REACTION SYSTEM RANKS FOR UNION-ADDITIVE FUNCTIONS UNDER VARIOUS RESOURCE CONSTRAINTS AND THEIR HIERARCHICAL ANALYSIS

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LIST OF SYMBOLS

$\mathbb{N}$	the set of natural numbers
S	background set, finite nonempty set
2^S	the power set of S
R_a	the reactant set
I_a	the inhibitor set
P_a	the product set
$\|T\|$	cardinality of the set T
$\emptyset$	null set (empty set)
Φ	a null function from 2^S to S^S
$\lceil\cdot\rceil$	the ceiling function
rsrank	reaction system rank or *rs* rank
minrsrank	minimal reaction system rank or minimal *rs* rank
alminrsrank	almost minimal reaction system rank or almost minimal *rs* rank
$\mathcal{RS}^*(m,n)$	hierarchical class based on rank witnessing reaction system
$\sim$	functional equivalence
$\mathcal{F}_U(S)$	a class of union-additive *rs* fucntions
$\mathcal{F}_U^k(S)$	the subclass of $\mathcal{F}_U(S)$ consisting of all functions with signature size k
$sig[f]$	the signature of $f \in \mathcal{F}_U(S)$
char$[f]$	the characteristic set of $f \in \mathcal{F}_U(S)$
$\wedge$	conjunction (AND operation) in Boolean logic
$\vee$	disjunction (OR operation) in Boolean logic
$\overline{v}$	negation of the boolean variable v

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PANGKAT SISTEM REAKSI BAGI FUNGSI BERDAYA TAMBAH KESATUAN DI BAWAH PELBAGAI KEKANGAN SUMBER DAN ANALISIS HIERARKI MEREKA

ABSTRAK

Sistem reaksi, yang diperkenalkan hampir dua dekad yang lalu oleh Ehrenfeucht dan Rozenberg, adalah rangka kerja pemodelan yang kukuh yang diilhamkan oleh interaksi kimia kompleks yang berlaku dalam sel hidup. Aspek penting sistem reaksi ialah fungsi *rs* yang berkaitan, yang menerangkan peralihan keadaan dalam proses interaktif. Kajian matematik terhadap fungsi *rs* telah menarik minat yang signifikan, terutamanya yang memberi tumpuan kepada fungsi yang ditentukan oleh sistem reaksi minimal. Konsep pangkat sistem reaksi sedang berkembang sebagai topik penyelidikan penting; ia mengukur kerumitan fungsi *rs* berdasarkan set reaksi terkecil yang boleh menentukannya. Karya ini mengkaji pangkat sistem reaksi bagi fungsi-fungsi yang tergolong dalam kelas fungsi *rs* berdaya tambah kesatuan, $\mathcal{F}_U(S)$, yang diperkenalkan oleh Salomaa. Kelas ini sangat menarik kerana setiap fungsi ditentukan sepenuhnya oleh imej bagi set singleton dan boleh ditentukan oleh sistem reaksi minimal. Untuk tujuan penyelidikan yang sistematik, kajian ini memperkenalkan tanggapan set ciri dan saiz tandatangan. Secara khususnya, kajian ini menentukan pangkat merentasi pelbagai saiz tandatangan, menetapkan pangkat malar untuk saiz tandatangan satu, mendedahkan kebergantungan pada saiz set dalam set ciri untuk saiz dua, dan menyediakan had bawah dan atas untuk saiz tiga dan untuk tandatangan satu-ke-satu. Di samping penyelidikan ini, tesis ini memperkenalkan dan menganalisis tiga konsep baharu: pangkat sistem reaksi minimal, yang mana formula amnya berjaya diterbitkan untuk semua fungsi dalam $\mathcal{F}_U(S)$; pangkat sistem reaksi hampir minimal, yang dikaji untuk saiz tandatangan tertentu; dan hierarki baharu, $\mathcal{RS}^*(m,n)$, di mana hasil kajian menetapkan bahawa fungsi dengan saiz tandatangan sehingga $k \leq 3$ tergolong secara khusus ke dalam kelas $\mathcal{RS}^*(k,1)$ dan bukan subkelas $\mathcal{RS}^*(k-1,1)$. Akhir sekali, tesis ini membincangkan aspek pengkomputeran bagi masalah ini. Atur cara Python telah dibangunkan untuk mengesahkan sama ada sistem reaksi yang diberi dapat menentukan sesuatu fungsi

dalam $\mathcal{F}_U(S)$ dan untuk menentukan pangkat *rs* bagi fungsi dalam kelas ini dengan tandatangan satu-ke-satu. Pendekatan pengkomputeran ini bukan sahaja mengesahkan penemuan teori tetapi juga melanjutkannya dengan kejayaan mengira pangkat untuk kes di mana saiz set latar belakang ialah lima, satu hasil yang tidak dicapai secara teori dalam kajian ini..

REACTION SYSTEM RANKS FOR UNION-ADDITIVE FUNCTIONS UNDER VARIOUS RESOURCE CONSTRAINTS AND THEIR HIERARCHICAL ANALYSIS

ABSTRACT

Reaction systems, introduced nearly two decades ago by Ehrenfeucht and Rozenberg, are a robust modeling framework inspired by the complex chemical interactions within living cells. A key aspect of reaction systems is the associated *rs* function, which describes the transition of states in an interactive process. Mathematical studies of *rs* functions have garnered significant interest, particularly focusing on functions specified by minimal reaction systems. The concept of reaction system rank is evolving as a significant research topic; it measures the complexity of an *rs* function based on the smallest set of reactions that can specify it. This work studies the reaction system ranks of functions belonging to the class of union-additive *rs* functions, $\mathcal{F}_U(S)$, introduced by Salomaa. This class is especially interesting because each function is entirely determined by the images of singletons and can be specified by a minimal reaction system. This study introduces the notions of characteristic set and signature size for systematic investigation. Specifically, this study determines the ranks across various signature sizes, establishing a constant rank for signature size one, revealing a dependency on the sizes of the sets in characteristic sets for size two, and providing lower and upper bounds for size three and for one-to-one signatures. Alongside this investigation, this thesis introduces and analyzes three novel concepts: minimal reaction system rank, for which a general formula is established for all functions in $\mathcal{F}_U(S)$; almost minimal reaction system rank, which is explored for specific signature sizes; and a new hierarchy, $\mathcal{RS}^*(m,n)$, where it is established that functions with signature sizes up to $k \leq 3$ strictly fall into the class $\mathcal{RS}^*(k,1)$ and not into the subclass $\mathcal{RS}^*(k-1,1)$. Finally, this thesis addresses the computational aspects of the problem. Python programs were developed to verify whether a given reaction system specifies a function in $\mathcal{F}_U(S)$ and to determine the *rs* rank for functions in this class with one-to-one signatures. This computational approach not only confirmed theoretical findings but also extended them

by successfully computing the rank for the case where the background set size is five, a result not achieved theoretically in this study.

