Reaction Systems Made Simple

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The plan

Introduction to RS

Classification: simulation

Classification: functions

The plan

Reaction Systems: definition

“Simulation” between RS

Classification: functions

The plan

Reaction Systems: definition

Classification: simulation

Functions defined by RS

Reaction Systems Definition

Reactions
Definition

$$a = (R_a, I_a, P_a)$$

- R_a: a set of *reactants*
- I_a: a set of *inhibitors*
- P_a: a set of *products*

Reactions
Definition

$$a = (R_a, I_a, P_a)$$

- R_a: a set of *reactants*
- I_a: a set of *inhibitors*
- P_a: a set of *products*

If there are all reactants and no inhibitors
then all products are generated

Reaction Systems
Definition

$$\mathcal{A} = (S, A)$$

- S: a finite set of entities
- A: a finite set of reactions

Reaction Systems

Next state function

- Let T be a subset of S

Reaction Systems

Next state function

- Let T be a subset of S
- For every reaction $a = (R_a, I_a, P_a) \in A$
  - $\mathrm{res}_a(T) = P_a$ if a is *enabled* in T
  - $\mathrm{res}_a(T) = \emptyset$ otherwise

Reaction Systems

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- $\mathrm{res}_A(T) = \bigcup_{a \in A} \mathrm{res}_a(T)$

Reaction Systems

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Reaction Systems

An example

Entities

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

Reactions

$$\begin{aligned} r_1 &= (\{a\}, \{b, c\}, \{a\}) \\ r_2 &= (\{a\}, \{b\}, \{c\}) \end{aligned}$$

Reaction Systems

An example

$\{a\}$

Entities

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

Reactions

$$
\begin{aligned}
r_1 &= (\{a\}, \{b, c\}, \{a\}) \\
r_2 &= (\{a\}, \{b\}, \{c\})
\end{aligned}
$$

Reaction Systems

An example

$$\{a\} \xrightarrow{r_1 \text{ and } r_2 \text{ are enabled}} \{a, c\}$$

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$$\begin{tikzcd} \{a\} \arrow[d, "r_1 \text{ and } r_2 \text{ are enabled}"] \\ \{a, c\} \arrow[d, "\text{Only } r_2 \text{ is enabled}"] \\ \{c\} \end{tikzcd}$$

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Reaction Systems

Bounding reactants and inhibitors

$$\mathcal{RS}(r,i)$$

All Reaction Systems whose reactions

- have at most r reactants
- and at most i inhibitors

Reaction Systems
Bounding reactants and inhibitors

- $\mathcal{RS}(\infty, 0)$ is all Reaction Systems without inhibitors
- $\mathcal{RS}(0, \infty)$ is all Reaction Systems without reactants
- $\mathcal{RS}(\infty, \infty)$ is all Reaction Systems

Classification: Simulation

k-simulation
Idea

$$\mathcal{A}: \quad \{a\} \longrightarrow \{a, c\} \longrightarrow \{c\} \longrightarrow \varnothing$$

k-simulation
Idea

$$\mathcal{A}: \quad \{a\} \longrightarrow \{a, c\} \longrightarrow \{c\} \longrightarrow \emptyset$$

$$\mathcal{B}: \quad \{a\}$$

The same initial state

k-simulation

Idea

$$\mathcal{A}: \quad \{a\} \longrightarrow \{a, c\} \longrightarrow \{c\} \longrightarrow \emptyset$$

$$\mathcal{B}: \quad \{a\} \to \{a, e\} \to \{a, c\} \to \{c, d\} \to \{c\} \longrightarrow \{d\} \longrightarrow \{e\}$$

The same initial state

k-simulation

Idea

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The same initial state

Every k steps. . .

k-simulation

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$$\mathcal{B}: \{a\} \to \{a, e\} \to \{a, c\} \to \{c, d\} \to \{c\} \to \{d\} \to \{e\}$$

The same initial state

Every k steps we obtain the "same" state

k-simulation
Definition

$$\mathcal{A} \preceq_k \mathcal{B}$$

For any subset of the substances of $\mathcal{A}$

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the state of $\mathcal{B}$ after kn steps
restricted to the substances of $\mathcal{A}$

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the state of $\mathcal{B}$ after kn steps
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$$\forall T \subseteq S \; \forall n \in \mathbb{N} \qquad \mathrm{res}^n_{\mathcal{A}}(T) = \mathrm{res}^{kn}_{\mathcal{B}}(T) \cap S$$

Reaction Systems

k-simulability relation

Q, Q': **classes** of reaction systems

Reaction Systems

k-simulability relation

Q, Q': **classes** of reaction systems

$$Q \preceq_k Q'$$

Every reaction systems of Q
is h-simulated ($h \leq k$) by some system in Q'

