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Complexity of fixed point counting problems in Boolean Networks*

Florian Bridoux^{†1}, Amélia Durbec^{‡1}, Kevin Perrot^{§1,2}, and Adrien Richard^{¶2,3}

¹Aix-Marseille Université, Université de Toulon, CNRS, LIS, Marseille, France

²Université Côte d’Azur, CNRS, I3S, Sophia Antipolis, France

³Universidad de Chile, CMM, Santiago, Chile

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Abstract

A *Boolean network* (BN) with n components is a discrete dynamical system described by the successive iterations of a function $f : \{0, 1\}^n \rightarrow \{0, 1\}^n$. This model finds applications in biology, where fixed points play a central role. For example, in genetic regulations, they correspond to cell phenotypes. In this context, experiments reveal the existence of positive or negative influences among components: component i has a positive (resp. negative) influence on component j meaning that j tends to mimic (resp. negate) i . The digraph of influences is called *signed interaction digraph* (SID), and one SID may correspond to a large number of BNs (which is, in average, doubly exponential according to n). The present work opens a new perspective on the well-established study of fixed points in BNs. When biologists discover the SID of a BN they do not know, they may ask: given that SID, can it correspond to a BN having at least/at most k fixed points? Depending on the input, we prove that these problems are in P or complete for NP, NP^{NP} , $\text{NP}^{\#\text{P}}$ or NEXPTIME. In particular, we prove that it is NP-complete (resp. NEXPTIME-complete) to decide if a given SID can correspond to a BN having at least two fixed points (resp. no fixed point).

Keywords: Complexity, Boolean networks, Fixed points, Interaction graph.

*This work extends some early results announced in [9].

[†]florian.bridoux@lis-lab.fr

[‡]amelia.durbec@lis-lab.fr

[§]kevin.perrot@lis-lab.fr

[¶]richard@unice.fr

1 Introduction

A *Boolean network* (BN) with n components is a discrete dynamical system described by the successive iterations of a function

$$f : \{0, 1\}^n \rightarrow \{0, 1\}^n, \quad x = (x_1, \dots, x_n) \mapsto f(x) = (f_1(x), \dots, f_n(x)).$$

The structure of the network is often described by a signed digraph D , called *signed interaction digraph* (SID) of f , catching effective positive and negative dependencies among components: the vertex set is $[n] = \{1, \dots, n\}$ and, for all $i, j \in [n]$, there is a positive (resp. negative) arc from j to i if $f_i(x) - f_i(y)$ is positive (resp. negative) for some $x, y \in \{0, 1\}^n$ that only differ in $x_j > y_j$. The SID provides a very rough information about f . Indeed, given a SID D , the set $F(D)$ of BNs whose SID is D is generally huge.

BNs have many applications. In particular, since the seminal papers of Kauffman [18, 19] and Thomas [40, 41], they are very classical models for the dynamics of gene networks. In this context, the first reliable experimental information often concern the SID of the network, while the actual dynamics are very difficult to observe [42, 22]. One is thus faced with the following question: *What can be said about the dynamics described by f according to D only?*

Among the many dynamical properties that can be studied, fixed points are of special interest. For instance, in the context of gene networks, they correspond to stable patterns of gene expression at the basis of particular cellular phenotypes [41, 2]. As such, they are arguably the property which has been the most thoroughly studied. The number of fixed points and its maximization in particular is the subject of a stream of work, *e.g.* in [34, 6, 30, 4, 14, 7, 13, 8].

From the computational complexity point of view, previous works essentially focused on decision problems of the following form: given f and a dynamical property P , what is the complexity of deciding if the dynamics described by f has the property P . For instance, it is well-known that deciding if f has a fixed point is NP-complete in general (see [21] and the references therein), and in P for some families of BNs, such as non-expansive BNs [10]. However, as mentioned above, in practice, f is often unknown while its SID is well approximated. Hence, a more natural question is: given a SID D and a dynamical property P , what is the complexity of deciding if the dynamics described by some $f \in F(D)$ has the property P . Up to our knowledge, there is, perhaps surprisingly, no work concerning this kind of questions.

In this paper, we study this class of decision problems, focusing on the maximum and minimum number of fixed points. More precisely, given a SID D , we respectively denote by $\phi^{\max}(D)$ and $\phi^{\min}(D)$ the maximum and minimum number of fixed points in a BN $f \in F(D)$, and we study the complexity of deciding if $\phi^{\max}(D) \geq k$ or $\phi^{\min}(D) < k$.

After the preliminaries given in Section 2, we first study the problem of deciding if $\phi^{\max}(D) \geq k$ when the positive integer k is fixed. In Section 3 we prove that this problem is in P when $k = 1$ and, in Section 4, we prove that it is NP-complete when $k \geq 2$. Furthermore, these results remain true if the maximum in-degree $\Delta(D)$ is bounded by any constant $d \geq 2$. The case $k = 2$ is of particular interest since many works have been devoted to finding necessary conditions for the existence of multiple fixed points, both in the discrete and continuous settings, see [37, 30, 37, 20, 33] and the references therein. Section 5 considers the case where k is part of the input. We prove that, given a SID D and a positive integer k , deciding if $\phi^{\max}(D) \geq k$ is NEXPTIME-complete, and becomes $\text{NP}^{\#\text{P}}$ -complete if $\Delta(D)$ is bounded by a constant $d \geq 2$. In Section 6, we study the minimum number of fixed points. We prove that, even for $k = 1$, deciding if $\phi^{\min}(D) < k$ is NEXPTIME-complete. It becomes NP^{NP} -complete when $\Delta(D)$ is bounded by a constant $d \geq 2$ and k is a constant, and $\text{NP}^{\#\text{P}}$ -complete when $\Delta(D)$ is bounded by a constant $d \geq 2$ and k is a parameter of the problem. Note that, from all these results, we immediately obtain complexity results for the dual decision problems $\phi^{\max}(D) < k$ and $\phi^{\min}(D) \geq k$. A summary is given in Table 1.

Problem	$\Delta(D) \leq d$	$k = 1$	$k \geq 2$	k given in input
$\phi^{\max}(D) \geq k$	no	P	NP-complete	NEXPTIME-complete
	yes			$\text{NP}^{\#\text{P}}$ -complete
$\phi^{\min}(D) < k$	no	NEXPTIME-complete		
	yes	NP^{NP} -complete	$\text{NP}^{\#\text{P}}$ -complete	

Table 1: Complexity results.

2 Preliminaries

2.1 Configurations

Given a finite set V (of components), a *configuration* on V is an element $x \in \{0, 1\}^V$ that assigns a *state* $x_i \in \{0, 1\}$ to every $i \in V$. For $a \in \{0, 1\}$, we write $x = a$ to mean that $x_i = a$ for all $i \in V$. Given an enumeration i_1, i_2, \dots, i_n of the elements of V , we write $x = x_{i_1}x_{i_2}\dots x_{i_n}$. For $I \subseteq V$, we denote by x_I the restriction of x on I , that is, the configuration $y \in \{0, 1\}^I$ such that $y_i = x_i$ for all $i \in I$; and x *extends* a configuration $y \in \{0, 1\}^I$ if $x_I = y$. For every $i \in V$, we denote the i -base vector e_i , that is, $(e_i)_i = 1$ and $(e_i)_j = 0$ for all $j \neq i$. Given $x, y \in \{0, 1\}^V$, we denote by $x \oplus y$ the configuration z on V such that $z_i = x_i \oplus y_i$ for all $i \in V$, where the addition is computed modulo two. Hence, $x \oplus e_i$ is the configuration obtained from x by flipping component i only. We write $x \leq y$ to mean that $x_i \leq y_i$ for all $i \in V$.

2.2 Boolean networks

A *Boolean network* (BN) with component set V is a function $f : \{0, 1\}^V \rightarrow \{0, 1\}^V$. Given an initial configuration x^0 on V , the dynamics of the network is described by the successive iterations of f , that is, $x^{t+1} = f(x^t)$ for all $t \in \mathbb{N}$. Hence, the state of component i evolves according to the *local function* $f_i : \{0, 1\}^V \rightarrow \{0, 1\}$, which is the coordinate i of f , that is, $f_i(x) = f(x)_i$. More generally, given $I \subseteq V$, we denote by f_I the function from $\{0, 1\}^V$ to $\{0, 1\}^I$ defined by $f_I(x) = f(x)_I$. If $y \in \{0, 1\}^I$ then $f_I = y$ means that f_I is a constant function that always returns y .

2.3 Signed digraphs

A *signed digraph* D consists of a finite set of vertices V , a set of arcs $A \subseteq V \times V$ and an arc-labeling function σ from A to $\{-1, 0, 1\}$, which gives a sign (negative, null or positive) to each arc (j, i) , denoted σ_{ji} . In the following, it will be convenient to set $\tilde{\sigma}_{ji} = 0$ if $\sigma_{ji} \geq 0$ and $\tilde{\sigma}_{ji} = 1$ otherwise. We say that D is *simple* if it has no null arc, and *full-positive* if it has only positive arcs. Given a vertex i , we denote by $N_D(i)$ the set of in-neighbors of i and, for $s \in \{-1, 0, 1\}$, we denote by $N_D^s(i)$ the set of in-neighbors j of i with $\sigma_{ji} = s$. We drop D in the previous notations when it is clear from the context. We call $N^1(i)$, $N^0(i)$ and $N^{-1}(i)$ the set of positive, null and negative in-neighbors of i , respectively. We say that i is a *source* if it has no in-neighbor. The maximum in-degree of D is denoted $\Delta(D)$. Cycles and paths are always directed and without repeated vertices. The *sign* of a cycle or a path is the product of the signs of its arcs. We say that i has a *positive loop* if D has a positive arc from i to itself (a positive cycle of length one). Given $I \subseteq V$, we denote by $D \setminus I$ the signed digraph obtained from D by deleting the vertices in I (with the attached arcs). We say that a signed digraph D' is a *spanning subgraph* of D if D' can be obtained from D by removing arcs only. We say that I is a *positive feedback vertex set* of D if $D \setminus I$ has only negative cycles (or is acyclic). The minimum size of a positive feedback vertex set of D is denoted $\tau^+(D)$. Given a signed digraph D , we denote by V_D its vertex set.

2.4 Signed interaction digraphs

The *signed interaction digraph* (SID) of a BN f with component set V is the signed digraph D_f with vertex set V defined as follows. First, given $i, j \in V$, there is an arc (j, i) if and only if there exists a configuration x on V such that $f_i(x \oplus e_j) \neq f_i(x)$ (*i.e.* the local function f_i depends on component j). Second, the sign σ_{ji} of an arc (j, i) depends on whether the local function f_i is increasing or decreasing with respect to component j , and is defined as

$$\sigma_{ji} = \begin{cases} 1 & \text{if } f_i(x \oplus e_j) \geq f_i(x) \text{ for all } x \in \{0, 1\}^V \text{ with } x_j = 0, \\ -1 & \text{if } f_i(x \oplus e_j) \leq f_i(x) \text{ for all } x \in \{0, 1\}^V \text{ with } x_j = 0, \\ 0 & \text{otherwise.} \end{cases}$$

A signed digraph is called a SID if it is the SID of at least one BN. Such signed digraphs are characterized below (as a consequence, every simple signed digraph is a SID).

Proposition 1 ([29]). *A signed digraph is a SID if and only if every vertex with a unique null in-neighbor has at least two non-null in-neighbors.*

A fundamental remark regarding the present work is that multiple BNs may have the same SID. Given a SID D with vertex set V , we denote by $F(D)$ the corresponding BNs:

$$F(D) = \{f : \{0, 1\}^V \rightarrow \{0, 1\}^V \mid D_f = D\}.$$

The size of $F(D)$ is generally large: there are 2^{n2^n} BNs with n components and only 3^n signed digraphs with n vertices. Given $i \in V$, we denote by $F_i(D)$ the possible local functions for i , that is,

$$F_i(D) = \{f_i \mid f \in F(D)\}.$$

The size of $F_i(D)$ is doubly exponential according to the in-degree d of i in D , thus it scales as the number of Boolean functions on d variables, 2^{2^d} . The precise value of $|F_i(D)|$ is not trivial and has been extensively studied when i has only positive in-neighbors, see A006126 on the OEIS [1].

In the following, we will often consider vertices with in-degree ≤ 2 and, in that case, the situation is clear. If i is a source, then there are only two possible local functions, the two constant local functions. If i has a unique in-neighbor, say j , then it is not null by Proposition 1, and there is a unique possible local function: we have $f_i(x) = x_j \oplus \tilde{\sigma}_{ji}$. If i has only positive or negative in-neighbors, we say that f_i is the AND (resp. OR) function if it is the ordinary logical and (resp. or) but inputs with a negative sign are flipped, that is,

$$f_i(x) = \bigwedge_{j \in N(i)} x_j \oplus \tilde{\sigma}_{ji} \quad (\text{resp. } f_i(x) = \bigvee_{j \in N(i)} x_j \oplus \tilde{\sigma}_{ji}).$$

(If i is of in-degree one, the AND and OR functions are identical.) Now, if i is of in-degree two and has no null in-neighbor, there are only two possible local functions: the AND function and the OR function.

2.5 Fixed points and basic results

A *fixed point* of f is a configuration x such that $f(x) = x$. We denote by $\phi(f)$ the number of fixed points of f . In this paper, we are interested in decision problems related to the maximum and minimum number of fixed points of BNs in $F(D)$, denoted

$$\begin{aligned} \phi^{\max}(D) &= \max \{\phi(f) \mid f \in F(D)\}, \\ \phi^{\min}(D) &= \min \{\phi(f) \mid f \in F(D)\}. \end{aligned}$$

Cycles of D are known to play a fundamental role concerning the number of fixed points. A basic result by Robert is that if D is acyclic, then every $f \in \mathbf{F}(D)$ has a unique fixed point (thus $\phi^{\max}(D) = \phi^{\min}(D) = 1$). Considering positive and negative cycles, Aracena [2] proved the following other basic results, that show a kind of duality between the two types of cycle (note that Robert's result is an immediate consequence of the first two items)

Theorem 1 ([2]). *Let D be a SID.*

1. *If D has only negative cycles then $\phi^{\max}(D) \leq 1$.*
2. *If D has only positive cycles then $\phi^{\min}(D) \geq 1$.*
3. *If D is strongly connected and has only negative cycles $\phi^{\max}(D) < 1$.*
4. *If D is strongly connected and has only positive cycles $\phi^{\min}(D) > 1$.*

The first item can be widely generalized into the following bound (many extensions or improvements for particular classes of SIDs exist; see [31, 13, 8] for instance).

Theorem 2 (Positive feedback bound [2]). *For every SID D we have $\phi^{\max}(D) \leq 2^{\tau^+(D)}$.*

An illustration is given in Figure 1. The positive feedback bound is an immediate consequence of the following lemma, used many times in the following.

Lemma 1 ([2]). *Let D be a SID, let I be a positive feedback vertex set of D and $f \in \mathbf{F}(D)$. If f has distinct fixed points x, y , then $x_I \neq y_I$.*

The proof of all the previous results uses at some point the following lemma, that we will also use intensively (the first item appears in [13] and the second is a consequence of the first; we give a proof for completeness). Given a SID D with vertex set V and $i \in V$, we define the partial order \leq_i^D on $\{0, 1\}^V$ by

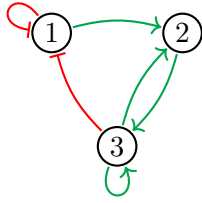
$$x \leq_i^D y \iff x_{N^1(i)} \leq y_{N^1(i)} \text{ and } y_{N^{-1}(i)} \leq x_{N^{-1}(i)} \text{ and } x_{N^0(i)} = y_{N^0(i)}.$$

Lemma 2. *Let D be a SID with vertex set V and sign function σ , and let $f \in \mathbf{F}(D)$. For every $i \in V$, we have the following properties:*

1. *The local function f_i is non-decreasing with respect to \leq_i^D , that is, for any configurations x, y on V we have*

$$x \leq_i^D y \implies f_i(x) \leq f_i(y).$$

2. *If i has at least one in-neighbor and at most one null in-neighbor then, for any configuration x on V , there is a non-null in-neighbor j of i such that $f_i(x) = x_j \oplus \tilde{\sigma}_{ji}$.*



x	$f^1(x)$	$f^2(x)$	$f^3(x)$	$f^4(x)$	$f^5(x)$	$f^6(x)$	$f^7(x)$	$f^8(x)$
000	100	100	100	100	100	100	100	100
001	000	001	010	011	100	101	110	111
010	100	101	100	101	100	101	100	101
011	001	001	011	011	101	101	111	111
100	000	000	010	010	100	100	110	110
101	010	011	010	011	010	011	010	011
110	000	001	010	011	100	101	110	111
111	011	011	011	011	011	011	011	011

Figure 1: Example of simple SID D with three vertices. Green arrows represent positive arcs and T-end red arrows represent negative arcs; this convention is used throughout the paper. D has two positive cycles (of length 1 and 2) and two negative cycles (of length 1 and 3). Each vertex is of in-degree two, so for each $f \in F(D)$ and $i \in \{1, 2, 3\}$ the local functions f_i is either the AND function or the OR function. Thus, $|F(D)| = 8$. The table of the 8 BNs in $F(D)$, denoted from f^1 to f^8 , is given; fixed points are in bold. These BNs have either 0 or 1 fixed point. Thus, $\phi^{\min}(D) = 0$ and $\phi^{\max}(D) = 1$. Note that $\{3\}$ is a positive feedback vertex set, hence $\tau^+(D) = 1$. The positive feedback bound gives $\phi^{\max}(D) \leq 2$; it is not reached.