CHAPTER 1

INTRODUCTION

1.1 Introduction

This chapter lays the foundation of this study by introducing the key concepts of reaction systems and providing the necessary background for this thesis. It begins by defining the terms and concepts relevant to this study, followed by a detailed discussion of the motivation for studying reaction system ranks and identifying gaps in the existing research. The chapter also presents the problem statements and outlines the primary research objectives. Lastly, it concludes with a summary of the thesis organization, offering a road map for the following chapters.

1.2 Background Studies

Imagine living cells as tiny biochemical factories, tirelessly transforming substances through a series of chemical reactions. These transformations are primarily governed by two key regulatory mechanisms: *facilitation* and *inhibition*, which control the interactions between biochemical reactions. Understanding these interactions is crucial, as they dictate various cellular functionalities, a topic that has been extensively studied over the years (see, for example, (Kitano, 2001; Păun, 2012; Schnell, 2006; Zenil, 2013)). Inspired by these natural regulatory processes, Ehrenfeucht and Rozenberg (2007) introduced *reaction systems*, a qualitative framework designed to model and analyze the complex biochemical interactions that regulate the behavior of living cells. In essence, a reaction system includes a set of entities and reactions that modulate how reactants are turned into products, depending on the presence or absence of certain factors.

To lay the groundwork for the concepts central to this thesis, the following section introduces key definitions and terminology related to reaction systems. A more detailed discussion of these concepts, along with their relevance in existing research, will be

provided in Chapter 2. These definitions aim to familiarize readers with the fundamental terms and framework for understanding the research problems and objectives.

1.2.1 Key Definitions and Terminology

Definition 1.1. *(Ehrenfeucht & Rozenberg, 2007) A* reaction *a in a nonempty finite set S, referred to as the* background set*, is an ordered triple* (R_a, I_a, P_a) *of subsets of S. The sets* R_a*,* I_a*, and* P_a *are referred to as the* reactant set*, the* inhibitor set*, and the* product set*, respectively. The sets* R_a *and* I_a *are disjoint (possibly empty), whereas* P_a *is a nonempty subset of S. The entities in* R_a *and* I_a *are referred to as the* resources *for the reaction a. A reaction a is said to be* enabled *by the state* $T \subseteq S$ *if* $R_a \subseteq T$ *and* $I_a \cap T = \emptyset$*.*

Definition 1.2. *(Ehrenfeucht & Rozenberg, 2007) A* reaction system over *S is formalized as an ordered pair* $\mathcal{A} = (S, A)$ *where A is a collection of reactions in S. A reaction system* $\mathcal{A} = (S, A)$ *is referred to as* nondegenerate *if both the reactant set* R_a *and the inhibitor set* I_a *are nonempty for all reactions in A, whereas a reaction system A is termed* degenerate *if the reactant set or the inhibitor set of any reaction in A is empty.*

Definition 1.3. *(Ehrenfeucht & Rozenberg, 2007) For any reaction system* $\mathcal{A} = (S, A)$*, the* result *function* $\mathrm{res}_{\mathcal{A}} : 2^S \to 2^S$ *defined as*

$$\mathrm{res}_{\mathcal{A}}(T) = \bigcup_{\substack{a \in A \\ R_a \subseteq T \text{ and } I_a \cap T = \emptyset}} P_a, \quad \text{for all } T \subseteq S,$$

is referred to as the function specified by $\mathcal{A}$*.*

Example 1.1. *Let* $S = \{1, 2, 3, 4, 5\}$ *and given the set of reactions:*

$$A = \big\{(\{1\}, \{2\}, \{3\}), (\{3, 4\}, \{5\}, \{4\}), (\emptyset, \{4\}, \{5\})\big\}.$$

Then $\mathcal{A} = (S, A)$ *is a reaction system. Moreover,* $\mathrm{res}_{\mathcal{A}}(\{1\}) = \{3, 5\}$*,* $\mathrm{res}_{\mathcal{A}}(\{1, 2\}) = \{5\}$*,* $\mathrm{res}_{\mathcal{A}}(\{1, 3, 4\}) = \{3, 4\}$*, and* $\mathrm{res}_{\mathcal{A}}(\{4\}) = \emptyset$*.*

Definition 1.4. *(Ehrenfeucht et al., 2012) Every power set function* $f : 2^S \to 2^S$*, where S is a finite nonempty set, is called an rs* function over *S.*

A function f is said to be specified by a reaction system $\mathcal{A} = (S, A)$ *over S if $f(T) = \mathrm{res}_{\mathcal{A}}(T)$ for all $T \subseteq S$.*

If f is specified by a nondegenerate reaction system $\mathcal{A} = (S, A)$, then $f(\emptyset) = f(S) = \emptyset$, because none of the reactions in A can be enabled by $\emptyset$ or S, as the reactant set and inhibitor set of each reaction in A are nonempty. In this case, f is termed a nondegenerate *rs* function*; otherwise, it is termed a* degenerate *rs* function*.*

An rs function f is called a null function *if and only if $f = \Phi_S$, where $\Phi_S(T) = \emptyset$ for all $T \subseteq S$.*

Definition 1.5. *(Ehrenfeucht et al., 2012; Salomaa, 2013b) Reaction systems $\mathcal{A} = (S, A)$ are categorized based on the number of resources available for each reaction. A nondegenerate reaction system is termed* minimal *if each reaction has a singleton reactant set and a singleton inhibitor set, specifically satisfying $|R_a| = 1 = |I_a|$ for all reactions $a \in A$. On the other hand, a nondegenerate reaction system is referred to as* almost minimal *if it involves up to three resources, meaning that for all reactions $a \in A$, either $1 \leq |R_a| \leq 2$ with $|I_a| = 1$, or $|R_a| = 1$ with $1 \leq |I_a| \leq 2$.*

Studies have also explored reaction systems with degeneracy due to their significance (Manzoni et al., 2014; Teh & Atanasiu, 2017b). If degeneracy is allowed in a reaction system, then the reactant set or inhibitor set of a reaction may be empty. In such cases, a minimal reaction system requires that the cardinality of each reaction's reactant and inhibitor sets be at most 1 (i.e., $|R_a| \leq 1$ and $|I_a| \leq 1$ for all $a \in A$). Similarly, an almost minimal reaction system allows up to three total resources, where for all reactions $a \in A$, either $|R_a| \leq 2$ and $|I_a| \leq 1$, or $|R_a| \leq 1$ and $|I_a| \leq 2$.

Definition 1.6. *(Manzoni et al., 2014) For all natural numbers m and n, the class $\mathcal{RS}(m, n)$ is defined as the collection of reaction systems $\mathcal{A} = (S, A)$ such that, for all $a \in A$, the reactant and inhibitor set sizes satisfy $|R_a| \leq m$ and $|I_a| \leq n$.*

A reaction system $\mathcal{A} = (S, A)$ is referred to as an (r, i) system if, for every reaction $a \in A$, the cardinalities of the reactant and inhibitor sets satisfy $|R_a| \leq r$ and $|I_a| \leq i$

(Salomaa, 2012a, 2013b). For instance, in Example 1.1, the reaction system $\mathcal{A}$ is a $(2, 1)$ system.