Reaction Systems
k-simulability relation

Q, Q': **classes** of reaction systems

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is h-simulated ($h \leq k$) by some system in Q'

$$Q \preceq Q'$$

$Q \preceq_k Q'$ for some k

Can we trade

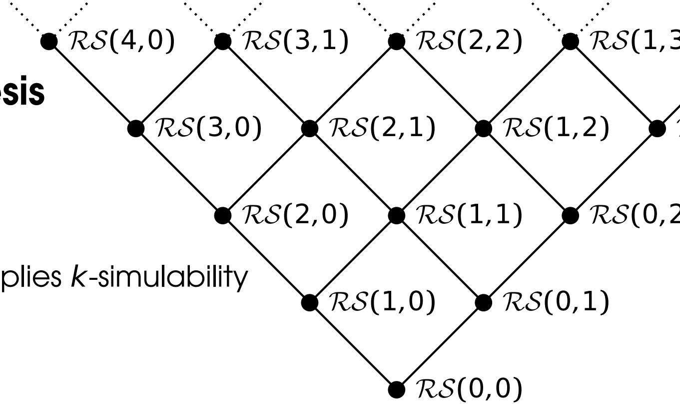
time

to obtain

simpler reactions

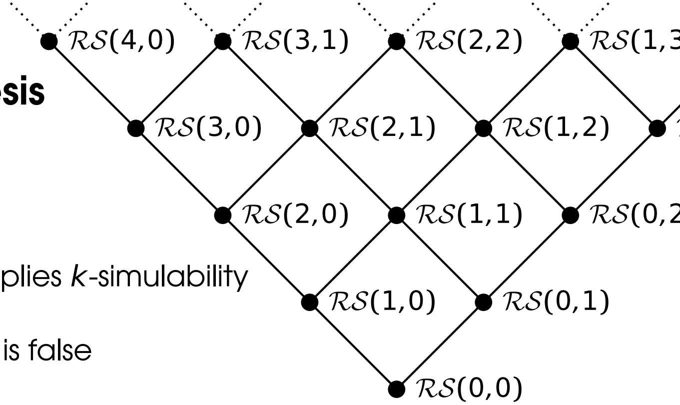
?

An hypothesis



Set inclusion implies k-simulability

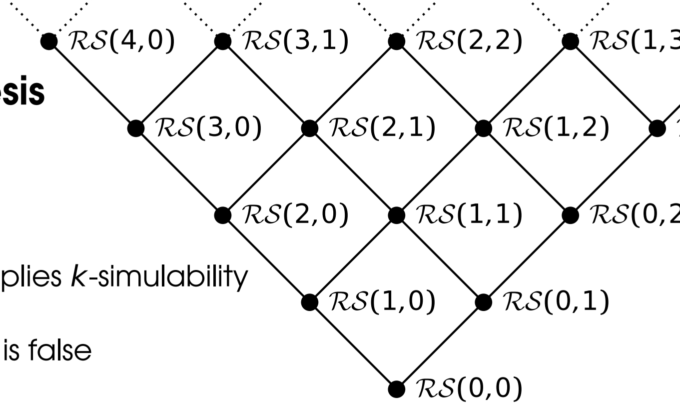
An hypothesis



Set inclusion implies k-simulability

But the reverse is false

An hypothesis



Set inclusion implies k-simulability

But the reverse is false

Theorem

$$\mathcal{RS}(r,i) \preceq_2 \mathcal{RS}(1,1)$$

How does it works?

An example with one reaction

$$\mathfrak{r} = (\{a, b\}, \{c\}, \{d\})$$

One reaction is replaced by a set of reactions
that produces the same results in 2 steps

How does it works?

New reactions

$(\emptyset, \{a\}, \{\mathfrak{r}\})$
$(\emptyset, \{b\}, \{\mathfrak{r}\})$

If some reactant is missing generates the object $\mathfrak{r}$

How does it works?

New reactions

$(\varnothing, \{a\}, \{\mathfrak{r}\})$
$(\varnothing, \{b\}, \{\mathfrak{r}\})$

If some reactant is missing generates the object $\mathfrak{r}$

$(\{c\}, \varnothing, \{\mathfrak{r}\})$

If some inhibitor is present generates the object $\mathfrak{r}$

How does it works?

