Complexity of the dynamics of resource-bounded reaction systems

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Reactions

Definition

Given a finite set S, a *reaction* a over S is a triple (R, I, P) of subsets of S:

- R is the set of *reactants*,
- I is the set of *inhibitors*,
- P is the set of *products*.

Reaction Systems

Definition

A *reaction system* (RS) is a pair $\mathcal{A} = (S, A)$ where:

- S is a finite set of *symbols* or *entities*, called the *background set*;
- A is a set of reactions over S.

A *state* of $\mathcal{A}$ is a subset of S.

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A *state* of $\mathcal{A}$ is a subset of S.

Any reaction system induces a discrete dynamical system where the state set is 2^S.

Result function

A reaction $a = (R, I, P)$ is *enabled* in a state $T \subseteq S$ when:

$$R \subseteq T \quad \text{and} \quad I \cap T = \varnothing.$$

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The *result function* of a on $T \subseteq S$ is:

$$\mathrm{res}_a(T) := \begin{cases} P & \text{if } a \text{ is enabled by } T \\ \varnothing & \text{otherwise.} \end{cases}$$

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Definition

The *result function* $\operatorname{res}_{\mathcal{A}}$ of a RS $\mathcal{A} = (S, A)$ is defined on any state $T \subseteq S$ as:

$$\operatorname{res}_{\mathcal{A}}(T) := \bigcup_{a \in A} \operatorname{res}_a(T).$$

Example of RS

Background set: $S = \{a, b\}$

Set of reactions: $r_1 = (\{a\}, \varnothing, \{a, b\})$

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$$\{b\} \subseteq T$$

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$$\{b\} \subseteq T, \quad \{a\} \cap T = \varnothing$$

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Result function on T:

$$\mathrm{res}_{\mathcal{A}}(T) = \mathrm{res}_{r_1}(T) \cup \mathrm{res}_{r_2}(T)$$

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$$\mathrm{res}_{\mathcal{A}}(\{b\}) = \{b\}$$

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$\mathrm{res}_{\mathcal{A}}(\{b\}) = \{b\} \Rightarrow \{b\}$ is a fixed point

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Representation of the dynamic:

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Result function on T:

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Discrete dynamical system:

RS vs Synchronous Boolean networks

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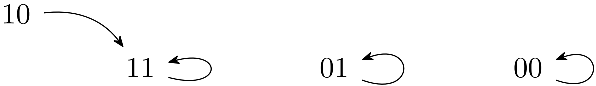
Discrete dynamical system:

$$x_a = \begin{cases} 1 \text{ if } a \in T \\ 0 \text{ if } a \notin T \end{cases} \qquad x_b = \begin{cases} 1 \text{ if } b \in T \\ 0 \text{ if } b \notin T \end{cases}$$



RS vs Synchronous Boolean networks

Background set: $S = \{a, b, c\}$

Set of reactions: $(\{a, c\}, \{b\}, \{a\})$

$(\{a, b\}, \{c\}, \{b\})$

$(\{c\}, \{a\}, \{b\})$

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$f : \{0, 1\}^3 \to \{0, 1\}^3$
$f(x_a, x_b, x_c) = (f_a(x_a, x_b, x_c), f_b(x_a, x_b, x_c), f_c(x_a, x_b, x_c))$

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Discrete dynamical system:

Example of RS: fixed points

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Fixed points attractor: $\{a, b\}$

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Fixed points attractor: $\{a, b\}$

Fixed points not attractor: $\{b\}, \varnothing$

Fixed Points: problems

Given a reaction system $\mathcal{A} = (S, A)$:

- does $\mathcal{A}$ have a fixed point?
- does $\mathcal{A}$ have a fixed point attractor?
- does $\mathcal{A}$ have a fixed point not attractor?
- ecc. . .

Fixed Points: problems

Given a reaction system $\mathcal{A} = (S, A)$:

- does $\mathcal{A}$ have a fixed point? **NP**-complete[1]
- does $\mathcal{A}$ have a fixed point attractor? **NP**-complete[1]
- and many more. . .

[1] Formenti, Manzoni, and Porreca 2014.

