A Categorial Approach to Reaction Systems: First Steps

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Abstract

In the literature, one encounters the intensely studied classical set-based reaction systems and the more recently introduced generalization to graph-based reaction systems where the considered graphs are directed, simple, and edge-labeled. In this paper, we propose a categorical approach to reaction systems so that a wider spectrum of data structures becomes available on which reaction systems can be based including various types of graphs and of graph-like structures like unlabeled graphs, vertex-labeled graphs, bipartite graphs, and a variety of types of hypergraphs. But also algebraic structures like monoids fit into the framework.

Keywords: category theory, reaction systems

1. Introduction

In 2007, the seminal concept of set-based reaction systems was introduced by Ehrenfeucht and Rozenberg in [1]. The original motivation was to provide a formal framework for the modeling of (a large number of) biochemical processes taking place in the living cell. Since then the framework has been intensely studied (see, e.g., [2][3][4][5][6][7]), and reaction systems turned out to be a novel paradigm of interactive and (massively) parallel computation suitable for modeling information processing in various fields beyond biochemistry. A set-based reaction system consists of a finite background set \( B \) and a set of reactions \( A \) each of which is a triple of subsets of \( B \) called reactant, inhibitor and product respectively. A reaction is enabled on a state (being a subset of \( B \)) if the reactant is inside the state and the inhibitor outside. All enabled reactions of \( A \) are applied to some state in parallel yielding the union of all their products as results. Starting from initial states, the iterated applications of enabled reactions of \( A \) define the dynamic semantics of a reaction system where, before each step, a context set can be added to the current state making the processes interactive in this way.

Kreowski and Rozenberg introduced in [8][9] graph-based reaction systems where the considered graphs are directed, simple, and edge-labeled. In both
papers various examples are discussed among them an approximation of the
Sierpinski triangle, cellular automata, and two shortest-path algorithms. Looking
at them, one can imagine that this type of graphs is not the only one of interest. The approximation of the Sierpinski triangle and cellular automata can
be based on hypergraphs in a natural way, too. For the two shortest-path al-

gorithms, directed simple edge-labeled graphs are well suited. But if one would
like to model other graph algorithms by reaction systems, then other types of
graphs like undirected graphs, graphs with multiple edges, vertex-labeled
graphs, or unlabeled graphs may be more appropriate. And there may be many
further structures on which reaction systems can be based in a meaningful way.
When the same kind of constructs and constructions can be considered for a
spectrum of underlying structures, it may be worthwhile to come up with a
categorical framework. In this way, the notions of interest can be defined once
and for all and then used whenever certain structures form a category fitting
into the framework.

In this paper, we propose a categorical approach to reaction systems so
that a wider spectrum of data structures becomes available on which reaction
systems can be based including, in particular, various types of graphs and of
graph-like structures. The categorical framework is tailored in such a way that
reaction systems over categories can be defined in close analogy to the set- and

graph-based cases. The basic ideas are explained at the beginning of the next
section in detail.

The paper is organized as follows. Section 2 provides the categorial frame-
work. In Section 3, we introduce reaction systems over categories exemplifying
the conception by sample reaction systems over the categories of hypergraphs
and monoids. In Section 4 and 5 we demonstrate that set-based and graph-
based reaction systems can be transformed into reaction systems over the cat-
egories of sets and graphs, respectively. We show that the transformations
preserve the semantics so that set-based and graph-based reaction systems fit
fully into the categorical framework. In Section 6 we take a further look at the
categorical framework by relating the concepts presented in Section 3 to other
concepts from category theory. Section 7 concludes the paper.

2. The categorial framework

In this section, we introduce the categorial notions and notations as far as
they are needed to define reaction systems over categories.

The ingredients of classical set-based reaction systems are finite sets, subsets
including the empty set, subset inclusions, the intersections of two subsets,
and the unions of finite numbers of subsets. Similarly, graph-based reaction
systems are defined by means of finite graphs, subgraphs including the empty
graph, subgraph inclusions, the intersections of two subgraphs, and the unions
of finite numbers of subgraphs. Aiming at a generalization of set- and graph-
based reaction systems to reaction systems over a suitable kind of categories,
one needs appropriate categorial counterparts. The problem is that objects in
categories are atomic and do not have any internal structure (there is nothing
like elements). If one wants to define objects with special properties or special operations on objects, then one must characterize them by their relations to other objects using morphisms.

