Inverse block-sequential operator in conjunctive networks.

J. Aracena[1], L. Cabrera-Crot[1], A. Richard[2], L. Salinas[1].
[1] Universidad de Concepción, Chile
[2] CNRS, Sophia Antipolis, France.

WAN 2021
July 15th

Contents

Boolean Network

Definition

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

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

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

We will say a Boolean network is conjunctive if $f_v(x) = \bigwedge_{i \in I_v} x_i$

Block-sequential schedule

Definition

A block-sequential schedule is an ordered partition of the components of a Boolean network which defines the order in which the states of the network are updated in one unit of time.

Examples

$$s_1 = \{3,4\}\{1\}\{2\},$$
$$s_2 = \{1,2,3,4\},$$
$$s_3 = \{2\}\{3\}\{4\}\{1\}.$$

Update a Boolean network

Definition (Robert 86)

Let f be a Boolean network and $s = B_1, B_2, \ldots, B_m$ a block-sequential update schedule. The dynamical behavior of f updated according s is given by:

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

$$\forall v \in B_i, i > 1, \qquad x_v^{t+1} = f_v(x_u^{t+1} : u \in \bigcup_{j=1}^{i-1} B_j ; x_u^t : u \in \bigcup_{j=i}^{m} B_j) \tag{2}$$

Update a Boolean network

Definition (Robert 86)

Let f be a Boolean network and $s = B_1, B_2, \ldots, B_m$ a block-sequential update schedule. The dynamical behavior of f updated according s is given by:

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

$$\forall v \in B_i, i > 1, \qquad x_v^{t+1} = f_v(x_u^{t+1} : u \in \bigcup_{j=1}^{i-1} B_j; x_u^t : u \in \bigcup_{j=i}^{m} B_j) \tag{2}$$

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

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

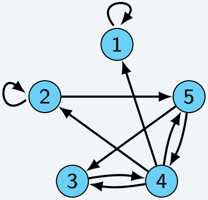
Where we define f^s as the composition of updating f block by block:

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

where:

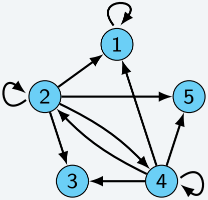
$$\forall x \in \{0,1\}^n, \quad f_v^{B_i}(x) = \begin{cases} x_v & \text{if } v \notin B_i \\ f_v(x) & \text{if } v \in B_i. \end{cases}$$

Example of f^s



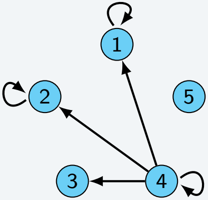
$$f_1 = x_1 \lor x_4$$
$$f_2 = x_2 \land x_4$$
$$f_3 = x_4 \land \neg x_5$$
$$f_4 = x_3 \land \neg x_5$$
$$f_5 = x_2 \land \neg x_4$$
$$s = \{2\}\{5\}\{3\}\{4\}\{1\}$$

(a)



$$f_1^s = x_1 \lor (x_4 \land \neg(x_2 \land x_4 \land \neg x_4))$$
$$f_2^s = x_2 \land x_4$$
$$f_3^s = x_4 \land \neg(x_2 \land x_4 \land \neg x_4)$$
$$f_4^s = x_4 \land \neg(x_2 \land x_4 \land \neg x_4)$$
$$f_5^s = x_2 \land x_4 \land \neg x_4$$

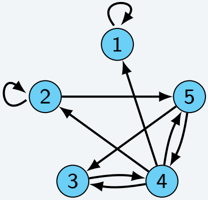
(b)



$$f_1^s = x_1 \lor x_4$$
$$f_2^s = x_2 \land x_4$$
$$f_3^s = x_4 \land \neg(0) = x_4$$
$$f_4^s = x_4 \land \neg(0) = x_4$$
$$f_5^s = (x_2 \land x_4) \land \neg x_4 = 0$$

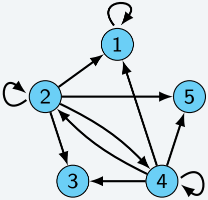
(c)

Example of f^s in a conjunctive network



$f_1 = x_1 \wedge x_4$
$f_2 = x_2 \wedge x_4$
$f_3 = x_4 \wedge x_5$
$f_4 = x_3 \wedge x_5$
$f_5 = x_2 \wedge x_4$
$s = \{2\}\{5\}\{3\}\{4\}\{1\}$

(a)



$f_1^s = x_1 \wedge x_4 \wedge x_2$
$f_2^s = x_2 \wedge x_4$
$f_3^s = x_4 \wedge x_2 \wedge x_4$
$f_4^s = x_4 \wedge x_2 \wedge x_4$
$f_5^s = x_2 \wedge x_4$

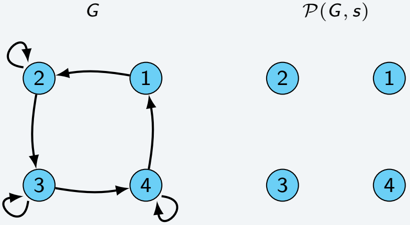
(b)

Goles and Noual, 2012.

