Dynamically equivalent disjunctive and linear Boolean networks

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Boolean network

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

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Interaction digraph

Definition

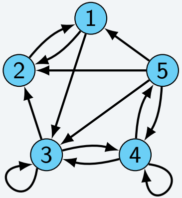
We define the interaction graph of a Boolean network $f : \{0,1\}^n \to \{0,1\}^n$, denoted by $G(f) = ([n], A(f))$, as:

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

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

Also, for each $u \in [n]$:

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



$$f_1(x) = \neg x_2 \wedge x_5$$
$$f_2(x) = (x_1 \wedge x_3) \vee (x_5 \wedge \neg x_3)$$
$$f_3(x) = (\neg x_1 \vee \neg x_5) \wedge x_3 \wedge x_4$$
$$f_4(x) = (x_4 \wedge x_3) \vee (x_5 \wedge \neg x_3)$$
$$f_5(x) = x_4$$

Update schedule

An *update schedule* is a function $s : \{1, \ldots, n\} \to \{1, \ldots, n\}$, where there exists $m \in \{1, \ldots, n\}$ such that $s(\{1, \ldots, n\}) = \{1, \ldots, m\}$.

Using this definition, we can write $s = B_1 \cdots B_m$, where each set B_j is a block of s, and $B_j = s^{-1}(\{j\}) = \{u \in \{1, \ldots, n\} : s(u) = j\}$.

Update schedule

Definition

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

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

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

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

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

where f^s is defined by:

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

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

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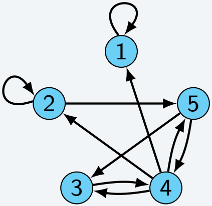
It is easy to prove that f^s is equivalent to:

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

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

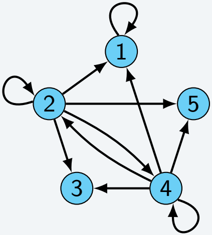
$$\forall x \in \{0,1\}^n, \quad f_v^{B_i}(x) = \begin{cases} x_v & \text{if } v \notin B_i \\ f_v(x) & \text{if } v \in B_i. \end{cases}$$

Dynamical behavior of a Boolean network



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

(a)



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

(b)

Figure: (a) f and an update schedule s (b) The parallel digraph $G_P(f, s)$.

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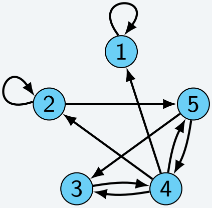

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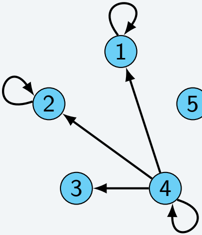

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f_4^s(x) &= x_4 \wedge \neg(0) = x_4 \\
f_5^s(x) &= (x_2 \wedge x_4) \wedge \neg x_4 = 0
\end{aligned}
$$

(c)

Figure: (a) f and an update schedule s (c) The effective network f^s.

Labelled digraph

Let $f : \{0,1\}^n \to \{0,1\}^n$ be a Boolean network and s an update schedule. We define the labeling function $\mathrm{lab}_s : A \to \{\ominus, \oplus\}$ in the following way:

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

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

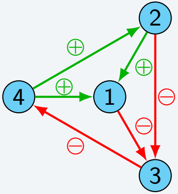

Figure: The associated digraph to f labeled by the function lab_s, with $s = \{1\}\{2\}\{3\}\{4\}$

Equivalence relation

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

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

We denote $[s]_f$ the equivalence class of s induced by $\sim_f$. It is kown that:

$$s \sim_f s' \implies f^s = f^{s'}. \tag{3}$$

Dynamically equivalent Boolean network problem

Definition

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

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

Preliminary results

Theorem

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.

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Notice that:

$$f^s = \underbrace{f^{B_k} \circ f^{B_{k-1}}}_{f^{B_k \cup B_{k-1}}} \circ f^{B_{k-2}} \circ \cdots \circ f^{B_1}$$

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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.

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Theorem

DEN is NP-Hard.

Disjunctive and linear Boolean networks

Definition

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

or, equivalently: $\forall u \in [n],\ f_u(x) = 1 \iff \left|\left\{v \in N_f^-(u) : x_v = 1\right\}\right| \geqslant 1.$

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Definition

Given $f : \{0,1\}^n \to \{0,1\}^n$ a Boolean network, f is called a linear Boolean network if: $\forall u \in [n],\ f_u(x) = \bigoplus_{v \in N_f^-(u)} x_v$, where $\oplus$ is the sum modulo 2

or, equivalently:

$\forall u \in [n],\ f_u(x) = 1 \iff \left|\left\{v \in N_f^-(u) : x_v = 1\right\}\right|$ is odd.