Proof. To prove the first property, let x, y be configurations on V such that $x \leq_i^D y$. Let $\Delta(x, y)$ be the set of $j \in V$ such that $x_j \neq y_j$. We proceed by induction on $|\Delta(x, y)|$, the Hamming distance between x and y . If $|\Delta(x, y)| = 0$ then $x = y$ so $f_i(x) = f_i(y)$. Otherwise, there exists $j \in \Delta(x, y)$ and we set $z = x \oplus e_j$. Since $z_j = y_j$, it is clear that $z \leq_i^D y$. Furthermore, we have $\Delta(z, y) = \Delta(x, y) \setminus \{j\}$ so $f_i(z) \leq f_i(y)$ by induction hypothesis. If $j \notin N(i)$, we have $f_i(x) = f_i(z) \leq f_i(y)$. Otherwise, j is either a positive or a negative in-neighbor of i (since $x_j \neq y_j$ and $x \leq_i^D y$). If j is a positive in-neighbor, then $x_j < y_j = z_j$ so $f_i(x) \leq f_i(z)$, and we deduce that $f_i(x) \leq f_i(y)$. If j is a negative in-neighbor, then $x_j > y_j = z_j$, so $f_i(x) \leq f_i(z)$ and we have again $f_i(x) \leq f_i(y)$. This concludes the induction step.

We now prove the second property. Suppose that $f_i(x) = 0$ and suppose, for a contradiction, that there is no non-null in-neighbor j of i such that $x_j \oplus \tilde{\sigma}_{ji} = 0$. This means that $x_{N^+(i)} = 1$ and $x_{N^-(i)} = 0$ or, equivalently, that x is a \leq_i^D -maximal configuration. If i has no null in-neighbor, for any configuration y we have $y \leq_i^D x$ and we deduce from the first property that $f_i(y) = 0$. Hence, f_i is the 0 constant function, which is a contradiction since i has at least one in-neighbor. Suppose now that i has a unique null in-neighbor, say k . For any configuration y with $y_k = x_k$ we have $y \leq_i^D x$ and we deduce from the first property that $f_i(y) = 0$, so that $f_i(y) \leq f_i(y \oplus e_k)$. It follows that k is a positive in-neighbor if $x_k = 0$

and a negative in-neighbor if $x_k = 1$, a contradiction. The case $f_i(x) = 1$ is similar. \square

2.6 Decision problems

We will study the complexity of deciding if $\phi^{\max}(D) \geq k$ or $\phi^{\min}(D) < k$, where k is a positive integer, fixed or not. This gives the following decision problems.

k -MAXIMUM FIXED POINT PROBLEM (k -MAXFPP)

Input: a SID D .

Question: $\phi^{\max}(D) \geq k$?

MAXIMUM FIXED POINT PROBLEM (MAXFPP)

Input: a SID D and an integer $k \geq 1$.

Question: $\phi^{\max}(D) \geq k$?

k -MINIMUM FIXED POINT PROBLEM (k -MINFPP)

Input: a SID D .

Question: $\phi^{\min}(D) < k$?

MINIMUM FIXED POINT PROBLEM (MINFPP)

Input: a SID D and an integer $k \geq 1$.

Question: $\phi^{\min}(D) < k$?

All these problems are in NEXPTIME (they can be decided in exponential time on a non-deterministic Turing machine). For instance the problem MAXFPP can be decided as follows. Given a SID D with vertex set V and an integer k :

1. Choose non-deterministically a BN f with component set V ; this can be done in exponential time since f can be represented using $|V|2^{|V|}$ bits.
2. Compute the SID D_f of f ; this can be done in exponential time by comparing $f_i(x)$ and $f_i(x \oplus e_j)$ for all configurations x on V and vertices $i, j \in V$.
3. Compute $\phi(f)$ by considering each of the $2^{|V|}$ configurations.
4. Accept if and only if $\phi(f) \geq k$ and $D_f = D$.

This non-deterministic exponential time algorithm has an accepting branch if and only if $\phi^{\max}(D) \geq k$. Therefore, the problem MAXFPP is in NEXPTIME. This algorithm can be adapted to the other problems.

However, as we will see later, this complexity bound can be refined for some problems or when we restrict the problems to some subclass of SIDs, such as SIDs with a maximum

in-degree bounded by a constant d . This is because the SIDs of this subclass only admit a simple exponential number of BNs. Indeed, if $f \in \mathbf{F}(D)$ and $\Delta(D) \leq d$, then each local function f_i can be regarded as a Boolean function with $|N(i)| \leq d$ inputs. Consequently, there are at most $c = 2^{2^d}$ possible choices for each local function, and $|\mathbf{F}(D)| \leq c^n$ is a simple exponential.

Remark 1 below shows that the restriction to SIDs D with maximum in-degree ≤ 1 reduces drastically the hardness of the problems. Therefore, in the rest of the article, we will only consider SIDs whose maximum in-degree is bounded by a constant $d \geq 2$ or not bounded at all.

Remark 1. *The decision problems k -MAXFPP, MAXFPP, k -MINFPP and MINFPP restricted to SIDs D such that $\Delta(D) \leq 1$ are in \mathbf{P} . Indeed, if $\Delta(D) \leq 1$ and D has exactly p positive cycles, then for any $f \in \mathbf{F}(D)$, one easily check that*

$$\phi(f) = \begin{cases} 0 & \text{if } D \text{ has a negative cycle,} \\ 2^p & \text{otherwise.} \end{cases}$$

As a consequence, computing $\phi(f)$, which is obviously equal to both $\phi^{\max}(D)$ and $\phi^{\min}(D)$, can be done in polynomial time, and it is sufficient to compare this value to k in order to answer any problem.

3 k -Maximum Fixed Point Problem for $k = 1$

In this Section, we are interested in the problem of deciding if a SID D admits a BN with at least one fixed point. This is the only decision problem we consider for which we do not prove tight complexity bounds. More precisely, Theorem 3 shows that the problem is in \mathbf{P} , but it remains open to know whether it is \mathbf{P} -hard.

Theorem 3. *1-MAXFPP is in \mathbf{P} .*

The next lemma shows that we can efficiently transform any SID D into a simple SID D' such that $\phi^{\max}(D) \geq 1$ if and only if $\phi^{\max}(D') \geq 1$. As a consequence, in order to prove that 1-MAXFPP is in \mathbf{P} , we can consider that the input SID is simple.

Lemma 3. *Let D be a SID and let D' be the simple SID obtained from D by deleting the set of arcs (j, i) such that i has at least two null in-neighbors in D or such that j is the unique null in-neighbor of i in D . We have*

$$\phi^{\max}(D) \geq 1 \iff \phi^{\max}(D') \geq 1.$$

Proof. Suppose that $\phi^{\max}(D) \geq 1$ and let $f \in \mathbf{F}(D)$ with a fixed point y . We define componentwise a BN $f' \in \mathbf{F}(D')$ that admits y as fixed point. Let i be any vertex. We consider three cases:

1. If i has no null in-neighbor in D , then i has the same in-coming arcs in D and D' thus we can set $f'_i = f_i$, so that $f'_i(y) = f_i(y) = y_i$.
2. If i has a unique null in-neighbor in D , then f'_i is defined as the AND function if $y_i = 0$, and the OR function otherwise. Suppose first that $y_i = 0$. Then $f_i(y) = 0$ so, by the second property of Lemma 2, there is a non-null in-neighbor j of i such that $y_j \oplus \tilde{\sigma}_{ji} = 0$, where σ is the sign function of D . Since f'_i is the AND function, we deduce that $f'_i(y) = 0$. We prove similarly that $f'_i(y) = 1$ when $y_i = 1$.
3. If i has at least two null in-neighbors in D , then i is a source of D' so f'_i has to be a constant function. We then set $f'_i = y_i$, so that $f'_i(y) = y_i$.

In this way, f' is a BN in $F(D')$ which has y as fixed point. Hence, $\phi^{\max}(D') \geq 1$.

Conversely, suppose that $\phi^{\max}(D') \geq 1$ and let $f' \in F(D')$ with a fixed point y . We define componentwise a BN $f \in F(D)$ that admits y as fixed point. Let i be any vertex. We consider three cases:

1. If i has no null in-neighbor in D , then i has the same in-coming arcs in D and D' thus we can set $f_i = f'_i$, so that $f_i(y) = f'_i(y) = y_i$.
2. Suppose that i has a unique null in-neighbor in D , say k . Note that i has at least two non-null in-neighbors in D by Proposition 1. Suppose that $y_i = 0$. Then $f'_i(y) = 0$ so, by the second property of Lemma 2, there is a non-null in-neighbor j of i such that $y_j \oplus \tilde{\sigma}_{ji} = 0$. We then define f_i by:

$$f_i(x) = ((x_j \oplus \tilde{\sigma}_{ji}) \vee (x_k \oplus y_k)) \wedge \bigwedge_{\ell \in N_D(i) \setminus \{j, k\}} ((x_\ell \oplus \tilde{\sigma}_{\ell i}) \vee (x_k \oplus \neg y_k)).$$

It is easy to check that $f_i \in F_i(D)$ and, since the first term of the conjunction vanishes for $x = y$, we have $f_i(y) = 0 = y_i$. If $y_i = 1$ we prove similarly that there is $f_i \in F_i(D)$ with $f_i(y) = 1$ (in that case, there is a non-null in-neighbor j such that $y_j \oplus \tilde{\sigma}_{ji} = 1$ and f_i is defined as above by swapping \wedge and \vee , and by swapping y_k and $\neg y_k$).

3. Suppose that i has at least two null in-neighbors in D . If $y_i = 0$ we define f_i by:

$$f_i(x) = \left(\bigoplus_{j \in N_D^0(i)} x_j \oplus y_j \right) \wedge \bigwedge_{j \in N_D(i) \setminus N_D^0(i)} (x_j \oplus \tilde{\sigma}_{ji}).$$

It is easy to check that $f_i \in F_i(D)$ and, since the first term of the conjunction vanishes for $x = y$, we have $f_i(y) = 0 = y_i$. The case $y_i = 1$ is symmetric (with \vee instead of \wedge and $\neg y_j$ instead of y_j).

In this way, f is a BN in $F(D)$ which has y as fixed point. Hence, $\phi^{\max}(D) \geq 1$. \square

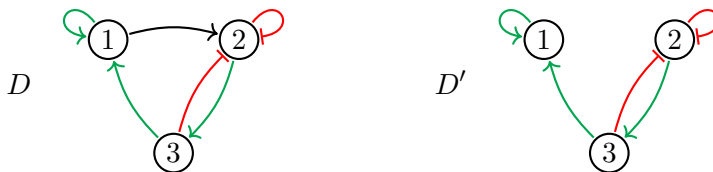
We now give a graph-theoretical characterization of the simple SIDs D such that $\phi^{\max}(D) \geq 1$. We need some additional definitions. A strongly connected component H in a signed digraph D is *trivial* if it has a unique vertex and no arc, and *initial* if D has no arc (i, j) where j is in H but not i .

Lemma 4. *Let D be a simple SID. We have $\phi^{\max}(D) \geq 1$ if and only if each non-trivial initial strongly connected component of D has a positive cycle.*

Proof. The left to right implication has been proven by Aracena in [4, Corollary 3] and is an easy consequence of the third item in Theorem 1. We present a version rewritten with the notations of this paper. Let σ be the sign function of D , and let $f \in F(D)$ with a fixed point x . Consider an arbitrary non-trivial initial strongly connected component H of D , and let us prove that H has a positive cycle. Since H is non-trivial, by the second property of Lemma 2, each vertex i in H has a non-null in-neighbor j such that $x_j \oplus \tilde{\sigma}_{ji} = f_i(x) = x_i$, and j is necessarily in H since H is initial. We deduce that H has a spanning subgraph H' in which each vertex is of in-degree one, and such that $x_j \oplus \tilde{\sigma}_{ji} = x_i$ for any arc (j, i) of H' . Hence, for any vertices i, j in H , if $x_j = x_i$ then any walk in H' from j to i visits an even number of negative arcs. In particular, any cycle of H' is positive. Since H' has no source, H' has a cycle, which is positive. Thus, H has a positive cycle as desired.

Conversely, suppose that each non-trivial initial strongly connected component of D has a positive cycle. Then it is easy to see that D has a spanning subgraph D' with only positive cycles, and with the same sources as D . Let any $f' \in F(D')$. By the second item of Theorem 1, f' has at least one fixed point, say x . We then define $f \in F(D)$ componentwise as follows. For any vertex i , if i is a source, then we set $f_i = x_i$, so that $f_i(x) = x_i$. Otherwise, by the second property of Lemma 2, i has an in-neighbor j in D' such that $x_j \oplus \tilde{\sigma}_{ji} = f'_i(x) = x_i$. We then define f_i as the AND function if $x_j \oplus \tilde{\sigma}_{ji} = x_i = 0$ and the OR function if $x_j \oplus \tilde{\sigma}_{ji} = x_i = 1$. It is then clear that $f_i(x) = x_i$. Hence, x is a fixed point of f . \square

Remark 2. *If D is not simple, we can have $\phi^{\max}(D) = 0$ even if each non-trivial initial strongly connected component of D has a positive cycle. Indeed, let D and D' be the following SIDs:*



The black arrow from vertex 1 to vertex 2 represents a null arc, thus D is not simple. Furthermore, D is strongly connected and has a positive cycle: the positive loop on vertex 1. However, $\phi^{\max}(D) = 0$. Indeed, by Lemma 3, $\phi^{\max}(D) \geq 1$ if and only if $\phi^{\max}(D') \geq 1$.

However, since D' is simple and has a non-trivial initial strongly connected component with only negative cycles, that containing vertices 2 and 3, by Lemma 4 we have $\phi^{\max}(D') = 0$ and thus $\phi^{\max}(D) = 0$.

The last ingredient for the proof of Theorem 3 is a difficult result independently proven by Robertson, Seymour and Thomas in [36], and McCuaig in [25].

Theorem 4 ([25, 36]). *There is a polynomial time algorithm to decide if a given digraph contains a cycle of even length.*

Proof of Theorem 3. As a consequence of Lemmas 3 and 4, to decide if $\phi^{\max}(D) \geq 1$, it is sufficient to compute the non-trivial initial strongly connected components of the simple SID D (this can be done in linear time [38]) and to check if each of them contains a positive cycle. Using the following transformation, the algorithm from Theorem 4 can be used to perform this in polynomial time.

Let D be a signed digraph with n vertices, and let \tilde{D} be the digraph obtained from D by replacing each positive arc by a path of length two (with one new vertex), and each negative arc by a path of length one. Then \tilde{D} has at most $n + n^2$ vertices, and D has a positive cycle if and only if \tilde{D} has a cycle of even length (this transformation also appears in [27]). This concludes the proof of Theorem 3. \square

4 k -Maximum Fixed Point Problem for $k \geq 2$

In this section we study k -MAXFPP for $k \geq 2$ and prove the following complexity result.

