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From kernels in directed graphs to fixed points and negative cycles in Boolean networks

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Abstract

We consider a class of Boolean networks called and-nets, and we address the question of whether the absence of negative cycle in local interaction graphs implies the existence of a fixed point. By defining correspondences with the notion of kernel in directed graphs, we prove a particular case of this question, and at the same time, we prove new theorems in kernel theory, on the existence and unicity of kernels.

Key words: Discrete dynamical system, Directed graph, Fixed point, Kernel, Negative cycle, Odd cycle.

1. Introduction

Boolean networks represent the dynamic interaction of components which can take two values, 0 and 1. Introduced by von Neumann in the context of automata theory [20], they have gained some recent interest through:

1. the study of relationships between the dynamics and the structure of these networks along the line developed by Robert [15], in particular the result of Shih and Dong [16] relating fixed points to cycles in local interaction graphs;
2. their applicability to gene regulatory networks (see, e.g., [6]), in particular rules conjectured by the biologist Thomas and relating positive or negative cycles in the local interaction graphs to non-unicity of fixed points or sustained oscillations [18, 19].

Arising from these two lines of research, a natural question is whether the absence of negative cycle in local interaction graphs implies the existence of a fixed point. While the answer to the general case is unknown, we approach in

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this article the case of and-nets, which are Boolean networks such that each component is a conjunction of its (positive or negative) inputs.

This is where kernels, a graph-theoretical notion introduced by von Neumann [21] in the context of game theory (see also [2, 1]), enter into play. In this article, by showing that fixed points of an and-net are in correspondence with kernels of some directed graph, we solve a particular case of the above question on and-nets, and at the same time, we prove new results on kernel theory itself, in particular generalizations of well-known theorems of von Neumann [21], Boros and Gurvich [3], Richardson [14] and Galeana-Sánchez and Neumann-Lara [4].

We finally complete the paper by explaining how the above results on and-nets can be proved to hold for the more general class of and-or-nets.

2. Fixed points in Boolean networks

2.1. Boolean networks and signed directed graphs

A *signed directed graph* S consists in a finite set of vertices $\mathcal{V}(S)$ and a set of *signed arcs* $\mathcal{A}(S) \subseteq \mathcal{V}(S) \times \{+, -\} \times \mathcal{V}(S)$. S is said to be *simple* when for any vertices u and v , $\mathcal{A}(S)$ does not contain both a positive and a negative arc from u to v . The directed graph underlying S , obtained by forgetting signs, is denoted by $|S|$. A signed directed graph S' is a *subgraph* of S if $\mathcal{V}(S') \subseteq \mathcal{V}(S)$ and $\mathcal{A}(S') \subseteq \mathcal{A}(S)$. A *cycle* of S is a simple subgraph C of S such that $|C|$ is an elementary directed cycle (the considered cycles are always elementary and directed). A cycle of S is *positive* (resp. *negative*) if it contains an even (resp. odd) number of negative arcs.

Let $\mathbb{B} = \{0, 1\}$ and V be a finite set. If $x \in \mathbb{B}^V$ and $v \in V$, then x_v denotes the image of v by x , and \bar{x}^v is the element of \mathbb{B}^V defined by $(\bar{x}^v)_v = 1 - x_v$ and $(\bar{x}^v)_u = x_u$ for every $u \neq v$. More generally, if $W \subseteq V$, \bar{x}^W is the element of \mathbb{B}^V defined by $(\bar{x}^W)_u = 1 - x_u$ for $u \in W$ and $(\bar{x}^W)_u = x_u$ otherwise.

A map $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ is often seen as a *Boolean network*. In this context, V corresponds to the set of components of the network, \mathbb{B}^V to the set of possible states (or configurations), and f to the global transition function. The local transition function associated with $v \in V$ is the map $f_v : \mathbb{B}^V \rightarrow \mathbb{B}$ defined by $f_v(x) = f(x)_v$. Given $u, v \in V$, the *discrete derivative* of f_v with respect to u is the map $f_{vu} : \mathbb{B}^V \rightarrow \{-1, 0, 1\}$ defined by:

$$f_{vu}(x) = \frac{f_v(\bar{x}^u) - f_v(x)}{(\bar{x}^u)_u - x_u}.$$

Given $x \in \mathbb{B}^V$, the *local interaction graph* of f at x , denoted by $\mathcal{G}(f)(x)$, is the signed directed graph with vertex set V and a positive (resp. negative) arc from u to v when $f_{vu}(x)$ is positive (resp. negative). The *global interaction graph* of f , denoted by $\mathcal{G}(f)$, is the signed directed graph with vertex set V and a positive (resp. negative) arc from u to v when $f_{vu}(x)$ is positive (resp. negative) for some $x \in \mathbb{B}^V$. For all $x \in \mathbb{B}^V$, $\mathcal{G}(f)(x)$ is therefore a subgraph of $\mathcal{G}(f)$.

2.2. Some results and a question

Since the seminal works of Kauffman [5, 6] and Thomas [17, 19], Boolean networks are extensively used to model gene regulatory networks. In this context, the most reliable biological informations often concern $\mathcal{G}(f)$; few informations on f itself are available. In addition, the fixed points of f are of great interest: they correspond to stable patterns of gene expressions that often characterize some biological functions. It is then interesting to try to deduce from $\mathcal{G}(f)$ some information about the fixed points of f , as in the three theorems below (in the first two theorems, the second assertion follows from the fact that each local interaction graph $\mathcal{G}(f)(x)$ is a subgraph of $\mathcal{G}(f)$).

Theorem 1 (Shih, Dong [16]) *If $\mathcal{G}(f)(x)$ has no cycle for all $x \in \mathbb{B}^V$, then f has a unique fixed point. As a consequence, if $\mathcal{G}(f)$ has no cycle, then f has a unique fixed point.*

Theorem 2 (Remy, Ruet, Thieffry [9]) *If $\mathcal{G}(f)(x)$ has no positive cycle for all $x \in \mathbb{B}^V$, then f has at most one fixed point. As a consequence, if $\mathcal{G}(f)$ has no positive cycle, then f has at most one fixed point.*

Theorem 3 (Richard [11]) *If $\mathcal{G}(f)$ has no negative cycle, then f has at least one fixed point.*

These three theorems lead to the following natural question.

Question 1 *Is it true that if $\mathcal{G}(f)(x)$ has no negative cycle for all $x \in \mathbb{B}^V$, then f has at least one fixed point?*

A positive answer would improve Theorem 3, and give, together with Theorem 2, a nice proof by dichotomy of Theorem 1. However, while Theorems 1, 2 and 3 hold in the non-Boolean discrete cases too, *i.e.*, when \mathbb{B} is replaced by a finite interval of integers of size more than two [8, 13, 10, 11], the question has a negative answer in the non-Boolean discrete case [11]. A positive answer has been given in the non-expansive Boolean case, *i.e.*, for maps $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ such that for all $x, y \in \mathbb{B}^V$, the Hamming distance between $f(x)$ and $f(y)$ is at most the Hamming distance between x and y [12]. Partial converses to Theorem 2 have been given in [7] by introducing a notion of chordless cycles.