New reactions

$(\varnothing, \{a\}, \{\mathfrak{r}\})$
$(\varnothing, \{b\}, \{\mathfrak{r}\})$

If some reactant is missing generates the object $\mathfrak{r}$

$(\{c\}, \varnothing, \{\mathfrak{r}\})$

If some inhibitor is present generates the object $\mathfrak{r}$

$(\varnothing, \{\mathfrak{r}\}, \{d\})$

If $\mathfrak{r}$ *is absent the products of* $\mathfrak{r}$ *are generated*

Does it work?

$\{a, b\}$

$\{a, b\}$

Does it work?

$$\{a, b\} \longrightarrow \{d\}$$

$$\{a, b\}$$

Does it work?

$$\{a, b\} \longrightarrow \{d\}$$

$$\{a, b\} \longrightarrow \{d\} \longrightarrow \{d\} \cup \{\mathfrak{r}\}$$

Does it work?

$$\begin{tikzcd}
\{a, b\} \arrow[rr] & & \{d\} \\
\{a, b\} \arrow[r] & \{d\} \arrow[r] & \{d\} \cup \{\mathfrak{r}\}
\end{tikzcd}$$

Does it work?

$$\{a, b\} \longrightarrow \{d\}$$

$$\{a, b\} \longrightarrow \{d\} \longrightarrow \{d\} \cup \boxed{\{\mathfrak{r}\}}$$

Another example

$\{a, c\}$

$\{a, c\}$

Another example

$$\{a, c\} \longrightarrow \emptyset$$

$$\{a, c\}$$

Another example

$$\{a, c\} \longrightarrow \emptyset$$

$$\{a, c\} \longrightarrow \emptyset \cup \{\mathfrak{r}\} \longrightarrow \emptyset \cup \{\mathfrak{r}\}$$

Another example

$$\begin{tikzcd}
\{a, c\} \arrow[rr] & & \varnothing \\
\{a, c\} \arrow[r] & \varnothing \cup \{\mathfrak{r}\} \arrow[r] & \varnothing \cup \{\mathfrak{r}\}
\end{tikzcd}$$

Another example

$$\{a, c\} \longrightarrow \emptyset$$

$$\{a, c\} \longrightarrow \emptyset \cup \{\mathfrak{r}\} \longrightarrow \emptyset \cup \boxed{\{\mathfrak{r}\}}$$

One is enough

A normal form for Reaction Systems

Theorem

Every Reaction System
can be 2-simulated
by a system in $\mathcal{RS}(1,1)$

One is enough

A normal form for Reaction Systems

Theorem

Every Reaction System
can be 2-simulated
by a system in $\mathcal{RS}(1,1)$

$\mathcal{RS}(1,1)$ is, in some sense,
a universal *class*

Minimality

Do we really need two steps?

Theorem

If $r' + i' < r + i$ then
$\mathcal{RS}(r, i) \not\preceq_1 \mathcal{RS}(r', i')$

Minimality

Do we really need two steps?

Theorem

If $r' + i' < r + i$ then
$\mathcal{RS}(r, i) \not\preceq_1 \mathcal{RS}(r', i')$

The 2-simulation is minimal in time

What is missing?

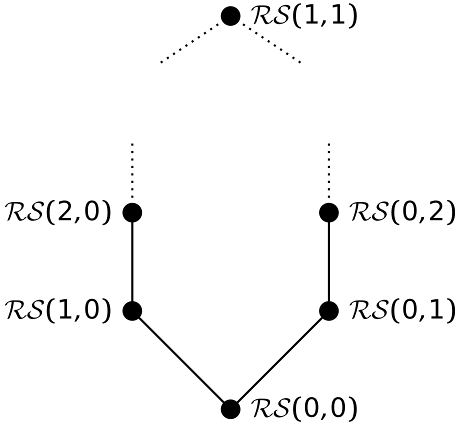
- When $r \geq 1$ and $i \geq 1$ we have:
  - $\mathcal{RS}(1, 1) \preceq \mathcal{RS}(r, i)$
  - $\mathcal{RS}(r, i) \preceq \mathcal{RS}(1, 1)$

What is missing?

- When $r \geq 1$ and $i \geq 1$ we have:
  - $\mathcal{RS}(1,1) \preceq \mathcal{RS}(r,i)$
  - $\mathcal{RS}(r,i) \preceq \mathcal{RS}(1,1)$
- But when $r = 0$ or $i = 0$ we only know:
  - $\mathcal{RS}(r,0) \preceq \mathcal{RS}(1,1)$
  - $\mathcal{RS}(0,i) \preceq \mathcal{RS}(1,1)$

Reactants

Do we need more than two?



