UNIVERSITÀ DEGLI STUDI DI TRIESTE

Natural Computing Laboratory

Reaction Systems and Their Dynamics

Luca Manzoni

Università degli Studi di Trieste

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Why Rection Systems?

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Reaction systems are a computational model inspired by *bio-chemical reactions*.

Why another bio-inspired model?

- A model abstract enough that is of theoretical interest. . .
- . . .but still useful to model biological processes

Example of Application

Ion Petre et al. have studied the *the eukaryotic heat shock response*[1]

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The heat shock response is a defense mechanism by which the cell reacts to elevated temperatures

They have reformulate the existing model in terms of reaction systems and studied biologically relevant properties

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Reactions

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If $R, I, P \subseteq S$ then a is a reaction over S

Reaction Systems

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

Example of a Reaction System

Background set:

$$S = \{a, b, c, d, e\}$$

Set of reactions:

$$A = \{(\{a\}, \{b, c\}, \{a, c\}) \\ (\{a, c, e\}, \{d\}, \{d, e\})\}$$

Enabled Reactions

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

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- *All the reactants* are present in T:

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- *None of the inhibitors* is present in T:

$$I \cap T = \varnothing$$

Result Function

Let $a = (R, I, P)$ be a reaction.

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

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

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

$$\text{res}_{\mathcal{A}} = \text{res}_A$$

Result Function: Example

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

Reactions: $r_1 = (\{a\}, \{b, c\}, \{a, c\})$
$r_2 = (\{a, c, e\}, \{d\}, \{d, e\})$

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State: $T = \{a, b, c, e\}$

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

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$$\mathrm{res}_{r_1}(T) = \varnothing$$

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$r_2 = (\{a, c, e\}, \{d\}, \{d, e\})$

State: $T = \{a, b, c, e\}$

$$\{a, c, e\} \subseteq T$$
$$\{d\} \cap T = \varnothing$$

$$\text{res}_{r_2}(T) = \{d, e\}$$

Result Function: Example

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

Reactions: $r_1 = (\{a\}, \{b, c\}, \{a, c\})$
$r_2 = (\{a, c, e\}, \{d\}, \{d, e\})$

State: $T = \{a, b, c, e\}$

$$\text{res}_A(T) = \text{res}_{r_1}(T) \cup \text{res}_{r_2}(T)$$

Result Function: Example

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Reactions: $r_1 = (\{a\}, \{b, c\}, \{a, c\})$
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$$\begin{aligned} \text{res}_A(T) &= \text{res}_{r_1}(T) \cup \text{res}_{r_2}(T) \\ &= \emptyset \cup \{d, e\} \end{aligned}$$

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This is a finite dynamical system:

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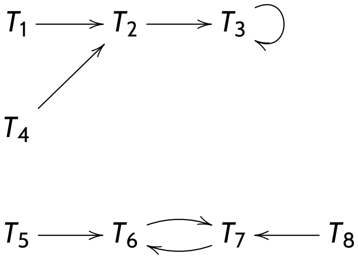
State sequence or *orbit* starting from $T \subseteq S$:

$$\left(T, \mathrm{res}_{\mathcal{A}}(T), \mathrm{res}_{\mathcal{A}}^2(T), \mathrm{res}_{\mathcal{A}}^3(T), \ldots\right)$$

Some Terminology

If $\text{res}_{\mathcal{A}}(T_i) = T_j$ then there is an arrow from T_i to T_j:



Some Dynamical Properties 1/3

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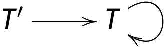

Some Dynamical Properties 1/3

- **Fixed Point.** $\text{res}_{\mathcal{A}}(T) = T$:

$$T \circlearrowright$$

- **Fixed Point Attractor.** “A fixed point with something going in”

$$T' \longrightarrow T \circlearrowright$$

- **Global Fixed Point Attractor.** “A fixed point where everything goes in”

$$\forall T' \subseteq S \qquad T' \longrightarrow T'' \longrightarrow \ldots \longrightarrow T \circlearrowright$$

Some Dynamical Properties 2/3

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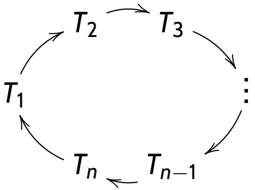
- **Cycle.** Every finite dynamical system has a cycle



