Extremal Combinatorics of Reaction Systems

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Outline

Reactions

Definition

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

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

Restriction: $R_a \cap I_a = \varnothing$.

Reactions

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- P_a: a non-empty set of *products*

Restriction: $R_a \cap I_a = \varnothing$.

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

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- For every reaction $a = (R_a, I_a, P_a) \in A$
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Reaction Systems

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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

$\{a\}$

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Reactions

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

Reaction Systems

An example

$$\{a\}$$

$\downarrow$ r_1 and r_2 are enabled

$$\{a, c\}$$

Entities

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Reactions

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Reaction Systems

An example

Entities

$\{a, b, c\}$

Reactions

$$r_1 = (\{a\}, \{b, c\}, \{a\})$$
$$r_2 = (\{a\}, \{b\}, \{c\})$$

$\{a\}$

↓ r_1 and r_2 are enabled

$\{a, c\}$

↓ Only r_2 is enabled

$\{c\}$

Reaction Systems

An example

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Reactions

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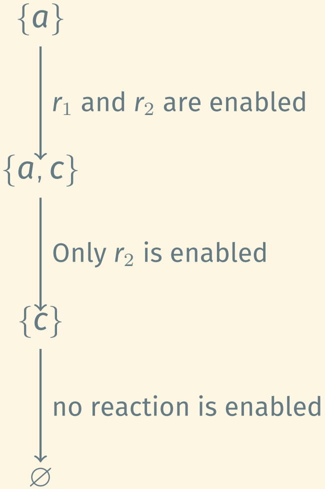

Threshold Properties

Definition

Fix n, the number of entities.

A property P is a threshold property if

No reaction — Size of the RS — All reactions

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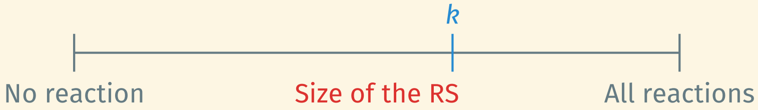

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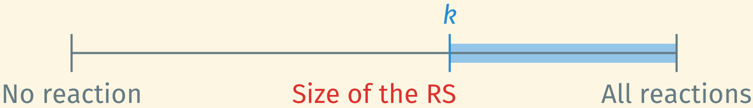

All RS with at least k reactions
have the property P

Threshold properties

Example

A threshold property

Having exactly one fixed point

A non-threshold property

Having a cycle of length 2

Threshold properties

Example

A threshold property

Having exactly one fixed point

- The RS with all the reactions has this property
- It is a threshold property

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Threshold properties

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A non-threshold property

Having a cycle of length 2

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Notation $R(P, n)$: Every RS with n entities and more than $R(P, n) = k$ reactions has property P.

Threshold Properties

Questions

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- Can we give the exact value of k in function of n?
- If not, can we obtain upper and lower bounds?

A Question about Concurrency

Always Parallel (AP)

In every $T \subseteq S$ either there are no reactions enabled or there are at least two distinct reaction enabled.

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Proposition

The threshold for AP is:

$$R(\mathsf{AP}, n) = (2^n - 1)(3^n - 5 \cdot 2^{n-1} + 2) + 2$$

Enabled Reactions

No-concurrency (NC)

In every $T \subseteq S$ not all reactions are enabled.

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Proposition

The threshold for NC is:

$$R(\mathsf{NC}, n) = (2^n - 1)(3^n - 2^{\lceil \frac{n}{2} \rceil} - 2^{\lfloor \frac{n}{2} \rfloor} + 1) + 1$$

Generation of Inhibitors

Inhibitors (Inh)

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Proposition

The threshold for Inh is:

$$(2^{n-1}-1)^2 < R(\mathsf{Inh}, n) < (2^n-1)(3^n-2^{\lceil \frac{n}{2} \rceil}-2^{\lfloor \frac{n}{2} \rfloor}+1)+1$$

Totality

Totality for RS (Tot)

For all $T \subset S$, $T \neq \varnothing$ implies $\mathrm{res}(T) \neq \varnothing$

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Proposition

The threshold for Tot is:

$$R(\mathrm{Tot}, n) = (2^n - 1)(3^n - 3 \cdot 2^n + 2^{\lceil \frac{n}{2} \rceil} + 2^{\lfloor \frac{n}{2} \rfloor}) + 1$$

Non-Decomposable (ND)

A RS $\mathcal{A} = (S, A)$ is decomposable if:

- There is a partition of S in S_1, S_2
- $\mathcal{A}_1 = (S_1, A_1)$, $\mathcal{A}_2 = (S_2, A_2)$ with $A_1 \cup A_2 = A$
- For each $T \subseteq S$
  $\text{res}_{\mathcal{A}}(T) = \text{res}_{\mathcal{A}_1}(T \cap S_1) \cup \text{res}_{\mathcal{A}_2}(T \cap S_2)$

Decomposable RS

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Proposition

The threshold for ND is:

$$R(\text{ND}, n) = (2^{n-1} + 1)(3^{n-1} - 2^n + 1) + 1$$

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When are two RS $\mathcal{A}$ and $\mathcal{B}$ equivalent?

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(S, A) is redundant if there exists $B \subset A$
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(S, A) contains unnecessary reactions.

Shrinkable RS

Ordering reactions

How to approach Red?

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Ordering of reactions

$a = (R_a, I_a, P_a) \preceq b = (R_b, I_b, P_b)$ when

- $R_a \supseteq R_b$ (a needs more reactants)
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If $a \prec b$ then a is not necessary.

Comparable (Comp)

A RS has property Comp if it contains two distinct comparable reactions

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Proposition

The threshold for Comp is:

$$\frac{n!(2^n - 2)}{\lceil \frac{n}{2} \rceil! \lfloor \frac{n}{2} \rfloor!} \leq R(\mathrm{Comp}, n) \leq \frac{n!(3^n - 2^{n+1} + 1)}{\lceil \frac{n}{2} \rceil! \lfloor \frac{n}{2} \rfloor!}$$

Shrinkable RS

Bounds (in a readable way)

What does the previous result means?

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Bounds (in a readable way)

What does the previous result means?

When the number of entities grows
the fraction of non-shrinkable RS goes to 0.

If RS do something
they do it with a small RS

Most of the RS are shrinkable

Conclusions

First study of extremal combinatorics in RS

- Interaction between reactions
- Functions defined by RS

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In the future:

- Length of cycles
- Length of preperiods
- Number of attraction basins

Questions?