Parallel digraph

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

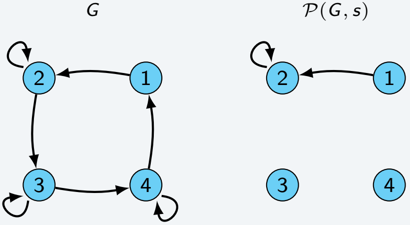
$s = \{2\}\{3\}\{4\}\{1\}$



Parallel digraph

The function that associates (G, s) with the digraph $\mathcal{P}(G, s)$ is called **block-sequential operator** and can be constructed in polynomial time.

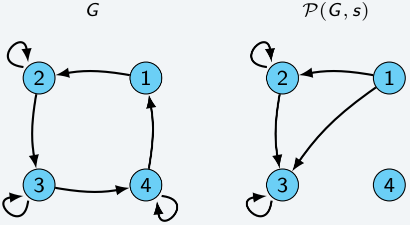
$s = \{2\}\{3\}\{4\}\{1\}$



Parallel digraph

The function that associates (G, s) with the digraph $\mathcal{P}(G, s)$ is called **block-sequential operator** and can be constructed in polynomial time.

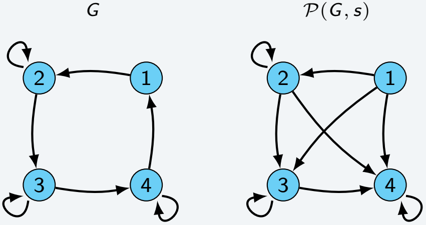
$s = \{2\}\{3\}\{4\}\{1\}$



Parallel digraph

The function that associates (G, s) with the digraph $\mathcal{P}(G, s)$ is called **block-sequential operator** and can be constructed in polynomial time.

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

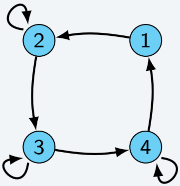


Parallel digraph

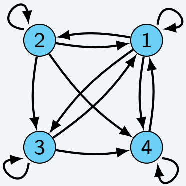
The function that associates (G, s) with the digraph $\mathcal{P}(G, s)$ is called **block-sequential operator** and can be constructed in polynomial time.

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

G



$\mathcal{P}(G, s)$



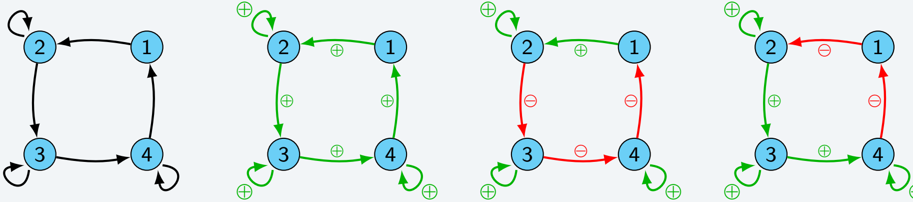
Labeled digraph

Given a interaction graph G and a block-sequential schedule s, a labeled digraph (G, s) is a digraph with a labeling function lab_s:

$$\mathrm{lab}_s : A(G) \to \{\oplus, \ominus\}$$
$$\mathrm{lab}_s(u, v) = \oplus \iff u \in B_i \wedge v \in B_j \wedge i \geqslant j$$

G $\quad s_1 = \{1, 2, 3, 4\}$ $\quad s_2 = \{2\}\{3\}\{4\}\{1\}$ $\quad s_3 = \{3, 4\}\{1\}\{2\}$

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



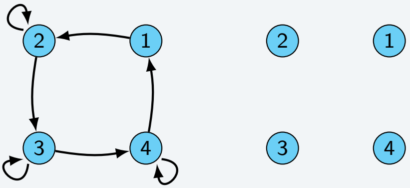
Aracena et al., 2009, 2011.