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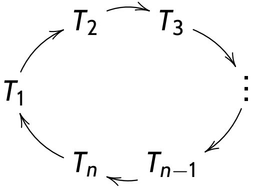
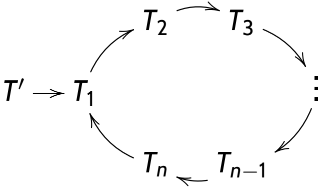


- **Attractor Cycle.** “A cycle with something going in”



Some Dynamical Properties 3/3

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- **Global Attractor Cycle.** “A cycle reachable from every state”

$$\forall T' \subseteq S \qquad T' \to \dots \to T_1$$

$$T_1 \to T_2 \to T_3 \to \cdots \to T_{n-1} \to T_n \to T_1$$

Some Dynamical Properties 3/3

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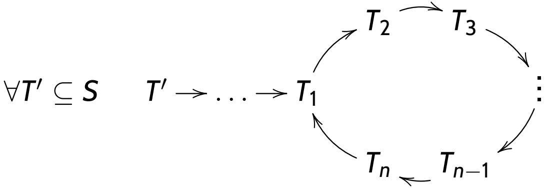

- **Gardens of Eden.** "A state with nothing going in"
  A state with no *preimages*

$$T' \overset{\text{never}}{\dashrightarrow} T$$

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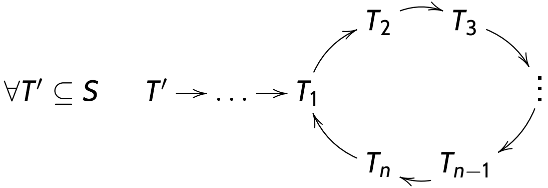

- **Gardens of Eden.** "A state with nothing going in"
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$$T' \overset{\text{never}}{\dashrightarrow} T$$

  Recall that: *garden of Eden* $\iff$ *attractor cycle*

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- does $\mathcal{A}$ have a fixed point that is a global attractor?

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

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Existence of a Fixed Point

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

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

We will build a reaction system with a fixed point *iff* φ is satisfiable

Background set: $S = \{x_1, x_2, x_3, \clubsuit, \spadesuit\}$

Encoding the Assignments

$$x_1 = \text{True}$$
$$x_2 = \text{False}$$
$$x_3 = \text{True}$$

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$$x_1 = \text{True}$$
$$x_2 = \text{False} \qquad \Rightarrow \{x_1, x_3\}$$
$$x_3 = \text{True}$$

Encoding the Assignments

$$\left.\begin{aligned} x_1 &= \text{True} \\ x_2 &= \text{False} \\ x_3 &= \text{True} \end{aligned}\right. \qquad \Rightarrow \{x_1, x_3\}$$

Idea: if T is a satisfying assignment then:

$$T \circlearrowright$$

else

$$T \longrightarrow T \cup \{\spadesuit\} \rightleftarrows T \cup \{\clubsuit\}$$

The Reactions

Preserve the assignment:

$$(\{x_i\}, \varnothing, \{x_i\})$$

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The Reactions

Preserve the assignment:

$$(\{x_i\}, \emptyset, \{x_i\})$$

Create a cycle with ♠ and ♣:

$$(\{\spadesuit\}, \emptyset, \{\clubsuit\})$$
$$(\{\clubsuit\}, \{\spadesuit\}, \{\spadesuit\})$$

Evaluate a clause (e.g., $x_1 \vee \neg x_2 \vee x_3$):

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

A Non-Satisfying Assignment

Evaluation of

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

with the assignment $x_1 = \text{False}, x_2 = \text{True}, x_2 = \text{False}$

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$$\{x_2\} \longrightarrow \{x_2, \spadesuit\}$$

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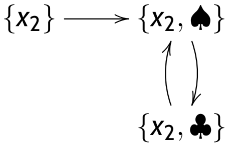

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$$\{x_1, x_2\} \longrightarrow \{\quad,\quad\}$$

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$$\{x_1, x_2\} \longrightarrow \{x_1, x_2\}$$

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With similar techniques we can find:

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Global Attractors

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For global attractors we need another approach:

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- The Turing Machine has a polynomially-sized tape
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- . . .unless the TM has already rejected the input

Global Attractors: Results

- Finding if there exists a global fixed point attractor is **PSPACE**-complete

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Global Attractors: Results

- Finding if there exists a global fixed point attractor is **PSPACE**-complete
- Finding if there exists a global attractor cycle is **PSPACE**-complete
- Reachability between two configurations is **PSPACE**-complete

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Bounding Reactants and Inhibitors

$\mathcal{RS}(r, i)$:
All Reaction Systems whose reactions

- have at most *r* reactants
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Classification

$\mathcal{RS}(\infty, \infty)$	Every function $2^S \to 2^S$
$\mathcal{RS}(0, \infty)$	Antitone functions: $T \subseteq T' \to \text{res}_{\mathcal{A}}(T) \supseteq \text{res}_{\mathcal{A}}(T')$
$\mathcal{RS}(\infty, 0)$	Monotone functions: $T \subseteq T' \to \text{res}_{\mathcal{A}}(T) \subseteq \text{res}_{\mathcal{A}}(T')$
$\mathcal{RS}(1, 0)$	Functions such that $\text{res}_{\mathcal{A}}(T \cup U) = \text{res}_{\mathcal{A}}(T) \cup \text{res}_{\mathcal{A}}(U)$

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$\mathcal{RS}(\infty, \infty)$	Every function $2^S \to 2^S$
$\mathcal{RS}(0, \infty)$	Antitone functions: $T \subseteq T' \to \text{res}_{\mathcal{A}}(T) \supseteq \text{res}_{\mathcal{A}}(T')$
$\mathcal{RS}(\infty, 0)$	Monotone functions: $T \subseteq T' \to \text{res}_{\mathcal{A}}(T) \subseteq \text{res}_{\mathcal{A}}(T')$
$\mathcal{RS}(1, 0)$	Functions such that $\text{res}_{\mathcal{A}}(T \cup U) = \text{res}_{\mathcal{A}}(T) \cup \text{res}_{\mathcal{A}}(U)$
$\mathcal{RS}(0, 0)$	All constant functions

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However for $\mathcal{RS}(1, 0)$ it is **NL**-hard and in **NP**.
We solved the similar problem of *sup-reachability*

Influence Graph

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\begin{aligned}
S &= \{a, b, c\} \\
A &= \{(\{a\}, \varnothing, \{b\}) \\
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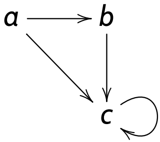

Sup-Reachability in $\mathcal{RS}(1, 0)$

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

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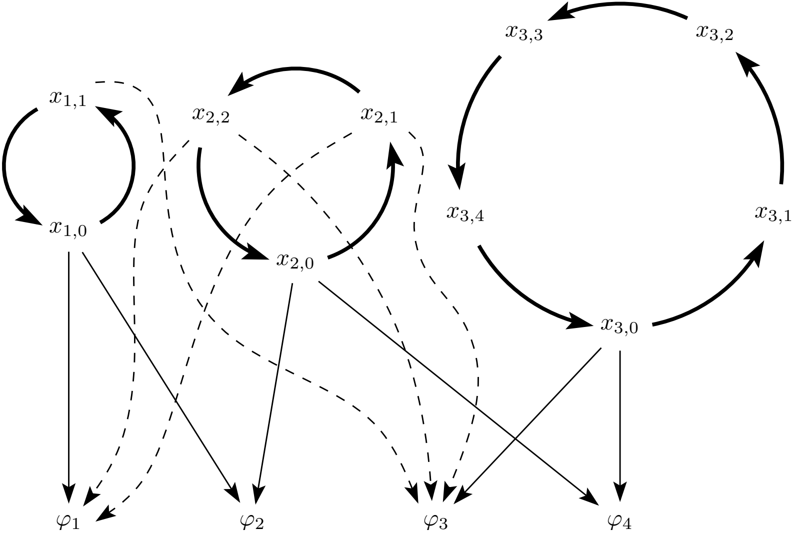
The set of all clauses appears iff φ is satisfiable

Reachability Influence Graph



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then we only need to guess a time step $t \in \mathbb{N}$ and check if

$$G^t X \geq Y$$

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Thank you
for your attention