Thus, the class $\mathcal{RS}(1, 1)$ corresponds to the collection of all minimal reaction systems, while the union $\mathcal{RS}(1, 2) \cup \mathcal{RS}(2, 1)$ represents the collection of all almost minimal reaction systems.

Definition 1.7. *(Ehrenfeucht & Rozenberg, 2007) Two reaction systems, $\mathcal{A} = (S, A)$ and $\mathcal{B} = (S, B)$, over the same background set S, are said to be* functionally equivalent*, denoted as $\mathcal{A} \sim \mathcal{B}$, if their specified functions produce the same result for every subset $T \subseteq S$. Formally, $\mathcal{A} \sim \mathcal{B}$ if $\text{res}_{\mathcal{A}}(T) = \text{res}_{\mathcal{B}}(T)$ for all $T \subseteq S$.*

Two reaction systems over the same background set can differ significantly; for example, they may belong to different classes, contain different numbers of reactions, or have distinct reaction structures. Despite these differences, their specified functions may produce the same result for every subset of the background set. It emphasizes the importance of functional equivalence, which enables the analysis and comparison of reaction systems despite their structural differences.

Definition 1.8. *(Teh & Atanasiu, 2017a) For any rs function f over S, the reaction system rank of f is given by:*

$$\text{rsrank}(f) = \min\{\, |A| : f = \text{res}_{\mathcal{A}}, \textit{where } \mathcal{A} \textit{ is a reaction system over } S \,\}.$$

We call $\mathcal{A}$ a witness *of the reaction system rank of f if $\mathcal{A}$ specifies f and $|A| = \text{rsrank}(f)$.*

The reaction system rank is abbreviated as rsrank (or simply *rs* rank).

The Definitions 1.9 and Definition 1.10 introduce our newly proposed concepts in the mathematical study of *rs* functions: minimal *rs* rank, almost minimal *rs* rank, and the hierarchy $\mathcal{RS}^*(m, n)$ based on rank witnessing reaction systems.

Definition 1.9. *Let f be an rs* function *over S. The* minimal *rs* rank *of f, denoted* $\mathrm{minrsrank}(f)$*, and the* almost minimal *rs* rank*, denoted* $\mathrm{alminrsrank}(f)$*, are defined as:*

$$\mathrm{minrsrank}(f) = \min\{|A| : f = \mathrm{res}_{\mathcal{A}}, \mathcal{A} \text{ is minimal reaction system over } S\};$$

$$\mathrm{alminrsrank}(f) = \min\{|A| : f = \mathrm{res}_{\mathcal{A}}, \mathcal{A} \text{ is an almost minimal reaction system over } S\}.$$

If $f = \mathrm{res}_{\mathcal{A}}$ and $\mathrm{minrsrank}(f) = |A|$ *(or* $\mathrm{alminrsrank}(f) = |A|$*), then $\mathcal{A}$ is called a* witness *of the minimal (or almost minimal) rs rank of f.*

Definition 1.10. *For all natural numbers m and n, $\mathcal{RS}^*(m,n)$ is the class of rs functions f such that there exists a reaction system belonging to $\mathcal{RS}(m,n)$ witnessing the rs rank of f.*

Definition 1.11. *(Salomaa, 2014) The class $\mathcal{F}_U(S)$ consists of rs functions over S satisfying:*

1. $f(S) = f(\emptyset) = \emptyset$;
2. *The image $f(\{s\})$ is a singleton for all $s \in S$;*
3. $f(T) = \bigcup_{s \in T} f(\{s\})$*, for every nonempty $T \subsetneq S$.*

The images of singletons fully characterize each function $f \in \mathcal{F}_U(S)$, which is captured by the following definition, referred to as the *signature* of f. This concept plays a fundamental role in this thesis, and its significance will be clarified in Theorems 3.2 and 4.1.

Definition 1.12. *Let $f \in \mathcal{F}_U(S)$. The function* $\mathrm{sgn}[f] : S \to S$*, defined by*

$$\mathrm{sgn}[f](x) = y \text{ if and only if } f(\{x\}) = \{y\} \text{ for all } x, y \in S,$$

is called the signature *of f.*

The characteristic set $\mathrm{char}[f]$ *of f is defined as*

$$\mathrm{char}[f] = \left\{ \{x \in S \mid f(\{x\}) = \{s\}\} \mid s \in S \right\} \setminus \{\emptyset\}.$$

Note that $|\operatorname{char}[f]|$ equals the number of distinct images of singletons under f. Hence, the *signature size* of f refers to the cardinality of its characteristic set, $\operatorname{char}[f]$.

Clearly, $1 \leq |\operatorname{char}[f]| \leq |S|$. For any integer k with $1 \leq k \leq |S|$, we define the subclass $\mathcal{F}_U^k(S)$ as the collection of functions in $\mathcal{F}_U(S)$ with signature size k. Thus, the class $\mathcal{F}_U(S)$ can be expressed as the disjoint union of the following subclasses:

$$\mathcal{F}_U(S) = \bigcup_{k=1}^{|S|} \mathcal{F}_U^k(S).$$

Specifically, the subclass $\mathcal{F}_U^1(S)$ consists of all constant functions, and the subclass $\mathcal{F}_U^{|S|}(S)$ consists of all bijective functions, both on nonempty proper subsets of S.

Example 1.2. *Consider a function $f \in \mathcal{F}_U(S)$ with $S = \{1, 2, 3, 4, 5\}$ such that $f(\{3\}) = \{1\}$, $f(\{1\}) = \{2\} = f(\{4\})$, and $f(\{2\}) = \{4\} = f(\{5\})$. Then $\operatorname{char}[f] = \big\{\{3\}, \{1, 4\}, \{2, 5\}\big\}$ and f has a signature size of three.*

1.3 Motivation of the Study

In the dynamical process of a reaction system, the transition of states is captured by a corresponding so-called *rs function*, and the mathematical study of *rs* functions is a growing research area initiated in (Ehrenfeucht et al., 2011). Numerous studies have addressed challenging mathematical and computational problems pertaining to the dynamics of reaction systems. These include problems such as reachability (Dennunzio et al., 2019), controllability (Ivanov & Petre, 2020), fixed points and attractors (Acone et al., 2024b; Formenti et al., 2014b), and convergence (Formenti et al., 2015), with complexities ranging from NP-complete to PSPACE-hard. This work studies the various mathematical aspects of *rs* functions.