Transitive property

Given $h, f : \{0,1\}^n \to \{0,1\}^n$ two disjunctive Boolean networks and s an update schedule such that $h^s = f$. then:

$$(u,v) \in A(f) \iff \begin{cases} ((u,v) \in A(h) \wedge s(u) \geqslant s(v)) & \vee \\ (\exists w \in N_h^-(v), s(w) < s(v) \wedge (u,w) \in A(f)) \end{cases}$$

Lemma

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 $u, v \in [n]$:

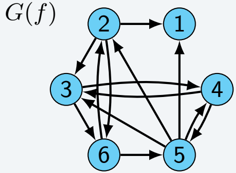
$$[(u,v) \in A(h) \wedge \mathrm{lab}_s(u,v) = \ominus] \implies N_f^-(u) \subseteq N_f^-(v).$$

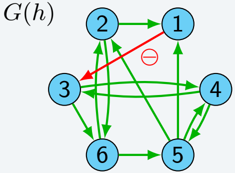
Solutions with one negative arc

Proposition

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





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Corollary

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.

Disjunctive Boolean network

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

Algoritmo: $\mathcal{G}_{\text{lab}}(f, A^-)$

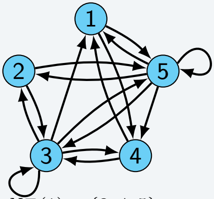
Input: A disjunctive Boolean network $f : \{0,1\}^n \to \{0,1\}^n$ and a subset $A^- \subseteq A^{\ominus}(f)$ of $G = G(f)$ such that $G[A^-]$ is acyclic.

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 $(A^+)^* \cap A^- = \varnothing$ **then return** $G([n], A^+ \cup A^-)$;

else return $\mathcal{G}_{\text{lab}}(f, A^- \backslash (A^+)^*)$;



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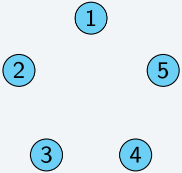

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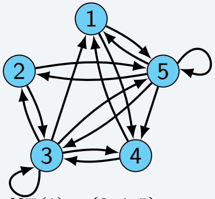

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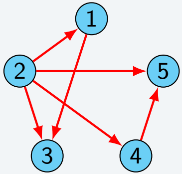

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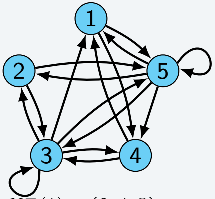

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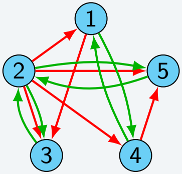

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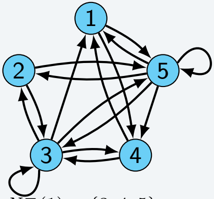

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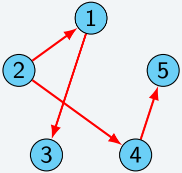

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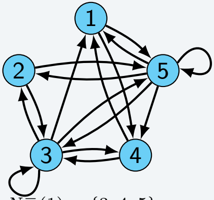

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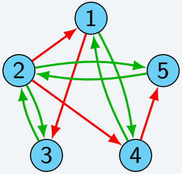


Disjunctive Boolean network

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

Algoritmo: $\mathcal{G}_{\text{lab}}(f, A^-)$

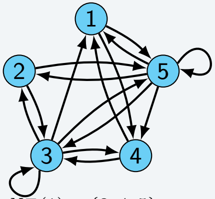
Input: A disjunctive Boolean network $f : \{0,1\}^n \to \{0,1\}^n$ and a subset $A^- \subseteq A^{\ominus}(f)$ of $G = G(f)$ such that $G[A^-]$ is acyclic.

Output: A labeled digraph $G[A^-, A^+]$.

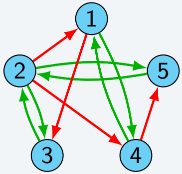
$A^+ \leftarrow \{(u,v) \in A(f) : \forall w \in N_f^+(u), (w,v) \notin A^-)\}$;

if $(A^+)^* \cap A^- = \varnothing$ **then return** $G([n], A^+ \cup A^-)$;

else return $\mathcal{G}_{\text{lab}}(f, A^- \backslash (A^+)^*)$;



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



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

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Lemma

Let $f : \{0,1\}^n \to \{0,1\}^n$ be a disjunctive Boolean network and $\{V_1, V_2\}$ an admissible partition of $\mathcal{G}_{\mathrm{lab}}(f, A^{\ominus}(f))$. 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 $\mathcal{G}_{\mathrm{lab}}(f, A^-)$ is an update digraph and $G_P(\mathcal{G}_{\mathrm{lab}}(f, A^-)) = G(f)$.

