Complexity of maximum and minimum fixed point problem in Boolean networks

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joint work with

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Workshop: Theory and applications of Boolean interaction networks
Freie Universität, Berlin, September 12-13, 2019
A Boolean network (BN) with \( n \) components is a function

\[
f : \{0, 1\}^n \rightarrow \{0, 1\}^n
\]

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x = (x_1, \ldots, x_n) \mapsto f(x) = (f_1(x), \ldots, f_n(x))
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- **Global** transition function
- **Locale** transition functions

\[
f_i : \{0, 1\}^n \rightarrow \{0, 1\}
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The **synchronous dynamics** is given by

\[
x^{t+1} = f(x^t).
\]

The **asynchronous dynamics** is more realistic in many cases.

**Fixed points** of \( f \) are **stable states** for both dynamics.
A **Boolean network (BN)** with $n$ components is a function

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$$x = (x_1, \ldots, x_n) \mapsto f(x) = (f_1(x), \ldots, f_n(x))$$

The **interaction graph (IG)** of $f$ is the **signed digraph** defined by

- the vertex set is $\{1, \ldots, n\}$,
- there is a positive edge $j \rightarrow i$ if there is $x \in \{0, 1\}^n$ such that

$$f_i(x_1, \ldots, x_{j-1}, 0, x_{j+1}, \ldots, x_n) = 0$$
$$f_i(x_1, \ldots, x_{j-1}, 1, x_{j+1}, \ldots, x_n) = 1$$

- there is a negative edge $j \rightarrow i$ if there is $x \in \{0, 1\}^n$ such that

$$f_i(x_1, \ldots, x_{j-1}, 0, x_{j+1}, \ldots, x_n) = 1$$
$$f_i(x_1, \ldots, x_{j-1}, 1, x_{j+1}, \ldots, x_n) = 0$$
Example with $n = 3$

\[
\begin{align*}
    f_1(x) &= x_2 \lor x_3 \\
    f_2(x) &= \overline{x_1} \land \overline{x_3} \\
    f_3(x) &= \overline{x_3} \land (x_1 \lor x_2)
\end{align*}
\]

Synchronous dynamics

Interaction graph
BNs are classical models for gene networks. When biologists study a gene network, the interaction graph is often the first reliable data.
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**Interaction Graph Consistency Problem**

**Input:** An interaction graph $G$ and a dynamical property $P$.

**Question:** Is there a BN on $G$ with a dynamics satisfying $P$?
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**Theorem** [Kosub 2008]

It is NP-complete to decide if a BN has a fixed point.
**Definitions**

\[
\begin{align*}
\max(G) & := \text{maximum number of fixed points in a BN on } G \\
\min(G) & := \text{minimum number of fixed points in a BN on } G
\end{align*}
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\begin{align*}
&\text{max}(G) = 3 \\
&\text{min}(G) = 1 \\
&(8 \text{ BNs})
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\[\text{max}(G) = 3 \quad \text{min}(G) = 1 \quad (8 \text{ BNs})\]

\[\text{max}(G') = 2 \quad \text{min}(G') = 2 \quad (8 \text{ BNs})\]
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(8 BNs)

\textit{k-MaxProblem: } Given \( G \), do we have \( \text{max}(G) \geq k \)?
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\text{*k-MaxProblem*: Given } G, \text{ do we have } \text{max}(G) \geq k? \text{*k-MinProblem*: Given } G, \text{ do we have } \text{min}(G) \leq k?
Theorem

\[ \max(G) \geq 1 \] iff each initial strong component of \( G \) has a positive cycle.
max\( (G) \geq 1? \)

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\[ \text{max}(G) \geq 1 \text{ iff each initial strong component of } G \text{ has a positive cycle.} \]

**Theorem** [Robertson, Seymour and Thomas 1999; McCuaig 2004]
We can decide in polynomial time if \( G \) has a positive cycle.
max(G) ≥ 1?

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**Corollary**

We can decide in polynomial time if max(G) ≥ 1.
max(G) ≥ 1?

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We can decide in polynomial time if \( G \) has a positive cycle.