Due to simplicity, mathematical studies of *rs* functions specified by minimal reaction systems have received significant attention due to their well-defined algebraic characterization (Ehrenfeucht et al., 2012; Farrell et al., 2024; Salomaa, 2013b, 2017). Manzoni et al. (2014) and Salomaa (2015) studied the simulation of *rs* functions and

demonstrated that any *rs* function can be simulated by some minimal reaction system over an extended background set. Later, Teh and Atanasiu (2020) strengthened studies on the simulation of *rs* functions by showing that the extended background set can be fixed beforehand independent of the provided *rs* function. The study also showed that the aforementioned simulation cannot be guaranteed by extending the background set by polynomially bounded elements. On the other hand, (Salomaa, 2014; Teh, 2018) investigated the generative power under compositions of *rs* functions specified by minimal reaction systems up to the specific size of the background set. These studies have shown that minimal reaction systems are remarkably versatile, including generating *rs* functions and simulating reaction systems.

Reaction systems are considered *functionally equivalent* if the *rs* functions specified by them are identical (Ehrenfeucht & Rozenberg, 2007). This concept is essential for comparing different reaction systems to see if they can be reduced or simplified without altering their functional behavior. Due to their inherent complexity, reaction systems are often difficult to compare. In particular, determining whether two sets of reactions are functionally equivalent is not trivial, and it is shown to be Co-NP-complete in (Ehrenfeucht & Rozenberg, 2007) due to the reduction to the tautology problem for Boolean formulas. Additionally, various aspects of functional and enabling equivalences, as well as their associated partial orders, have been extensively studied (Genova et al., 2017, 2021; Kleijn et al., 2018). An important question to investigate is determining the minimal (reduced size) reaction system among functionally equivalent ones.

The aspect of minimizing reaction systems, including reducing the number of reactions and the resources involved in reactions, was explored in (Corolli et al., 2012a) using their associated Boolean functions while preserving functional behavior. Genova et al. (2020) also investigated the minimization of reaction systems through Boolean minimization techniques, such as Karnaugh maps and Boolean expressions. Furthermore, they proposed an Espresso-type algorithm that produces a functionally

equivalent reaction system with a reduced number of reactions and minimal resource usage. A distinct approach to minimizing reaction systems was examined in (Farrell et al., 2024), focusing on reducing the number of resources per reaction, referred to as the degree of the reaction system. This study applied minimization techniques to cycles within reaction systems, leveraging the fact that functions can be effectively represented using zero-context graphs, where each component of these graphs terminates in a cycle (Formenti et al., 2014a, 2014b; Genova et al., 2017).

In the theoretical study of *rs* functions, the concept of *rs* rank has emerged as a significant research topic. Independently introduced in (Teh & Atanasiu, 2017a), it quantifies the complexity of an *rs* function based on the smallest attainable cardinality of a set of reactions that specifies the function. The study established that, for any background set S, the *rs* rank of an *rs* function is tightly bounded above by $2^{|S|}$. However, for any bijective *rs* function, the maximum attainable *rs* rank is $2^{|S|} - 1$, which is also attainable. Despite these findings, determining the *rs* rank for functions specified by minimal reaction systems remains an open problem (Teh & Atanasiu, 2017b). Since each reaction system can be represented as a Boolean formula (Ehrenfeucht & Rozenberg, 2007; Genova et al., 2020), the complexity of determining the equivalence of Boolean formulas is directly related to the complexity of establishing the equivalence of reaction systems. As a result, computing the *rs* rank becomes increasingly challenging for larger background sets due to the inherent difficulty of identifying functionally equivalent reaction systems. However, by focusing on reaction systems with restricted resources, specifically those with at most one resource, referred to as *strictly minimal reaction systems*, some progress has been made in determining the *rs* ranks of functions specified by these reaction systems for specific background set sizes, leaving an open problem for larger sizes of the background set S (Teh et al., 2021).

Our study provides new insights into the mathematical study of *rs* functions, specifically those belonging to the class $\mathcal{F}_U(S)$ of union-additive functions introduced by Salomaa (2014). This class is particularly significant because every function in $\mathcal{F}_U(S)$

can be specified by a minimal reaction system. Furthermore, the composition of functions from this class can also be specified by a minimal reaction system, a property that does not hold for *rs* functions in general. Additionally, Salomaa (2014) demonstrated that three fixed members of $\mathcal{F}_U(S)$ are sufficient to express every function in the class through composition. Building on this, Teh (2018) extended these findings by incorporating degeneracy in reaction systems, showing that, over a ternary alphabet, all *rs* functions can be constructed through the composition of three fixed functions corresponding to minimal reaction systems. However, this result does not extend to quaternary alphabets.

Despite the significant contributions and unique properties of functions in the class $\mathcal{F}_U(S)$, the concept of *rs* rank for these functions has not been explored. This study addresses this gap by investigating the *rs* ranks of functions within $\mathcal{F}_U(S)$. Additionally, this thesis introduces and studies three novel concepts in the mathematical study of *rs* functions: minimal *rs* ranks, almost minimal *rs* ranks, and a hierarchy based on rank witnessing reaction systems. These concepts are specifically explored for *rs* functions from the class $\mathcal{F}_U(S)$ to provide a deeper understanding of their structural complexity and rank behavior in the context of minimal and almost minimal reaction systems.

1.4 Research Problems

The class $\mathcal{F}_U(S)$ of *rs* functions plays a significant role in reaction systems research (Salomaa, 2014; Teh, 2018). While prior studies have investigated *rs* ranks and minimization for *rs* functions (Corolli et al., 2012a; Genova et al., 2020; Teh & Atanasiu, 2017a; Teh et al., 2021), none have specifically examined the *rs* ranks of functions in $\mathcal{F}_U(S)$. This gap in the literature motivates the need for a systematic framework to study the *rs* ranks of functions within this class. The fact that functions in the subclasses $\mathcal{F}_U^k(S)$ of $\mathcal{F}_U(S)$, for a fixed signature size k where $k \neq 1$ and $k \neq |S|$, may contain distinct characteristic sets provides a richer structure for analysis, yet the relationship between these variations and the corresponding *rs* ranks remains an open area for investigation.

Minimal and almost minimal reaction systems have attracted considerable interest due to their distinct algebraic properties and their capacity for simulation and generation within reaction systems (Ehrenfeucht et al., 2012; Manzoni et al., 2014; Salomaa, 2013b, 2014, 2015, 2017; Teh, 2018; Teh & Atanasiu, 2020). This study contributes to the theoretical development of these systems by defining the concepts of minimal *rs* rank and almost minimal *rs* rank, which measure the smallest size of a reaction system among all specifying minimal and almost minimal reaction systems, respectively. Particularly, this research focuses on investigating the minimal and almost minimal ranks of functions from the class $\mathcal{F}_U(S)$ across various signature sizes, excluding one-to-one signatures, with particular emphasis on how these ranks depend on the characteristic sets of functions in this class. Additionally, this study investigates our novel new hierarchy $\mathcal{RS}^*(m,n)$ of *rs* functions based on rank witnessing reaction systems, which provides a more refined classification than the existing one based on the maximum number of resources used in specifying reaction systems introduced in (Ehrenfeucht et al., 2011). This hierarchy is particularly explored for functions within the class $\mathcal{F}_U(S)$ according to their signature sizes by leveraging minimal and almost minimal *rs* ranks.