3. Results

3.1. And-nets

We are interested in solving Question 1 for a particular class of Boolean networks, called *and-nets*. In such networks, each local transition function is a conjunction of literals.

Definition (And-net) A map $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ is called an *and-net* when for each $v \in V$, f_v is an *and-map*, i.e. there exist disjoint sets $P_v, N_v \subseteq V$ such that

$$f_v(x) = \prod_{u \in P_v} x_u \prod_{u \in N_v} (1 - x_u),$$

with the convention that the empty product is 1. Vertices in P_v (resp. N_v) are called *positive* (resp. *negative*) *inputs* of f_v .

The following immediate property gives a correspondence between and-nets and simple signed directed graphs.

Proposition 1 1. If $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ is an *and-net*, then $\mathcal{G}(f)$ has a *positive* (resp. *negative*) *arc* from u to v if and only if u is a *positive* (resp. *negative*) *input* of f_v . In particular, since P_v and N_v are disjoint for all v , $\mathcal{G}(f)$ is a *simple*.
2. Conversely, for any *simple signed directed graph* S with vertex set V , there is a *unique and-net* $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ such that $S = \mathcal{G}(f)$; we call it the *and-net* associated with S .

Our interest for and-nets f comes from the fact that, as shown by the previous proposition, f and $\mathcal{G}(f)$ share the same information, so that local conditions of Theorems 1, 2 and Question 1 can be translated into (much simpler) conditions on cycles of the global interaction graph $\mathcal{G}(f)$. This translation involves the notion of delocalizing triple.

Definition (Delocalizing triple) Given a signed directed graph S , a cycle C of S and vertices u, v_1, v_2 of S , (u, v_1, v_2) is said to be a *delocalizing triple* of C when

1. v_1, v_2 are distinct vertices of C ,
2. $(u, +, v_1)$ is an arc of S that is not in C ,
3. $(u, -, v_2)$ is an arc of S that is not in C .

A delocalizing triple (u, v_1, v_2) of C is *internal* when u is a vertex of C , *external* otherwise.

This definition is illustrated in Figure 3. The following property shows that, for and-nets, the absence of delocalizing triples for a given cycle is equivalent to its locality.

Proposition 2 Let $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ be an *and-net*, and let C be a cycle of $\mathcal{G}(f)$. There exists $x \in \mathbb{B}^V$ such that C is a cycle of $\mathcal{G}(f)(x)$ if and only if C has no delocalizing triple.

PROOF. It is sufficient to show that, given an arc (w, s, v) of $\mathcal{G}(f)$ and $x \in \mathbb{B}^V$, (w, s, v) is an arc of $\mathcal{G}(f)(x)$ if and only if f_v has no positive input $u \neq w$ such that $x_u = 0$, and no negative input $u \neq w$ such that $x_u = 1$.

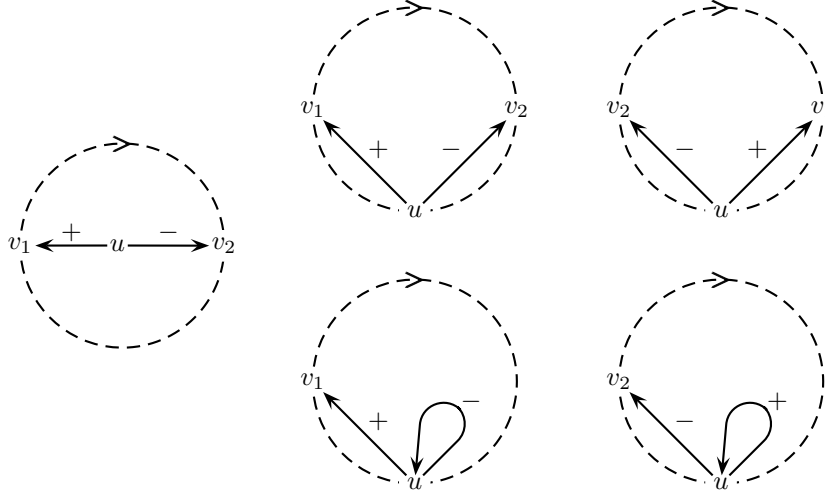


Figure 1: External and internal delocalizing triples of a cycle in a signed directed graph.

1. On one hand, if (w, s, v) is an arc of $\mathcal{G}(f)(x)$, then $f_v(x) \neq f_v(\bar{x}^w)$, so either $f_v(x) = 1$ or $f_v(\bar{x}^w) = 1$, and we deduce that $x_u = (\bar{x}^w)_u = 1$ for every positive input $u \neq w$ of f_v , and $x_u = (\bar{x}^w)_u = 0$ for every negative input $u \neq w$ of f_v .
2. On the other hand, if f_v has no positive input $u \neq w$ such that $x_u = 0$, and no negative input $u \neq w$ such that $x_u = 1$, then $f_v(x) \neq f_v(\bar{x}^w)$ and we deduce that (w, s, v) is an arc of $\mathcal{G}(f)(x)$.

□

As an easy consequence of this proposition, we have a reformulation of Theorems 1, 2 and Question 1 for and-nets, in terms of global interaction graphs and delocalizing triples.

Theorem 1' *Let f be an and-net. If every cycle of $\mathcal{G}(f)$ has a delocalizing triple, then f has a unique fixed point.*

Theorem 2' *Let f be an and-net. If every positive cycle of $\mathcal{G}(f)$ has a delocalizing triple, then f has at most one fixed point.*

Question 1' *Let f be an and-net. Is it true that if every negative cycle of $\mathcal{G}(f)$ has a delocalizing triple, then f has at least one fixed point?*

We have not been able to solve this question. However, in Section 5, by using tools from kernel theory in directed graphs, we shall provide the following partial answer (which generalizes Theorem 3 for and-nets).

Theorem 3' *Let f be an and-net. If every negative cycle of $\mathcal{G}(f)$ has an internal delocalizing triple, then f has at least one fixed point.*

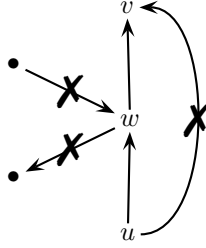


Figure 2: A subdivision of (u, v) .

3.2. Kernels in directed graphs

Let D be a directed graph. We shall only consider simple directed graphs and therefore assume that $\mathcal{A}(D) \subseteq \mathcal{V}(D) \times \mathcal{V}(D)$. A vertex u *dominates* a vertex v when D has an arc from u to v . A set I of vertices of D is called *independent* when no arc of D links two vertices in I , and *absorbent* when every vertex not in I dominates at least one vertex in I . A *kernel* is an independent and absorbent set of vertices. Kernels have many applications and several interesting relations with other areas, in particular with game theory; see [3] for a survey.