Theorem 5. *k -MAXFPP is NP-complete for every $k \geq 2$, even when restricted to SIDs D such that $\Delta(D) \leq 2$.*

We first prove the upper bound and then the lower bound.

4.1 Upper bound

Lemma 5. *k -MAXFPP is in NP for any $k \geq 2$.*

Proof. Let D be a SID with vertex set V . Suppose that $k \leq 2^{|V|}$, otherwise D is obviously a false instance. The algorithm we consider is fairly simple. It first guesses k fixed points and, for each non-negative (resp. non-positive) arc (j, i) in D , it guesses a configuration in which an increase of component j produces an increase (rep. decrease) of the local function f_i . It finally checks that these non-deterministic guesses do not contradict the first property of Lemma 2. If so, this partial knowledge of the local functions can be extended into a BN in $F(D)$ with the k guessed fixed points, *i.e.* D is a true instance. More precisely, the algorithm is as follows:

1. Choose non-deterministically k distinct configurations x^1, \dots, x^k on V and, for every $i \in V$, compute the sets $F_i = \{x^\ell \mid x_i^\ell = 0, \ell \in [k]\}$ and $T_i = \{x^\ell \mid x_i^\ell = 1, \ell \in [k]\}$.
2. For each non-negative arc (j, i) of D , choose non-deterministically a configuration $x^{j^{i+}}$ on V with $x_j^{j^{i+}} = 0$. Then add $x^{j^{i+}}$ in the set F_i and $x^{j^{i+}} \oplus e_j$ in the set T_i .
3. For each non-positive arc (j, i) of D , choose non-deterministically a configuration $x^{j^{i-}}$ on V with $x_j^{j^{i-}} = 0$. Then add $x^{j^{i-}}$ in the set T_i and $x^{j^{i-}} \oplus e_j$ in the set F_i .
4. Accept if and only if there is no $i \in V$, $x \in F_i$ and $y \in T_i$ such that $y \leq_i^D x$.

This algorithm runs in $O(|V|\Delta(D)^3)$, which is actually the time complexity of the last item, the most consuming one. Indeed, we have $|F_i||T_i| \leq (\Delta(D) + k)^2$, and the relation $y \leq_i^D x$ can be checked in $O(\Delta(D))$.

We will prove that there is an accepting branch if and only if $\phi^{\max}(D) \geq k$.

Suppose first that there is $f \in F(D)$ with at least k fixed points. One can consider the following execution. First, the configurations x^1, \dots, x^k chosen in the first step are fixed points of f . Second, for each non-negative arc (j, i) of D , the configuration $x^{j^{i+}}$ chosen in the second step is such that $f_i(x^{j^{i+}}) < f_i(x^{j^{i+}} \oplus e_j)$; this configuration exists since D is the SID of f . Third, for each non-positive arc (j, i) , the configuration $x^{j^{i-}}$ chosen in the third step is such that $f_i(x^{j^{i-}}) > f_i(x^{j^{i-}} \oplus e_j)$; this configuration exists since D is the SID of f . Hence, for all $i \in V$, $x \in F_i$ and $y \in T_i$ we have $f_i(x) = 0$ and $f_i(y) = 1$ and we deduce from the first property of Lemma 2 that $y \not\leq_i^D x$, so the algorithm has an accepting branch.

For the other direction, suppose that the algorithm has an accepting branch. Let us prove that there is $f \in F(D)$ with at least k fixed points. For each $i \in V$, we define f_i as follows: for all configurations x on V ,

$$f_i(x) = \begin{cases} 1 & \text{if there is } y \in T_i \text{ such that } y \leq_i^D x, \\ 0 & \text{otherwise.} \end{cases}$$

Clearly, $f_i(x) = 1$ if $x \in T_i$. Furthermore, if $x \in F_i$ then, since we are considering an accepting branch, there is no $y \in T_i$ such that $y \leq_i^D x$, and we deduce that $f_i(x) = 0$. Consequently, $f_i(x^\ell) = x_i^\ell$ for $1 \leq \ell \leq k$. Thus, x^1, \dots, x^k are fixed points of f .

It remains to prove that the SID D_f of f is equal to D . Suppose first that D_f has a non-negative arc (j, i) . Then there is a configuration x with $x_j = 0$ such that $f_i(x) < f_i(x \oplus e_j)$. We deduce that $x \not\leq_i^D y \leq_i^D x \oplus e_j$ for some $y \in T_i$. So (j, i) is an arc of D and, since $x_j \leq y_j$ and $y \leq_i^D x \oplus e_j$, if this arc is negative then $y \leq_i^D x$, a contradiction. Thus, (j, i) is a non-negative arc of D . We prove similarly that every non-positive arc of D_f is a non-positive arc of D . Now, suppose that D has a non-negative arc (j, i) and let $x = x^{j^{i+}}$ be the corresponding configuration chosen in the second step. We have $x \in F_i$ and $x \oplus e_j \in T_i$, so $f_i(x) < f_i(x \oplus e_j)$ and since $x_j = 0$ we deduce that (j, i) is a non-negative arc of D' . We prove similarly that every non-positive arc of D is a non-positive arc of D_f . This proves that $D_f = D$. \square

4.2 Lower bound

We now prove the lower bound. We first show that the problem can be reduced to $k = 2$: by the following lemma, 2-MAXFPP is as hard as k -MAXFPP for all $k > 2$.

Lemma 6. *Let $k > 2$ and let D be any SID. Let D' be the SID obtained from D by adding $\lceil \log_2 k \rceil - 1$ new vertices and a positive loop on each new vertex. We have*

$$\phi^{\max}(D') \geq k \iff \phi^{\max}(D) \geq 2.$$

Proof. Let $\ell = \lceil \log_2 k \rceil$ so that $2^{\ell-1} < k \leq 2^\ell$ and $\ell \geq 2$. Let H be the SID with $\ell - 1$ vertices and a positive loop on each vertex. Then $F(H)$ contains a unique BN, which is the identity, thus $\phi^{\max}(H) = 2^{\ell-1}$. Since D' is the disjoint union of D and H ,

$$\phi^{\max}(D') = \phi^{\max}(D) \cdot \phi^{\max}(H) = \phi^{\max}(D) \cdot 2^{\ell-1}.$$

Thus, $\phi^{\max}(D') \geq 2^\ell \geq k$ if $\phi^{\max}(D) \geq 2$, and $\phi^{\max}(D') \leq 2^{\ell-1} < k$ otherwise. \square

It remains to prove the case $k = 2$: it is NP-hard to decide if $\phi^{\max}(D) \geq 2$. This is the main contribution of the paper. First, from a technical point of view, the reduction used for this decision problem will be adapted for all the other hardness results of this paper. Second, from a more general point of view, many works have been devoted to the study of the SID of dynamical systems with multiple steady states, both in the continuous and discrete setting, see [37, 30, 37, 20, 33] and the references therein. The basic observation, answering a conjecture of the biologist Thomas, is that a non-negative cycle must be present. The biological motivation behind is that dynamical systems (in particular BNs) with multiple steady states (fixed points in the discrete setting) should account for very important biological phenomena: cell differentiation processes. In our setting, the principal observation we just mention is the first item of Theorem 1: if $\phi^{\max}(D) \geq 2$ then D has a non-negative cycle. This necessary condition for $\phi^{\max}(D) \geq 2$ (which can be checked in polynomial time) is obviously not sufficient, and it is natural to seek for a characterization. By proving that it is NP-hard to decide that $\phi^{\max}(D) \geq 2$, we show that any such characterization is difficult to check. Together with the complexity upper bound established above, this answers a question stated in [32].

The rough idea is the following. We know that if a SID D_1 has no source and is full-positive then $\phi^{\min}(D_1) \geq 2$ (this is an easy consequence of the last item of Theorem 1). More precisely, every $f \in F(D_1)$ has two distinct fixed points x and y such that $x \leq y$. If, in addition, D_1 has a positive feedback vertex set of size one, then $\phi^{\max}(D_1) \leq 2$ thus every $f \in F(D_1)$ has *exactly* two distinct fixed points x and y such that $x \leq y$. The simplest example is the full-positive cycle. Now, if we add some negative arcs in D_1 , without producing additional positive cycles, this can only reduce the maximum number of fixed points. In many cases the reduction is effective: the resulting SID D_2 is such that $\phi^{\max}(D_2) \leq 1$. The simplest example is a full-positive cycle plus any negative arc. The

idea then to add to D_2 some additional sources that “control” the negative arcs in such a way that some BNs behave as if their SID were D_1 (the negative arcs are “dynamically absent”) and have thus two fixed points, while some others behave as if their SID were D_2 (the negative arcs are “dynamically present”) and have at most one fixed point. If this “control” is possible if and only if rather particular graphical conditions are satisfied, then some complexity lower bound should be obtained. Actually, the reduction consists in encoding, in these graphical conditions, a 3-SAT formula.

So consider a 3-SAT formula ψ over a set λ of n variables and with a set of m clauses μ . To each variable $\lambda \in \lambda$ is associated a positive literal λ^+ and a negative literal λ^- . The resulting sets of positive and negative literals are denoted λ^+ and λ^- , and each clause is regarded as a triplet of elements taken in $\lambda^+ \cup \lambda^-$. An *assignment* for ψ is regarded as a configuration z on a set V such that $\lambda \subseteq V$. A positive literal λ^+ is satisfied by z if $z_\lambda = 1$, and a negative literal λ^- is satisfied by z if $z_\lambda = 0$. A clause is satisfied by z if at least one of its literals is satisfied by z . The formula ψ is *satisfied* by z (or z is a *satisfying assignment* for ψ) if every clause in μ is satisfied by z . We say that ψ is *satisfiable* if it has at least one satisfying assignment.

The reduction from the 3-SAT problem is based on the following definition; see Figure 2 for an illustration.

Definition 1 (D_ψ). *Let ψ be a 3-CNF formula over a set λ of n variables and with a set of m clauses μ . Given an enumeration $\lambda = \{\lambda_1, \dots, \lambda_n\}$ of the variables and an enumeration $\mu = \{\mu_1, \dots, \mu_m\}$ of the clauses, we define a SID D_ψ with $4n + 2m + 1$ vertices as follows:*

- *The vertex set is*

$$V_\psi = \lambda \cup U_\psi \quad \text{with} \quad U_\psi = \lambda^+ \cup \lambda^- \cup \ell \cup \mu \cup \mathbf{c},$$

where $\ell = \{\ell_0, \dots, \ell_n\}$ and $\mathbf{c} = \{c_1, \dots, c_m\}$.

- *The arcs are, for all $r \in [n]$ and $s \in [m]$,*
 - $(\lambda_r, \lambda_r^+), (\ell_{r-1}, \lambda_r^+),$
 - $(\lambda_r, \lambda_r^-), (\ell_{r-1}, \lambda_r^-),$
 - $(\lambda_r^+, \ell_r), (\lambda_r^-, \ell_r),$
 - $(c_1, \ell_0),$
 - (i, μ_s) for all $i \in \lambda^+ \cup \lambda^-$ such that i is a literal in $\mu_s,$
 - $(\mu_s, c_s), (c_{s+1}, c_s),$ where c_{m+1} means $\ell_n.$
- *For all $r \in [n]$ and $s \in [m]$, the arcs (λ_r, λ_r^-) and (μ_s, c_s) are negative, and all the other arcs are positive.*

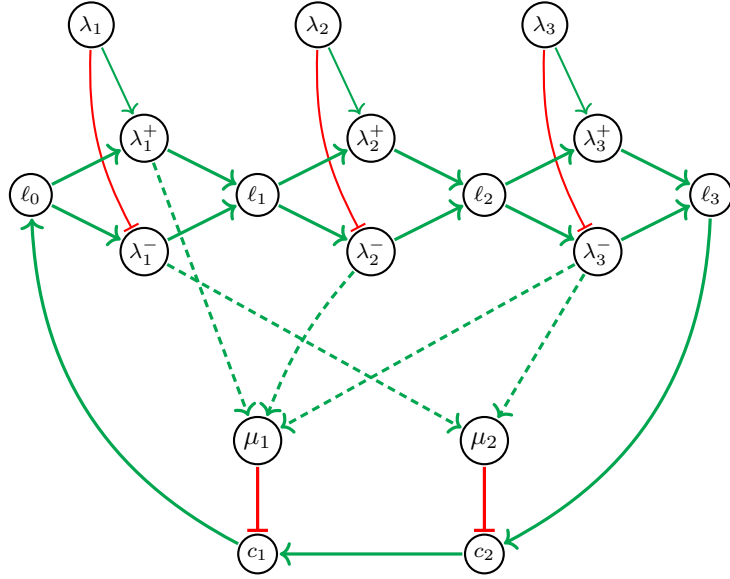


Figure 2: SID D_ψ of Definition 1 for the 3-CNF formula $\psi = (\lambda_1 \vee \neg\lambda_2 \vee \neg\lambda_3) \wedge (\neg\lambda_1 \vee \neg\lambda_3)$. Using our notations, the set of variables is $\lambda = \{\lambda_1, \lambda_2, \lambda_3\}$ and the set of clauses is $\mu = \{\mu_1, \mu_2\}$ where, for instance, $\mu_1 = (\lambda_1^+, \lambda_2^-, \lambda_3^-)$ and $\mu_2 = (\lambda_1^-, \lambda_3^-, \lambda_3^-)$ (what matter is that $\lambda_1^+, \lambda_2^-, \lambda_3^-$ appear in μ_1 and λ_1^-, λ_3^- appear in μ_2). Clauses are encoded in D_ψ through dashed arrows.

Note that $\Delta(D_\psi) \leq 3$. More precisely, vertices in λ (variables) have in-degree 0 (they are sources), vertices in μ (clauses) have in-degree at most 3, and all the other vertices have in-degree 2, excepted ℓ_0 which has in-degree 1.

Intuitively, the SID $D_{\psi,1}$ obtained from D_ψ by deleting the sources and the negative arcs corresponds to the SID D_1 in the above rough description of the construction: $D_{\psi,1}$ has no source and is full-positive, so that $\phi^{\min}(D_{\psi,1}) \geq 2$, and since any vertex in $\ell \cup \mathbf{c}$ is a positive feedback vertex set we have $\phi^{\min}(D_{\psi,1}) = \phi^{\max}(D_{\psi,1}) = 2$. Let $D_{\psi,2}$ be obtained from $D_{\psi,1}$ by adding the negative arcs (μ_s, c_s) . One can check that the addition of these negative arcs decreases the maximum number of fixed points: we have $\phi^{\max}(D_{\psi,2}) \leq 1$ (see [32], Theorem 3). This SID $D_{\psi,2}$ plays the role of SID D_2 in the above rough description of the construction.

This construction works intuitively as follows. For the first direction, we consider an assignment $z \in \{0,1\}^\lambda$ and we construct $f \in \mathbf{F}(D_\psi)$, in such a way that, at the first iteration, each source λ_r is “fixed” to the state z_{λ_r} . By taking the OR function for the local functions associated with the positive and negative literals, it results that, at the second iteration, exactly one of λ_r^+, λ_r^- is “fixed” to state 1: the positive literal if $z_{\lambda_r} = 1$, and the negative literal otherwise. At this point, if z is a true assignment, each clause μ_s has at least one in-neighbor “fixed” to state 1, and by taking f_{μ_s} as the OR function, μ_s is fixed at state 1 at the third iteration. By taking f_{c_s} as the OR function, each vertex c_s is still “free”, and by taking f_{ℓ_r} as the AND function, each vertex ℓ_r is still “free”. Hence, there is a positive cycle containing only “free” vertices, which “produces” two fixed points. This is like if, in three iterations, all the negative arcs “disappear” leaving “free” a full-positive cycle. In this construction, only the local functions associated with the sources depend on the assignment z , and f has at least one fixed point even if z is not a true assignment. These two properties will be very useful for the other hardness results. Below, we do not described formally this “three iterations process”. We only prove what we need for the following.