Finally, the problem of rank determination becomes particularly acute for the specific subclass of functions in $\mathcal{F}_U(S)$ with one-to-one signatures. It is known that these functions are bijective on all nonempty proper subsets of S and that each can be specified by a minimal reaction system. While the *rs* rank of general bijective functions has been investigated (Teh & Atanasiu, 2017a), the investigation of the *rs* rank for functions specified by minimal reaction systems remains largely unexplored, except for specific background set sizes (Teh & Atanasiu, 2017b; Teh et al., 2021). This foundational gap applies directly to the newly introduced concepts of minimal *rs* rank and almost minimal *rs* rank. Consequently, determining the exact values for all three of these ranks for this subclass of functions, and analyzing how the smallest size of specifying reaction systems changes under varying resource constraints, remains an open question for investigation.

1.4.1 Research Objectives

The primary objective of this study is to explore the *rs* ranks, minimal and almost minimal *rs* ranks, and the hierarchy of *rs* functions in the class $\mathcal{F}_U(S)$. Specifically, this research aims to investigate these ranks comprehensively, analyze their relationships with characteristic sets, and establish a structured classification based on rank witnessing reaction systems. The following objectives outline the key aspects of this study.

1. To analyze the *rs* ranks of functions in $\mathcal{F}_U(S)$ across various signature sizes, excluding one-to-one signatures, with the aim of understanding the relationship between characteristic sets and *rs* ranks.

2. To establish the minimal and almost minimal *rs* ranks of functions within the class $\mathcal{F}_U(S)$ across various signature sizes, excluding one-to-one signatures, with the aim of understanding the relationship between characteristic sets and these ranks. Additionally, to examine the hierarchy of functions in $\mathcal{F}_U(S)$ based on signature sizes by utilizing these ranks.

3. To determine the *rs* rank, minimal *rs* rank, and almost minimal *rs* rank for functions in the class $\mathcal{F}_U(S)$ with one-to-one signatures, and consequently analyze how these ranks differ under resource constraints in specifying reaction systems.

1.5 Thesis Outline

The outline of the thesis is as follows. **Chapter 1** provides the foundational elements of the thesis. It begins with a review of the background studies, including the basic definitions and terminology of reaction systems. The motivation for the research is then discussed, followed by a formal statement of the research problems and the corresponding objectives. The chapter concludes with this outline of the thesis structure.

Chapter 2 explores the key concepts and properties of reaction systems. It begins with the foundational definitions of reactions, reaction systems, and the underlying model, before moving to a discussion of interactive processes and their interpretations. The chapter then examines the classification of reaction systems, with a specific focus on minimal and almost minimal reaction systems. The core theoretical concepts are then introduced, including the function specified by reaction systems, the classification theorem, the class $\mathcal{F}_U(S)$, and functional equivalence. The chapter culminates in an examination of irreducibility, minimization, and *rs* rank, covering Boolean representations and minimization techniques to establish the theoretical groundwork for the contributions of this thesis.

Chapter 3 presents the results for the first research objective, analyzing the *rs* ranks of functions within the class $\mathcal{F}_U(S)$ across various signature sizes. The chapter begins by determining the *rs* ranks for signature sizes one and two, revealing how these ranks are influenced by the sizes of the sets within the characteristic sets. The analysis is then extended to functions with signature size three, where both general lower and upper bounds are provided. Additionally, the *rs* ranks are determined for specific characteristic sets over any size of the background set S. The chapter concludes by summarizing these findings to offer insights into the relationship between *rs* ranks and the structure of characteristic sets.

Chapter 4 presents the results for the second objective of this study, focusing on the minimal *rs* rank, almost minimal *rs* rank, and the hierarchy of *rs* functions. After establishing the necessary background, motivation, and preliminary results, the chapter explores its main contributions. The investigation first focuses on the minimal *rs* ranks for functions in $\mathcal{F}_U(S)$ across various signature sizes, offering a general formula that connects these ranks to the sizes of sets in the characteristic sets. The chapter then introduces the hierarchical class $\mathcal{RS}^*(m,n)$ and covers the almost minimal *rs* ranks for functions with signature size three, with results that apply to any background set size. The chapter concludes by demonstrating how these contributions provide a more

refined framework for understanding the complexity of functions in this class.

Chapter 5 presents the results for the third objective, investigating the *rs* rank, minimal *rs* rank, and almost minimal *rs* rank for functions from the class $\mathcal{F}_U(S)$ with one-to-one signatures. The analysis begins with the *rs* rank, presenting results for specific background set sizes and establishing general lower and upper bounds. It then moves to the minimal and almost minimal *rs* ranks, providing results applicable to any size of the background set. The chapter culminates in a comparison of these three ranks under various restrictions on resources, offering insights into how their behaviors differ and summarizing the key findings of this investigation.

Chapter 6 discusses two computational approaches for functions in $\mathcal{F}_U(S)$. The first approach addresses whether a given reaction system can specify a function in this class, presenting a series of algorithms that form the foundation for the Python program in Appendix A. The second approach explores the computational determination of the *rs* rank for functions from the subclass $\mathcal{F}_U^{|S|}(S)$. For this task, the chapter details the relevant algorithms and their corresponding Python program (Appendix B), which is then used to determine the *rs* ranks for a background set with five elements, a result that was previously unobtainable by purely theoretical means. The chapter concludes by demonstrating the power of these computational methods to solve problems that are otherwise intractable.

Finally, **Chapter 7** concludes this thesis by summarizing the key contributions and findings of this work. It reiterates the novel concepts introduced, such as minimal *rs* ranks, almost minimal *rs* ranks, and the hierarchical class $\mathcal{RS}^*(m,n)$, and emphasizes their significance in advancing the mathematical study of reaction systems, particularly for functions in the class $\mathcal{F}_U(S)$. The thesis closes by presenting several open problems that arose from this study, offering potential directions for future research in this domain.

CHAPTER 2

PRELIMINARIES

2.1 Introduction

This chapter provides a comprehensive review of reaction systems and their associated functions, laying the groundwork for this study. It begins by introducing fundamental concepts related to reactions, reaction systems, and their underlying assumptions, including the threshold and non-permanency assumptions, before extending the discussion to interactive processes within reaction systems, emphasizing their interpretations and functional behavior. The chapter then explores functions characterized by reaction systems, with a particular focus on the classification of reaction systems and functions specified by minimal reaction systems. A detailed discussion follows on the special class $\mathcal{F}_U(S)$, which plays a central role in this study. Additionally, key concepts such as functional equivalence, irreducibility, minimization, and *rs* ranks are reviewed to highlight their significance in characterizing reaction systems. Lastly, this chapter presents our contributions to *rs* ranks, minimal *rs* ranks, almost minimal *rs* ranks, and the hierarchy of functions in the class $\mathcal{F}_U(S)$, and it concludes by identifying existing challenges and open problems in reaction systems research, providing a foundation for the subsequent development of the study.