In the next section, we shall relate the notion of delocalizing triple (of a signed directed graph) to the following notion of killing triple (of a directed graph), which requires the following definition of *subdivisions*.

Definition (Subdivision) Let D be a directed graph. Given vertices u, v of D (not necessarily distinct), a vertex $w \neq u, v$ is said to be a *subdivision* of (u, v) when:

1. (u, w) and (w, v) are arcs of D ,
2. (u, v) is not an arc of D ,
3. the in-degree and out-degree of w both equal 1.

A vertex is a *subdivision* when it is a subdivision of some pair of vertices.

See Figure 2.

Definition (Killing triple) Given a directed graph D , a cycle C of D and vertices u, v_1, v_2 of D , (u, v_1, v_2) is called a *killing triple* of C when:

1. v_1 and v_2 are distinct vertices of C ,
2. (v_1, u) has a subdivision in D , but no subdivision of (v_1, u) belongs to C .
3. (v_2, u) is an arc of D that is not in C ,

A killing triple (u, v_1, v_2) of C is *internal* when u is a vertex of C , *external* otherwise.

The *parity* of a cycle is the parity of the number of its arcs. The next section will establish correspondences between positive (resp. negative) cycles and even (resp. odd) cycles, and between fixed points and kernels. These correspondences

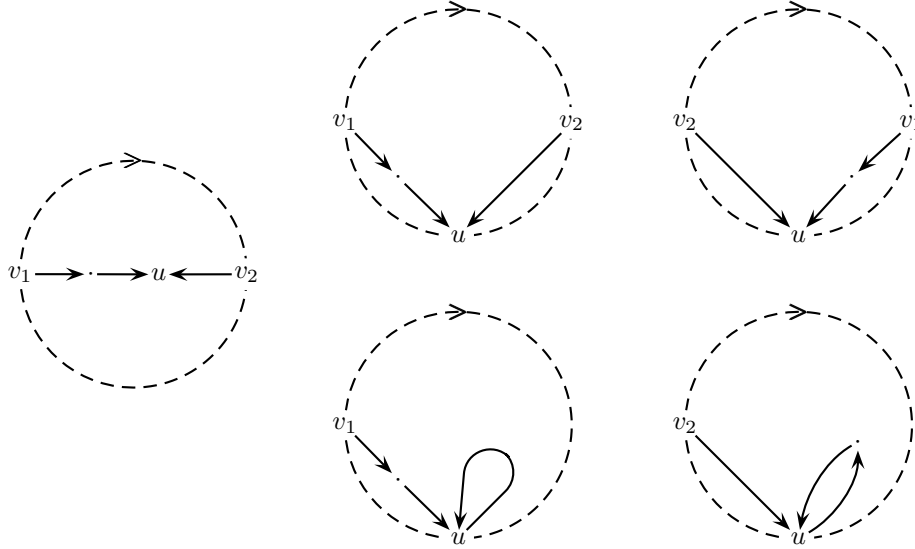


Figure 3: External and internal killing triples of a cycle in a directed graph. The dots (\cdot) are subdivisions.

will allow us to prove that Theorem 1', Theorem 2', Question 1', and Theorem 3' are respectively equivalent to Theorem 1'', Theorem 2'', Question 1'', and Theorem 3''.

Theorem 1'' *Let D be a directed graph. If every cycle of D has a killing triple, then D has a unique kernel.*

Theorem 2'' *Let D be a directed graph. If every even cycle of D has a killing triple, then D has at most one kernel.*

Question 1'' *Let D be a directed graph. Is it true that if every odd cycle of D has a killing triple, then D has at least one kernel?*

Theorem 3'' *Let D be a directed graph. If every odd cycle of D has an internal killing triple, then D has at least one kernel.*

The interest of these reformulations is twofold. Firstly, it will enable us to prove Theorem 3' (equivalently Theorem 3'') by using techniques from graph theory (Section 5). Secondly, it gives new results on kernel theory itself, as Theorems 1'', 2'' and 3'' generalize respectively the well-known theorems of von Neumann, Boros and Gurvich, and Richardson.

Theorem 4 (von Neumann [21]) *If a directed graph has no cycle, then it has a unique kernel.*

Theorem 5 (Boros, Gurvich [3]) *If a directed graph has no even cycle, then it has at most one kernel.*

Theorem 6 (Richardson [14]) *If a directed graph has no odd cycle, then it has at least one kernel.*

4. Reformulation in terms of kernels

In this section, we prove the equivalences, mentioned above, between statements on and-nets and directed graphs.

Theorem 7

Theorem 1'	\iff	Theorem 1''
Theorem 2'	\iff	Theorem 2''
Theorem 3'	\iff	Theorem 3''
Question 1'	\iff	Question 1''

4.1. Negative and-nets

We start by introducing a class of and-nets, called negative and-nets, which is in natural correspondence with directed graphs (Proposition 3), and by proving that this correspondence relates fixed points of negative and-nets and kernels of directed graphs (Proposition 4).

Definition (Negative and-net) A *negative and-net* is an and-net $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ such that for each $v \in V$, all inputs of f_v are negative.

Proposition 3 *For every directed graph D with vertex set V , there is a unique negative and-net $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ such that $D = |\mathcal{G}(f)|$; we call it the negative and-net associated with D .*

The *opposite* of a directed graph D (or a signed directed graph S), obtained by reversing the direction of arcs, is denoted by D^{op} (or S^{op}).

Proposition 4 *Let D be a directed graph and f be the negative and-net associated with D . There is a bijection between the set of fixed points of f and the set of kernels of D^{op} .*

PROOF. Let V be the vertex set of D , and let $\mathbf{1} : \mathbb{B}^V \rightarrow \mathcal{P}(V)$ be the bijection defined by mapping any point $x \in \mathbb{B}^V$ to the set $\mathbf{1}(x) \subseteq V$ of $u \in V$ such that $x_u = 1$. We prove that x is a fixed point of f if and only if $\mathbf{1}(x)$ is a kernel of D^{op} .

1. Let x be a fixed point of f . If $(v, u) \in \mathcal{A}(D^{\text{op}})$ and $u \in \mathbf{1}(x)$, then u is a negative input of v and $x_u = 1$, so $x_v = f_v(x) = 0$, hence $v \notin \mathbf{1}(x)$. Therefore $\mathbf{1}(x)$ is an independent set of vertices in D^{op} . Moreover, if $v \notin \mathbf{1}(x)$, then $0 = x_v = f_v(x)$ and f_v has at least one negative input u such that $x_u = 1$. Therefore $(v, u) \in \mathcal{A}(D^{\text{op}})$ and $u \in \mathbf{1}(x)$. We conclude that $\mathbf{1}(x)$ is an absorbent set of D^{op} , hence a kernel.