Lemma 7. *Let $z \in \{0,1\}^\lambda$ and $f \in \mathbf{F}(D_\psi)$ defined by: $f_\lambda = z$ and, for all $i \in U_\psi$, f_i is the AND function if $i \in \ell$ and the OR function otherwise. Then f has at least one fixed point, and if ψ is satisfied by z , then f has at least two fixed points.*

Proof. Let x be the configuration on V_ψ defined by $x_\lambda = z$ and $x_{U_\psi} = 1$. First, $f(x)_\lambda = z = x_\lambda$. Second, $f_{\ell_0}(x) = x_{c_1} = 1 = x_{\ell_0}$ and, for all $r \in [n]$, $f_{\ell_r}(x) = x_{\lambda_r^+} \wedge x_{\lambda_r^-} = 1 \wedge 1 = 1 = x_{\ell_r}$. Third, any vertex $i \in U_\psi \setminus \ell$ has a positive in-neighbor $j \in U_\psi$. Since f_j is the OR function and $x_j = 1$, we have $f_i(x) = 1 = x_i$. Thus, $f(x) = x$.

Let y be the configuration on V_ψ be defined by: $y_\lambda = z$ and, for all $i \in U_\psi$,

$$y_i = 1 \iff \begin{cases} i \text{ is a clause } \mu_s, \text{ or} \\ i \text{ is a positive literal } \lambda_r^+ \text{ such that } z_{\lambda_r} = 1, \text{ or} \\ i \text{ is a negative literal } \lambda_r^- \text{ such that } z_{\lambda_r} = 0. \end{cases}$$

Note that $y_{\lambda_r^+} = z_{\lambda_r} \neq y_{\lambda_r^-}$ for all $r \in [n]$, so $x \neq y$. Suppose that ψ is satisfied by z , and let us prove that y is a fixed point of f . It is clear that $f(y)_\lambda = z = y_\lambda$. Let $r \in [n]$. Since exactly one of $y_{\lambda_r^+}, y_{\lambda_r^-}$ is 0, we have $f_{\ell_r}(y) = y_{\lambda_r^+} \wedge y_{\lambda_r^-} = 0 = y_{\ell_r}$; and $f_{\ell_0}(y) = y_{c_1} = 0 = y_{\ell_0}$. Then

$$\begin{aligned} f_{\lambda_r^+}(y) &= y_{\lambda_r} \vee y_{\ell_{r-1}} = z_{\lambda_r} \vee 0 = z_{\lambda_r} = y_{\lambda_r^+}, \\ f_{\lambda_r^-}(y) &= \neg y_{\lambda_r} \vee y_{\ell_{r-1}} = \neg z_{\lambda_r} \vee 0 = \neg z_{\lambda_r} = y_{\lambda_r^-}. \end{aligned}$$

Let $s \in [m]$. Since ψ is satisfied by z , μ_s has at least one in-neighbor which is a positive literal λ_r^+ with $z_{\lambda_r} = 1$ or a negative literal λ_r^- such that $z_{\lambda_r} = 0$. Hence, μ_s has an in-neighbor i with $y_i = 1$ and since f_{μ_s} is the OR function we deduce that $f_{\mu_s}(y) = 1 = y_{\mu_s}$. We finally prove that $f_{c_s}(y) = 0 = y_{c_s}$ by induction on s from $m+1$ to 1. Since c_{m+1} means ℓ_n , the case $s = m+1$ is already proven. Then, for $s \in [m]$, we have $y_{c_{s+1}} = 0$ by induction so $f_{c_s}(y) = \neg y_{\mu_s} \vee y_{c_{s+1}} = \neg 1 \vee 0 = 0 = y_{c_s}$. Thus, $f(y) = y$. \square

For the other direction, we suppose that there is $f \in F(D_\psi)$ with two distinct fixed points x and y . Then we prove that either $x \leq y$ or $y \leq x$, exactly as if the SID of f where $D_{\psi,1}$ (or any full-positive SID without two vertex-disjoint positive cycles); this results from Lemma 8 below. Furthermore, for each clause μ_s it appears that $x_{\mu_s} = y_{\mu_s}$, the clause is “fixed”. Since $x \leq y$ or $y \leq x$, this is possible only if μ_s has an in-neighbor (a positive or negative literal associated to some variable λ_r) which is also “fixed”; this results from Lemma 9 below. Beside, an easy consequence of $x \neq y$ is that at most one λ_r^+, λ_r^- is “fixed” and from that point we easily obtain a satisfying assignment.

Lemma 8. *Let D be a simple SID, without two vertex-disjoint positive cycles, such that every positive cycle is full-positive and, for any negative arc (j, i) , either j is a source or every positive cycle contains i . Let $f \in F(D)$ with two fixed point x and y . The following holds:*

- We have $x \leq y$ or $y \leq x$.
- If (j, i) is a negative arc and i is of in-degree two, then $x_j = y_j$.

Proof. Let I be the set of vertices i in D such that $x_i \neq y_i$. We prove that each $i \in I$ has an in-neighbor $j \in I$ such that $x_j \oplus \tilde{\sigma}_{ji} = x_i$. Let $i \in I$ and suppose that $x_i < y_i$, the other case being similar. Then $f_i(x) < f_i(y)$ and thus $y \not\leq_i^D x$ by Lemma 2. Hence, i has at least one in-neighbor j such that: (j, i) is positive and $x_j < y_j$, or (j, i) is negative and $x_j > y_j$. In both cases, $j \in I$ and $x_j \oplus \tilde{\sigma}_{ji} = x_i$.

We deduce that D has a subgraph D' with vertex set I , in which each vertex is of in-degree one, and such that $x_j \oplus \tilde{\sigma}_{ji} = x_i$ for any arc (j, i) of D' . Hence, for any $i, j \in I$, if $x_j = x_i$ then any walk in D' from j to i visits an even number of negative arcs. In particular, any cycle of D' is positive. Thus, by hypothesis, any cycle of D' is full-positive.

Since, in D' , each vertex is of in-degree one, D' has a cycle C (which is full-positive). Furthermore, D' has no other cycle (since otherwise D has two vertex-disjoint positive

cycles). Thus, D' is connected. Furthermore, D' is full-positive: if (j, i) is a negative arc of D' then j is not a source (since $j \in I$) so, by hypothesis, i is in C , and thus j too. But then C has a negative arc, and it is a contradiction. So D' is full-positive and we deduce that $x_j = x_i$ for any arc (j, i) of D' . Since D' is connected, we deduce that $x_j = x_i$ for any $i, j \in I$ and this implies that $y_j = y_i$ for any $i, j \in I$. Thus, either $x \leq y$ or $y \leq x$. Suppose, without loss, that $x \leq y$.

Let (j, i) be a negative arc of D . Suppose that i is of in-degree two in D and, for a contradiction, that $x_j \neq y_j$. Then $x_j < y_j$ since $x \leq y$. By hypothesis, i is in C thus $x_i < y_i$. Since i is of in-degree two, f_i is either the AND function or the OR function. If f_i is the OR function, then $f_i(x) = 1$ since $x_j = 0$ and (j, i) is negative, which is a contradiction since $x_i = 0$. If f_i is the AND function, then $f_i(y) = 0$ since $y_j = 1$ and (j, i) is negative, which is a contradiction since $y_i = 1$. Thus, $x_j = y_j$. \square

Lemma 9. *Let D be a SID and $f \in F(D)$ with two fixed points x, y such that $x \leq y$. Every vertex i with only positive in-neighbors such that $x_i = y_i$ has a positive in-neighbor j such that $x_j = y_j$.*

Proof. Let i be as in the statement. If $x_i = y_i = 0$ then, by Lemma 2, i has a positive in-neighbor j such that $y_j = f_i(y) = y_i = 0$, and since $x \leq y$ we have $x_j = y_j = 0$. If $x_i = y_i = 1$ then, by Lemma 2, i has a positive in-neighbor j such that $x_j = f_i(x) = x_i = 1$, and since $x \leq y$ we have $x_j = y_j = 1$. \square

We go back to our construction D_ψ and prove a kind of converse of Lemma 7. We need a definition. For every $r \in [n]$, ℓ_r is of in-degree two in D_ψ , so f_{ℓ_r} is either the AND function or the OR function; we then define $\epsilon(f) \in \{0, 1\}^\lambda$ as follows: for all $r \in [n]$,

$$\epsilon(f)_{\lambda_r} = \begin{cases} 0 & \text{if } f_{\ell_r} \text{ is the OR function,} \\ 1 & \text{if } f_{\ell_r} \text{ is the AND function.} \end{cases}$$

Lemma 10. *If $f \in F(D_\psi)$ has distinct fixed points x and y , then ψ is satisfied by $x_\lambda \oplus \epsilon(f)$.*

Proof. Let $f \in F(D_\psi)$ and $\epsilon = \epsilon(f)$. Suppose that f has distinct fixed points x and y . By Lemma 8, we have $x \leq y$ or $y \leq x$. Suppose, without loss, that $x \leq y$. Since vertices in λ are sources, there is $z \in \{0, 1\}^\lambda$ such that $x_\lambda = y_\lambda = z$. Note also that, for every $i \in \ell$, $\{i\}$ is a positive feedback vertex, and thus $x_i < y_i$ by Lemma 1.

Consider any clause μ_s , and let us prove that it is satisfied by $z \oplus \epsilon$. By Lemma 8, we have $x_{\mu_s} = y_{\mu_s}$ and, by Lemma 9, μ_s has an in-neighbor i such that $x_i = y_i$. This in-neighbor i is a positive or negative literal contained in μ_s and associated with some variable, say λ_r . We prove that this literal is satisfied by $z \oplus \epsilon$, and so is μ_s . We consider two cases:

1. Suppose that $i = \lambda_r^+$. Since $x_{\ell_{r-1}} < y_{\ell_{r-1}}$, if f_i is the OR function we have

$$x_i = f_i(x) = x_{\lambda_r} \vee x_{\ell_{r-1}} = x_{\lambda_r} \vee 0 = x_{\lambda_r} = z_{\lambda_r},$$

and if f_i is the AND function we have

$$y_i = f_i(y) = y_{\lambda_r} \wedge y_{\ell_{r-1}} = y_{\lambda_r} \wedge 1 = y_{\lambda_r} = z_{\lambda_r}.$$

Since $x_i = y_i$, we have $z_{\lambda_r} = x_i = y_i$ and consider two cases.

(a) If $z_{\lambda_r} = 1$ then $x_i = 1$ so, if f_{ℓ_r} is the OR function, then

$$x_{\ell_r} = f_{\ell_r}(x) = x_i \vee x_{\lambda_r^-} = 1 \vee x_{\lambda_r^-} = 1,$$

and this contradicts $x_{\ell_r} < y_{\ell_r}$. Hence, f_{ℓ_r} is the AND function so $\epsilon_{\lambda_r} = 0$.

(b) If $z_{\lambda_r} = 0$ then $y_i = 0$ so, if f_{ℓ_r} is the AND function, then

$$x_{\ell_r} = f_{\ell_r}(y) = y_i \wedge y_{\lambda_r^-} = 0 \wedge y_{\lambda_r^-} = 0,$$

and this contradicts $x_{\ell_r} < y_{\ell_r}$. Hence, f_{ℓ_r} is the OR function so $\epsilon_{\lambda_r} = 1$.

In both cases we have $z_{\lambda_r} \oplus \epsilon_{\lambda_r} = 1$ thus $i = \lambda_r^+$ is satisfied by $z \oplus \epsilon$.

2. Suppose that $i = \lambda_r^-$. Since $x_{\ell_{r-1}} < y_{\ell_{r-1}}$, if f_i is the OR function we have

$$x_i = f_i(x) = \neg x_{\lambda_r} \vee x_{\ell_{r-1}} = \neg x_{\lambda_r} \vee 0 = \neg x_{\lambda_r} = \neg z_{\lambda_r},$$

and if f_i is the AND function we have

$$y_i = f_i(y) = \neg y_{\lambda_r} \wedge y_{\ell_{r-1}} = \neg y_{\lambda_r} \wedge 1 = \neg y_{\lambda_r} = \neg z_{\lambda_r}.$$

We deduce that $z_{\lambda_r} \neq x_i = y_i$. If $z_{\lambda_r} = 0$ then $x_i = 1$ and we deduce as in the first case that $\epsilon_{\lambda_r} = 0$. If $z_{\lambda_r} = 1$ then $y_i = 0$ and we deduce as in the first case that $\epsilon_{\lambda_r} = 1$. In both cases we have $z_{\lambda_r} \oplus \epsilon_{\lambda_r} = 0$ thus $i = \lambda_r^-$ is satisfied by $z \oplus \epsilon$.

□

We can now prove the main property of D_ψ .

Lemma 11.

$$\phi^{\max}(D_\psi) = \begin{cases} 2 & \text{if } \psi \text{ is satisfiable,} \\ 1 & \text{otherwise.} \end{cases}$$

Proof. By Lemma 7 and the positive feedback bound, we have $1 \leq \phi^{\max}(D_\psi) \leq 2$. By Lemma 10, if $\phi^{\max}(D_\psi) = 2$ then ψ is satisfiable, and the converse is given by Lemma 7. □

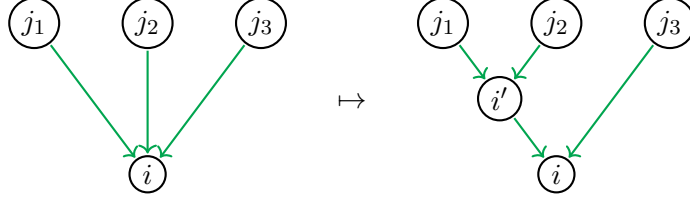


Figure 3: Transformation in Lemma 12 used to reduce the maximum in-degree.

The following lemma is useful to reduce the maximum in-degree without modifying the maximum and minimum number of fixed points. The proof is a simple exercise and is omitted.

Lemma 12. *Let D be a SID and let I be the set of vertices with exactly three in-neighbors, all positive. Let D' be obtained from D by doing the following transformation for every $i \in I$: denoting j_1, j_2, j_3 the three in-neighbors of i , the arcs $(j_1, i), (j_2, i)$ are replaced by positive arcs $(j_1, i'), (j_2, i')$, where i' is a new vertex, and a positive arc (i', i) is added (see Figure 3). Suppose that there is $f_i^{\max}, f_i^{\min} \in F(D)$ with $\phi^{\max}(D)$ and $\phi^{\min}(D)$ fixed points, respectively, where each of f_i^{\max}, f_i^{\min} is the OR function for every $i \in I$. We have*

$$\phi^{\max}(D') = \phi^{\max}(D) \quad \text{and} \quad \phi^{\min}(D') = \phi^{\min}(D).$$

We then deduce the NP-hardness of 2-MAXFPP.

Lemma 13. *2-MAXFPP is NP-hard, even when restricted to SIDs D such that $\Delta(D) \leq 2$.*

Proof. Given a 3-SAT formula ψ with n variables and m clauses, D_ψ has $4n + 2m + 1$ vertices and, by Lemma 11, we have $\phi^{\max}(D_\psi) \geq 2$ if and only if ψ is satisfiable. Since $\Delta(D_\psi) \leq 3$ and since vertices of in-degree three correspond to clauses and have only positive in-neighbors, the SID D'_ψ be obtained from D_ψ as in Lemma 12 has at most $4n + 3m + 1$ vertices and $\Delta(D'_\psi) \leq 2$. By Lemmas 7 and 11, there is $f \in F(D_\psi)$ with $\phi^{\max}(D_\psi)$ fixed points such that f_i is the OR function for every vertex i of in-degree three. Hence, by Lemma 12, we have $\phi^{\max}(D'_\psi) = \phi^{\max}(D_\psi)$ and the lemma is proven. \square

The proof of Theorem 5 is an obvious consequence of Lemmas 5, 6 and 13.

Remark 3. *Let D''_ψ be obtained from D'_ψ by adding: two new vertices u, v ; a positive arcs (ℓ_0, u) ; a negative arc (ℓ_0, v) ; and, for every $r \in [n]$, the positive arcs $(u, \lambda_r), (v, \lambda_r)$. One can check that these operations does not change the maximum number of fixed points, that is, $\phi^{\max}(D''_\psi) = \phi^{\max}(D'_\psi)$. Since D''_ψ is strongly connected this shows that 2-MAXFPP is NP-hard, even when restricted to strongly connected SIDs D with $\Delta(D) \leq 2$. By adapting conveniently Lemma 6, we obtain that, for all $k \geq 2$, k -MAXFPP is NP-hard, even when restricted to strongly connected SIDs D such that $\Delta(D) \leq 2$.*

4.3 Extensions

We now present easy extensions of the key Lemmas 7 and 10, which will be useful for the other hardness results. We start some definitions.