Parallel digraph

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

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

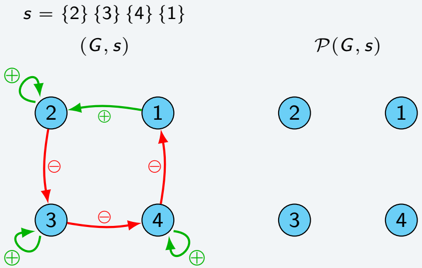
G $\mathcal{P}(G, s)$



Parallel digraph

Can be obtained from the labeled digraph.
$\forall (u, v) \in V(G) \times V(G), (u, v) \in A(\mathcal{P}(G, s))$ if and only if:

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

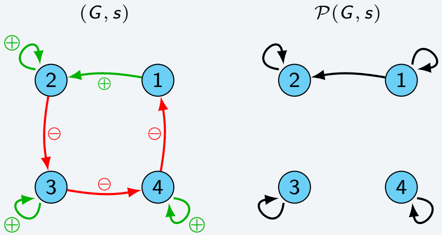


Parallel digraph

Can be obtained from the labeled digraph.
$\forall (u,v) \in V(G) \times V(G), (u,v) \in A(\mathcal{P}(G,s))$ if and only if:

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

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

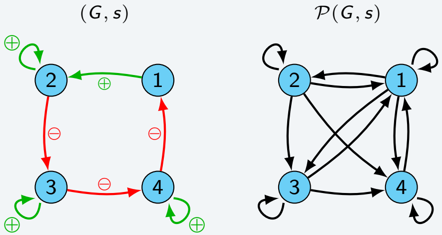


Parallel digraph

Can be obtained from the labeled digraph.
$\forall (u,v) \in V(G) \times V(G), (u,v) \in A(\mathcal{P}(G,s))$ if and only if:

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

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

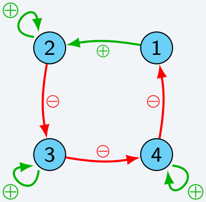


Parallel digraph

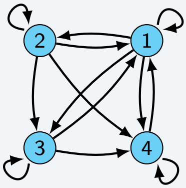
The function that associates (G, s) with the digraph $\mathcal{P}(G, s)$ is called **block-sequential operator** and can be constructed in polynomial time.

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

(G, s)



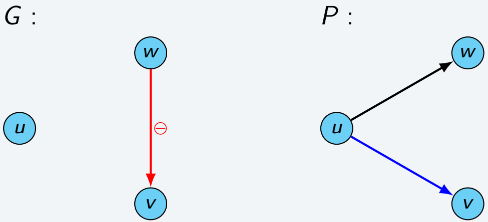
$\mathcal{P}(G, s)$



Transitive property

Let $u, v, w \in V(G)$:

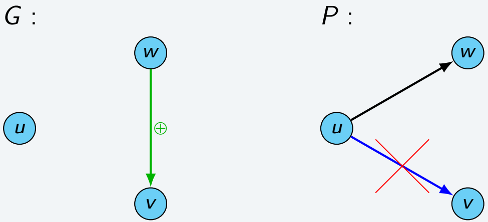
1. $(u, w) \in A(P) \wedge (w, v) \in A(G) \wedge \text{lab}_s(w, v) = \ominus \implies (u, v) \in A(P)$.



Transitive property

Let $u, v, w \in V(G)$:

1. $(u, w) \in A(P) \wedge (w, v) \in A(G) \wedge \text{lab}_s(w, v) = \ominus \implies (u, v) \in A(P)$.
2. $(u, w) \in A(P) \wedge (u, v) \notin A(P) \wedge (w, v) \in A(G) \implies \text{lab}_s(w, v) = \oplus$.

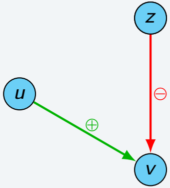


Transitive property

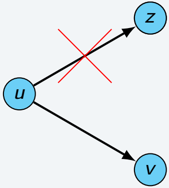
Let $u, v, w \in V(G)$:

1. $(u,w) \in A(P) \wedge (w,v) \in A(G) \wedge \text{lab}_s(w,v) = \ominus \implies (u,v) \in A(P)$.
2. $(u,w) \in A(P) \wedge (u,v) \notin A(P) \wedge (w,v) \in A(G) \implies \text{lab}_s(w,v) = \oplus$.
3. $(u,v) \in A(G) \cap A(P) \wedge (\nexists z \in V(G), (u,z) \in A(P) \wedge (z,v) \in A(G) \wedge \text{lab}_s(z,v) = \ominus) \implies \text{lab}_s(u,v) = \oplus$.