2. Assume on the other hand that $\mathbf{1}(x)$ is a kernel of D^{op} , and let v be any vertex of D^{op} . If $v \in \mathbf{1}(x)$, then any vertex u dominated by v in D^{op} is not in $\mathbf{1}(x)$. In other words, f_v has no input u in $\mathbf{1}(x)$, and we deduce that $f_v(x) = 1 = x_v$. On the other hand, if $v \notin \mathbf{1}(x)$, then v dominates some vertex $u \in \mathbf{1}(x)$ in D^{op} . Hence f_v has an input u such that $x_u = 1$, and we deduce that $f_v(x) = 0 = x_v$. Therefore x is a fixed point of f .

□

4.2. Removing signs

In this section, we prove direction \Leftarrow of Theorem 7. To this end, we shall associate with every simple signed directed graph S , a directed graph S^* such that: (i) the and-net associated with S and the negative and-net associated with S^* have the same number of fixed points; (ii) if S satisfies the conditions of Theorems 1'-3' and Question 1', then $S^{*\text{op}}$ satisfies the conditions of Theorems 1''-3'' and Question 1''.

The desired directed graph S^* is obtained by replacing each positive arc of S by two successive arcs (and removing all signs).

Definition (S^*) Let S be a simple signed directed graph, and let

$$\begin{aligned}\mathcal{A}^-(S) &= \{(u, v) \mid (u, -, v) \in \mathcal{A}(S)\}, \\ \mathcal{A}^+(S) &= \{(u, v) \mid (u, +, v) \in \mathcal{A}(S)\}.\end{aligned}$$

Then S^* is the directed graph whose vertex set is the disjoint union $\mathcal{V}(S) \cup \mathcal{A}^+(S)$, and whose arcs are those in $\mathcal{A}^-(S)$, plus (u, a) and (a, v) for each $a = (u, v) \in \mathcal{A}^+(S)$.

Proposition 5 *If S is a simple signed directed graph, then the vertices in $\mathcal{A}^+(S)$ are subdivisions in S^* .*

Proposition 6 *Let S be a simple signed directed graph. The and-net associated with S and the negative and-net associated with S^* have the same number of fixed points.*

PROOF. Let V be the vertex set of S and $V^* = V \cup \mathcal{A}^+(S)$ be the vertex set of S^* . Let $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ be the and-net associated with S and $f^* : \mathbb{B}^{V^*} \rightarrow \mathbb{B}^{V^*}$ the negative and-net associated with S^* . Let

$$X = \{x \in \mathbb{B}^{V^*} \mid x_{(u,v)} = 1 - x_u \text{ for all } (u, v) \in \mathcal{A}^+(S)\}.$$

Since $f_{(u,v)}^*(x) = 1 - x_u$, every fixed point of f^* is in X . Consider the bijection from X to \mathbb{B}^V mapping each point $x \in X$ to the restriction x' of x on V . Since all the fixed points of f^* are in X , it is sufficient to prove that, for all $x \in X$,

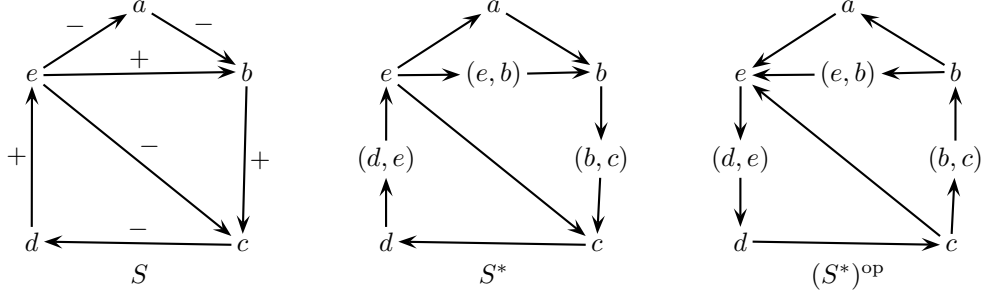


Figure 4: The cycle C of $(S^*)^{\text{op}}$ with vertex sequence $a, e, (d, e), d, c, (b, c), b, a$ comes from the cycle H of S with vertex sequence a, b, c, d, e, a . H has a delocalizing triple (e, b, c) in S , but C has no killing triple in $(S^*)^{\text{op}}$ ((e, b, c) is not a killing triple of C since a is a subdivision of (b, e) that belongs to C).

$f^*(x) = x$ if and only if $f(x') = x'$. Let $x \in X$. For all $v \in V$, we have

$$\begin{aligned}
f_v^*(x) &= \prod_{(u,v) \in \mathcal{A}^-(S^*)} 1 - x_u \\
&= \prod_{(u,v) \in \mathcal{A}^-(S)} 1 - x_u \prod_{(u,v) \in \mathcal{A}^+(S)} 1 - x_{(u,v)} \\
&= \prod_{(u,v) \in \mathcal{A}^-(S)} 1 - x_u \prod_{(u,v) \in \mathcal{A}^+(S)} x_u \quad \text{since } x \in X \\
&= \prod_{(u,v) \in \mathcal{A}^-(S)} 1 - x'_u \prod_{(u,v) \in \mathcal{A}^+(S)} x'_u \\
&= f_v(x').
\end{aligned}$$

Thus, if $f^*(x) = x$ then $f(x') = x'$. Conversely, if $f(x') = x'$, then $f_v^*(x) = f_v(x') = x'_v = x_v$ for all $v \in V$. Moreover, for any $(u, v) \in \mathcal{A}^+(S) = V^* \setminus V$ and $x \in X$, $f_{(u,v)}^*(x) = 1 - x_u = x_{(u,v)}$. Consequently, $f^*(x) = x$. \square

It is very easy to see that every even (resp. odd) cycle C of $S^{*\text{op}}$ can be obtained from a positive (resp. negative) cycle H of S by replacing each positive arc by two successive arcs, and by reversing every arcs: $(H^*)^{\text{op}} = C$. The situation is less straightforward for the correspondence between delocalizing and killing triples: it is possible for C to have no killing triple, whereas H has delocalizing triples; see Figure 4. However, nothing is lost for our purpose, thanks to the introduction of good delocalizing triples, which are sufficient to express the conditions of Theorems 1'-3' and Question 1' (Proposition 7), and become killing triples through the transformation $S \mapsto S^{*\text{op}}$ (Proposition 8).

Definition (Good delocalizing triple) Given a simple signed directed graph S and a cycle C of S , a delocalizing triple (u, v_1, v_2) of C is said to be *good* when either it is external, or the path from u to v_1 in C is not $(u, -, w), (w, -, v_1)$ for a vertex w whose in-degree and out-degree both equal 1.