Definition 2 (Extensions of D_ψ and partial fixed points). *An extension of D_ψ is a SID D which is the union of D_ψ and a SID H with $V_H \cap V_\psi \subseteq \lambda$; equivalently:*

- D_ψ is a subgraph of D (i.e. each arc of D_ψ is in D with the same sign), and
- in- and out-neighbors of vertices in U_ψ are identical in D and D_ψ .

Let D be an extension of D_ψ and $I = V_D \setminus U_\psi$. Given $f \in \mathbf{F}(D)$, we say that a configuration z on I is a partial fixed point of f if $f(x)_I = x_I = z$ for some configuration x on V_D (which thus extends z); since there is no arc from U_ψ to I , if z is a partial fixed point, then $f(x)_I = z$ for every configuration x on V_D extending z .

Note that every fixed point extends a partial fixed point. Note also that D_ψ is an extension of itself with $I = \lambda$, and each $f \in \mathbf{F}(D_\psi)$ has a unique partial fixed point: the configuration z on λ such that $f_\lambda = z$. If f is as in Lemma 7 and ψ is satisfied by z , then z can be extended into two (global) fixed points. Conversely, in any case, by Lemma 10, if z can be extended into two (global) fixed points, then ψ is satisfied by $z \oplus \epsilon(f)$. The next two lemmas show that, more generally, if the SID of f is an extension of D_ψ , then these properties remain true for every partial fixed point z .

Lemma 14. *Let D be an extension of D_ψ . Let $f \in \mathbf{F}(D)$ such that, for all $i \in U_\psi$, f_i is the AND function if $i \in \ell$ and the OR function otherwise. Let z be a partial fixed point of f . Then f has at least one fixed point extending z and, if ψ is satisfied by z_λ , then f has at least two fixed points extending z .*

Proof. Let $I = V_D \setminus U_\psi$ and let $\tilde{f} \in \mathbf{F}(D_\psi)$ be defined by $\tilde{f}_\lambda = z_\lambda$ and, for all $i \in U_\psi$, \tilde{f}_i is the AND function if $i \in \ell$ and the OR function otherwise. By Lemma 7, \tilde{f} has a fixed point \tilde{x} . Let x be the configuration on V_D defined by $x_I = z$ and $x_{U_\psi} = \tilde{x}_{U_\psi}$. Since z is a partial fixed point, we have $f(x)_I = x_I$, and since each vertex $i \in U_\psi$ has the same in-neighbors in D and D_ψ , and since f_i and \tilde{f}_i are either both AND functions or both OR functions, we have $f_i(x) = \tilde{f}_i(\tilde{x}) = \tilde{x}_i = x_i$. Thus, x is a fixed point of f . By Lemma 7, if ψ is satisfied by z_λ , then \tilde{f} has a fixed point $\tilde{y} \neq \tilde{x}$. Similarly, the configuration y on V_D defined by $y_I = z$ and $y_{U_\psi} = \tilde{y}_{U_\psi}$ is a fixed point of f . Since $\tilde{y}_\lambda = \tilde{x}_\lambda = z_\lambda$, we have $\tilde{x}_{U_\psi} \neq \tilde{y}_{U_\psi}$ and thus $x \neq y$. \square

If D is an extension of D_ψ , each vertex ℓ_r is of in-degree two in D thus, for each $f \in \mathbf{F}(D)$, f_{ℓ_r} is either the AND function or the OR function. Then, as previously, we define $\epsilon(f) \in \{0, 1\}^\lambda$ by $\epsilon(f)_{\lambda_r} = 0$ if f_{ℓ_r} is the OR function and $\epsilon(f)_{\lambda_r} = 1$ otherwise.

Lemma 15. *Let D be an extension of D_ψ . Let $f \in \mathbf{F}(D)$ and let z be a partial fixed point of f . Then f has at most two fixed points extending z , and if f has two fixed points extending z , then ψ is satisfied by $z_{\lambda \oplus \epsilon}(f)$.*

Proof. Let $I = V_D \setminus U_\psi$. Since $z \in \{0,1\}^I$ and $D \setminus I$ has a positive feedback vertex set of size one, by Lemma 1, f has at most two fixed points extending z . Let \tilde{f} be the BN with component set V_ψ defined by: $\tilde{f}_\lambda = z_\lambda$ and for all configurations x on V_D , $\tilde{f}(x_{V_\psi})_{U_\psi} = f(x)_{U_\psi}$; there is no ambiguity since all the in-neighbors of vertices in U_ψ are in V_ψ . Since vertices in λ are sources of D_ψ and since every vertex in U_ψ have exactly the same in-neighbors in D and D_ψ it is clear that $\tilde{f} \in \mathbf{F}(D_\psi)$. Suppose now that f has two distinct fixed points x, y extending z . We easily check that the restrictions \tilde{x}, \tilde{y} of x, y on V_ψ are fixed points of \tilde{f} and that $\epsilon(\tilde{f}) = \epsilon(f)$. Since $x_I = y_I = z$ and $x \neq y$, we have $\tilde{x} \neq \tilde{y}$ thus, by Lemma 10, ψ is satisfied by $\tilde{x}_{\lambda \oplus \epsilon}(\tilde{f}) = z_{\lambda \oplus \epsilon}(f)$. \square

5 Maximum Fixed Point Problem

In this section, we study the case where k is not a constant but a parameter of the problem. Contrary to the two previous sections, we will see here that the restriction to SIDs with a bounded maximum in-degree reduces the complexity of the problem.

5.1 $\Delta(D)$ bounded

In this first subsection, we study the problem MAXFPP for the family of SIDs with a maximum in-degree bounded by a constant $d \geq 2$, and prove that it is $\mathbf{NP}^{\#\mathbf{P}}$ -complete. To introduce this complexity class, let us first recall that problems in $\#\mathbf{P}$ consist in counting the number of certificates of decision problems in \mathbf{NP} (the number of accepting branches of a non-deterministic polynomial time algorithm). The canonical $\#\mathbf{P}$ -complete problem is $\#\mathbf{SAT}$, which asks for the number of satisfying assignments of an input 3-CNF formula. The class $\mathbf{NP}^{\#\mathbf{P}}$ then corresponds to decision problems computable in polynomial time by a non-deterministic Turing machine with an oracle in $\#\mathbf{P}$ (a “black box” answering any problem in the class $\#\mathbf{P}$ without using any resource).

Theorem 6. *When $\Delta(D) \leq d$, MAXFPP is $\mathbf{NP}^{\#\mathbf{P}}$ -complete.*

We first prove the upper bound.

Lemma 16. *When $\Delta(D) \leq d$, MAXFPP is in $\mathbf{NP}^{\#\mathbf{P}}$.*

Proof. Let $d \geq 2$ be a fixed integer. Consider the algorithm, which takes as input a SID D with vertex set V such that $\Delta(D) \leq d$ and an integer k , and proceeds as follows.

1. Choose non-deterministically a BN f with component set V such that, for all $i \in V$, the local function f_i only depends on components in $N(i)$; this can be done in linear time since each local function f_i can be represented using $2^{|N(i)|} \leq 2^d$ bits.

2. Compute the SID D_f of f ; this can be done in quadratic time since, to compute the in-neighbors of each $i \in V$ and the corresponding signs, we only have to consider $2^{|N(i)|} \leq 2^d$ configurations (for each configuration x on $N(i)$ and $j \in N(i)$, we compare $f_i(\tilde{x})$ and $f_i(\tilde{x} \oplus e_j)$ where \tilde{x} is any configuration on V extending x).
3. Compute $\phi(f)$, the number of fixed points of f , with a call to the $\#P$ oracle (the problem of deciding if f has a fixed point is trivially in NP : choose non-deterministically a configuration, and accept if and only if it is a fixed point).
4. Accept if and only if $\phi(f) \geq k$ and $D_f = D$.

This non-deterministic polynomial time algorithm has an accepting branch if and only if $\phi^{\max}(D) \geq k$, so MAXFPP is in $NP^{\#P}$. \square

For the lower bound, it is convenient to define $NP^{\#P}$ in another way. The class PP regroups decision problems decided by a probabilistic Turing machine in polynomial time, with a probability of error less than a half. The canonical PP -complete decision problem is MAJORITY-SAT, which asks if the majority of the assignments of a given 3-CNF formula are satisfying. The class NP^{PP} then corresponds to decision problems computable in polynomial time by a non-deterministic Turing machine with an oracle in PP . It is well known that $P^{\#P} = P^{PP}$ [28], and from that we easily deduce that $NP^{\#P} = NP^{PP}$. The following problem is known to be NP^{PP} -complete [24], and thus also $NP^{\#P}$ -complete.

EXISTENTIAL-MAJORITY-3SAT (E-MAJ3SAT)
Input: a 3-CNF formula ψ over $\lambda = \{\lambda_1, \dots, \lambda_n\}$ and $s \in [n]$.
Question: does there exist $z' \in \{0, 1\}^{\lambda'}$, where $\lambda' = \{\lambda_1, \dots, \lambda_s\}$, such that ψ is satisfied by the majority of the assignments $z \in \{0, 1\}^\lambda$ extending z' ?

Lemma 17. *When $\Delta(D) \leq d$, MAXFPP is $NP^{\#P}$ -hard.*

Proof. We present a reduction from E-MAJ3SAT. Let ψ be a 3-CNF formula over the set of variables $\lambda = \{\lambda_1, \dots, \lambda_n\}$. Let $s \in [n]$ and $\lambda' = \{\lambda_1, \dots, \lambda_s\}$. Given $z' \in \{0, 1\}^{\lambda'}$, we denote by $E(z')$ the 2^{n-s} assignments $z \in \{0, 1\}^\lambda$ extending z' . Then we denote by $\alpha(z')$ the number of $z \in E(z')$ satisfying ψ , and α^* is the maximum of $\alpha(z')$ for $z' \in \{0, 1\}^{\lambda'}$. Thus, (ψ, s) is a true instance of E-MAJ3SAT if and only if $\alpha^* \geq 2^{n-s-1}$.

Let $D_{\psi,s}$ be obtained from D_ψ by adding, for every $i \in \lambda \setminus \lambda'$, a positive loop on i . Thus, $D_{\psi,s}$ is an extension of D_ψ . Let us prove that:

$$\phi^{\max}(D_{\psi,s}) = 2^{n-s} + \alpha^*.$$

Let $z' \in \{0, 1\}^{\lambda'}$ such that $\alpha(z') = \alpha^*$. Let $f \in F(D_{\psi,s})$ such that $f_{\lambda'} = z'$ and, for all $i \in U_\psi$, f_i is the AND function if $i \in \ell$ and the OR function otherwise. Since each vertex

in $\lambda \setminus \lambda'$ has a positive loop and no other in-coming arc, $E(z')$ is the set of partial fixed points of f . Hence, by Lemma 14, for every $z \in E(z')$, f has a fixed point extending z and, if ψ is satisfied by z , then f has another fixed point extending z . We deduce that f has at least $2^{n-s} + \alpha(z')$ fixed points, and thus $\phi^{\max}(D_{\psi,s}) \geq 2^{n-s} + \alpha(z') = 2^{n-s} + \alpha^*$.

For the other direction, let any $f \in F(D_{\psi,s})$ and set $\epsilon = \epsilon(f)$. Since vertices in λ' are sources, $f_{\lambda'} = z'$ for some $z' \in \{0,1\}^{\lambda'}$. Since each vertex in $\lambda \setminus \lambda'$ has a positive loop and no other in-coming arc, $E(z')$ is the set of partial fixed points of f . By Lemma 15, for every $z \in E(z')$, f has at most two fixed points extending z , and if f has two fixed points extending z , then ψ is satisfied by $z \oplus \epsilon$. Since every fixed point extends a partial fixed point, we deduce that f has at most $2^{n-s} + \beta$ fixed points, where β is the number of $z \in E(z')$ such that $z \oplus \epsilon$ is satisfying. Since $\beta = \alpha(z' + \epsilon_{\lambda'}) \leq \alpha^*$, we deduce that f has at most $2^{n-s} + \alpha^*$ fixed points. Hence, $\phi^{\max}(D_{\psi,s}) \leq 2^{n-s} + \alpha^*$.

Consequently, we have $\alpha^* \geq 2^{n-s-1}$ if and only if $\phi^{\max}(D_{\psi,s}) \geq 3 \cdot 2^{n-s-1}$. Thus, (ψ, s) is a true instance of E-MAJ3SAT if and only if $(D_{\psi,s}, k)$ is a true instance of MAXFPP, where $k = 3 \cdot 2^{n-s-1}$.

We have $\Delta(D_{\psi,s}) \leq 3$ but, using Lemma 12, we can obtain from $D_{\psi,s}$ a SID $D'_{\psi,s}$ (by adding at most one vertex and one arc per clause) with $\Delta(D'_{\psi,s}) \leq 2$ and $\phi^{\max}(D'_{\psi,s}) = \phi^{\max}(D_{\psi,s})$ (for that we use the fact, showed above, that there is $f \in F(D_{\psi,s})$ with $\phi^{\max}(D_{\psi,s})$ fixed points where f_i is the OR function for every vertex i of in-degree three). \square

5.2 $\Delta(D)$ unbounded

In this second subsection, we study MAXFPP without restriction on the maximum in-degree, and prove the following.

Theorem 7. *MAXFPP is NEXPTIME-complete.*

In Section 2 we proved that MAXFPP is in NEXPTIME, so we only have to prove its NEXPTIME-hardness; this is done with a reduction from SUCCINT-3SAT, which is a basic complete problem for this class (see Theorem 20.2 of [28]).

SUCCINT-3SAT takes as input a succinct representation of a 3-CNF formula Ψ , under the form of a circuit, and asks if Ψ is satisfiable. To give details, we need to introduce circuits and, to work in a single framework, it is convenient to introduce circuits in the language of BNs.

Let C be a SID obtained from an acyclic SID by adding a positive loop on some sources. Let I be the set of vertices with a positive loop, called *input vertices*, and let O the set of vertices of out-degree zero, called *output vertices*. We say that C is a *circuit structure*. Then any $h \in F(C)$ is a *circuit* that encodes a map g from $\{0,1\}^I$ to $\{0,1\}^O$ as follows. Since input vertices have a positive loop and no other in-coming arc, we have $h(x)_I = x_I$ for every

configuration x on V_C . Then, since $C \setminus I$ is acyclic, for any *input configuration* $z \in \{0, 1\}^I$, h has exactly one fixed point x extending z (and thus h has exactly $2^{|I|}$ fixed points). We then call $\tilde{z} = x_O$ the *output configuration computed by h from z* . Thus, h encodes the map g from $\{0, 1\}^I$ to $\{0, 1\}^O$ defined by $g(z) = \tilde{z}$ or, equivalently, by $g(x_I) = x_O$ for every fixed point x of h . We say that C is a *basic circuit structure* if $\Delta(C) \leq 2$ and every vertex i of in-degree two has only positive in-neighbors, so that h_i is either the AND gate or the OR gate. In that case, the fixed points of h can be characterized by a short 3-CNF formula.

Lemma 18. *Let C be a basic circuit structure and $h \in F(C)$. There is a 3-CNF formula ω , which can be computed in polynomial time with respect to $|V_C|$, whose variables are in V_C , and containing at most $3|V_C|$ clauses, such that, for all configurations x on V_C :*

$$h(x) = x \iff \omega \text{ is satisfied by } x.$$

Proof. Since input vertices have a positive loop and no other incoming arc, we only have to prove that ω is satisfied by x if and only if $h_i(x) = x_i$ for all non-input vertex i . We construct ω as follows, for every non-input vertex i , and simultaneously prove the lemma.