Resource-bounded systems

Class of RS

$\mathcal{RS}(\infty, \infty)$

$\mathcal{RS}(0, \infty)$

$\mathcal{RS}(\infty, 0)$

$\mathcal{RS}(1, 0)$

Resource-bounded systems: classification[2]

Class of RS	Subclass of $2^S \to 2^S$
$\mathcal{RS}(\infty, \infty)$	all
$\mathcal{RS}(0, \infty)$	antitone
$\mathcal{RS}(\infty, 0)$	monotone
$\mathcal{RS}(1, 0)$	additive

[2] Manzoni, Pocas, and Porreca 2014.

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$\mathcal{RS}(\infty, \infty)$	all
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$\mathcal{RS}(0, \infty)$	antitone: $T \subseteq T' \Rightarrow \mathrm{res}(T) \supseteq \mathrm{res}(T')$
$\mathcal{RS}(\infty, 0)$	monotone: $T \subseteq T' \Rightarrow \mathrm{res}(T) \subseteq \mathrm{res}(T')$
$\mathcal{RS}(1, 0)$	additive: $\mathrm{res}(T \cup T') = \mathrm{res}(T) \cup \mathrm{res}(T')$

[2] Manzoni, Pocas, and Porreca 2014.

$\exists$ fixed point for $\mathcal{RS}(0, \infty)$

Theorem

Given $\mathcal{A} \in \mathcal{RS}(0, \infty)$, it is **NP**-*complete to decide if $\mathcal{A}$ has a fixed point.*

Python code: Colab notebook

$\exists$ fixed point for $\mathcal{RS}(0, \infty)$ is **NP**-complete
Sketch of the proof

$\varphi = (x_1 \vee \neg x_2 \vee x_3) \wedge (x_1 \vee x_2 \vee \neg x_3)$ in CNF

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Sketch of the proof

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We will build a $\mathcal{A} \in \mathcal{RS}(0,\infty)$ with a fixed point iff φ is satisfiable.

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Sketch of the proof

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We will build a $\mathcal{A} \in \mathcal{RS}(0, \infty)$ with a fixed point iff φ is satisfiable.
Background set: $S = \{x_1, x_2, x_3, \overline{x_1}, \overline{x_2}, \overline{x_3}, \clubsuit, \spadesuit\}$.

$\varphi = (x_1 \vee \neg x_2 \vee x_3) \wedge (x_1 \vee x_2 \vee \neg x_3)$ in CNF

We will build a $\mathcal{A} \in \mathcal{RS}(0,\infty)$ with a fixed point iff φ is satisfiable.
Background set: $S = \{x_1, x_2, x_3, \overline{x_1}, \overline{x_2}, \overline{x_3}, \clubsuit, \spadesuit\}$.
Reactions:

$$(\varnothing, \{x_1, \overline{x}_2, x_3\}, \{\spadesuit\}) \tag{4.1}$$
$$(\varnothing, \{x_1, x_2, \overline{x}_3\}, \{\spadesuit\}) \tag{4.2}$$
$$\overline{a_i} := (\varnothing, \{x_i\}, \{\overline{x_i}\}) \quad \text{for } 1 \le i \le 3 \tag{4.3}$$
$$a_i := (\varnothing, \{\overline{x_i}\}, \{x_i\}) \quad \text{for } 1 \le i \le 3 \tag{4.4}$$
$$(\varnothing, \{\clubsuit\}, \{\clubsuit, \spadesuit\}) \tag{4.5}$$
$$(\varnothing, \{\spadesuit\}, \{\clubsuit\}). \tag{4.6}$$

$\exists$ fixed point for $\mathcal{RS}(0, \infty)$ is **NP**-complete

Encoding the assignments

$\varphi = (x_1 \vee \neg x_2 \vee x_3) \wedge (x_1 \vee x_2 \vee \neg x_3)$
Encoding the assignments:

$$\begin{aligned} x_1 &= \text{False} \\ x_2 &= \text{True} \qquad \Rightarrow \{\overline{x}_1, x_2, x_3\} \\ x_3 &= \text{True} \end{aligned}$$

$X = \{\overline{x}_1, x_2, x_3\}$ satisfies φ if and only if both

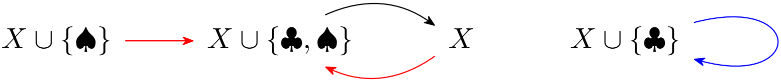
$$(\varnothing, \{x_1, \overline{x}_2, x_3\}, \{\spadesuit\}) \quad \text{and} \quad (\varnothing, \{x_1, x_2, \overline{x}_3\}, \{\spadesuit\})$$

are not enabled.