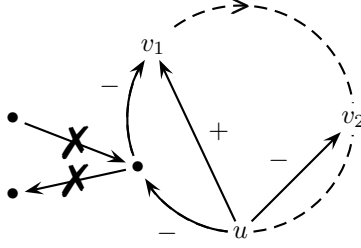


Figure 5: Forbidden configuration in the definition of internal good delocalizing triples.

This definition is illustrated in Figure 5.

Proposition 7 *Let S be a signed directed graph. Every positive cycle of S has a delocalizing triple (resp. an internal delocalizing triple) if and only if every positive cycle of S has a good delocalizing triple (resp. an internal good delocalizing triple). The assertion remains true if positive is replaced by negative.*

PROOF. We concentrate on the statements on positive cycles, the case of negative cycles is similar. The if part is immediate. In order to prove the only if part, we distinguish between the statement on internal good triples and the statement on arbitrary good triples.

1. Assume for a contradiction that every positive cycle of S has an internal delocalizing triple, and that the set X of positive cycles of S which do not have an internal good delocalizing triple is non-empty. Let C be an element of X of minimal length, and (u, v_1, v_2) be an internal delocalizing triple of C . As (u, v_1, v_2) is not a good delocalizing triple, there exists a vertex w whose in-degree and out-degree both equal 1 and such that the path from u to v_1 in C is $(u, -, w), (w, -, v_1)$. The cycle C' obtained from C by replacing this path by the arc $(u, +, v_1)$ is positive and has smaller length. Since an internal good delocalizing triple for C' would be an internal good delocalizing triple for C too, $C' \in X$, in contradiction with the minimality of C .
2. To prove the statement on arbitrary delocalizing triples, it suffices to observe that external delocalizing triples are good delocalizing triples and proceed as above.

□

Proposition 8 *Let S be a simple signed directed graph. For every even (resp. odd) cycle C in $(S^*)^{\text{op}}$, there is a positive (resp. negative) cycle H in S such that $(H^*)^{\text{op}} = C$. Furthermore, every external (resp. internal) good delocalizing triple of H in S is an external (resp. internal) killing triple of C in $(S^*)^{\text{op}}$.*

PROOF. The first assertion is obvious, and the second is straightforward for external good delocalizing triples. We therefore consider the statement on internal good delocalizing triples. Let (u, v_1, v_2) be an internal good delocalizing triple

of H . Clearly, u is a vertex of C , and v_1 and v_2 are distinct vertices of C . Since $(u, -, v_2)$ is an arc of S that is not in H , it is also obvious that (v_2, u) is an arc of $(S^*)^{\text{op}}$ that is not in C . It remains to prove that, in $(S^*)^{\text{op}}$, (v_1, u) has a subdivision and no subdivision of (v_1, u) is a vertex of C . Since $(u, +, v_1)$ is an arc of S that is not in H , $a = (u, v_1)$ is a subdivision of (v_1, u) in $(S^*)^{\text{op}}$ that is not a vertex of C . If (v_1, u) has a subdivision w that is a vertex of C , w is a vertex of S (since $w \neq a$), so $(u, -, w), (w, -, v_1)$ is the path from u to v_1 in H and both the in- and out-degree of w in S is one. Therefore, the delocalizing triple (u, v_1, v_2) is not good, a contradiction. \square

PROOF (OF DIRECTION \Leftarrow OF THEOREM 7). Let us prove that Theorem 1'' implies Theorem 1', the other cases being similar. Assume that Theorem 1'' holds. Let S be a simple signed directed graph such that every cycle of S has a delocalizing triple. Then, by Proposition 7, every cycle of S has a good delocalizing triple. We deduce from Proposition 8 that every cycle of $(S^*)^{\text{op}}$ has a killing triple. By Theorem 1'', $(S^*)^{\text{op}}$ has a unique kernel, and by Proposition 4, the negative and-net associated with S^* has a unique kernel. Hence, by Proposition 6, the and-net associated with S has a unique fixed point, and Theorem 1' is proved. \square

4.3. Adding signs

In this section, we prove direction \Rightarrow of Theorem 7. The general idea is similar: it consists in associating with every directed graph D , a simple signed directed graph D^* such that: (i) the negative and-net associated with D and the and-net associated with D^* have the same number of fixed points; (ii) if D^{op} satisfies the conditions of Theorems 1''-3'' and Question 1'', then D^* satisfies the conditions of Theorems 1'-3' and Question 1'.

The rough idea, in order to define D^* , is to consider the inverse of the graph transformation introduced in the previous case, *i.e.* to replace, when w is a subdivision of (u, v) , the two successive arcs $(u, w), (w, v)$, by a positive arc $(u, +, v)$, and two add a negative sign to the other arcs. As u, v may be subdivisions as well, this transformation may not be well-defined, but it is sufficient to restrict it to pairs (u, v) such that neither u nor v is itself a subdivision.

Definition (D^*) Let D be a simple directed graph. Let $\mathcal{C}(D)$ denote the set of pairs (u, v) of vertices with at least one subdivision and such that neither u nor v is a subdivision, and $\mathcal{W}(D)$ denote the set of vertices which are subdivision of some $(u, v) \in \mathcal{C}(D)$. Then D^* is the signed directed graph whose vertex set is $\mathcal{V}(D) \setminus \mathcal{W}(D)$ and whose arcs are:

$$\begin{aligned} &(u, -, v) \text{ for each } (u, v) \in \mathcal{A}(D) \text{ with } u, v \notin \mathcal{W}(D), \text{ and} \\ &(u, +, v) \text{ for each } (u, v) \in \mathcal{C}(D). \end{aligned}$$

Observe that D^* is simple because, by definition of a subdivision, $\mathcal{A}(D) \cap \mathcal{C}(D) = \emptyset$.

Proposition 9 *Let D be a directed graph. The negative and-net associated with D and the and-net associated with D^* have the same number of fixed points.*

PROOF. Let $V^* = \mathcal{V}(D^*) \subseteq \mathcal{V}(D) = V$, let $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ be the negative and-net associated with D , and let $f^* : \mathbb{B}^{V^*} \rightarrow \mathbb{B}^{V^*}$ be the and-net associated with D^* . For every $w \in \mathcal{W}(D) = V \setminus V^*$, there exists a unique pair $(u, v) \in \mathcal{C}(D)$ such that w is a subdivision of (u, v) ; we denote this unique pair by (u_w, v_w) (note that vertices u_w and v_w are not in $\mathcal{W}(D)$, since, by the definition of $\mathcal{C}(D)$, they are not subdivisions). Let

$$X = \{x \in \mathbb{B}^V \mid x_w = 1 - x_{u_w} \text{ for all } w \in \mathcal{W}(D)\}.$$