- If i is a source and h_i is the 1 constant function, we add the clause (i^+, i^+, i^+) . This clause is satisfied by x if and only if $x_i = 1 = h_i(x)$.
- If i is a source and h_i is the 0 constant function, we add the clause (i^-, i^-, i^-) . This clause is satisfied by x if and only if $x_i = 0 = h_i(x)$.
- If i has a unique in-neighbor j , which is positive, we add the clauses (i^+, j^-, j^-) and (i^-, j^+, j^+) . These clauses are simultaneously satisfied by x if and only if $x_i = x_j = h_i(x)$.
- If i has a unique in-neighbor j , which is negative, we add the clauses (i^+, j^+, j^+) and (i^-, j^-, j^-) . These clauses are simultaneously satisfied by x if and only if $x_i = \neg x_j = h_i(x)$.
- If i has two in-neighbors j, k , and h_i is the AND gate, we add three clauses: (i^-, j^+, j^+) , (i^-, k^+, k^+) and (i^+, j^-, k^-) . These clauses are simultaneously satisfied by x if and only if $x_i = x_j \wedge x_k = h_i(x)$.
- If i has two in-neighbors j, k , and h_i is the OR gate, we add three clauses: (i^+, j^-, j^-) , (i^+, k^-, k^-) and (i^-, j^+, k^+) . These clauses are simultaneously satisfied by x if and only if $x_i = x_j \vee x_k = h_i(x)$.

□

Consider a 3-CNF formula Ψ over a set \mathbf{A} of 2^n variables and with a set \mathbf{M} of 2^m clauses. To simplify notations, we take two sets W, U of size n and m respectively, and write:

$$\mathbf{A} = \{\Lambda_w\}_{w \in \{0,1\}^W}, \quad \mathbf{M} = \{M_u\}_{u \in \{0,1\}^U}, \quad M_u = (M_{u,01}, M_{u,10}, M_{u,11}).$$

A *succinct representation* of Ψ is then a couple (h, C) , where C is a basic circuit structure and $h \in \mathbf{F}(C)$, with the following specifications: the set of input vertices is $U \cup P$, where $P = \{p_1, p_2\}$, and the set of output vertices is $W \cup \{\rho\}$ (these four sets are pairwise disjoint); and for every fixed point x of h with $x_P \neq 00$, we have:

$$M_{x_U, x_P} = \begin{cases} \Lambda_{x_W}^+ & \text{if } x_\rho = 1, \\ \Lambda_{x_W}^- & \text{if } x_\rho = 0. \end{cases} \quad (*)$$

Hence, each input configuration with $x_P \neq 00$ corresponds to a clause (x_U) and a valid position in that clause (x_P) , and the output configuration gives the corresponding positive or negative literal: the involved variable (x_W) and the polarity of the literal (x_ρ) . See Figure 4 for an illustration. In all the following, (h, C) is a given succinct representation of Ψ .

The next definition provides some flexibility regarding the representation of Ψ .

Definition 3 (ϵ -fixed points and consistency). *Let C, C' be circuit structures with $V_C \subseteq V_{C'}$, $h' \in \mathbf{F}(C')$ and ϵ be a configuration on $V_{C'}$. A configuration x on $V_{C'}$ is an ϵ -fixed point of h' if $x \oplus \epsilon$ is a fixed point of h' . We say that h' is ϵ -consistent if every ϵ -fixed point x of h' extends a fixed point of h and has a valid position, that is, $x_P \neq 00$ (thus $(*)$ holds for every ϵ -fixed point x , so h' embeds in some way the calculations performed by h). We say that h' is consistent if it is ϵ -consistent with $\epsilon = 0$.*

We will construct, from the succinct representation (h, C) of Ψ , a SID D_Ψ with a number of vertices linear in $|V_C|$ such that $\phi^{\max}(D_\Psi) \geq 2^{m+1}$ if and only if Ψ is satisfiable; and since D_Ψ will have a positive feedback vertex set of size $m + 1$, the inequality in this equivalence is actually an equality (by Theorem 2). We first give a sketch of the construction, proceeding in three steps.

First, we construct a circuit structure C' over C , whose input configurations correspond to the clauses of Ψ (so the corresponding BNs have 2^m fixed points, one per clause) and with two output vertices: ρ (which is already in C) and ν . We then show two properties.

- (1) Given an assignment $\zeta \in \{0, 1\}^{\mathbf{A}}$, there is a consistent BN $h' \in \mathbf{F}(C')$ such that, for every fixed point x , the clause M_{x_U} is satisfied by ζ if and only if $x_\rho = x_\nu$.
- (2) Conversely, for every ϵ -consistent BN $h' \in \mathbf{F}(C')$ there is an assignment $\zeta \in \{0, 1\}^{\mathbf{A}}$ such that, for every ϵ -fixed point x , the clause M_{x_U} is satisfied by ζ whenever $x_\rho = x_\nu$.

The trick is then to encode the consistency conditions and the condition “ $x_\rho = x_\nu$ ” into a 3-CNF formula. First consider the formula ω characterizing the fixed points of h . Then configuration x on $V_{C'}$ extends a fixed point of h if and only if ω is satisfied by x_{V_C} . By adding few clauses in ω , we can then obtain a formula ψ which is satisfied by x if and only if x extends a fixed point of h , $x_P \neq 00$ and $x_\rho = x_\nu$. In particular, if ψ is satisfied

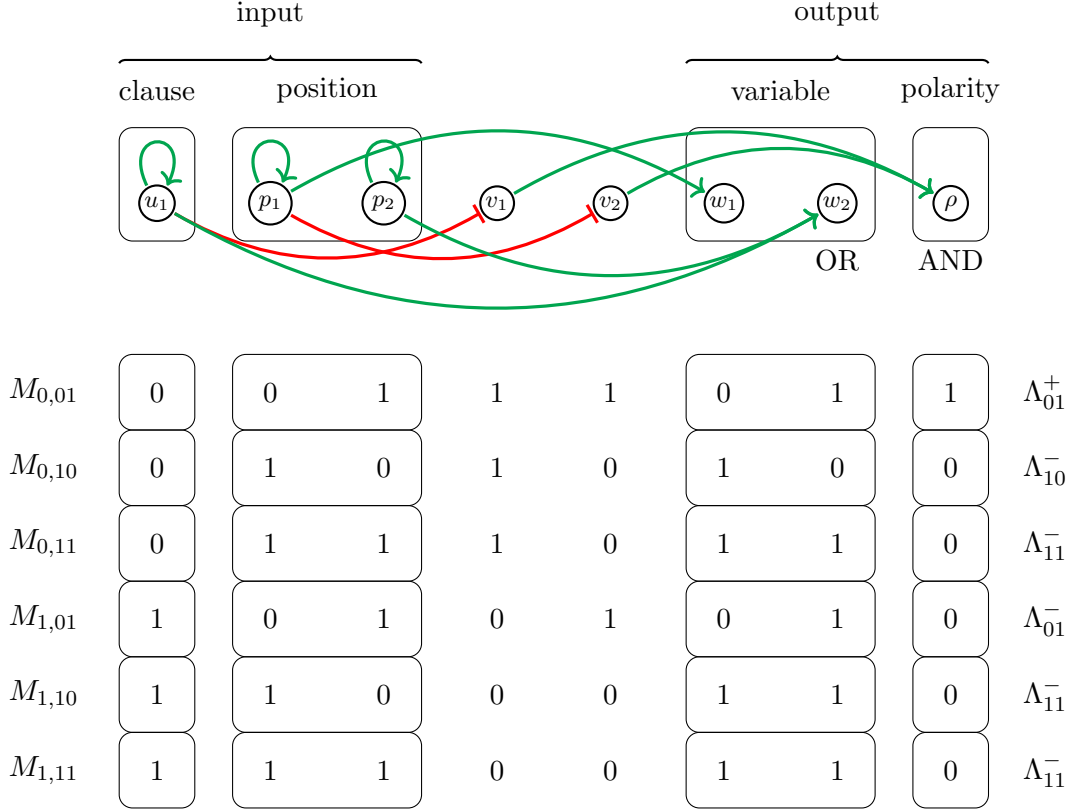


Figure 4: A circuit $h \in F(C)$ encoding a 3-CNF formula Ψ over the set of variables $\Lambda = \{\Lambda_{00}, \Lambda_{01}, \Lambda_{10}, \Lambda_{11}\}$ and containing the clauses $M_0 = (M_{0,01}, M_{0,10}, M_{0,11}) = (\Lambda_{01}^+, \Lambda_{10}^-, \Lambda_{11}^-)$ and $M_1 = (M_{1,01}, M_{1,10}, M_{1,11}) = (\Lambda_{01}^-, \Lambda_{11}^-, \Lambda_{11}^-)$. In other words $\Psi = (\Lambda_{01} \vee \neg \Lambda_{10} \vee \neg \Lambda_{11}) \wedge (\neg \Lambda_{01} \vee \neg \Lambda_{11})$; this formula is equivalent to the formula ψ of Figure 2. The circuit structure C , which is basic, is drawn on the top; the set of input vertices is $U \cup P$ with $U = \{u_1\}$ and $P = \{p_1, p_2\}$, and the set of output vertices is $W \cup \{\rho\}$ with $W = \{w_1, w_2\}$. The circuit h is the BN in $F(C)$ such that h_{w_2} is the OR function and h_ρ is the AND function (there is a unique possible local function for the other vertices). The 6 fixed points x of h with $x_P \neq 00$ are displayed. They encode the formula Ψ as indicated.

by the 2^m ϵ -fixed points of h' , then h' is ϵ -consistent. Now, if Ψ is satisfied by ζ , then ψ is satisfied by the 2^m fixed points of the consistent BN h' described in (1). Conversely, for any $h' \in F(C')$ and ϵ , if ψ is satisfied by the 2^m ϵ -fixed points of h' , then Ψ is satisfied by the assignment ζ described in (2). Hence, we obtain:

- (3) The following conditions are equivalent: (a) Ψ is satisfiable; (b) there is $h' \in F(C')$ such that ψ is satisfied by the 2^m fixed points of h' ; (c) there are $h' \in F(C')$ and ϵ such that ψ is satisfied by the 2^m ϵ -fixed points of h' .

The last step is to consider D_ψ . Actually, we define D_Ψ as the extension of D_ψ resulting from the union of C' and D_ψ . If Ψ is satisfiable, there is a BN $f \in F(D_\Psi)$, satisfying the conditions of Lemma 14, whose partial fixed points are the fixed points of the BN $h' \in F(C')$ described in (b). Then, since the 2^m partial fixed points are satisfying assignments of ψ , they give rise to 2^{m+1} fixed points for f . Conversely, for any $f \in F(D_\Psi)$, the partial fixed points of f are the fixed points of some $h' \in F(C')$, and if f has 2^{m+1} fixed points, then each fixed point x of h' gives rise to two fixed points of f . We then deduce from Lemma 15 that this is possible only if there is ϵ such that, for every fixed point x of h' , ψ is satisfied by $x \oplus \epsilon$. This is equivalent to say that ψ is satisfied by the 2^m ϵ -fixed points of h' , so (c) holds and we deduce that Ψ is satisfiable.

We now proceed to the details.

Definition 4 (C'). We denote by C' the circuit structure obtained from C by removing the positive loops on vertices p_1, p_2 , and by adding three new vertices, s_1, s_2, ν , and the following arcs:

- a null arc (j, p_1) and a null arc (j, p_2) , for all $j \in U \cup \{s_1, s_2\}$;
- a null arc (j, ν) , for all $j \in W \cup \{s_1, s_2\}$.

So C' is a circuit structure where U is the set of input vertices (input configurations correspond to clauses of Ψ) and $\{\rho, \nu\}$ is the set of output vertices. The vertices s_1, s_2 are sources. See the top of Figure 5 for an illustration.

The following lemma is a formal statement of the property (1) discussed above.

Lemma 19. For every assignment $\zeta \in \{0, 1\}^\Lambda$ there is a consistent circuit $h' \in F(C')$ such that, for every fixed point x of h' ,

$$M_{x_U} \text{ is satisfied by } \zeta \iff x_\rho = x_\nu.$$

Proof. For every configuration x on $V_{C'}$, we define $h'(x)$ componentwise as follows. Since every non-input vertex i of C has exactly the same incoming arcs in C' and C , we can set $h'_i(x) = h_i(x_{V_C})$. Next we define h'_{s_1} and h'_{s_2} as the 0 constant function. Since each $i \in U$

has a positive loop and nothing else, we necessarily set $h'_i(x) = x_i$. It remains to define the local functions of p_1, p_2 and ν . Let $S = \{s_1, s_2\}$.

First, we set

$$h'_{p_1}(x) = \begin{cases} \bigoplus_{i \in U \cup S} x_i & \text{if } x_S \neq 00, \\ 0 & \text{if } x_S = 00 \text{ and } M_{x_U, 01} \text{ is satisfied by } \zeta, \\ 1 & \text{otherwise.} \end{cases}$$

$$h'_{p_2}(x) = \begin{cases} \bigoplus_{i \in U \cup S} x_i & \text{if } x_S \neq 00, \\ 0 & \text{if } x_S = 00 \text{ and } M_{x_U, 10} \text{ is satisfied by } \zeta \text{ but not } M_{x_U, 01}, \\ 1 & \text{otherwise.} \end{cases}$$

It is clear h'_{p_1} and h'_{p_2} only depend on components in $U \cup S$, and the first case in each definition ensures that these dependencies are effective and neither positive nor negative, so that $h'_{p_1} \in F_{p_1}(C')$ and $h'_{p_2} \in F_{p_2}(C')$. Furthermore, if $h'(x) = x$ then $x_S = 00$, and it is easy to check that this implies $x_P \neq 00$ and the following equivalence:

$$M_{x_U} \text{ is satisfied by } \zeta \iff M_{x_U, x_P} \text{ is satisfied by } \zeta.$$

Second, we set

$$h'_\nu(x) = \begin{cases} \bigoplus_{i \in W \cup S} x_i & \text{if } x_S \neq 00 \\ \zeta_{\Lambda_{x_W}} & \text{otherwise.} \end{cases}$$

Similarly, h'_ν only depends on components in $W \cup S$, and the first case ensures that these dependencies are effective and neither positive nor negative, so that $h'_\nu \in F_\nu(C')$.

Suppose that $h'(x) = x$. As said above, we have $x_S = 00$ and $x_P \neq 00$. Furthermore, for each non-input vertex i of C we have $h_i(x_{V_C}) = h'_i(x) = x_i$, thus x_{V_C} is a fixed point of h . Hence, h' is consistent, and M_{x_U, x_P} is $\Lambda_{x_W}^+$ if $x_P = 1$ and $\Lambda_{x_W}^-$ otherwise. Since $x_\nu = h'_\nu(x) = \zeta_{\Lambda_{x_W}}$, the literal M_{x_U, x_P} is satisfied by ζ if and only if $x_P = x_\nu$, and by the equivalence above, the clause M_{x_U} is satisfied by ζ if and only if $x_P = x_\nu$. \square

We now prove a kind of converse, which is a formal statement of the property (2) discussed above.

Lemma 20. *For every ϵ -consistent circuit $h' \in F(C')$ there is an assignment $\zeta \in \{0, 1\}^\Lambda$ such that, for every ϵ -fixed point x of h' ,*

$$x_P = x_\nu \implies M_{x_U} \text{ is satisfied by } \zeta.$$

Proof. Since s_1, s_2 are sources, for every fixed points x, y of h' we have $x_{s_1} = y_{s_1}$ and $x_{s_2} = y_{s_2}$. Thus, if $x_W = y_W$ then $x_\nu = h'_\nu(x) = h'_\nu(y) = y_\nu$, because all the in-neighbors

of ν are in $W \cup \{s_1, s_2\}$. In other words, there is a function g from $\{0, 1\}^W$ to $\{0, 1\}$ such that $g(x_W) = x_\nu$ for every fixed point x of h' . Let any $\zeta \in \{0, 1\}^\Lambda$ satisfying

$$\zeta_{\Lambda_{x_W} \oplus \epsilon_W} = g(x_W) \oplus \epsilon_\nu = x_\nu \oplus \epsilon_\nu$$

for every fixed point x of h' . This is equivalent to say that, for every ϵ -fixed point x of h' ,

$$\zeta_{\Lambda_{x_W}} = x_\nu.$$

Now, since h' is ϵ -consistent, for every ϵ -fixed point x of h' we have $x_P \neq 00$ and M_{x_U, x_P} is $\Lambda_{x_W}^+$ if $x_\rho = 1$ and $\Lambda_{x_W}^-$ otherwise. If $x_\rho = x_\nu = \zeta_{\Lambda_{x_W}}$, then this literal M_{x_U, x_P} is satisfied by ζ , and so is the clause M_{x_U} . \square

Here is the definition of the formula ψ encoding the consistency conditions and the condition “ $x_\rho = x_\nu$ ”.