$\exists$ fixed point for $\mathcal{RS}(0,\infty)$ is **NP**-complete

A satisfying assignment

Thus, $X = \{\overline{x}_1, x_2, x_3\}$ satisfies φ then $X \cup \{\clubsuit\}$ is a fixed point:



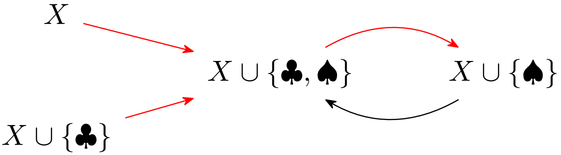
Enabled reactions:

$$(\varnothing, \{x_1\}, \{\overline{x_1}\})$$
$$(\varnothing, \{\overline{x_2}\}, \{x_2\})$$
$$(\varnothing, \{\overline{x_3}\}, \{x_3\})$$
$$(\varnothing, \{\clubsuit\}, \{\clubsuit, \spadesuit\})$$
$$(\varnothing, \{\spadesuit\}, \{\clubsuit\})$$

$\exists$ fixed point for $\mathcal{RS}(0, \infty)$ is **NP**-complete

A non-satisfying assignment

$X = \{\overline{x}_1, x_2, \overline{x}_3\}$ does not satisfy φ then there are no fixed points:



Enabled reactions:

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$$(\varnothing, \{\overline{x_2}\}, \{x_2\})$$
$$(\varnothing, \{x_3\}, \{\overline{x_3}\})$$
$$(\varnothing, \{\clubsuit\}, \{\clubsuit, \spadesuit\})$$
$$(\varnothing, \{\spadesuit\}, \{\clubsuit\})$$

$\exists$ fixed point for $\mathcal{RS}(0,\infty)$ is **NP**-complete

Spurious cases

- $X = \{x_1, \overline{x_1}, x_2, x_3\}$ then neither

  $$(\varnothing, \{x_1\}, \{\overline{x_1}\}) \quad \text{or} \quad (\varnothing, \{\overline{x_1}\}, \{x_1\})$$

  are enabled, thus $x_1, \overline{x_1} \notin \text{res}_{\mathcal{A}}(X)$
  $\Rightarrow X$ cannot be a fixed point.

$\exists$ fixed point for $\mathcal{RS}(0, \infty)$ is **NP**-complete

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  are enabled, thus $x_1, \overline{x_1} \notin \mathrm{res}_{\mathcal{A}}(X)$
  $\Rightarrow X$ cannot be a fixed point.
- $X = \{x_2, x_3\}$ then both

  $$(\varnothing, \{x_1\}, \{\overline{x_1}\}) \quad \text{and} \quad (\varnothing, \{\overline{x_1}\}, \{x_1\})$$

  are enabled, thus $x_1, \overline{x_1} \in \mathrm{res}_{\mathcal{A}}(X)$
  $\Rightarrow X$ cannot be a fixed point.

$\exists$ fixed point for $\mathcal{RS}(\infty, 0)$

$\exists$ fixed point for $\mathcal{RS}(\infty, 0)$

Always True!
Recall that given $\mathcal{A} \in \mathcal{RS}(\infty, 0)$ then $f = \mathrm{res}_{\mathcal{A}}$ is monotone, i.e. $T_1 \subseteq T_2 \Rightarrow f(T_1) \subseteq f(T_2)$.

Theorem (Knaster Tarski)

Given $f : 2^S \to 2^S$ monotone, there exists a fixed point.