With respect to sets, a subset of a set $B$ can be characterized by the set of injective mappings into $B$ with the same image and $B$ is finite if it has only a finite number of subsets. The empty set has only itself as subset, the intersection of two subsets of $B$ is the largest subset of $B$ that is included into each of the given subsets, and the union of a finite number of subsets of $B$ is the smallest subset of $B$ that contains all the given subsets. All these characterizations carry over to graphs. The introduced categorical framework is based on these observations providing categorical notions that correspond to these characterizations. Table 1 lists the categorial concepts used in this paper in synopsis with the corresponding set and graph concepts.

We introduce the categorical framework in three steps. In 2.1, categories, subobjects and finite objects are defined. This allows to introduce reaction systems over a category with finite background objects, states, and reactions in Section 3. In 2.2, intersection of two subobjects and empty subobjects are defined. This allows to specify whether a reaction is enabled on a state or not, and the result of the application of a single reaction to a state. In 2.3, the union of a finite number of subobjects is defined so that the result of the application of a finite set of reactions on a state can be introduced in Section 3. Based on the notion of results, the interactive-process semantics of reaction systems over categories is given there.

For all the introduced concepts, we list several useful properties. Some of them are just stated as facts if they are easy to prove or standard results in category theory. Other statements are proved by providing the basic arguments. Moreover, we discuss a variety of categories that fit into the introduced framework.

For further categorial notions and notations we refer to [10, 11, 12] and for a comprehensive introduction into category theory see, e.g., [13].

### 2.1. Categories, subobjects, and finite objects

A category $\mathbf{C} = (\text{Ob}_C, \text{Mor}_C, \circ, 1)$ consists of a class of objects $\text{Ob}_C$, a set of morphisms $\text{Mor}_C(A, B)$ for each pair of objects $A, B \in \text{Ob}_C$, an associative
Monomorphisms are closed under composition, i.e., a composition operation \( \circ : \text{Mor}_C(B, C) \times \text{Mor}_C(A, B) \rightarrow \text{Mor}_C(A, C) \) for each triple of objects \( A, B, C \in \text{Ob}_C \), and, an identity morphism \( 1_A \in \text{Mor}_C(A, A) \) for each object \( A \in \text{Ob}_C \) such that \( f \circ 1_A = f \) and \( 1_B \circ f = f \) for each \( f \in \text{Mor}_C(A, B) \) holds.

We may write \( f : A \rightarrow B \) or \( A \xrightarrow{f} B \) for \( f \in \text{Mor}_C(A, B) \) and \( A \xrightarrow{k} B \) for pairs of morphisms with same domain and codomain. Let \( f : A \rightarrow B \) and \( g : B \rightarrow C \). We may write \( A \xrightarrow{f} B \xrightarrow{g} C \) instead of \( g \circ f \).

A morphism \( f : A \rightarrow B \) is a monomorphism if, for all pairs \( C \xrightarrow{i} A \) of morphisms, \( f \circ h = f \circ k \) implies \( h = k \).

A morphism \( f : A \rightarrow B \) is an isomorphism if there exists an inverse morphism \( f^{-1} : B \rightarrow A \) with \( f^{-1} \circ f = 1_A \) and \( f \circ f^{-1} = 1_B \). Two objects \( A, B \) are isomorphic, denoted \( A \cong B \), if there is an isomorphism \( f : A \rightarrow B \).

Monomorphisms and isomorphisms have some well-known properties that are easy to prove, but very useful.

Properties 1.

1. Monomorphisms are closed under composition, i.e., a composition \( g \circ f \) of monomorphisms \( f : A \rightarrow B \) and \( g : B \rightarrow C \) is a monomorphism.
2. If the composition \( g \circ f \) of \( f : A \rightarrow B \) and \( g : B \rightarrow C \) is a monomorphism, then \( f \) is a monomorphism.
3. Each isomorphism is a monomorphism.
4. The inverse morphism of an isomorphism is unique and an isomorphism.
5. Isomorphisms are closed under composition.
6. Each identity is an isomorphism with itself as inverse morphism.
7. Given a category \( C \), the restriction of each set \( \text{Mor}_C(A, B) \) to its monomorphisms yields a subcategory of \( C \), denoted by \( C_{\text{mono}} \).

A subobject of \( B \) for some \( B \in \text{Ob}_C \) is an equivalence class of the following equivalence of monomorphisms with codomain \( B \): Two monomorphisms \( m_1 : A_1 \rightarrow B, m_2 : A_2 \rightarrow B \) are equivalent, denoted by \( m_1 \cong m_2 \), if there is an isomorphism \( i : A_1 \rightarrow A_2 \) such that \( m_1 = m_2 \circ i \).