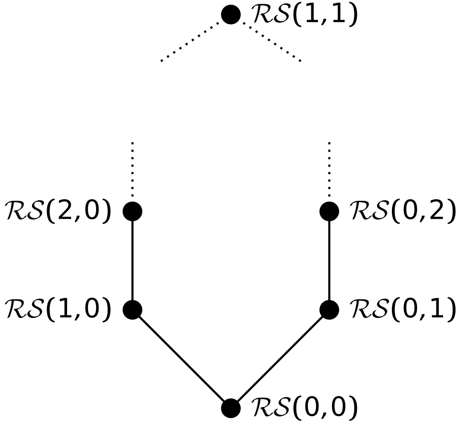
Reactants

Do we need more than two?

Lemma

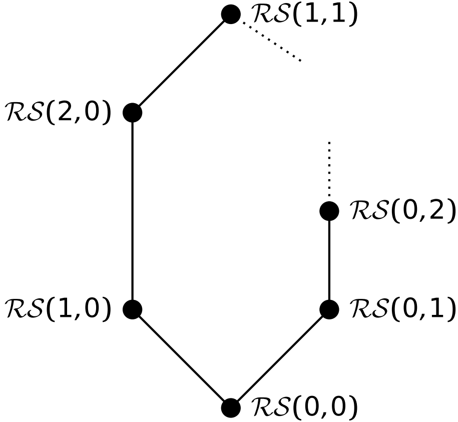
For every $r > 2$

$$\mathcal{RS}(r,0) \preceq_{\lceil \log r \rceil} \mathcal{RS}(2,0)$$



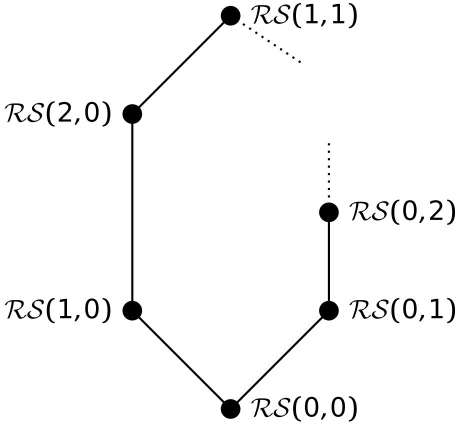
Inhibitors

Do we need more than ~~two~~ one?



Inhibitors

Do we need more than ~~two~~ one?

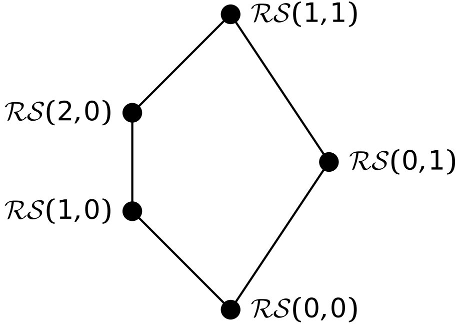


Lemma

For every $i \in \mathbb{N}$
$\mathcal{RS}(0,i) \preceq_3 \mathcal{RS}(0,1)$

Reactants and Inhibitors

Who is stronger?

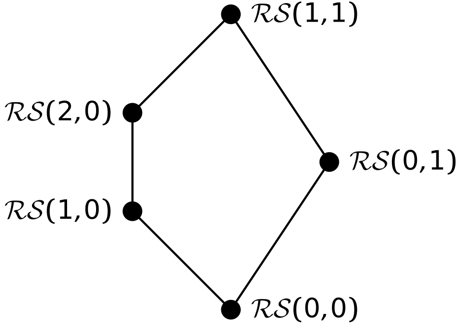


Reactants and Inhibitors

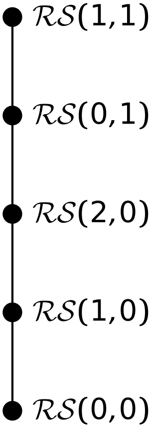
Who is stronger?

Lemma

$$\mathcal{RS}(2,0) \preceq_2 \mathcal{RS}(0,1)$$



Classification Theorem (k-simulability)



Classification Theorem (k-simulability)

- $\mathcal{RS}(1,1)$
- $\mathcal{RS}(0,1)$
- $\mathcal{RS}(2,0)$
- $\mathcal{RS}(1,0)$
- $\mathcal{RS}(0,0)$

Classification Theorem (k-simulability)

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

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- All classes are distinct

Classification Theorem (k-simulability)

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

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$\mathcal{RS}(2,0)$

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

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

- All classes are distinct
- All the simulations are minimal in time

Classification:
functions

Result function

Every Reaction Systems $\mathcal{A} = (S, A)$ *defines* a function.

$$\begin{aligned} \text{res}_{\mathcal{A}}: \quad & 2^S \rightarrow 2^S \\ & T \mapsto \text{res}_A(T) \end{aligned}$$

Result function

Every Reaction Systems $\mathcal{A} = (S, A)$ *defines* a function.

$$\begin{aligned} \mathrm{res}_{\mathcal{A}}: \quad & 2^S \to 2^S \\ & T \mapsto \mathrm{res}_A(T) \end{aligned}$$

What are the functions defined by Reaction Systems?