∃ fixed point: summary

Problem	$\mathcal{RS}(\infty,\infty)$	$\mathcal{RS}(0,\infty)$	$\mathcal{RS}(\infty,0)$
∃ fixed point	**NP**-c[1]	**NP**-c[2]	**P** [3]

[1] Formenti, Manzoni, and Porreca 2014
[2] Ascone, Bernardini, and Manzoni 2024b
[3] Knaster-Tarski Theorem

Results: studied problems

Inhibitorless and Reactantless RS

Problem	$\mathcal{RS}(\infty,\infty)$	$\mathcal{RS}(0,\infty)$	$\mathcal{RS}(\infty,0)$
A given state is a fixed point attractor	**NP**-c[1]	**NP**-c[2]	**NP**-c[2]
$\exists$ fixed point	**NP**-c[1]	**NP**-c[2]	**P** [3]
$\exists$ common fixed point	**NP**-c[1]	**NP**-c[2]	**NP**-c[2]
sharing all fixed points	**coNP**-c[1]	**coNP**-c[2]	**coNP**-c[2]
$\exists$ fixed point attractor	**NP**-c[1]	**NP**-c[2]	Unknown
$\exists$ common fixed point attractor	**NP**-c[1]	**NP**-c[2]	**NP**-c[2]
sharing all fixed points attractor	$\Pi_2^{\mathbf{P}}$-c[1]	$\Pi_2^{\mathbf{P}}$-c[2]	$\Pi_2^{\mathbf{P}}$-c[2]
$\exists$ fixed point not attractor	$\Sigma_2^{\mathbf{P}}$-c[2]	$\Sigma_2^{\mathbf{P}}$-c[2]	$\Sigma_2^{\mathbf{P}}$-c[2]
$\exists$ common fixed point not attractor	$\Sigma_2^{\mathbf{P}}$-c[2]	$\Sigma_2^{\mathbf{P}}$-c[2]	$\Sigma_2^{\mathbf{P}}$-c[2]
sharing all fixed points not attractor	**coNP**-c[2]	**coNP**-c[2]	**coNP**-c[2]
$\mathrm{res}_{\mathcal{A}} = \mathrm{res}_{\mathcal{B}}$	**coNP**-c[2]	**P** [2]	**P** [2]

1 Formenti, Manzoni, and Porreca 2014

2 Ascone, Bernardini, and Manzoni 2024b

3 Knaster-Tarski Theorem

Additive RS: $\mathcal{RS}(1, 0)$

Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

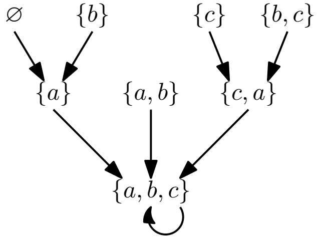


Figure: Discrete dynamical system of $\mathcal{A}$, size $\mathcal{O}(2^{|S|})$.

Additive RS

Influence graph

Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

Influence graph $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$:

$\varnothing_G$

a

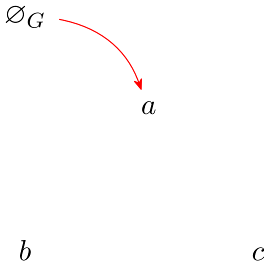
b c

Additive RS
Influence graph

Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

Influence graph $G_\mathcal{A} = (V_\mathcal{A}, E_\mathcal{A})$:

$$\mathrm{res}_\mathcal{A}(\varnothing) = \{a\}$$

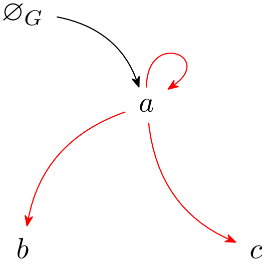


Additive RS
Influence graph

Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

Influence graph $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$:

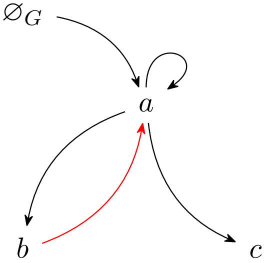
$$\text{res}_{\mathcal{A}}(\{a\}) = \{a, b, c\}$$



Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

Influence graph $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$:

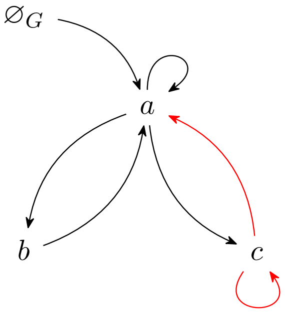
$$\mathrm{res}_{\mathcal{A}}(\{b\}) = \{a\}$$



Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

Influence graph $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$:

$$\text{res}_{\mathcal{A}}(\{c\}) = \{a, c\}$$



Background set: $S = \{a, b, c\}$
Reactions: $(\varnothing, \varnothing, \{a\})$ $(\{a\}, \varnothing, \{b, c\})$ $(\{c\}, \varnothing, \{c\})$

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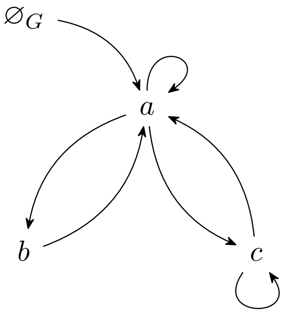
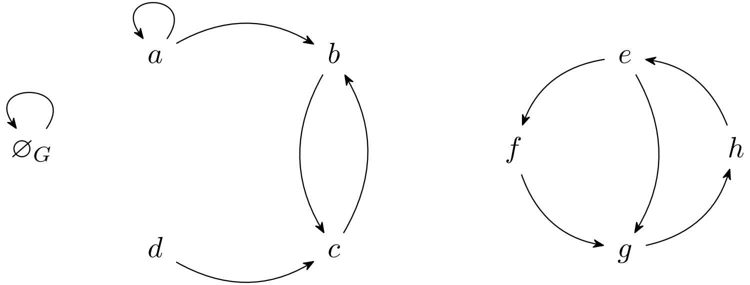
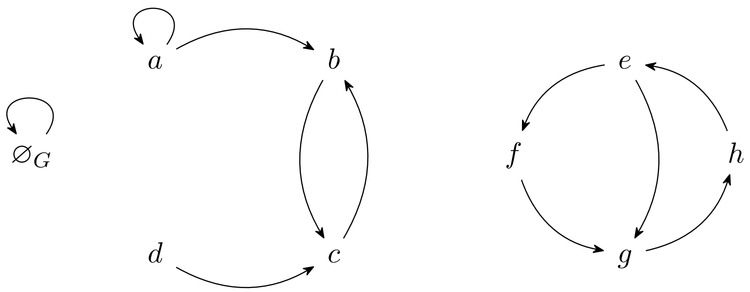