Observe that X and \mathbb{B}^{V^*} have the same cardinality. Furthermore, since $f_w(x) = 1 - x_{u_w}$, every fixed point of f is in X . Consider the bijection from X to \mathbb{B}^{V^*} mapping each point $x \in X$ to the restriction x' of x on V^* , i.e. $x'_v = x_v$ for all $v \in V^*$. Since all the fixed points of f are in X , it is sufficient to prove that, for all $x \in X$, $f(x) = x$ if and only if $f^*(x') = x'$. Let $x \in X$. For all $v \in V^*$, we have

$$\begin{aligned} f_v(x) &= \prod_{(u,v) \in \mathcal{A}(D)} 1 - x_u \\ &= \prod_{(u,v) \in \mathcal{A}(S), u \notin \mathcal{W}(D)} 1 - x_u \quad \prod_{(w,v) \in \mathcal{A}(D), w \in \mathcal{W}(D)} 1 - x_w \\ &= \prod_{(u,-,v) \in \mathcal{A}(D^*)} 1 - x_u \quad \prod_{(w,v) \in \mathcal{A}(D), w \in \mathcal{W}(D)} x_{u_w} \quad \text{since } x \in X \\ &= \prod_{(u,-,v) \in \mathcal{A}(D^*)} 1 - x_u \quad \prod_{(u,v) \in \mathcal{C}(D)} x_u \\ &= \prod_{(u,-,v) \in \mathcal{A}(D^*)} 1 - x_u \quad \prod_{(u,+,v) \in \mathcal{A}(D^*)} x_u \\ &= \prod_{(u,-,v) \in \mathcal{A}(D^*)} 1 - x'_u \quad \prod_{(u,+,v) \in \mathcal{A}(D^*)} x'_u \\ &= f_v^*(x'). \end{aligned}$$

Thus, if $f(x) = x$ then $f^*(x') = x'$. Conversely, if $f^*(x') = x'$, then $f_v(x) = f_v^*(x') = x'_v = x_v$ for all $v \in V^*$. And if $w \in \mathcal{W}(D) = V \setminus V^*$, we have $f_w(x) = x_w$ because $f_w(x) = 1 - x_{u_w}$ and $x \in X$. Thus $f(x) = x$. \square

Proposition 10 *Let D be a directed graph. For every positive (resp. negative) cycle C in D^* , there is an even (resp. odd) cycle H in D such that every external (resp. internal) killing triple of H^{op} in D^{op} is an external (resp. internal) delocalizing triple of C in D^* .*

PROOF. Let C be a cycle of D^* . For every $(u, v) \in \mathcal{A}^+(C)$, we have $(u, v) \in \mathcal{C}(D)$, therefore (u, v) has at least one subdivision in D , say w_{uv} . Consider

the cycle H whose vertices are those in $\mathcal{V}(C)$ plus vertex w_{uv} for each $(u, v) \in \mathcal{A}^+(C)$, and whose arcs are those in $\mathcal{A}^-(C)$ plus (u, w_{uv}) and (w_{uv}, v) for each $(u, v) \in \mathcal{A}^+(C)$. Then H is a cycle of D , which is even if C is positive and odd if C is negative.

Let (u, v_1, v_2) be a killing triple of H^{op} in D^{op} . Since u, v_1 and v_2 are not subdivisions in D , v_1 and v_2 are distinct vertices of C , and $u \in \mathcal{V}(H)$ if and only if $u \in \mathcal{V}(C)$. It remains to prove that $(u, +, v_1)$ and $(u, -, v_2)$ are arcs of D^* that are not in C . By definition of a killing triple, (u, v_1) has a subdivision in D , and no subdivision of (u, v_1) is a vertex of H . Therefore $(u, v_1) \in \mathcal{C}(D)$ and $(u, +, v_1) \in \mathcal{A}(D^*)$; moreover, if $(u, +, v_1) \in \mathcal{A}(C)$, then w_{uv_1} is a subdivision of (u, v_1) that is a vertex of H , a contradiction. By definition of a killing triple, (u, v_2) is an arc of D that is not in H . Since (u, v_2) cannot have a subdivision, $(u, v_2) \notin \mathcal{C}(D)$ and we deduce that $(u, -, v_2)$ is an arc of D^* which is not in C (since otherwise (u, v_2) would be in H). \square

PROOF (OF DIRECTION \Rightarrow OF THEOREM 7). Let us prove that Theorem 1' implies Theorem 1'', the other cases being similar. Let D be directed graph such that every cycle of D^{op} has a delocalizing triple, and let us prove, assuming Theorem 1', that D^{op} has a unique kernel. According to Proposition 10, every cycle of D^* has a delocalizing triple. Thus, according to Theorem 1', the and-net associated with D^* has a unique fixed point, and we deduce from Proposition 9 that the negative and-net associated with D has a unique fixed point. Following Proposition 4, D^{op} has a unique kernel and Theorem 1'' is proved. \square

5. Proof of Theorem 3'

Let D be a directed graph and C be a cycle of D of length $l \geq 1$. We recall that an arc (u, v) of D is said to be a *chord* C when u and v are distinct vertices of C and $(u, v) \notin \mathcal{A}(C)$.

Definition (Bad vertex) Given a vertex u of C , C may be uniquely written as a sequence of vertices $C = v_0, v_1, v_2, \dots, v_{l-1}, v_0$ with $v_0 = u$. The set of vertices v_i , with i odd, $0 \leq i \leq l-1$, is then denoted by C_u . We shall say that u is a *bad vertex* of C if C has no chord (v, w) with $w \in C_u \cup \{u\}$.

Galeana-Sánchez and Neumann-Lara have proved the following extension of Richardson's theorem.

Theorem 8 (Galeana-Sánchez, Neumann-Lara [4]) *Let D be a directed graph. If every odd cycle of D has no bad vertex, then D has at least one kernel.*

In this section, we prove the following theorem, which implies the theorem of Galeana-Sánchez and Neumann-Lara, as well as Theorem 3'' (equivalently Theorem 3'). The proof follows the idea of Galeana-Sánchez and Neumann-Lara, while being a bit more technical.

Theorem 9 *Let D be a directed graph. If every odd cycle of D with a bad vertex has an internal killing triple, then D has at least one kernel.*

We shall first need the following lemma.

Lemma 1 *Let D be a directed graph and D' a spanning subgraph of D obtained:*

1. *either by removing all arcs starting from a vertex w with out-degree at least two;*
2. *or by removing an arc (u, w) such that, for some vertices v and x , w and x are distinct subdivisions of (u, v) .*

If every even (resp. odd) cycle of D with a bad vertex has an internal killing triple, then every even (resp. odd) cycle of D' with a bad vertex has an internal killing triple.