2.2 Reactions, Reaction Systems, and Interactive Processes

2.2.1 Reactions

Living cells undergo biochemical reactions that result in the production of biochemical products if all the necessary reactants are present and there are no inhibiting entities to prevent the production of the products. As previously defined in Definition 1.1, a reaction in a finite nonempty set S is formally represented as a triple $a = (R_a, I_a, P_a)$ of finite sets, where R_a is the reactant set, I_a is the inhibitor set, and P_a is the product set. The sets R_a and I_a are disjoint subsets of S, while P_a is a nonempty subset of S.

When the conditions favor a reaction to occur, it transforms the reactants into products, and the result of a reaction a on a subset $T \subseteq S$, denoted $\mathrm{res}_a(T)$, is formally defined in (Ehrenfeucht & Rozenberg, 2007) as follows:

$$\mathrm{res}_a(T) = \begin{cases} P_a, & \text{if } R_a \subseteq T \text{ and } I_a \cap T = \emptyset, \\ \emptyset, & \text{otherwise.} \end{cases}$$

A reaction a occurs in a state $T \subseteq S$, or is enabled by T, if $R_a \subseteq T$ and $I_a \cap T = \emptyset$, denoted $\mathrm{ena}_a(T)$. Otherwise, a is not enabled by T. When a is enabled, the outcome is given by the *result function* $\mathrm{res}_a : 2^S \to 2^S$, which maps T to the product set P_a, i.e., $\mathrm{res}_a(T) = P_a$. If a is not enabled, then $\mathrm{res}_a(T) = \emptyset$.

Remark 2.1. *In this chapter, there is no restriction on the reactant and inhibitor sets of a reaction being nonempty throughout the discussion. This condition was originally imposed in the definition of reaction systems due to biological motivations. However, more recently, reactions that do not adhere to this restriction have been explored, particularly in mathematically oriented studies (see, e.g., Manzoni et al., 2014; Teh and Atanasiu, 2017a; Teh et al., 2021).*

Recall that the elements of the set $R_a \cup I_a$ are referred to as the resources of a, denoted by M_a. If both R_a and I_a are nonempty, then $|M_a| \geq 2$. On the other hand, if $R_a = I_a = \emptyset$, then $|M_a| = 0$.

The following examples are now discussed, including a biological example of a reaction.

Example 2.1. *Suppose* $S = \{1, 2, 3, 4\}$. *Then* $a = (\{1, 2\}, \{4\}, \{1, 3\})$ *is a reaction in* S *where* $R_a = \{1, 2\}$, $I_a = \{4\}$, $P_a = \{1, 3\}$, *and* $M_a = \{1, 2, 4\}$. *Moreover, for a selection of subsets* $T \subseteq S$, *the following table illustrates the behavior of reaction* a*:*

Table 2.1: Reaction: res_a, ena_a

T	$\{1,2,3\}$	$\{1,2,4\}$	$\{1,2\}$	$\{3\}$	$\{4\}$
$\text{ena}_a(T)$	yes	no	yes	no	no
$\text{res}_a(T)$	$\{1,3\}$	$\emptyset$	$\{1,3\}$	$\emptyset$	$\emptyset$

Example 2.2. *In E. coli cells, the metabolism of lactose is controlled by the expression of a specific set of genes in a complex genetic regulatory system. The reaction system modeling this regulatory process is discussed in (Ehrenfeucht & Rozenberg, 2007). One of the key reactions in this system determines whether the gene is expressed, enabling lactose digestion.*

The biochemical environment in which the reaction occurs involves the following molecular entities: lac (lactose), cAMP-CAP, I-OP, Z, Y, and A. If the reactants lac and cAMP-CAP are present and the inhibitor I-OP is absent, then Z, Y, and A are produced, allowing gene expression for lactose digestion.

To model this reaction, let $S = \{lac, cAMP\text{-}CAP, I\text{-}OP, Z, Y, A\}$ *and define the reaction as:*

$$a = (\{lac, cAMP\text{-}CAP\}, \{I\text{-}OP\}, \{Z, Y, A\}).$$

For any state $T \subseteq S$*, the result of the reaction is given by:*

$$res_a(T) = \begin{cases} \{Z, Y, A\}, & \text{if } a \text{ is enabled by } T, \\ \emptyset, & \text{otherwise.} \end{cases}$$

2.2.2 Reaction Systems

Over the past few decades, exploring the functionality of living cells has been a prominent research topic; see, for example, (Bower & Bolouri, 2004; Kitano, 2001; Păun, 2005; Zenil, 2013). The primary determinant of these functionalities is the in-

teraction between biochemical reactions, making their understanding crucial. Reaction systems, first introduced in (Ehrenfeucht & Rozenberg, 2007), provide a qualitative framework for modeling these interactions, based on two key regulatory mechanisms within a cell: facilitation and inhibition. Recall from Definition 1.2 that a reaction system over S is formally defined as a pair $\mathcal{A} = (S, A)$, where S is a finite set, and A is a (possibly empty) set of reactions in S.

The set S is called the background set of $\mathcal{A}$, and its elements are referred to as entities. The subsets of S are known as the states of $\mathcal{A}$. Since S is finite, the set of reactions A is also finite, and consequently, each state of $\mathcal{A}$ is finite as well.

As discussed earlier, if a reaction a in S is enabled by a state $T \subseteq S$, then $\text{res}_a(T) = P_a$. In the context of a reaction system $\mathcal{A} = (S, A)$, the result function $\text{res}_{\mathcal{A}} : 2^S \to 2^S$ (see Definition 1.3) is cumulative on a state $T \subseteq S$. It is defined as the union of the results of all reactions $a \in A$ that are enabled by T, formally, $\text{res}_{\mathcal{A}}(T) = \bigcup\{\text{res}_a(T) \mid a \in A \text{ and } \text{ena}_a(T)\}$.

Note that if no reaction $a \in A$ is enabled by T, the result of the reaction system is the empty set, i.e., $\text{res}_{\mathcal{A}}(T) = \emptyset$. The result function $\text{res}_{\mathcal{A}} : 2^S \to 2^S$ acts as a state transition function, mapping the current state $T \subseteq S$ to its successor state $\text{res}_{\mathcal{A}}(T)$.

When S is understood, we may identify $\mathcal{A}$ with A and use res_A to denote $\text{res}_{\mathcal{A}}$.

Example 2.3. *Suppose* $S = \{a, b, c\}$. *Let*

$$A = \{(\{a\}, \{b\}, \{a, b\}), (\{a\}, \{b, c\}, \{c\}), (\{a, b\}, \emptyset, \{b, c\}), (\emptyset, \{b, c\}, \{c\})\}.$$

Then $\mathcal{A} = (S, A)$ *is a reaction system in* S. *If* $T = \{a, b\}$ *is a state of* S, *then the only reaction in* A *that is enabled by* T *is* $(\{a, b\}, \emptyset, \{b, c\})$. *Thus,* $\text{res}_A(T) = \{b, c\}$.