Fixed points through Influence Graph



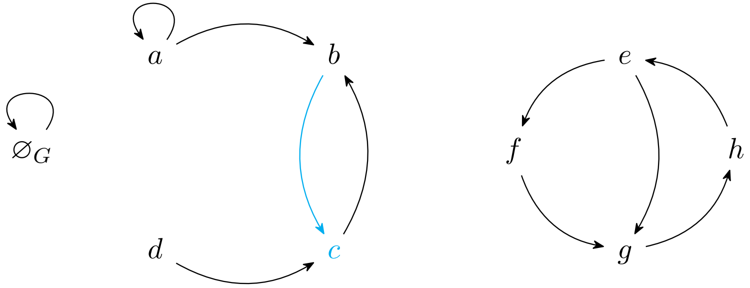
Fixed points through Influence Graph

$V_b = \{\} \longrightarrow$ vertices reachable by b



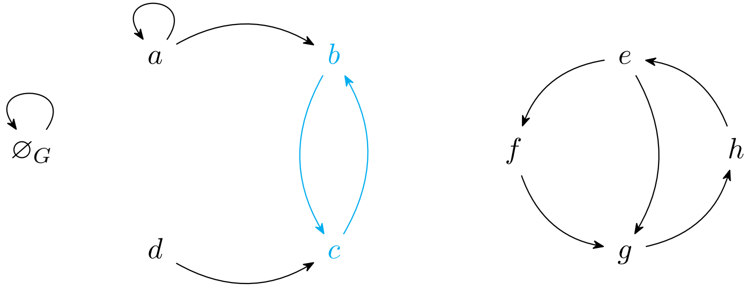
Fixed points through Influence Graph

$V_b = \{c\} \longrightarrow$ vertices reachable by b



Fixed points through Influence Graph

$V_b = \{c, b\} \longrightarrow$ vertices reachable by b



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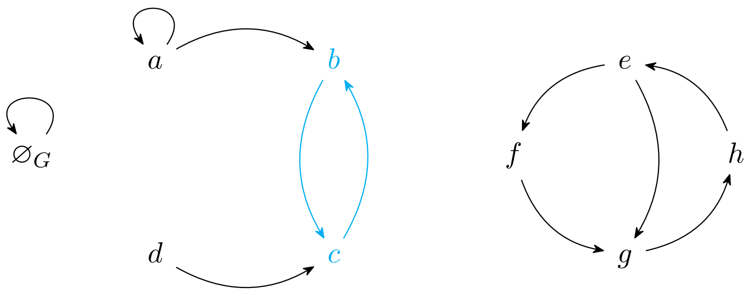

$b \in V_b$ if and only if b belongs to a cycle

Fixed points through Influence Graph

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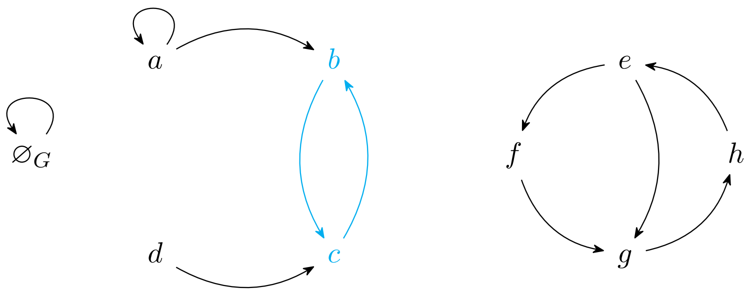

$b \in V_b$ if and only if b belongs to a cycle
$\Rightarrow \mathrm{res}_{\mathcal{A}}(\{b, c\}) = \{b, c\}$ i.e. $\mathrm{res}_{\mathcal{A}}(V_b) = V_b$

Fixed point *basis*

Let $\mathcal{A} \in \mathcal{RS}(1,0)$ and let $G_{\mathcal{A}} = (V_{\mathcal{A}}, E_{\mathcal{A}})$ be the influence graph of $\mathcal{A}$.

Lemma

For any vertex $u \in V_{\mathcal{A}}$, if $u \in V_u$ then V_u is a fixed point of $\mathcal{A}$.

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Lemma

For any vertex $u \in V_{\mathcal{A}}$, if $u \in V_u$ then V_u is a fixed point of $\mathcal{A}$.

Remark

Given $\mathrm{res} : 2^S \to 2^S$ additive, V_a, V_b fixed points, then $V_a \cup V_b$ is a fixed point:

$$\mathrm{res}(V_a \cup V_b) = \mathrm{res}(V_a) \cup \mathrm{res}(V_b) = V_a \cup V_b\,.$$

Fixed point *basis*

Is the converse also true?

Fixed point *basis*

Is the converse also true? Yes!

Proposition

Given $\varnothing \subsetneq T \subseteq S$ *a fixed point, then*

$$T = \bigcup_{u \in C_T} V_u$$

Fixed point *basis*

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Proposition

Given $\emptyset \subsetneq T \subseteq S$ *a fixed point, then*

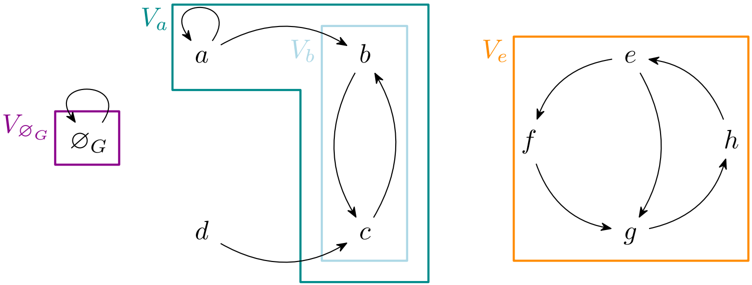
$$T = \bigcup_{u \in C_T} V_u$$

Given $\mathcal{A} \in \mathcal{RS}(1, 0)$, let us define

$$F_{\mathcal{A}} \coloneqq \{V_u \mid u \in V_u\}$$

Fixed point *basis*

$$F_{\mathcal{A}} = \{V_{\varnothing_G}, V_a, V_b, V_e\}$$



Fixed point *basis*: application

Corollary

Given $\mathcal{A}, \mathcal{B} \in \mathcal{RS}(1,0)$ *with a common background set* S*, it is in* **P** *to decide whether* $\mathcal{A}$ *and* $\mathcal{B}$ *share all fixed points.*

Fixed point *basis*: application

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Proof.