G :



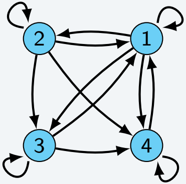
P :



Inverse problem

Given a digraph P, does there exist a digraph G and a block-sequential s such that $\mathcal{P}(G, s) = P$?

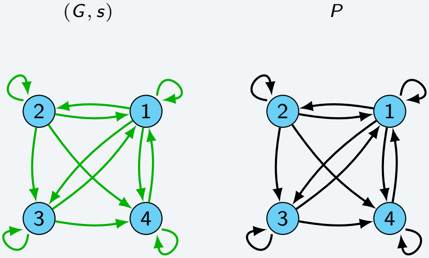
P



Inverse problem

Given a digraph P, does there exist a digraph G and a block-sequential s such that $\mathcal{P}(G, s) = P$?

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



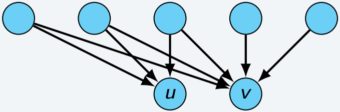
Parallel digraph preimage problem

Let P be a digraph, does there exists a digraph G and an update schedule s non equivalent to s_p such that $\mathcal{P}(G, s) = P$?

Necessary condition

Lemma

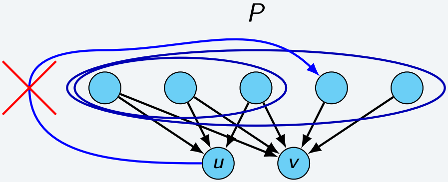
Let P be digraph, if there exists a preimage different to the trivial one, then there are vertices $u, v \in V(P)$ such that $N_P^-(u) \subseteq N_P^-(v)$.

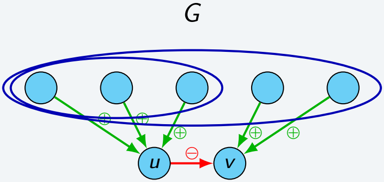


Sufficient condition

Lemma

Let P be a digraph, if there exists $u, v \in V(P)$ such that $N_P^-(u) \subseteq N_P^-(v)$ and for every vertex $w \in N_P^-(v) \backslash N_P^-(u)$ there is no path from u to w in $G - v$, then there exists a non trivial preimage (G, s) such that $\mathcal{P}(G, s) = P$.

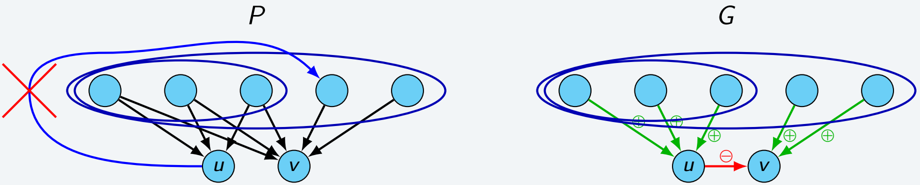




Sufficient condition

Lemma

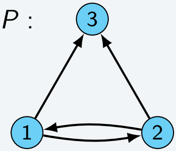
Let P be a digraph, if there exists $u, v \in V(P)$ such that $N_P^-(u) \subseteq N_P^-(v)$ and for every vertex $w \in N_P^-(v) \setminus N_P^-(u)$ there is no path from u to w in $G - v$, then there exists a non trivial preimage (G, s) such that $\mathcal{P}(G, s) = P$.

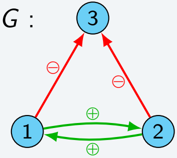


Corollary

Let P be a digraph, if there exists $u, v \in V(P)$ such that $N_P^-(u) = N_P^-(v)$, then there exists a non trivial preimage (G, s) such that $\mathcal{P}(G, s) = P$.

Example

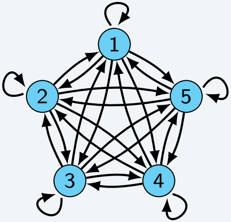




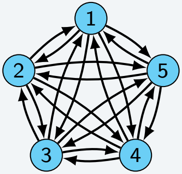
$$N^{-}(1) = \{2\}$$
$$N^{-}(2) = \{1\}$$
$$N^{-}(3) = \{1, 2\}$$

Example

K_n

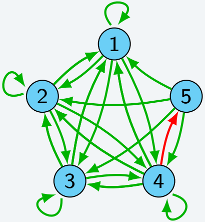


K_n°



$\forall v \in V(K_n), N^{-}(v) = V(K_n)$ $\qquad$ $\forall v \in V(K_n^{\circ}), N^{-}(v) = V(K_n^{\circ}) \setminus \{v\}$