Algorithm

Algoritmo: AdmissiblePartition(G, lab)

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

$G^{\oplus} \leftarrow \mathrm{lab}^{\oplus}[(G, \mathrm{lab})]$;
$(\hat{V}, \hat{A}) \leftarrow \mathrm{ComponentDigraph}(G^{\oplus})$;
$Q \leftarrow \{G_i \in \hat{V} : \nexists G_j \in \hat{V}, (G_j, G_i) \in \hat{A}\}$; `// initial components`
$v^* \leftarrow \mathrm{Null}$;
while $v^* = \mathrm{Null}$ **do**
  $G_q \leftarrow$ first element of Q;
  if $\exists u \in G_q \wedge \exists (w, u) \in A(G), \mathrm{lab}(w, u) = \ominus$ **then** $v^* \leftarrow u$;
  else $Q \leftarrow Q \cup \{G_i \in \hat{V} : (G_q, G_i) \in \hat{A}\}$;
$V_2 \leftarrow \{v \in V(G)$: $\exists$ a path in $G^{\oplus}$ from v to some vertex in the same component of $v^*\}$;
$V_1 \leftarrow V(G) \backslash V_2$;
return $\{V_1, V_2\}$

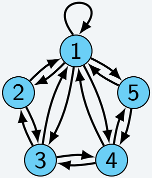
Algorithm for D-DEN Problem

Algoritmo: D-DENPSolve(f)

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

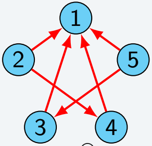
if $A^{\ominus}(f)$ has a cycle **then**
  Let u and v be two vertices such that $N_f^-(u) = N_f^-(v)$;
  return $G[\{(u,v)\}, A(f) \setminus \left\{(x,v) : x \in N_f^-(v)\right\}]$
else
  $(G, \mathrm{lab}) \leftarrow \mathcal{G}_{\mathrm{lab}}(f, A^{\ominus}(f))$;
  if $\mathrm{lab}^{\ominus}(G, \mathrm{lab}) = \varnothing$ **then return** Null;
  if (G, lab) is update **then return** (G, lab);
$\{V_1, V_2\} \leftarrow \mathrm{AdmissiblePartition}(G, \mathrm{lab})$;
$A^- \leftarrow \{(u,v) \in A(G, \mathrm{lab}) : u \in V_1 \wedge v \in V_2\}$;
return $\mathcal{G}_{\mathrm{lab}}(f, A^-)$;

Example of the algorithm

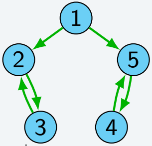


$$
\begin{aligned}
N^-(1) &= \{1,2,3,4,5\} \\
N^-(2) &= \{1,3\} \\
N^-(3) &= \{1,2,4\} \\
N^-(4) &= \{1,3,5\} \\
N^-(5) &= \{1,4\}
\end{aligned}
$$

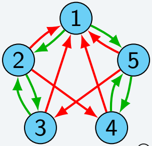
(a) Digraph $G(f)$



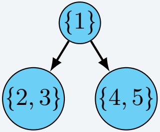
(b) $A^{\ominus}(f)$



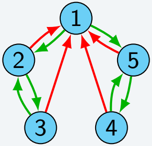
(c) A^+ according $\mathcal{G}_{\text{lab}}$



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



(e) The Poset digraph Adm. Partition



(f) Labeled digraph V_1 and V_2

Transitive property for linear Boolean network

Lemma

Let $f,\ h : \{0,1\}^n \to \{0,1\}^n$ *be two linear Boolean networks and* $s = B_1 \dots B_m$ *a block sequential update schedule such that* $h^s = f$*. Then, given* $k \in \{1, \dots, m-1\}$*, it follows,*

$$M(h)^{B_1} = M(f)^{B_1}$$
$$M(h)^{B_{k+1}} M(f)^{B_k^*} = M(f)^{B_{k+1}^*},$$

where $B_k^* = \bigcup_{j=1}^{k} B_j$.

Notice that this lemma solve the problem:

Given $f : \{0,1\}^n \to \{0,1\}^n$ a linear Boolean network and s an update schedule. Does there exist h a linear Boolean network such that $h^s = f$?