**Corollary**
We can decide in polynomial time if \( \max(G) \geq 1 \).

Recall that it is **NP-complete** to decide if a BN has a fixed point.
max($G$) ≥ 2?

According to Thomas, $\max(G) \geq 2$ means that $G$ can be the interaction graph of a gene network controlling a cell differentiation process.
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**Theorem** [Aracena 2008]

1. If $\max(G) \geq 2$, then $G$ has a positive cycle. [Thomas’ 1st rule]
max($G$) $\geq$ 2?

According to Thomas, $\max(G) \geq 2$ means that $G$ can be the interaction graph of a gene network controlling a cell differentiation process.

**Theorem** [Aracena 2008]

1. If $\max(G) \geq 2$, then $G$ has a positive cycle.
2. If $G$ has *only* positive cycles and no source, then $\min(G) \geq 2$. 
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Can we hope for a simple characterization of $\max(G) \geq 2$?
**max(G) ≥ 2?**

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**Theorem**

It is **NP-complete** to decide if $\max(G) \geq 2$.

It is **NP-complete** to decide if $\max(G) \geq k$, for every fixed $k \geq 2$. 
\[ \text{max}(G) \geq k? \text{ is in NP} \]

**Theorem**

There is an algorithm with the following specifications:

**Input:** \( G \) and \( k \) couples of states \((x^1, y^1) \ldots (x^k, y^k)\).

**Output:** A BN \( f \) on \( G \) with \( f(x^\ell) = y^\ell \) for \( 1 \leq \ell \leq k \), if it exists.

**Running time:** \( O(k^2n^2) \).
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**Running time:** $O(k^2n^2)$.

If $\max(G) \geq k$, there is a BN $f$ on $G$ with $k$ fixed points $x^1, \ldots, x^k$.

Then $(x^1, \ldots, x^k)$ is a certificat of size $O(kn)$ which can be checked in $O(k^2n^2)$-time by giving as input $G$ and the couples $(x^1, x^1), \ldots, (x^k, x^k)$. 

$\max(G) \geq k$? is in NP
max(G) ≥ k? is in NP

**Theorem**

There is an algorithm with the following specifications:

**Input:** G and k couples of states \((x^1, y^1) \ldots (x^k, y^k)\).

**Output:** A BN \(f\) on G with \(f(x^\ell) = y^\ell\) for \(1 ≤ \ell ≤ k\), if it exists.

**Running time:** \(O(k^2 n^2)\).

If \(\max(G) ≥ k\), there is a BN \(f\) on G with \(k\) fixed points \(x^1, \ldots, x^k\).

Then \((x^1, \ldots, x^k)\) is a certificate of size \(O(kn)\) which can be checked in \(O(k^2 n^2)\)-time by giving as input G and the couples \((x^1, x^1), \ldots, (x^k, x^k)\).

Thus \(\max(G) ≥ k?\) is in **NP**.
$\max(G) \geq 2 ?$ is NP-hard
Theorem

Given a SAT formula $\phi$ with $n$ variables and $m$ clauses, we can built in $O(n + m)$-time an interaction graph $G_\phi$ with $O(n + m)$ vertices s.t.

$$\max(G_\phi) \geq 2 \iff \phi \text{ is satisfiable}$$
max\(G\) ≥ 2? is NP-hard

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Basic observation:

- 2 fixed points
- 1 fixed point

The idea is to “control” with \(\phi\) the “effectiveness” of the negative chord, so that the chord can be “ineffective” if and only if \(\phi\) is satisfiable.
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max(G) \geq 2? is NP-hard

Example with \( \phi = (a \lor \bar{b} \lor c) \land (\bar{a} \lor \bar{c}). \)
max(G) ≥ 2? is NP-hard

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\(\phi\) is sat. \(\Rightarrow\) max(\(G\)) \(\geq\) 2

Consider a true assignment:
\(a = 1,\ b = 1,\ c = 0\)
max(G) \geq 2? is NP-hard

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Example with $\phi = (a \lor \overline{b} \lor c) \land (\overline{a} \lor \overline{c})$.