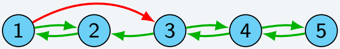
K_n



Example

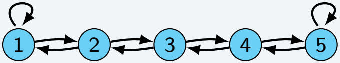
P :

G :



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

P :

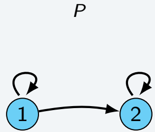


$$N^-(1) = \{1,2\}$$
$$N^-(2) = \{1,3\}$$
$$N^-(3) = \{2,4\}$$
$$N^-(4) = \{3,5\}$$
$$N^-(5) = \{4,5\}$$

Inverse problem

Given a digraph P and a block-sequential schedule s, does there exist a digraph G such that $\mathcal{P}(G, s) = P$?

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



Inverse problem

Given a digraph P and a block-sequential schedule s, does there exist a digraph G such that $\mathcal{P}(G,s) = P$?

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

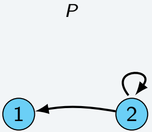
(G,s) P

Unique solution

Inverse problem

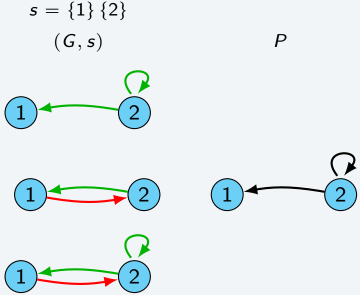
Given a digraph P and a block-sequential schedule s, does there exist a digraph G such that $\mathcal{P}(G, s) = P$?

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



Inverse problem

Given a digraph P and a block-sequential schedule s, does there exist a digraph G such that $\mathcal{P}(G, s) = P$?

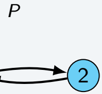


Multiple solutions

Inverse problem

Given a digraph P and a block-sequential schedule s, does there exist a digraph G such that $\mathcal{P}(G, s) = P$?

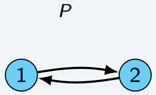
$s = \{1\}\{2\}$



Inverse problem

Given a digraph P and a block-sequential schedule s, does there exist a digraph G such that $\mathcal{P}(G, s) = P$?

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



No solution

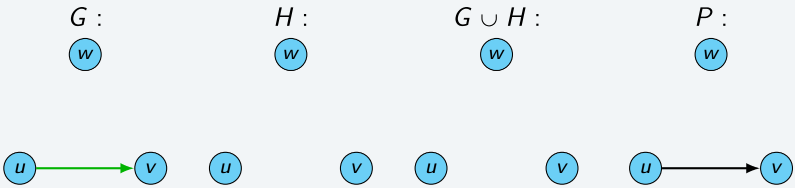
Complexity

Theorem

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

Proposition

Let s be an update schedule, and let P, G and H be three digraphs such that $\mathcal{P}(G, s) = \mathcal{P}(H, s) = P$, then $\mathcal{P}(G \cup H, s) = P$.



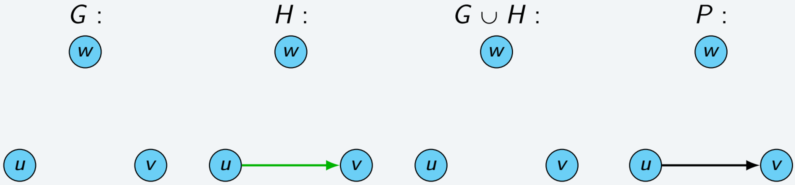
Complexity

Theorem

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

Proposition

Let s be an update schedule, and let P, G and H be three digraphs such that $\mathcal{P}(G,s) = \mathcal{P}(H,s) = P$, then $\mathcal{P}(G \cup H, s) = P$.



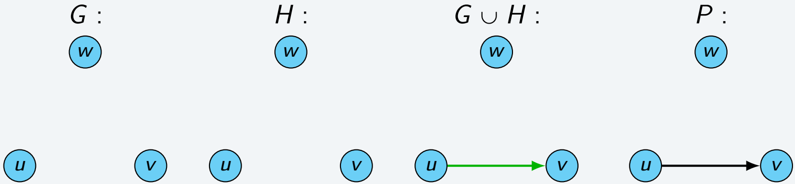
Complexity

Theorem

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

Proposition

Let s be an update schedule, and let P, G and H be three digraphs such that $\mathcal{P}(G, s) = \mathcal{P}(H, s) = P$, then $\mathcal{P}(G \cup H, s) = P$.