To deal with subobjects, we use their elements as representatives. This does not cause any problem because most categorial concepts and constructions are unique up to isomorphism.

Given subobjects \( p_1 : P_1 \rightarrow B \) and \( p_2 : P_2 \rightarrow B \), a monomorphism \( m : P_1 \rightarrow P_2 \) is a subobject inclusion from \( p_1 \) to \( p_2 \) if \( p_1 = p_2 \circ m \). The subobjects of some object \( B \) as objects and the subobject inclusions form a category denoted by \( \text{Sub}(B, C) \). Note that a subobject inclusion \( m : P_1 \rightarrow P_2 \) from \( p_1 : P_1 \rightarrow B \) to \( p_2 : P_2 \rightarrow B \) is unique as \( p_2 \) is a monomorphism. Therefore, the category \( \text{Sub}(B, C) \) is a preorder with respect to subobject inclusion as order relation like the set of subsets of a set, and we may write \( p_1 \subseteq p_2 \).

An object is finite if its set of subobjects is finite.

Example 1. The most frequently used category is the category of sets, denoted by \( \text{Sets} \), with sets as objects and mappings as morphisms. The composition is
given by the usual sequential composition \( g \circ f : A \to C \) of mappings \( g : B \to C \) and \( f : A \to B \) with \( g \circ f(x) = g(f(x)) \) for all \( x \in A \). The identities are the identity mappings, i.e., \( 1_A : A \to A \) with \( 1_A(x) = x \) for all \( x \in A \) and all sets \( A \).

The monomorphisms in \textbf{Sets} are the injective mappings. The isomorphisms are the bijective mappings. A subobject of a set \( B \) consists of all injective mappings with the same image in \( B \) and it is uniquely represented by the inclusion of this image and the image itself. Therefore, there is a one-to-one-correspondence between the categorial subobjects of a set and its subsets so that subobjects of sets can be handled as subsets (where their inclusions define the corresponding subobject uniquely). Consequently, the finite objects in \textbf{Sets} are the finite sets.

There are various categories that can be derived from \textbf{Sets} in such a way that they inherit the concepts of composition, monomorphisms, isomorphisms, subobjects, subobject inclusion, and finiteness from \textbf{Sets}. In the context of this paper, the following examples are interesting.

1. The product category \textbf{Sets} \times \textbf{Sets}: Its objects are ordered pairs \((A,B)\) of sets and the morphisms are respective pairs of mappings \((f : A \to A', g : B \to B')\).

2. The category \( \Sigma\)-\textbf{Sets} of \( \Sigma \)-labeled sets for some alphabet (finite set) \( \Sigma \): Its objects are mappings \( h : A \to \Sigma \) for some set \( A \) and the morphisms from \( h : A \to \Sigma \) to \( h' : A' \to \Sigma \) are the mappings \( f : A \to A' \) with \( h' \circ f = h \).

3. The category \textbf{Maps} of mappings: Its objects are mappings \( k : A \to B \) and the set of morphisms \( \text{Mor}_{\text{Maps}}(k : A \to B, k' : A' \to B') \) consists of the set of pairs of mappings \((f : A \to A', g : B \to B')\) with \( k' \circ f = g \circ k \) for each pair \( k, k' \) of objects.

4. The category \( \Sigma\)-\textbf{Graphs} of \( \Sigma \)-graphs for some alphabet \( \Sigma \): Its objects are \( \Sigma \)-graphs and its morphisms are \( \Sigma \)-graph morphisms defined as follows. A \( \Sigma \)-\textbf{graph} \( G = (V,E,s,t,l) \) consisting of a set \( V \) of \textit{vertices}, a set \( E \) of \textit{edges}, \textit{source} and \textit{target} mappings \( s : E \to V \) and \( t : E \to V \), and a \textit{labeling} mapping \( l : E \to \Sigma \). A \( \Sigma \)-\textbf{graph} morphism \( f = (f_V, f_E) : G \to G' \) for \( \Sigma \)-graphs \( G = (V,E,s,t,l) \) and \( G' = (V',E',s',t',l') \) consists of two mappings \((f_V : V \to V', f_E : E \to E')\) with \( f_V \circ s = s' \circ f_E, f_V \circ t = t' \circ f_E \), and \( l = l' \circ f_E \).