Check $F_{\mathcal{A}} = F_{\mathcal{B}}$. □

Fixed point *basis*: application

Problem	$\mathcal{RS}(\infty, \infty)$	$\mathcal{RS}(0, \infty)$	$\mathcal{RS}(\infty, 0)$	$\mathcal{RS}(1, 0)$
sharing all fixed points	**coNP**-c[1]	**coNP**-c[2]	**coNP**-c[2]	**P** [4]

1 Formenti, Manzoni, and Porreca 2014

2 Ascone, Bernardini, and Manzoni 2024b

4 Ascone, Bernardini, and Manzoni 2024a

All results

Problem	$\mathcal{RS}(\infty, \infty)$	$\mathcal{RS}(0, \infty)$	$\mathcal{RS}(\infty, 0)$	$\mathcal{RS}(1, 0)$
A given state is a fixed point attractor	NP-c[1]	NP-c[2]	NP-c[2]	P [4]
∃ fixed point	NP-c[1]	NP-c[2]	P [3]	
∃ common fixed point	NP-c[1]	NP-c[2]	NP-c[2]	P [4]
sharing all fixed points	coNP-c[1]	coNP-c[2]	coNP-c[2]	P [4]
∃ fixed point attractor	NP-c[1]	NP-c[2]	Unknown	P [4]
∃ common fixed point attractor	NP-c[1]	NP-c[2]	NP-c[2]	P [4]
sharing all fixed points attractor	Π_2^{P}-c[1]	Π_2^{P}-c[2]	Π_2^{P}-c[2]	P [4]
∃ fixed point not attractor	Σ_2^{P}-c[2]	Σ_2^{P}-c[2]	Σ_2^{P}-c[2]	P [4]
∃ common fixed point not attractor	Σ_2^{P}-c[2]	Σ_2^{P}-c[2]	Σ_2^{P}-c[2]	P [4]
sharing all fixed points not attractor	coNP-c[2]	coNP-c[2]	coNP-c[2]	P [4]
$\mathrm{res}_{\mathcal{A}} = \mathrm{res}_{\mathcal{B}}$	coNP-c[2]	P [2]	P [2]	

1 Formenti, Manzoni, and Porreca 2014

2 Ascone, Bernardini, and Manzoni 2024b

3 Knaster-Tarski Theorem

4 Ascone, Bernardini, and Manzoni 2024a

Open problems

- Is $\exists$ *fixed point attractor* for $\mathcal{RS}(\infty, 0)$ **NP**-complete?

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- Is *Reachability* for $\mathcal{RS}(1, 0)$ **NP**-complete? (Only supreachability is known)

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- Is *Reachability* for $\mathcal{RS}(1, 0)$ **NP**-complete? (Only supreachability is known)

Problem	$\mathcal{RS}(\infty, \infty)$	$\mathcal{RS}(0, \infty)$	$\mathcal{RS}(\infty, 0)$	$\mathcal{RS}(1, 0)$
Reachability[3]	**PSPACE**-c	**PSPACE**-c	**PSPACE**-c	**NP**-c?

[3] Dennunzio et al. 2016.

Future directions

- Study similar problems related to cycles and global attractors (to complete).

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- Study similar problems related to cycles and global attractors (to complete).
- Study what happens for $\mathcal{RS}(2,0), \mathcal{RS}(3,0), \dots$
- Use multisets and allow inputs $\rightarrow$ automaton equivalent to the Turing machine.

References

- Ascone, Rocco, Giulia Bernardini, and Luca Manzoni (Mar. 2024a). "Fixed points and attractors of additive reaction systems". In: *Natural Computing*.
- — (2024b). "Fixed points and attractors of reactantless and inhibitorless reaction systems". In: *Theoretical Computer Science*.
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