Definition 5 (Formula ψ associated with h). *Let ω be the 3-CNF formula characterizing the fixed points of h , as in Lemma 18. The formula ψ associated with h is the 3-CNF formula obtained from ω by adding the following three clauses: (p_1^+, p_2^+, p_2^+) , (ρ^+, ν^-, ν^-) and (ρ^-, ν^+, ν^+) . So ψ is a formula over the set of variables $\lambda = V_C \cup \{\nu\}$.*

Note that, given a fixed point x of h' , ω is satisfied by x if and only if x extends a fixed point of h (since ω is satisfied by x if and only if ω is satisfied by x_{V_C} if and only if x_{V_C} is a fixed point of h), and the three additional clauses are simultaneously satisfied by x if and only if $x_P \neq 00$ and $x_\rho = x_\nu$. In particular, if ψ is satisfied by every ϵ -fixed point of h' , then h' is ϵ -consistent.

We now prove a formal statement of the property (3) discussed above.

Lemma 21. *The following conditions are equivalent:*

- (a) Ψ is satisfiable;
- (b) there is $h' \in F(C')$ such that ψ is satisfied by every fixed point of h' ;
- (c) there are $h' \in F(C')$ and $\epsilon \in \{0, 1\}^{V_{C'}}$ such that ψ is satisfied by every ϵ -fixed point of h' .

Proof. Suppose that Ψ is satisfied by $\zeta \in \{0, 1\}^\Lambda$. By Lemma 19, there is a BN $h' \in F(C')$ consistent with h such that $x_\rho = x_\nu$ for every fixed point x of h . By consistency, $x_P \neq 00$ and x extends a fixed point of h , thus ω is satisfied. We deduce that ψ is satisfied by every fixed point of h' . This proves that (a) implies (b). Since (b) trivially implies (c), it remains to prove that (c) implies (a).

Suppose h' and ϵ are as in (c). Then h' is ϵ -consistent, and $x_\rho = x_\nu$ for every ϵ -fixed point x of h' . Hence, by Lemma 20, there is an assignment $\zeta \in \{0, 1\}^\Lambda$ such that, for every

ϵ -fixed point x of h' , M_{x_U} is satisfied by ζ . Since U is the set of input vertices of C' , any input configuration, that is any member of in $\{0, 1\}^U$, is extended by a fixed point of h' . Hence, for any input configuration u , the input configuration $u \oplus \epsilon_U$ is extended by a fixed point x of h' , so u is extended by $x \oplus \epsilon$, which is an ϵ -fixed point of h' . Hence, all the clauses of Ψ are satisfied by ζ . This proves that (c) implies (a). \square

The formal definition of our construction D_Ψ follows, see Figure 5 for an illustration.

Definition 6 (D_Ψ). *Let C' be the circuit structure of Definition 4. Let ψ be the 3-CNF formula associated with h given in Definition 5, which is a formula over the set of variables $\lambda = V_C \cup \{\nu\}$. Let D_ψ be the SID defined from ψ as in Definition 1. We define D_Ψ as the extension of D_ψ obtained by taking the union of C' and D_ψ (supposing naturally that vertices s_1, s_2 are not in $D_\psi \setminus \lambda$). We denote by V_Ψ the vertex set of D_Ψ .*

Since ψ has at most $3|V_C| + 3$ clauses and $|\lambda| = |V_C| + 1$, we have

$$|V_\Psi| = |V_\psi| + 2 \leq (4|\lambda| + 2(3|V_C| + 3) + 1) + 2 = 10|V_C| + 13,$$

which is linear according to the size of the succinct representation of Ψ .

Since C' has m positive loops and no other cycle, and since $D_\Psi \setminus V_{C'}$ has a positive feedback vertex set of size one, we deduce that D_Ψ has a positive feedback vertex set of size $m + 1$. Thus, $\phi^{\max}(D_\Psi) \leq 2^{m+1}$ by the positive feedback bound. Actually, since D_Ψ has $m + 1$ vertex-disjoint positive cycles, we have $\tau^+(D) = m + 1$ (since C' has m positive loops and $D_\psi \setminus \lambda$ has a positive cycle). Putting things together, we prove that the positive feedback bound is reached if and only if Ψ is satisfiable, and this proves Theorem 7.

Lemma 22. $\phi^{\max}(D_\Psi) = 2^{m+1}$ if and only if Ψ is satisfiable.

Proof. Suppose that Ψ is satisfied by an assignment $\zeta \in \{0, 1\}^\Lambda$. By Lemma 21 there is $h' \in F(C')$ such that ψ is satisfied by all the 2^m fixed points of h' . Let $f \in F(D_\Psi)$ be defined as follows. First, $f(x)_{V_{C'}} = h'(x_{V_{C'}})$ for every configuration x on V_Ψ . Second, for every $i \in V_\Psi \setminus V_{C'}$, we define f_i has the AND function if $i \in \ell$ and the OR function otherwise (vertices in ℓ are those with two in-neighbors corresponding to the positive and negative literals associated with a variable in λ). By the first part of the definition, the set of fixed points of h' is the set of partial fixed points of f . So ψ is satisfied by the 2^m partial fixed points of f , and we deduce from Lemma 14 that f has at least 2^{m+1} fixed points. Thus, $\phi^{\max}(D_\Psi) \geq 2^{m+1}$ and $\phi^{\max}(D_\Psi) = 2^{m+1}$ by the positive feedback bound.

Conversely, suppose that $\phi^{\max}(D_\Psi) = 2^{m+1}$. Let $f \in F(D_\Psi)$ with 2^{m+1} fixed points. Let h' be the BN with component set $V_{C'}$ defined by $h'(x_{V_{C'}}) = f(x)_{V_{C'}}$ for all configurations x on V_Ψ ; there is no ambiguity since vertices in C' have only in-neighbors in C' and, thanks to this property, the SID of h' is $D_\Psi \setminus U_\psi = C'$. Furthermore, the set of fixed points of h' is the set of partial fixed points of f . Hence, f has 2^m partial fixed points. Since f has

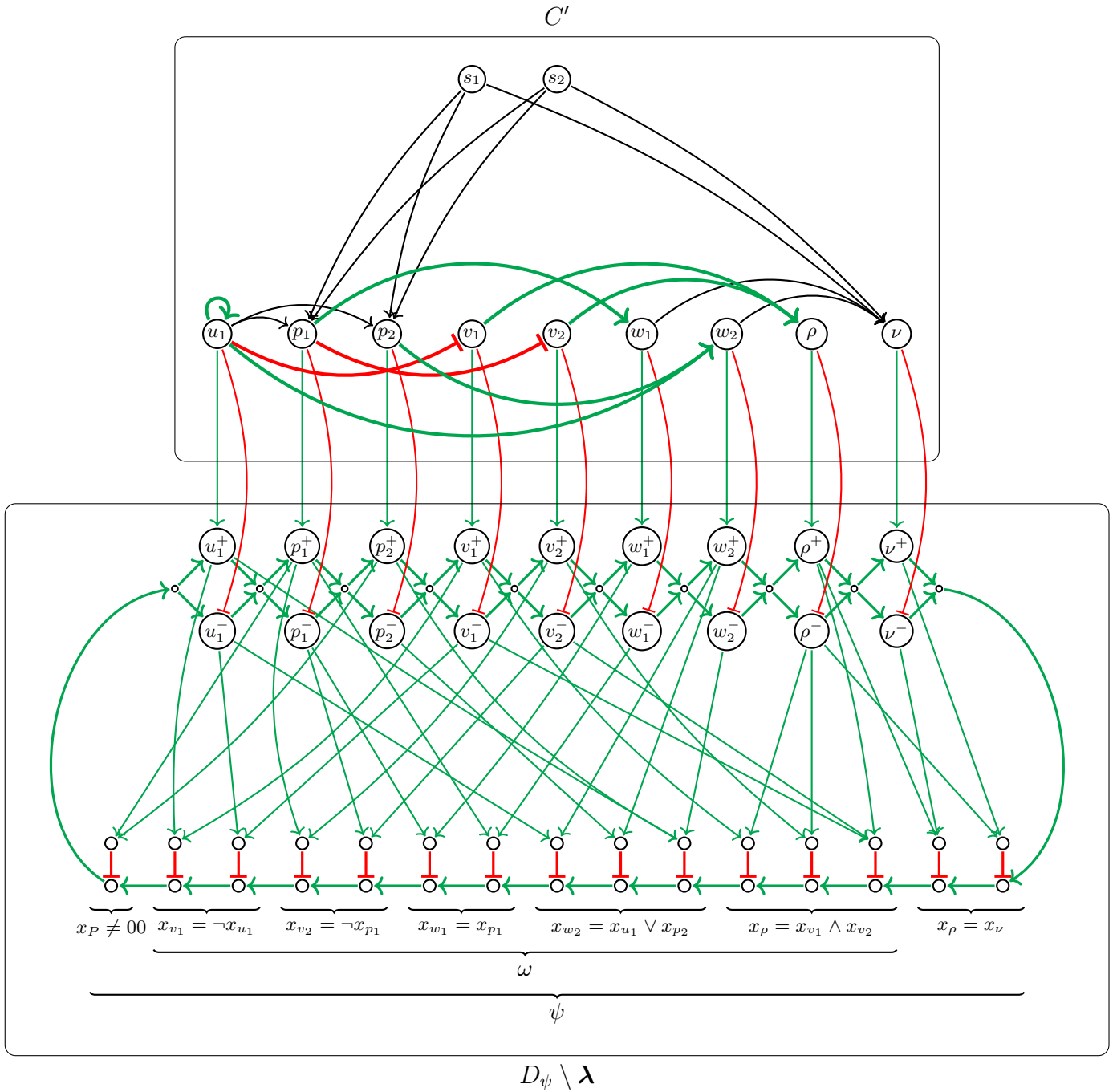


Figure 5: The SID D_Ψ constructed from the circuit $h \in F(C)$ described in Figure 4. Black arrows represent null arcs. Braces correspond to sets of clauses contained in ψ , and below each brace the necessary and sufficient conditions for the corresponding clauses to be simultaneously satisfied by an assignment x are given.

at most two fixed points extending the same partial fixed point, and since every fixed point of f extends a partial fixed point, we deduce that, for every partial fixed point x , f has exactly two fixed points extending x . Hence, by Lemma 15, ψ is satisfied by $x_{\lambda \oplus \epsilon}(f)$ for every fixed point x of h' . This is equivalent to say that ψ is satisfied by every ϵ -fixed point of h' , where ϵ is any configuration on $V_{C'}$ extending $\epsilon(f)$, and we deduce from Lemma 21 that Ψ is satisfiable. \square

Remark 4. *By this lemma, the problem of deciding if $\phi^{\max}(D) = 2^{\tau^+(D)}$ is NEXPTIME-complete. This is interesting since many works have been devoted to study the conditions for similar bounds to be reached, see [14, 12, 8] and the references therein. In particular, [8] gives a graph-theoretical characterization of the SIDs D with only positive arcs such that $\phi^{\max}(D) = 2^{\tau^+(D)}$, and we may ask if the problem remains as hard under this restriction. Furthermore, the much studied network coding problem in information theory can be restated as a problem concerning BNs that consists in deciding if a bound similar to the positive feedback bound is reached [14].*

Remark 5. *With slightly more precise arguments, we can prove that $\phi^{\max}(D_{\Psi}) = 2^{m+1} + \alpha$, where α is the maximum number of clauses contained in Ψ that can be simultaneously satisfied.*

6 Minimum Fixed Point Problem

In this section, we study decision problems related to the minimum number of fixed points, and we obtain the following tight complexity results. A new complexity class is involved: NP^{NP} (often denoted by Σ_2^{P}), which contains decision problems computable in polynomial time on a non-deterministic Turing machine with an oracle in NP.

Theorem 8. *Let $k \geq 1$ and $d \geq 2$ be fixed integers.*

- k -MINFPP and MINFPP are NEXPTIME-complete.
- When $\Delta(D) \leq d$, k -MINFPP is NP^{NP} -complete.
- When $\Delta(D) \leq d$, MINFPP is $\text{NP}^{\#\text{P}}$ -complete.

We first prove the upper bounds.

Lemma 23. *Let $k \geq 1$ and $d \geq 2$ be fixed integers.*

- k -MINFPP and MINFPP are in NEXPTIME.
- When $\Delta(D) \leq d$, k -MINFPP is in NP^{NP} .
- When $\Delta(D) \leq d$, MINFPP is in $\text{NP}^{\#\text{P}}$.

Proof. As argued in Section 2, k -MINFPP and MINFPP are in NEXPTIME. We now consider the restrictions to SIDs with bounded maximum in-degree.

For k -MINFPP, consider the algorithm that takes as input a SID D with vertex set V and such that $\Delta(D) \leq d$, and proceeds as follows.

1. Choose non-deterministically a BN f with component set V such that, for all $i \in V$, the local function f_i only depends on components in $N(i)$; this can be done in linear time since each local function f_i can be represented using $2^{|N(i)|} \leq 2^d$ bits.
2. Compute the SID D_f of f ; this can be done in quadratic time since, to compute the in-neighbors of each $i \in V$ and the corresponding signs, we only have to consider $2^{|N(i)|} \leq 2^d$ configurations (for each configuration x on $N(i)$ and $j \in N(i)$, we compare $f_i(\tilde{x})$ and $f_i(\tilde{x} \oplus e_j)$ where \tilde{x} is any configuration on V extending x).
3. Decide, with a call to the NP-oracle, if f has at least k fixed points (this decision problem is trivially in NP: choose non-deterministically k distinct configurations, and accept if and only if they are all fixed points).
4. Accept if and only if the oracle's answer is no and $D_f = D$.

This non-deterministic polynomial time algorithm has an accepting branch if and only if $\phi^{\min}(D) < k$. Thus, when $\Delta(D) \leq d$, k -MINFPP is in NP^{NP} .

For MINFPP, the algorithm we consider is the one described in Lemma 16, excepted that it accepts if and only if $\phi(f) < k$ and $D_f = D$. With this modification, we obtain a non-deterministic polynomial time algorithm which calls the $\#\text{P}$ oracle and has an accepting branch if and only if $\phi^{\min}(D) < k$. Thus, when $\Delta(D) \leq d$, MINFPP is in $\text{NP}^{\#\text{P}}$. \square

For the lower bounds, we use reductions based on the construction D_ψ given in Section 4. We thus use the notations of that section, and we start with an adaptation of that construction suited for the study of the minimum number of fixed points.

Definition 7 (D_ψ^- , extension of D_ψ^-). *We denote by D_ψ^- the SID obtained from the SID D_ψ of Definition 1 by making negative the arc (c_1, ℓ_0) . An extension of D_ψ^- is defined as in Definition 2 with D_ψ^- instead of D_ψ .*

As previously, given $f \in \text{F}(D)$ and setting $I = V_D \setminus U_\psi$, we say that a configuration z on I is a *partial fixed point* of f if $f(x)_I = x_I = z$ for some configuration x on V_D (and since there is no arc from U_ψ to I , if z is a partial fixed point, then $f(x)_I = z$ for *every* extension x of z).

The following lemmas are adaptations of Lemmas 14 and 15 to the above definition. Together, they show that $\phi^{\min}(D_\psi^-) = 0$ if and only if ψ is satisfiable.

Lemma 24. *Let D be an extension of D_ψ^- . Let $f \in \mathbf{F}(D)$ such that, for all $i \in U_\psi$, f_i is the AND function if $i \in \ell$ and the OR function otherwise. Let z be a partial fixed point of f . Then f has at most one fixed point extending z and, if ψ is satisfied by z_λ , then f has no fixed point extending z .*

Proof. Let $I = V_D \setminus U_\psi$, and let f^0, f^1 be the BNs with component set V_D defined as follows. First, $f_I^0 = f_I^1 = z$. Second, $f_{\ell_0}^0 = 0, f_{\ell_0}^1 = 1$. Third, $f_i^0 = f_i^1 = f_i$ for all $i \in U_\psi \setminus \{\ell_0\}$. Then f^0, f^1 have the same SID, which is the SID obtained from D by removing all the arc (j, i) with $i \in I \cup \{\ell_0\}$, and which is thus acyclic. Hence, f^0 has a unique fixed point x^0 and f^1 has a unique fixed point x^1 .