PROOF. If C is a cycle of D' with a bad vertex, then it is clearly a cycle of D , and w is not a vertex of C since it has either out-degree 0 or in-degree 0 in D' . Therefore, C has the same chords in D and in D' , and it has a bad vertex in D too. The hypothesis of the lemma then implies that C has an internal killing triple (u, v_1, v_2) in D , and to prove that it is an internal killing triple of C in D' , it is sufficient to prove that (v_1, u) has a subdivision in D' . This is obvious if w is not a subdivision of (v_1, u) . If w is a subdivision of (v_1, u) then we are in the second case (since in the first case w has out-degree at least 2 in D), and by hypothesis, (v_1, u) also has, in D , a subdivision $x \neq w$, which is clearly a subdivision of (v_1, u) in D' . \square

The remainder of the section is devoted to prove Theorem 9. Assume for a contradiction that D is a minimal counterexample with respect to the number of arcs.

Claim 1 *For any vertices u and v , (u, v) has at most one subdivision in D .*

PROOF. Suppose for a contradiction that (u, v) has two distinct subdivisions, say w and x , and let D' be the subgraph of D obtained by removing the arc (u, w) . By Lemma 1, every odd cycle of D' with a bad vertex has an internal good triple, hence D' has a kernel K . Clearly, K is absorbent in D , and since K may not be a kernel of D , K is not independent in D , i.e., $u, w \in K$. As K is independent in D' , $x, v \notin K$. As x has out-degree 1 and K is absorbent in D' , $v \in K$, and we have a contradiction. This proves Claim 1. \square

It is clear that the maximal out-degree of D is at least 2 (otherwise, D would have no odd cycle, and by Richardson's theorem, it would have a kernel). Let therefore:

- u be a vertex of D with out-degree at least 2,
- X be the set of arcs (u, v) of D for all $v \in \mathcal{V}(D)$,

- D' be the spanning subgraph of D obtained by removing all arcs of X .

By Lemma 1, every odd cycle of D' with a bad vertex has an internal good triple, therefore D' has a kernel. Let:

- K be a kernel of D' ,
- I be the set of vertices of K dominated by u ,
- U be the set of vertices of D distinct from u that dominate a vertex in I .

Since u is of out-degree 0 in D' , $u \in K$. Moreover, since K is not a kernel of D , $I \neq \emptyset$. And since $u \notin U$ and K is an independent set of D' , we have $K \cap U = \emptyset$.

Definition (Perfect path) A *perfect path* is an elementary directed path $P = v_0, v_1, \dots, v_l$ of D of length $l \geq 0$ such that:

- $v_0 \in I$ and $v_l \in K$,
- $v_i \in K$ if and only if i is even,
- $v_0, \dots, v_l \notin U$,
- for all $i < j$ with i even and j odd, $(v_j, v_i) \notin \mathcal{A}(D)$,
- for all $i \leq j < l - 2$ with i and j odd, (v_j, v_i) has no subdivision,
- for all i odd, if $v_{l-1}v_i$ has a subdivision, then it is v_l .

v_l is the *endpoint* of P .

Observe that conditions (a) and (b) imply that l is even, and that for each even $k < l$, the prefix path v_0, v_1, \dots, v_k is perfect too. Finally, let

- K' be the set of $v \in K$ such that there exists a perfect path with v as endpoint.

Claim 2 *There is no perfect path with endpoint u . Therefore $u \notin K'$.*

PROOF. Given a vertex v , $d(v)$ denotes the total degree (sum of in-degree and out-degree) of v in D' , and the *weight* of a path is defined as the sum of the degrees of its vertices. Now, suppose, for a contradiction, that the set of perfect paths with endpoint u is non-empty, and take in this set the a perfect path

$$P = v_0, v_1, \dots, v_l$$

of minimal weight. Since $v_l = u$ and $v_0 \in I$,

$$C = v_0, v_1, \dots, v_l, v_0$$

is an odd cycle of D .

We first prove that if (v_j, v_i) is a chord of C , then i is odd, *i.e.*, $v_i \notin K$. Suppose for a contradiction, that C has a chord (v_j, v_i) with $v_i \in K$. Since

$v_j \notin U$ and $v_0 \in I$, we have $i \neq 0$, and since K is an independent set, $v_j \notin K$. Therefore i is even, j is odd, hence $j < i$ according to (d). Since $j \neq i - 1$,

$$P' = v_0, v_1, \dots, v_{j-1}, v_j, v_i, v_{i+1}, \dots, v_l$$

is a perfect path with endpoint u , whose weight is smaller than the weight of P , a contradiction. We conclude that $v_i \notin K$, *i.e.*, i is odd.

Consequently, u is a bad vertex of C and C has an internal good triple (v_i, v_j, v_k) . Let w be a (actually the unique by Claim 1) subdivision of (v_j, v_i) . Observe that $w \neq u$ and $w \neq v_0$ because by definition of good triples, w is not a vertex of C . Furthermore, as (v_k, v_i) is a chord of C , i is odd, *i.e.*, $v_i \notin K$. Since K is an absorbent set of D' and v_i is the unique vertex dominated by w , this implies that $w \in K$. There are now two cases.

1. If $j = l$, then $v_j = u$ and $w \in I$, therefore

$$P' = w, v_i, v_{i+1}, \dots, v_l$$

is a perfect path with endpoint u . If $i = 1$, its weight is smaller than the weight of P : indeed, by Claim 1, v_0 and w cannot be two distinct subdivisions of (v_l, v_1) , hence $d(w) = 2 < d(v_0)$. If $i > 1$, the weight of P' is clearly smaller than the weight of P too, and in both cases, we have a contradiction with the minimality of P .

2. If $j < l$, then by minimality of P , $v_j \neq u$, and $v_j \notin K$ because $w \in K$ and K is independent in D' , *i.e.*, j is odd. By (f), we have $j < l - 1$ because i is odd and $w \neq u$. From (e), we may then deduce that $j < i$. Now, the path

$$P' = v_0, v_1, \dots, v_j, w, v_i, v_{i+1}, \dots, v_l$$

is a perfect path with endpoint u . If $j = i - 2$, its weight is smaller than the weight of P : indeed, by Claim 1, v_{i-1} and w cannot be two distinct subdivisions of (v_{i-2}, v_i) , hence $d(w) = 2 < d(v_{i-1})$. If $j < i - 2$, the weight of P' is clearly smaller than the weight of P too, and in both cases, we have a contradiction with the minimality of P .

This completes the proof of Claim 2. □

Claim 3 K' is an independent set of D , and it is semi-absorbent: every vertex $w \notin K'$ dominated by a vertex in K' dominates some vertex in K' .