The following definition introduces a specific type of reaction system, as formalized by Salomaa (2012a).

Definition 2.1. *Let $\mathcal{A} = (S, A)$ be a reaction system. A reaction $a \in A$ is called* maximally inhibited *if its inhibitor set satisfies $I_a = S \setminus R_a$. A reaction system $\mathcal{A}$ is said to be* maximally inhibited *if every reaction $a \in A$ satisfies $I_a = S \setminus R_a$.*

Example 2.4. *Suppose $S = \{a, b, c\}$. Let*

$$A = \{(\{a\}, \{b, c\}, \{c\}), (\{a, b\}, \{c\}, \{b, c\}), (\emptyset, \{a, b, c\}, \{c\})\}.$$

Then $\mathcal{A} = (S, A)$ is a maximally inhibited reaction system since, for every reaction $a \in A$, the inhibitor set satisfies $I_a = S \setminus R_a$.

2.2.3 Assumptions of Reaction System Model

The reaction system model outlined in (Ehrenfeucht & Rozenberg, 2007) is based on fundamental assumptions that provide an abstraction of biochemical processes while preserving key biological principles. These assumptions are generally valid for most biological reactions and form the foundation of the model. Notably, they distinguish reaction systems from standard models of concurrent systems, such as Petri nets (e.g., see (Reisig, 2016)), which model conflicts arising from concurrent interactions.

The reaction system framework is based on two main assumptions, outlined as follows:

The Threshold Assumption

The *threshold assumption* states that if a resource is present in a state $T \subseteq S$, it is available in sufficient quantity to enable all reactions requiring it. The model does not consider concentrations or quantitative variations; instead, resource availability is treated as a *binary condition*, ensuring that any present resource is adequate for all relevant reactions. This assumption simplifies the analysis of reaction systems by focusing on *qualitative availability* rather than *quantitative measures*.

An illustration of this assumption appears in Example 2.2, which describes a biological mechanism involving lactose in a living cell. The example considers only

the *presence or absence* of lactose, rather than its molecular quantity, reflecting the *threshold assumption's qualitative approach* to resource availability.

The Non-Permanency Assumption

The *non-permanency assumption* is the principle that formalizes the dynamic turnover of entities in biochemical systems. It establishes that entities do not persist by default; their presence in a subsequent state must be actively justified. Formally, this means that for any entity x present in a state T, it remains in the next state T' if and only if it is produced by an enabled reaction (that is, $x \in \mathrm{res}_A(T)$) or it is provided by the environment (the external inputs). Therefore, any entity not regenerated by a reaction or supplied by the environment will not persist. This principle aligns with the transient nature of molecular components in living cells, where stability depends on continuous synthesis or replenishment.

For instance, in Example 2.2, lactose acts as a reactant in certain reactions. These reactions convert lactose into products, and it will persist in the system only if it appears in the product set of enabled reactions. This illustrates the non-permanency assumption, where entities are retained only if they are actively regenerated or externally sustained.

The non-permanency assumption establishes that once the enabled reactions in a reaction system transform reactants into products, a new state, $\mathrm{res}_A(T)$, is generated. This new state defines the biochemical environment, consisting solely of entities produced by the enabled reactions. As emphasized in (Ehrenfeucht & Rozenberg, 2007), reactions serve as the fundamental components of the system, while structures are considered secondary.

In this framework, reactions do not merely modify existing states; they construct new states based on the dynamics of facilitation and inhibition. As a result, any entity or structure unrelated to the enabled reactions is not carried forward into the new state. This characteristic distinguishes reaction systems from traditional models, where structural components or state elements may persist independently of active processes. Thus,

reaction systems prioritize dynamic interactions over static configurations, capturing the transient and process-driven nature of biochemical systems.

2.2.4 Interactive Processes in Reaction Systems

To fully understand how a system functions, it is essential to examine how its reactions interact and the outcomes they produce. In the reaction systems framework, *interactive processes* serve as key tools for this understanding. This concept was originally introduced in (Ehrenfeucht & Rozenberg, 2007).

The following definition formalizes an interactive process for a given number of steps, n, wherein the system's evolution depends on contextual inputs at each step. Consequently, the resulting sequence of states is not necessarily periodic, even over prolonged execution. Furthermore, since the iterative procedure may proceed indefinitely, the standard definition, irrespective of contextual considerations, does not impose an upper bound on the number of steps, n.

Definition 2.2. *Let $\mathcal{A} = (S, A)$ be a reaction system. For some integer $n \geq 1$, an (n-step) interactive process in $\mathcal{A}$ is a pair $\pi = (\gamma, \delta)$ of finite sequences such that $\gamma = C_0, \ldots, C_n$ and $\delta = D_0, \ldots, D_n$, where $C_0, \ldots, C_n, D_0, \ldots, D_n \subseteq S$, $D_0 = \emptyset$, and $D_i = \mathrm{res}_A(D_{i-1} \cup C_{i-1})$ for all $i \in \{1, \ldots, n\}$.*

The sequence γ is called the context sequence of π, the sequence δ is the result sequence of π, and the sequence $\tau = W_0, \ldots, W_n$ such that $W_0 = C_0$ and $W_i = C_i \cup D_i$ for all $i \in \{1, \ldots, n\}$ is referred to as the state sequence of π, where W_0 is the initial state of π.

The interactive process π begins at the initial state W_0. The reactions from A, enabled by W_0, produce the result D_1, which, together with the context C_1, forms the state $W_1 = D_1 \cup C_1$. The state sequence τ is generated through the iteration of this procedure: for each state W_i with $i \in \{0, \ldots, n-1\}$, its successor is defined as:

$$W_{i+1} = D_{i+1} \cup C_{i+1}, \text{ where } D_{i+1} = \mathrm{res}_A(W_i).$$

In Figure 2.1, this process is illustrated.

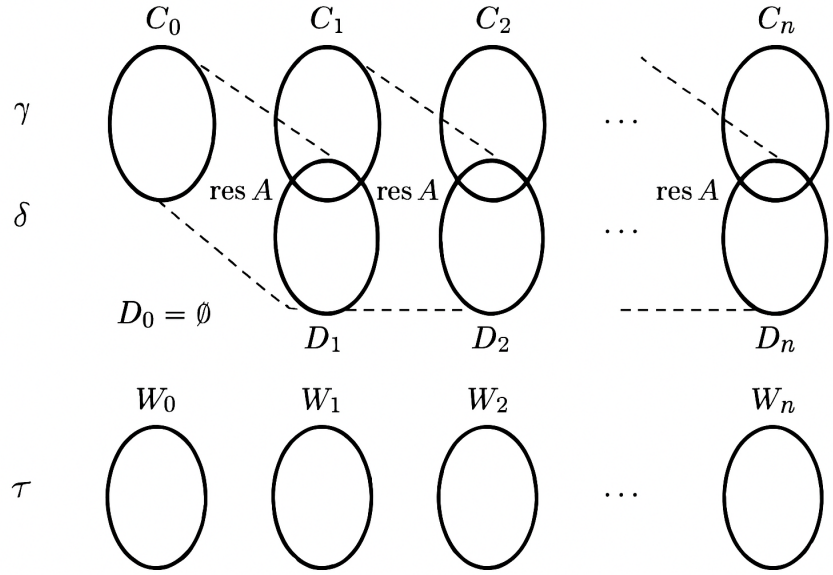

Figure 2.1: Interactive Process in Reaction Systems

The context sequence γ formalizes the idea that the living cell is an open system, meaning it interacts with its environment, that is, with the larger system.