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max($G$) $\geq$ 2? is NP-hard

**Example** with $\phi = (a \lor \neg b \lor c) \land (\neg a \lor \neg c)$.

Consider a true assignment: $a = 1$, $b = 1$, $c = 0$

$\phi$ is sat. $\Rightarrow$ max($G$') $\geq$ 2
max(G) ≥ 2? is NP-hard

Example with \( \phi = (a \lor \bar{b} \lor c) \land (\bar{a} \lor \bar{c}) \).

\( \phi \) is sat. \( \Rightarrow \) max(G) ≥ 2

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max(\(G\)) ≥ 2? is NP-hard

Example with \(\phi = (a \lor \overline{b} \lor c) \land (\overline{a} \lor \overline{c})\).

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\( G_\phi \)

\[ \begin{array}{c}
1 \quad f_s = 1 \\
\end{array} \]

\( \phi \) is sat. \( \Rightarrow \) \( \max(G') \geq 2 \)

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max(G) ≥ 2? is NP-hard

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**Isolated positive cycle**

\[ \Downarrow \]

2 fixed points
max($G$) $\geq 2$? is NP-hard

**Example** with $\phi = (a \lor \overline{b} \lor c) \land (\overline{a} \lor \overline{c})$.

Let $f$ be a BN on $G$ with two fixed points: $x$ and $y$.
max($G$) \geq 2? is NP-hard

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$G_\phi$

max($G$) \geq 2 \Rightarrow \phi \text{ is sat.}$

Let $f$ be a BN on $G$ with two fixed points: $x$ and $y$

- $x_i < y_i$
- $x_i > y_i$
- $x_i = y_i$
- $x_i \leq y_i$

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max(\(G\)) \(\geq\) 2? is NP-hard

**Example** with \(\phi = (a \lor \overline{b} \lor c) \land (\overline{a} \lor \overline{c})\).

Let \(f\) be a BN on \(G\) with two fixed points: \(x\) and \(y\).

Since all the positive cycles are full-positive, by a thm of Aracena there is a positive cycle where vertices are all \(\bigcirc\) or all \(\bullet\).
max(\(G\)) \(\geq 2\) is NP-hard

Example with \(\phi = (a \lor \overline{b} \lor c) \land (\overline{a} \lor \overline{c})\).

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Since all the positive cycles are full-positive, by a thm of Aracena there is a positive cycle where vertices are all ● or all ○.
\textbf{Example} with $\phi = (a \lor \overline{b} \lor c) \land (\overline{a} \lor \overline{c})$.

\[
\begin{align*}
\text{max}(G) \geq 2 \Rightarrow \phi \text{ is sat.}
\end{align*}
\]

Let $f$ be a BN on $G$ with two fixed points: $x$ and $y$

\begin{itemize}
  \item $x_i < y_i$
  \item $x_i > y_i$
  \item $x_i = y_i$
  \item $x_i \leq y_i$
\end{itemize}

Since all the positive cycles are full-positive, by a thm of Aracena there is a positive cycle where vertices are all \textcolor{green}{\bullet} or all \textcolor{red}{\bullet}.
max($G$) $\geq 2$? is NP-hard

**Example** with $\phi = (a \lor \bar{b} \lor c) \land (\bar{a} \lor \bar{c})$.

$G_{\phi}$

max($G$) $\geq 2 \implies \phi$ is sat.

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Since all the positive cycles are full-positive, by a thm of Aracena there is a positive cycle where vertices are all $\bullet$ or all $\circ$. 
max(G) ≥ 2? is NP-hard

Example with \( \phi = (a \lor \neg b \lor c) \land (\neg a \lor \neg c) \).
max\( (G) \geq 2 \) is NP-hard

**Example** with \( \phi = (a \lor \bar{b} \lor c) \land (\bar{a} \lor \bar{c}) \).

Let \( f \) be a BN on \( G \) with two fixed points: \( x \) and \( y \)

\[
\begin{align*}
\circ \quad x_i &< y_i \\
\circ \quad x_i &> y_i \\
\circ \quad x_i &= y_i \\
\bullet \quad x_i &\leq y_i
\end{align*}
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Since all the positive cycles are full-positive, by a thm of Aracena there is a positive cycle where vertices are all \( \circ \) or all \( \bullet \).
max(G) ≥ 2? is NP-hard