PROOF. By Claim 2, $u \notin K'$, therefore $I \subseteq K' \subseteq K \setminus \{u\}$, and K' is thus an independent set of D . Suppose for a contradiction that K' is not semi-absorbent. Let (v, w) be an arc of D such that $v \in K'$, $w \notin K'$ and w dominates no vertex in K' . Then $w \neq u$, and since $K \setminus \{u\}$ is independent, $w \notin K$. Since K is a kernel of D' , w dominates at least one vertex $x \in K \setminus K'$. Let $P = v_0, v_1, \dots, v_l$ be a perfect path with endpoint $v_l = v$, and consider the path

$$P' = v_0, v_1, \dots, v_{l-1}, v_l, v_{l+1}, v_{l+2}, \quad v_{l+1} = w, \quad v_{l+2} = x.$$

Clearly, $v_0, v_2, \dots, v_l \in K'$, hence v_{l+1} dominates no v_i with i even, $i \leq l$. As a consequence, P' satisfies conditions (a), (b), (c), (d) of the definition of a perfect path. Since $x \notin K'$, P' is not a perfect path.

1. If P' does not enjoy condition (e), there exist $i \leq j < l$, such that i, j are odd and (v_j, v_i) has a subdivision in D , say y . Since P is perfect, $j = l - 1$ and $y = v_l = v$. Therefore v has out-degree 1, hence $w = v_i$, and w dominates $v_{i+1} \in K'$, a contradiction.
2. If P' does not enjoy condition (f), there exists i odd such that (v_{l+1}, v_i) has a subdivision $y \neq v_{l+2} = x$ in D . As y is dominated by $v_{l+1} = w$, $y \notin K'$. Since, moreover, the only vertex dominated by y is $v_i \notin K$ and K is absorbent, $y \in K \setminus K'$. But then, setting $v_{l+2} = y$ instead of x , P' becomes a perfect path, because by Claim 1, y is the unique subdivision of (v_{l+1}, v_i) . Hence $y \in K'$ and we have a contradiction.

This completes the proof of Claim 3. \square

We are now in position to prove Theorem 9. Let L be the set of vertices that are not in K' and dominate no vertex in K' .

Let $D[L]$ be the subgraph of D induced by L . Let $u, v \in L$, and suppose that (u, v) has, in D , a subdivision w . Since $u \in L$, w is not a vertex of K' , and since the only vertex that w dominates is v , which is not in K' , we have $w \in L$. We deduce that every odd cycle of $D[L]$ with a bad vertex has an internal good triple. Since $\emptyset \neq I \subseteq K'$, $D[L]$ is a strict subgraph of D , and as a consequence, $D[L]$ has a kernel M .

Since K' is an independent and semi-absorbent set of D , by construction, K' is a kernel of $D[\mathcal{V}(D) \setminus L]$. Since K' is semi-absorbent and by the definition of L , there is no arc between $D[L]$ and $D[K']$, thus $K' \cup M$ is an independent set of D . For every vertex $v \notin K' \cup M$, either $v \in L$ and it dominates some vertex in M (because M is a kernel of $D[L]$) or $v \notin L$ and it dominates some vertex of K' (because K' is a kernel of $D[\mathcal{V}(D) \setminus L]$). Therefore $K' \cup M$ is absorbent in D . As a consequence, $K' \cup M$ is a kernel of D , and we have a contradiction with the hypothesis that D is a counterexample to Theorem 9.

6. And-or-nets

We finish this paper by mentioning an easy but significant generalization of Theorem 1', Theorem 2', Question 1', and Theorem 3'. Recall that a map $\varphi : \mathbb{B}^V \rightarrow \mathbb{B}$ is said to be a clause when it is a disjunction of literals, *i.e.*, there exist disjoint sets P and $N \subseteq V$ such that

$$\varphi(x) = \bigvee_{u \in P} x(u) \vee \bigvee_{u \in N} (1 - x(u)),$$

where \vee denotes supremum and the empty supremum is 0. As in the case of and-maps, vertices in P (resp. in N) are called *positive (resp. negative) inputs* of φ . A map $f : \mathbb{B}^V \rightarrow \mathbb{B}^V$ is called an *and-or-net* when for each $v \in V$, f_v is either an and-map or a clause.

Given an and-or-net f , let V_1, V_2 be the partition of V such that $v \in V_1$ if and only if f_v is an and-map. Let C be a cycle of $\mathcal{G}(f)$, and $u, v_1, v_2 \in V$. Then (u, v_1, v_2) is said to be a *delocalizing triple* of C when v_1, v_2 are distinct vertices of C and $(u, s_1, v_1), (u, s_2, v_2)$ are two arcs of $\mathcal{G}(f)$ that are not in C and such that

$$\begin{aligned} s_1 = + \text{ and } s_2 = - \text{ if } v_1, v_2 \in V_1 \text{ or } v_1, v_2 \in V_2, \\ s_1 = s_2 \text{ in all other cases.} \end{aligned}$$

If in addition, u is a vertex of C , then (u, v_1, v_2) is called an *internal delocalizing triple* of C . Clearly, $V_1 = V$ if and only if f is an and-net, and we recover the definition of delocalizing triples for and-nets. It is also easy to see that point 2 of Proposition 2 can be extended to and-or-nets.

Now, given an and-or-net f as above, consider the map

$$\tilde{f} : \mathbb{B}^V \rightarrow \mathbb{B}^V \text{ defined by } \tilde{f}(x) = \overline{f(\bar{x}^{V_2})}^{V_2}.$$

Then \tilde{f} is an and-net, and x is a fixed point of f if and only if \bar{x}^{V_2} is a fixed point of \tilde{f} . Moreover, $|\mathcal{G}(\tilde{f})| = |\mathcal{G}(f)|$ and the signs of arcs are given by the following rules:

- for $u, v \in V_1$ or $u, v \in V_2$, $(u, s, v) \in \mathcal{A}(\mathcal{G}(\tilde{f}))$ if and only if $(u, s, v) \in \mathcal{A}(\mathcal{G}(f))$;
- for $(u, v) \in (V_1 \times V_2) \cup (V_2 \times V_1)$, $(u, +, v) \in \mathcal{A}(\mathcal{G}(\tilde{f}))$ if and only if $(u, -, v) \in \mathcal{A}(\mathcal{G}(f))$, and $(u, -, v) \in \mathcal{A}(\mathcal{G}(\tilde{f}))$ if and only if $(u, +, v) \in \mathcal{A}(\mathcal{G}(f))$.

In more intuitive terms, $\mathcal{G}(\tilde{f})$ is obtained from $\mathcal{G}(f)$ by iteratively flipping signs of arcs around each \vee -vertex (*i.e.*, each vertex in V_2). Therefore $\mathcal{G}(f)$ and $\mathcal{G}(\tilde{f})$ have the same cycles, and these cycles have the same signs. It is also easy to see that a cycle has a delocalizing triple (resp. an internal delocalizing triple) in $\mathcal{G}(f)$ if and only if it has a delocalizing triple (resp. an internal delocalizing triple) in $\mathcal{G}(\tilde{f})$. As a consequence, Theorem 1', Theorem 2', Question 1', and Theorem 3' can be extended to the class of and-or-nets.

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