The first element C_0 in the context sequence represents the initial state, while the remaining elements $C_1, \ldots, C_n$ are referred to as the proper context. If the current proper context set C_i is contained in D_i (i.e., $C_i \subseteq D_i$), then this context does not impact the current state W_i. This is because all entities in C_i are already accounted for by the system's reactions, as $D_i = \mathrm{res}_A(D_{i-1})$. Therefore, the sequence $C_1 - D_1, \ldots, C_n - D_n$ is defined as the significant context sequence. In practice, to calculate the result sequence and the state sequence, one can replace the proper context sequence with the significant context sequence.

An interactive process π is said to be context-independent *if its significant context sequence, $C_1 - D_1, \ldots, C_n - D_n$, contains only empty sets. In other words, at every step of the process, the environment does not contribute any new information beyond what is already generated internally by the system itself. Formally, this is captured by the condition $C_i \subseteq D_i$ for all $i > 0$, indicating that the external context C_i is entirely*

subsumed by the system's own output D_i from the previous state. If π is such a process and

$$\tau = W_0, \ldots, W_i, W_{i+1}, \ldots, W_n$$

is the state sequence, then during the transition from W_i to W_{i+1}, all elements in $W_i - \mathrm{res}_A(W_i)$ disappear (they are no longer present in W_{i+1}). This demonstrates the non-permanency property of reaction systems discussed earlier. For a general (not necessarily context-independent) interactive process, the non-permanency property states that, as the system transitions from W_i to W_{i+1}, an entity $x \in W_i$ will disappear (i.e., not appear in W_{i+1}) unless it is produced by the system ($x \in \mathrm{res}_A(W_i)$) or is introduced by the context ($x \in C_{i+1}$).

An interpretation of interactive processes in reaction systems is often illustrated through biochemical systems. For example, the eukaryotic heat shock response in cells is frequently conceptualized as an interactive process (see (Azimi et al., 2014)). The reaction system modeling the heat shock response within a cell operates as part of a larger system encompassing the entire organism and its environment. This broader system interacts with the reaction system by modulating heat stress by introducing or alleviating it through the context sequence. This provides a foundational framework for understanding interactive processes.

An alternative interpretation, discussed in (Ehrenfeucht & Rozenberg, 2007), posits that the result sequence encapsulates our knowledge of the modeled system, whereas the state sequence captures the observed behaviors of the system. Each observation facilitates the prediction of subsequent system states, offering a dynamic and iterative perspective on system analysis. Furthermore, as elaborated in (Ehrenfeucht & Rozenberg, 2007), interactive processes can also be examined through the lens of transition systems, such as finite automata, which can be associated with reaction systems.

We now present an example, adapted from Brijder et al. (2011), to illustrate context-independent interactive processes in reaction systems.

Example 2.5. *Consider the reaction system $\mathcal{A} = (\{a, b, c, d\}, A)$, where the set of reactions A is defined as follows:*

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

Then the sequence $\tau = \{\{a, b, d\}, \{a, b, c\}, \emptyset\}$ is a context-independent state sequence of $\mathcal{A}$. This is because, at the first step,

$$D_1 = \mathrm{res}_A(D_0 \cup C_0) = \mathrm{res}_A(W_0) = \mathrm{res}_A(\{a, b, d\}) = \{a, b, c\},$$

which implies that $C_1 = \emptyset$, as no additional entities from the context are required. Similarly, at the next step,

$$D_2 = \mathrm{res}_A(D_1 \cup C_1) = \mathrm{res}_A(\{a, b, c\}) = \emptyset,$$

which again implies $C_2 = \emptyset$.

The following example, adapted from (Kleijn et al., 2018), illustrates a context-dependent interactive process in a reaction system, starting from the initial state $\{d\}$, where the entities c and d are not produced by the system itself but are instead supplied by the environment as context.

Example 2.6. *Consider a reaction system $\mathcal{A} = (S, A)$ over the background set $S = \{a, b, c, d\}$ and the set of reactions A as:*

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

In Table 2.2, we demonstrate the interactive process of A, where the entities c and d are not produced by the system itself but are instead provided by the environment as a context.

Table 2.2: Interactive Process in the Reaction System with a Context-Dependent Sequence

γ	$\{d\}$	$\{d\}$	$\{c\}$	$\{d\}$
δ	$\emptyset$	$\{a\}$	$\{a, b\}$	$\{a\}$
τ	$\{d\}$	$\{a, d\}$	$\{a, b, c\}$	$\{a, d\}$

The following biological example demonstrates how genetic regulatory networks can be modeled using reaction systems, as outlined in (De Jong, 2002). It illustrates the construction of complex reaction systems from individual components, providing a foundation for understanding intricate biological processes.

Example 2.7. *Genetic regulatory networks play a crucial role in understanding cellular functions, as they regulate gene expression through interactions among genes and proteins. Consider a simplified genetic regulatory network consisting of three genes, x, y, and z, which express proteins P_1, P_2, and P_3, respectively. These genes and proteins interact dynamically to regulate gene expression.*

Protein P_1 interacts with another protein P_4 to form a complex C_1. Protein P_1 inhibits the expression of gene z, while proteins P_2 or P_3 inhibit the expression of gene x. Additionally, the protein complex C_1 inhibits the expression of gene y.

These interactions can be modeled using reaction systems, where the following sets of reactions define the expression of each gene and the formation of the protein complex:

$$A_x = \{(\{x\}, I_x, \{x\}), (\{x\}, \{P_2, P_3\}, \{x'\}), (\{x, x'\}, I_{expr1}, \{P_1\})\},$$
$$A_y = \{(\{y\}, I_y, \{y\}), (\{y\}, \{C_1\}, \{y'\}), (\{y, y'\}, I_{expr2}, \{P_2\})\},$$
$$A_z = \{(\{z\}, I_z, \{z\}), (\{z\}, \{P_1\}, \{z'\}), (\{z, z'\}, I_{expr3}, \{P_3\})\},$$
$$A_{C_1} = \{(\{P_1, P_4\}, I_{C_1}, \{C_1\})\}.$$