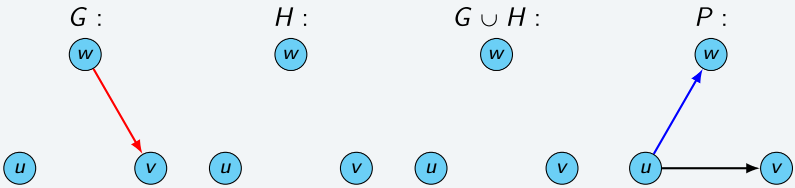
Complexity

Theorem

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

Proposition

Let s be an update schedule, and let P, G and H be three digraphs such that $\mathcal{P}(G, s) = \mathcal{P}(H, s) = P$, then $\mathcal{P}(G \cup H, s) = P$.



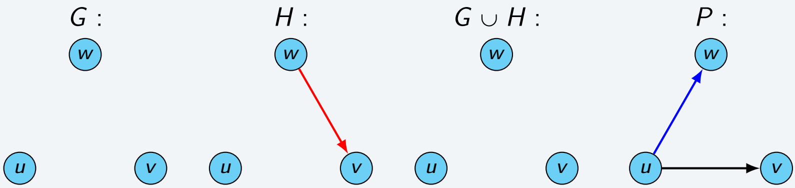
Complexity

Theorem

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

Proposition

Let s be an update schedule, and let P, G and H be three digraphs such that $\mathcal{P}(G, s) = \mathcal{P}(H, s) = P$, then $\mathcal{P}(G \cup H, s) = P$.



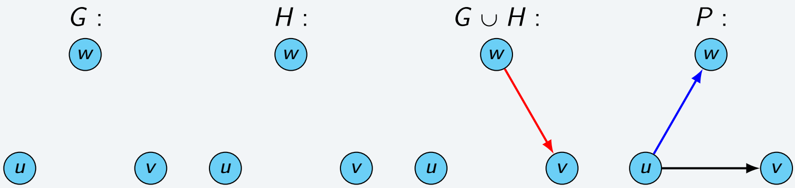
Complexity

Theorem

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

Proposition

Let s be an update schedule, and let P, G and H be three digraphs such that $\mathcal{P}(G, s) = \mathcal{P}(H, s) = P$, then $\mathcal{P}(G \cup H, s) = P$.



Algorithm

Algoritmo 1: MaximumPreImage(P, s)

$M \leftarrow \{(u, v) \in V \times V : s(u) < s(v)\}$;
for $(u, v) \notin A$ **do**
  for $w \in V$ **do**
    if $((u, w) \in A) \wedge ((w, v) \in M)$ **then**
      $M \leftarrow M \backslash \{(w, v)\}$
$GA \leftarrow \{(u, v) \in A : s(u) \geqslant s(v)\}$;
$RA \leftarrow \{(u, v) \in A : s(u) < s(v)\}$;
for $(u, v) \in RA$ **do**
  if $\forall w \in V, (u, w) \notin GA \vee (w, v) \notin M$ **then return** NULL;
$A' \leftarrow M \cup GA$;
return $G \leftarrow (V, A')$;

Algorithm

Algoritmo 2: enumerationPreImages(P, s)

$G \leftarrow \mathrm{MaximumPreImage}(P, s)$;
$S \leftarrow \{G\}$;
$Q \leftarrow \{G\}$;
while $Q \neq \emptyset$ **do**
    Let G be an element of Q;
    $Q \leftarrow Q \setminus \{G\}$;
    for $(u, v) \in A(G)$ **do**
        $G' \leftarrow G - (u, v)$;
        if $\mathcal{P}(G', s) = P$ **then**
            $S \leftarrow S \cup \{G'\}$;
            $Q \leftarrow Q \cup \{G'\}$;
return S

References

1. Julio Aracena, Eric Fanchon, Marco Montalva, and Mathilde Noual. Combinatorics on updatedigraphs in boolean networks. Discrete Applied Mathematics, 159(6):401–409, 2011.
2. Julio Aracena, Eric Goles, Andrés Moreira, and Lilian Salinas. On the robustness of updateschedules in boolean networks. Biosystems, 97(1):1–8, 2009.
3. Eric Goles and Mathilde Noual. Disjunctive networks and update schedules. Advances in Applied Mathematics, 48(5):646–662, 2012.
4. F. Robert.Discrete iterations: a metric study, volume 6 of Series in Computational Mathematics. Springer, 1986.

Thanks!