**Example** with \( \phi = (a \lor \overline{b} \lor c) \land (\overline{a} \lor \overline{c}) \).

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\[
\begin{align*}
\text{if } x_i &< y_i \\
\text{if } x_i &> y_i \\
\text{if } x_i &= y_i \\
\text{if } x_i &\leq y_i
\end{align*}
\]

max($G$) \( \geq 2 \) \( \Rightarrow \) \( \phi \) is sat.
\[ \max(G) \geq 2? \text{ is NP-hard} \]

**Example** with \[ \phi = (a \lor \overline{b} \lor c) \land (\overline{a} \lor \overline{c}) \].

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\[ \Rightarrow \]
\( \text{max}(G) \geq 2? \) is NP-hard

**Example** with \( \phi = (a \lor \bar{b} \lor c) \land (\bar{a} \lor \bar{c}) \).

\[ G_\phi \]

\[
\begin{align*}
G_\phi & = (a \lor \bar{b} \lor c) \land (\bar{a} \lor \bar{c}) \\
S & \quad a \\
\bar{a} & \quad b \\
\bar{b} & \quad c \\
\bar{c} & \quad \text{C}_1 \\
\text{C}_2
\end{align*}
\]

\( \text{max}(G) \geq 2 \Rightarrow \phi \text{ is sat.} \)

Let \( f \) be a BN on \( G \) with two fixed points: \( x \) and \( y \)

\[
\begin{align*}
& x_i < y_i \\
& x_i > y_i \\
& x_i = y_i \\
& x_i \leq y_i
\end{align*}
\]

\[ \Rightarrow \]
max($G$) $\geq 2$? is NP-hard

Example with $\phi = (a \lor \overline{b} \lor c) \land (\overline{a} \lor \overline{c})$.

Let $f$ be a BN on $G$ with two fixed points: $x$ and $y$

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\]
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\[
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&x_i < y_i \\
&x_i > y_i \\
&x_i = y_i \\
&x_i \leq y_i
\end{align*}
\]

\[
\begin{align*}
a = 1, \ b = 0, \ c = 0 \\
a = 1, \ b = 1, \ c = 0
\end{align*}
\]

are true assignments of \(\phi\)
**$k$-MaxProblem:** Given $G$, do we have $\max(G) \geq k$?

**Theorem**

$k$-MaxProblem is in P if $k \leq 1$ and NP-complete if $k \geq 2$. 

**MinProblem:** Given $G$, do we have $\min(G) \leq k$?

This problem is much more difficult:

**Theorem**

$k$-MinProblem is NP-hard for every $k$. But to prove the NEXPTIME-hardness, we use a much more technical reduction from SuccintSAT.
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This problem is much more difficult:

**Theorem**

$k$-MinProblem is $\text{NEXPTIME}$-complete for every $k$.

With a construction very similar to $G_\phi$, we can prove that $\min(G) \leq k$ is $NP$-hard. But to prove the $\text{NEXPTIME}$-hardness, we use a much more technical reduction from SuccinctSAT.
MaxProblem: Given $G$ and $k$, do we have $\max(G) \geq k$?

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**Theorem**

MaxProblem and MinProblem are NEXPTIME-complete.
Conclusion

We study, from a complexity point of view, a natural class of problems.

**Interaction Graph Consistency Problem**

**Input:** An interaction graph $G$ and a dynamical property $P$.

**Question:** Is there a BN on $G$ with a dynamics satisfying $P$?

We obtain exact classes of complexity for this problem when

$$P = \text{“to have at least/most } k \text{ fixed points”}$$

Our main result is about bistability:

It is **NP-complete** to decide if there is a BN on $G$ with two fixed points.
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**Perspectives**

1. **Other dynamical properties.**
   
   $\leftrightarrow$ number/size of cyclic attractors in the (a)synchronous case.

2. **Non-Boolean case** and **unsigned case**.