Functions defined by $\mathcal{RS}(\infty, \infty)$

Theorem

For every finite S, for every $f : 2^S \to 2^S$

there exists $\mathcal{A} \in \mathcal{RS}(\infty, \infty)$ s.t.

$$\mathrm{res}_{\mathcal{A}} = f$$

Functions defined by $\mathcal{RS}(\infty, \infty)$

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What happens if we limit resources?

Functions defined by Reaction Systems

- Antitone

  $T_1 \subseteq T_2 \implies f(T_1) \supseteq f(T_2)$

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

Functions defined by Reaction Systems

- Antitone

  $T_1 \subseteq T_2 \implies f(T_1) \supseteq f(T_2)$

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

- $f, f^3, f^5, \ldots$ are all antitone
- $f^2, f^4, f^6, \ldots$ are all isotone
- Hence the simulation in $\mathcal{RS}(0,\infty) \preceq_3 \mathcal{RS}(0,1)$ is *minimal* in time

Functions defined by Reaction Systems

- Isotone

  $T_1 \subseteq T_2 \implies f(T_1) \subseteq f(T_2)$

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

Functions defined by Reaction Systems

- Isotone

  $T_1 \subseteq T_2 \implies f(T_1) \subseteq f(T_2)$

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

- $f, f^2, f^3, \ldots$ are all isotone
- This explains why $\mathcal{RS}(\infty, 0)$ cannot simulate $\mathcal{RS}(0, \infty)$

Functions defined by Reaction Systems

- Additive

  $f(T_1 \cup T_2) = f(T_1) \cup f(T_2)$

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

Functions defined by Reaction Systems

- Additive

  $f(T_1 \cup T_2) = f(T_1) \cup f(T_2)$

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

- $f, f^2, f^3, \ldots$ are all additive
- There exist isotone functions that are not additive
- This explains the difference between $\mathcal{RS}(1,0)$ and $\mathcal{RS}(\infty,0)$.

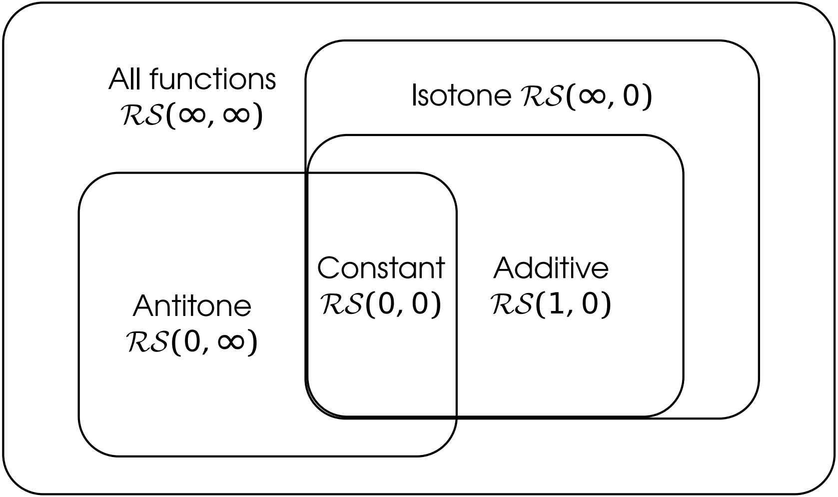
Functions defined by Reaction Systems

- Constant

  $f(T_1) = f(T_2)$

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

The big picture



Conclusions

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of the classes of reaction systems
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- based on *k*-simulability
- based on functions defined by RS

All the simulations are *minimal* in time
The results *need* auxiliary entities

There are many other

interesting

questions

about

Reaction

Systems

Combinatorics

There are many other

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Reaction Systems

Dynamics

Combinatorics

Dynamics of Reaction Systems
People involved

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Present

Complexity of the dynamics of Reaction Systems

What is the difficulty to determine

- the existence of a fixed point?
- If two reactions systems have the same local fixed point attractors?
- the existence of a global attractor?
- ...

Present

Complexity of the dynamics of Reaction Systems

What is the difficulty to determine

- the existence of a fixed point?

  NP-**complete**

- If two reactions systems have the same local fixed point attractors?

  Π_2^p-**complete**

- the existence of a global attractor?

  $PSPACE$-**complete**

- $\cdots$

?

Questions