Acyclic linear Boolean network

Proposition

Let $f : \{0,1\}^n \to \{0,1\}^n$ be a linear Boolean network. There exists a linear Boolean network $h : \{0,1\}^n \to \{0,1\}^n$ 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 $G(f) - v$*

Corollary

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

Acyclic linear Boolean network

Corollary

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

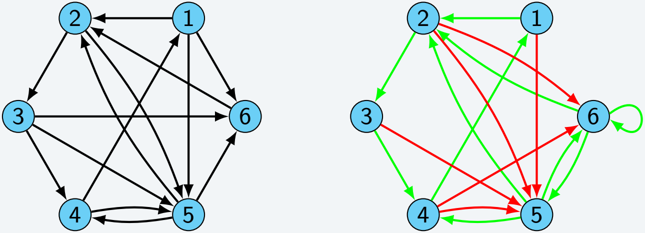
Corollary

Let $f : \{0,1\}^n \to \{0,1\}^n$ be a linear Boolean network. If $G(f)$ is acyclic and for all $u \neq v \in V(f)$, $N_f^-(u) \neq N_f^-(v)$, then there exists a non-trivially pre-image (h, s) such that $h^s = f$.

Strongly connected linear Boolean network

Proposition

Let $f : \{0,1\}^n \to \{0,1\}^n$ be a linear Boolean network. If there exist a simple cycle $C = [v_0, \ldots, v_{k-1}, v_k = v_0]$ in $G(f)$ such that $N_f^+(C) \neq \varnothing$, then there exists a non-trivially pre-image (h, s) such that $h^s = f$.



Example of proposition where the cycle is defined by the vertices {1,2,3,4}

Linear Boolean network

Theorem

Let $f : \{0,1\}^n \to \{0,1\}^n$ be a linear Boolean network, and let $P = \{u \in V(f) : u$ is not a vertex of a cycle in $G(f)\}$. There exists a solution for L-DEN problem if and only if one of the following conditions is satisfied:

1. *There exists a simple cycle C such that $|N_f^+(C)| > 0$*
2. $|P| > 1$
3. *$G(f)$ is disconnected and $|P| = 1$*

Besides, if a solution exists, it can be found in polynomial time.

Disjunctive Boolean network

Theorem

Preimage problem with fixed update schedule can be solved in polynomial time.

Algoritmo: MaximumPreImage(f, s)

Input: A disjunctive Boolean network f and an update schedule s.
Output: The maximum preimage h or Null if it does not exist.

$A^- \leftarrow \{(u,v) \in A^{\ominus}(f) : s(u) < s(v)\}$;

if $A^- = \varnothing$ **then return** Null;

$A^+ \leftarrow \{(u,v) \in A(f) : s(u) \geqslant s(v)\}$;

$h \leftarrow \mathrm{BN}([n], A^- \cup A^+)$;

if $h^s = f$ **then return** h;

else return Null;

Algorithm

Algoritmo: $s(h, f)$

Input: Two disjunctive Boolean networks $f, h : \{0,1\}^n \to \{0,1\}^n$.
Output: If there exists an update schedule s such that $h^s = f$, it returns s. Otherwise, returns Null.

$s \leftarrow s_p$;
$k \leftarrow 0$;
while $h^s \neq f$ **do**
    $s' \leftarrow$ s-divider(f, h, s, k);
    if $s' = s$ **then return** Null;
    $k \leftarrow k + 1$;
    $s \leftarrow s'$;
return s;

Disjunctive Boolean network

Algoritmo: s-divider(f, h, s, k)

Input: Two disjunctive Boolean networks $f, h : \{0,1\}^n \to \{0,1\}^n$ and s is a k-valid update schedule.

Output: s as a $(k+1)$-valid update schedule.

$V \leftarrow \emptyset$;
forall $v \in [n], s(v) = k+1$ **do**
    $B \leftarrow \{u \in N_f^-(w) : w \in N_h^-(v) \wedge s(w) \leqslant k\}$;
    $F \leftarrow \{u \in N_h^-(v) : s(u) > k\}$;
    if $N_f^-(v) = B \cup F$ **then** $V \leftarrow V \cup \{v\}$;
$s' \leftarrow s$;
repeat
    for $v \notin V \wedge s(v) = k+1$ **do** $s'(v) \leftarrow k+2$;
    $V^{\ominus} \leftarrow \{v \in V : \exists (u,v) \in A^-(h,f), s'(u) \geqslant s'(v)\}$;
    $V^{\oplus} \leftarrow \{v \in V : \exists (v,u) \in A^+(h,f), s'(v) < s'(u)\}$;
    $V^p \leftarrow \{v \in V : \exists (v,u) \in A(f), (v,u) \notin \text{potential}(f,h,s',k+1)\}$;
    $V \leftarrow V \backslash (V^{\ominus} \cup V^{\oplus} \cup V^p)$;
until $(V^{\ominus} \cup V^{\oplus} \cup V^p) = \emptyset$;

Linear Boolean networks

Until now, we do not have a polynomial time solution

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