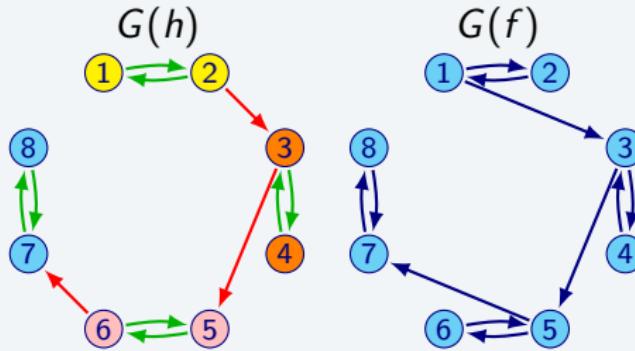


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What occurs when $h = f$?

- A solution based on the s-divider procedure returns the parallel update schedule.
- A new strategy, based on two-block solutions, is generated, which gives us a non-trivial solution (if it exists).



Remarks



- Fixing one of the parameters of the original D-DEN problem does not generate a higher cost in its resolution.
- Moreover, in the case where the update schedule is fixed, a certain monotony is described that allows us to list all the solutions to the problem.
- The next step will be to find monotonicity in the case when we fix the Boolean network h so that we can find an algorithm that allows us to enumerate all the solutions.



Contents



- 1 Definitions
- 2 Motivation
- 3 Properties of parallel digraph
- 4 Algorithms to find fixed points
- 5 Dynamically equivalent networks
- 6 Subproblems of dynamically equivalent networks
- 7 Final conclusions



Final conclusions



- In this thesis we have addressed different issues that allow us to satisfy the goal of studying how interaction graphs change when evaluated with different update schedules.
- All these results are interesting new tools that, combined in the right way, would allow to explore a number of topics in the field of Boolean networks that have yet to be explored.



Future Work: Open problems



- For FixedPoint algorithm, exploring methods to reduce the size of a network while conserving τ^+ .
- Analyzing the comprehensive complexity of the DEN problem.
- Evaluating whether restricting conditions on the output of the D-DEN problem increases or decreases its time cost.
- Studying whether by applying D-DEN on a non-disjunctive network, it is possible to reconstruct its DEN.

Thank You!