Let D' be obtained from D by making positive the arc (c_1, ℓ_0) , so that D' is an extension of D_ψ . Let $f' \in \mathbf{F}(D')$ such that $f'_i = f_i$ for all vertices $i \neq \ell_0$. By Lemma 14, f' has a fixed point extending z , and another fixed point extending z if ψ is satisfied by z_λ .

It is clear that if x is a fixed point of f or f' extending z , then $f^0(x) = x$ if $x_{\ell_0} = 0$ and $f^1(x) = x$ if $x_{\ell_0} = 1$, so x is one of x^0, x^1 . Thus, the set of fixed points of f extending z is included in $\{x^0, x^1\}$, and similarly for f' . Furthermore, if $f'(x) = x$ then $f(x) \neq x$ (because $f_{\ell_0}(x) = \neg x_{c_1}$ and $f'_{\ell_0}(x) = x_{c_1}$). Since f' has a fixed point extending z , we deduce that f has at most one fixed point extending z and, since f' has two fixed points extending z if ψ is satisfied by z_λ , we deduce that f has no fixed point extending z if ψ is satisfied by z_λ . \square

Given an extension D of D_ψ^- and $f \in \mathbf{F}(D)$, we define the assignment $\epsilon(f)$ exactly as previously: for $r \in [n]$, $\epsilon(f)_{\lambda_r} = 0$ if f_{ℓ_r} is the OR function, and $\epsilon(f)_{\lambda_r} = 1$ otherwise.

Lemma 25. *Let D be an extension of D_ψ^- . Let $f \in \mathbf{F}(D)$ and let z be a partial fixed point of f . If f has no fixed point extending z , then ψ is satisfied by $z_\lambda \oplus \epsilon(f)$.*

Proof. Let f^0, f^1, f' be the BNs defined from f as in the previous proof, and let x^0, x^1 be the fixed points of f^0, f^1 , respectively (which extend z). For all vertices $i \neq \ell_0$ and all $a \in \{0, 1\}$ we have $f_i(x^a) = f'_i(x^a) = f_i^a(x^a) = x_i^a$. Suppose that f has no fixed point extending z . Then, for all $a \in \{0, 1\}$ we have $\neg x_{c_1}^a = f_{\ell_0}(x^a) \neq x_{\ell_0}^a$ and thus $f'_{\ell_0}(x^a) = x_{c_1}^a = x_{\ell_0}^a$. Consequently, x^0 and x^1 are distinct fixed points of f' extending z and, according to Lemma 15, ψ is satisfied by $z_\lambda + \epsilon(f')$. Since $\epsilon(f') = \epsilon(f)$, this proves the lemma. \square

The following lemma shows that 1-MINFPP is as hard as k -MINFPP for every $k \geq 2$.

Lemma 26. *Let $k \geq 2$ and let D be any SID. Let D' be the SID obtained from D by adding $\lceil \log_2 k \rceil$ new vertices and a positive loop on each new vertex. Then*

$$\phi^{\min}(D') < k \iff \phi^{\min}(D) = 0.$$

Proof. Let $\ell = \lceil \log_2 k \rceil$ so that $k \leq 2^\ell$. Let H be the SID with ℓ vertices and a positive loop on each vertex. Then $F(H)$ contains a unique BN, which is the identity, thus $\phi^{\min}(H) = 2^\ell$. Since D' is the disjoint union of D and H ,

$$\phi^{\min}(D') = \phi^{\min}(D) \cdot \phi^{\min}(H) = \phi^{\min}(D) \cdot 2^\ell.$$

Thus, $\phi^{\min}(D') = 0 < k$ if $\phi^{\min}(D) = 0$, and $\phi^{\min}(D') \geq 2^\ell \geq k$ otherwise. \square

We now prove that, for SIDs with a bounded maximum in-degree, k -MINFPP and MINFPP are NP^{NP} -hard and $\text{NP}^{\#\text{P}}$ -hard, respectively. The proof is very similar to that of Lemma 17. The hardness of k -MINFPP is obtained with a reduction from the following decision problem, known to be NP^{NP} -complete [28, Theorem 17.10].

QUANTIFIED SATISFIABILITY with 2 alternating quantifiers (QSAT₂)
Input: a 3-CNF formula ψ over $\lambda = \{\lambda_1, \dots, \lambda_n\}$ and $s \in [n]$.
Question: does there exist $z' \in \{0, 1\}^{\lambda'}$, where $\lambda' = \{\lambda_1, \dots, \lambda_s\}$, such that ψ is satisfied by all the assignments $z \in \{0, 1\}^\lambda$ extending z' ?

Lemma 27. *Let $k \geq 1$ and $d \geq 2$ be fixed integers.*

- *When $\Delta(D) \leq d$, k -MINFPP is NP^{NP} -hard.*
- *When $\Delta(D) \leq d$, MINFPP is $\text{NP}^{\#\text{P}}$ -hard.*

Proof. For the second item, we present a reduction from E-MAJ3SAT. Let ψ be a 3-CNF formula over the set of variable $\lambda = \{\lambda_1, \dots, \lambda_n\}$. Let $s \in [n]$ and $\lambda' = \{\lambda_1, \dots, \lambda_s\}$. Given $z' \in \{0, 1\}^{\lambda'}$, we denote by $E(z')$ the 2^{n-s} assignments $z \in \{0, 1\}^\lambda$ extending z' . Then we denote by $\alpha(z')$ the number of $z \in E(z')$ satisfying ψ , and α^* is the maximum of $\alpha(z')$ for $z' \in \{0, 1\}^{\lambda'}$. Thus, (ψ, s) is a true instance if and only if $\alpha^* \geq 2^{n-s-1}$.

Let $D_{\psi,s}$ be the extension of $D_{\bar{\psi}}$ obtained by adding, for every $i \in \lambda \setminus \lambda'$, a positive loop on i . Let us prove that:

$$\phi^{\min}(D_{\psi,s}) = 2^{n-s} - \alpha^*.$$

Let $z' \in \{0, 1\}^{\lambda'}$ such that $\alpha(z') = \alpha^*$. Let $f \in F(D_{\psi,s})$ such that $f_{\lambda'} = z'$ and, for all $i \in U_\psi$, f_i is the AND function if $i \in \ell$ and the OR function otherwise. Since each vertex in $\lambda \setminus \lambda'$ has a positive loop and no other in-coming arc, $E(z')$ is the set of partial fixed points of f . Hence, by Lemma 24, for every $z \in E(z')$, f has at most one fixed point extending z and, if ψ is satisfied by z , then f has no fixed point extending z . Since every fixed point extends a partial fixed point, we deduce that f has at most $2^{n-s} - \alpha(z')$ fixed points, and thus $\phi^{\min}(D_{\psi,s}) \leq 2^{n-s} - \alpha(z') = 2^{n-s} - \alpha^*$.

For the other direction, let any $f \in F(D_{\psi,s})$ and set $\epsilon = \epsilon(f)$. Since vertices in λ' are sources, $f_{\lambda'} = z'$ for some $z' \in \{0, 1\}^{\lambda'}$. Since each vertex in $\lambda \setminus \lambda'$ has a positive loop

and no other in-coming arc, $E(z')$ is the set of partial fixed points of f . By Lemma 25, for every $z \in E(z')$, if ψ is not satisfied by $z \oplus \epsilon$, then f has a fixed point extending z . Thus, f has at least $2^{n-s} - \alpha(z' \oplus \epsilon_{\mathcal{X}'})$ fixed points, and since $\alpha(z' \oplus \epsilon_{\mathcal{X}'}) \leq \alpha^*$, we deduce that $\phi^{\min}(D_{\psi,s}) \geq 2^{n-s} - \alpha^*$.

We have $\Delta(D_{\psi,s}) \leq 3$ but, using Lemma 12, we can obtain from $D_{\psi,s}$ a SID $D'_{\psi,s}$ (by adding at most one vertex and one arc per clause) with $\Delta(D'_{\psi,s}) \leq 2$ and

$$\phi^{\min}(D'_{\psi,s}) = \phi^{\min}(D_{\psi,s}) = 2^{n-s} - \alpha^*.$$

(For that we use the fact, showed above, that there is $f \in F(D_{\psi,s})$ with $\phi^{\min}(D_{\psi,s})$ fixed points where f_i is the OR function for every vertex i of in-degree three.)

Consequently, we have $\alpha^* \geq 2^{n-s-1}$ if and only if $\phi^{\min}(D'_{\psi,s}) \leq 2^{n-s-1}$. Thus, (ψ, s) is a true instance of E-MAJ3SAT if and only if $(D'_{\psi,s}, k)$ is a true instance of MINFPP, where $k = 2^{n-s-1} + 1$ if $s < n$ and $k = 1$ otherwise. Thus, when $\Delta(D) \leq d$, MINFPP is $\text{NP}^{\#P}$ -hard.

An other consequence is that $\phi^{\min}(D'_{\psi,s}) = 0$ if and only if $\alpha^* = 2^{n-s}$, that is, there is a partial assignment z' of the variables in \mathcal{X}' such that ψ is satisfied by all the assignments extending z' . Thus, (ψ, s) is a true instance of QSAT₂ if and only if $D'_{\psi,s}$ is a true instance of 1-MINFPP, and therefore 1-MINFPP is NP^{NP} -hard. We then deduce from Lemma 26 that, when $\Delta(D) \leq d$, k -MINFPP is NP^{NP} -hard for all $k \geq 2$. \square

It remains to prove that, in the general case, k -MINFPP and MINFPP are NEXPTIME-hard. We proceed with a reduction from SUCCINCT-3SAT, which is very similar to the one given in Section 5.2 to obtain the hardness of MAXFPP. We thus use the notations from that section. We consider a succinct representation of a 3-CNF formula Ψ with a set Λ of 2^n variables (indexed by configurations on W) and with a set M of 2^m clauses (indexed by configurations on U). The following is an adaptation of the construction D_Ψ suited for the study of the minimum number of fixed points.

Definition 8 ($D_{\bar{\Psi}}$). We denote by $D_{\bar{\Psi}}$ the SID obtained from the SID D_Ψ of Definition 6 by making negative the arc (c_1, ℓ_0) .

The main property is the following. The proof is almost identical to that of Lemma 22, using Lemmas 24 and 25 instead of Lemmas 14 and 15.

Lemma 28. $\phi^{\min}(D_{\bar{\Psi}}) = 0$ if and only if Ψ is satisfiable.

Proof. Suppose that Ψ is satisfied by an assignment $\zeta \in \{0,1\}^\Lambda$. By Lemma 21 there is $h' \in F(C')$ such that ψ is satisfied by all the 2^m fixed points of h' . Let $f \in F(D_{\bar{\Psi}})$ be defined as follows. First, $f(x)_{V_{C'}} = h'(x_{V_{C'}})$ for every configuration x on $V_{\bar{\Psi}}$. Second, for every $i \in V_{\bar{\Psi}} \setminus V_{C'}$, we define f_i has the AND function if $i \in \ell$ and the OR function

otherwise (vertices in ℓ are those with two in-neighbors corresponding to the positive and negative literals associated with a variable in λ). By the first part of the definition, the set of fixed points of h' is set of partial fixed points of f . So ψ is satisfied by any partial fixed point x of f , and we deduce from Lemma 24 that f has no fixed point extending x . Since every fixed point extends a partial fixed point, we deduce that f has no fixed point and thus $\phi^{\min}(D_{\Psi}^-) = 0$.

Conversely, suppose that $\phi^{\max}(D_{\Psi}) = 0$. Let $f \in F(D_{\Psi})$ without fixed point. Let h' be the BN with component set $V_{C'}$ defined by $h'(x_{V_{C'}}) = f(x)_{V_{C'}}$ for all configurations x on V_{Ψ} ; there is no ambiguity since vertices in C' have only in-neighbors in C' and, thanks to this property, the SID of h' is $D_{\Psi} \setminus U_{\psi} = C'$. Furthermore, the set of fixed points of h' is the set of partial fixed points of f . Let x be a fixed point of h' . Since f has no fixed point extending x , by Lemma 25, ψ is satisfied by $x_{\lambda \oplus \epsilon(f)}$. This is equivalent to say that ψ is satisfied by every ϵ -fixed point of h' , where ϵ is any configuration on $V_{C'}$ extending $\epsilon(f)$, and we deduce from Lemma 21 that Ψ is satisfiable. \square

Remark 6. *With slightly more precise arguments, we can prove that $\phi^{\min}(D_{\Psi}^-) = 2^{m+1} - \alpha$, where α is the maximum number of clauses contained in Ψ that can be simultaneously satisfied.*

The following hardness results, the last we need to obtain, are immediate consequences.

Lemma 29. *MINFPP and k -MINFPP for every $k \geq 1$, are NEXPTIME-hard.*

Proof. By the previous lemma, D_{Ψ}^- is a true instance of 1-MINFPP if and only if (h, C) , the succinct representation of Ψ , is a true instance of SUCCINT-3SAT. Therefore, 1-MINFPP is NEXPTIME-hard. We then deduce from Lemma 26 that k -MINFPP is NEXPTIME-hard for all $k \geq 2$. Consequently, MINFPP is also NEXPTIME-hard. \square

7 Conclusion and perspectives

In this paper, we studied the algorithmic complexity of many decision problems related to counting the number of fixed points of a BN from its SID only. Except for 1-MAXFPP, we proved exact complexity bounds for each one of these problems, revealing a large range of complexities, some classes having a pretty scarce literature.

The function problems of computing $\phi^{\max}(D)$ or $\phi^{\min}(D)$ can, quite classically, be seen as n (since the result ranges from 0 to 2^n , but the case 2^n can be treated separately) decision problems providing the bits of the answer by binary search. Table 1 gives the worst case complexity of computing each of these bits in the different cases (minimum/maximum, degree bounded/unbounded). Note that, even though they do not intuitively correspond to counting problems, computing $\phi^{\max}(D)$ or $\phi^{\min}(D)$ are proven to be #P-hard problems even for bounded degree, from the proofs of Lemmas 17 and 27.

Even if the problems we studied are natural, they have not been considered before. Indeed, most of the works on the complexity of BNs are of the form: does a BN f satisfies a given dynamical property P ? Here, we studied problems of the form: does a SID D corresponds to a BN $f \in F(D)$ satisfying a given property P ? In some cases, this new problem can be easier. For instance, the problem of deciding if a BN (encoded as a concatenation of local functions in conjunctive normal form) has at least one fixed point is NP-complete [21], but we showed that deciding if there exists a BN $f \in F(D)$ with at least one fixed point is in P. Conversely, the problem of deciding if a BN f has no fixed point is in coNP, whereas it is NEXPTIME-complete to decide if there is a BN $f \in F(D)$ without fixed point.

This new theme opens many further investigations. First, we proved that 1-MAXFPP is equivalent (up to a polynomial reduction) to the problem of finding an even cycle in a digraph. This problem is known to be in P [25, 36] but, to the best of our knowledge, no work has been done to show its C-hardness for any complexity class C. It would be interesting to find such lower bounds, because this problem is equivalent to many other decision problems of graph theory ([36] lists several of them).

Furthermore, we could study the effect of other restrictions on the SIDs considered. For instance, what happens for the family of SIDs with positives arcs only? It is an interesting problem, because the BN having such SIDs are monotone, and since Tarski [39] monotone networks received great attention [8, 35, 3, 5, 26, 15, 16, 17]. We hope to be able to adapt our constructions in order to fit this new constraint. We conjecture that, in this case, there is an integer k_0 such that k -MAXFPP is in P if $k \leq k_0$, and NP-complete otherwise.

As further variations, we could study unsigned interaction digraph, or consider *automata network* instead of Boolean network (where a component can take more than two states), or consider BNs that may ignore some arcs of the SID to get closer to real experimental conditions (where arcs of the SID are not always a hundred percent accurate). This could affect the problems' difficulties drastically, and may reveal relations to *network coding* problems in information theory [23, 14, 12].

Finally, we could think of new problems where, given a SID D , we want to decide other properties shared by all $f \in F(D)$. Indeed, there are many other interesting BN properties, such as the number or the size of the limit cycles, the size of their transients... we could also look for properties of their basins of attraction, some complexity results already being known for threshold networks [11].

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