5. The category \( \Sigma\)-\textbf{Hypergraphs} of \( \Sigma \)-hypergraphs for some alphabet \( \Sigma \): Its objects are \( \Sigma \)-hypergraphs and its morphisms are \( \Sigma \)-hypergraph morphisms defined as follows. A \( \Sigma \)-\hypergraph \( H = (V,E,\text{att},l) \) over a given set \( \Sigma \) of \textit{labels} is a system consisting of a set \( V \) of \textit{vertices}, a set \( E \) of \textit{hyperedges}, an \textit{attachment} mapping \( \text{att} : E \to V^* \) (assigning a string of attachment vertices to each hyperedge) and a \textit{labeling} mapping \( l : E \to \Sigma \). The length of the attachment is called \textit{type}. A \textit{hypergraph morphism} \( f \) from \( H = (V,E,\text{att},l) \) to \( H' = (V',E',\text{att}',l') \) is a pair \((f_V : V \to V', f_E : E \to E')\) of two mappings such that \( f_V \circ \text{att} = \text{att}' \circ f_E \) and \( l = l' \circ f_E \), where \( V^* \) is the set of all string over \( V \) and \( f_V^* : V^* \to V'^* \) is the canonical extension of \( f_V \) to strings defined by \( f_V^*(v_1 \cdots v_n) = f_V(v_1) \cdots f_V(v_n) \) for all \( v_1 \cdots v_n \in V^* \).

6. The category \textbf{Monoids} of monoids: The objects are monoids \((M,+,0)\) with a base set \( M \), an associative inner operation \(+ : M \times M \to M \) and
a neutral element 0 ∈ M with \( x + 0 = x = 0 + x \) for all \( x \in M \). The morphisms are the monoid morphisms, i.e., mappings \( f: M \rightarrow M' \) with \( f(x + y) = f(x) + f'(y) \) for all \( x, y \in M \) and \( f(0) = 0' \) for monoids \((M, +, 0)\) and \((M', +', 0')\).

In all six cases, the sequential composition is given componentwise by the sequential composition of the respective mappings. If the underlying mappings of morphisms in these categories are injective, then the morphisms are monomorphisms obviously. If the underlying mappings are bijective, then the morphisms are isomorphisms. That the converse holds, too, is more difficult to see. Consider, for example, the category \( \Sigma\text{-Graphs} \). A singleton set \( \mathcal{T} = \{1\} \) induces the \( \Sigma\text{-graph} \( gr(1) = (\mathcal{T}, \emptyset, \emptyset, \emptyset_T, \emptyset_S) \), where \( \emptyset \) denotes the empty set and \( \emptyset_X: \emptyset \rightarrow X \) for a set \( X \) the empty mapping. Let \( G = (V,E,s,t,l) \) be some \( \Sigma\text{-graph} \) and \( v_0 \in V \). Then the pair of mappings \((v_0 \in V)\{1\} = v_0\) defines a graph morphism \( \text{mor}(v_0,G): gr(1) \rightarrow G \).

Let \( g = (g_V,g_E): G \rightarrow G' = (V',E',s',t',l') \) be a graph morphism where \( g_V \) is not injective. Then there are vertices \( v_1,v_2 \in V \) with \( v_1 \neq v_2 \), but \( g_V(v_1) = g_V(v_2) \). And one gets: \( g \circ \text{mor}(v_1,G) = (g_V \circ [v_1 \in V],\emptyset) = ((g_V(v_1) \in V'),\emptyset) = ((g_V(v_2) \in V'),\emptyset) = (g_V \circ [v_2 \in V],\emptyset) = g \circ \text{mor}(v_1,G) \).

As \( \text{mor}(v_1,G) \neq \text{mor}(v_2,G), \) \( g \) is not a monomorphism. Similarly, one can show that \( g \) is not a monomorphism if \( g_E \) is not injective. As a test graph, one can use the \( \Sigma\text{-graph} \) with two vertices and a single \( a \)-labeled edge for \( a \in \Sigma \) \( gr(a) = (\{b,e\},\mathcal{T},[b \in \{b,e\}],[e \in \{b,e\}],[a \in \Sigma]) \). Altogether, the monomorphisms in the category \( \Sigma\text{-Graphs} \) are the morphisms both components of which are injective mappings.

Adapted reasoning works for all other examples. That the isomorphism must have bijective component mappings follows from the fact that their compositions with their inverse morphisms yield identities which are defined componentwise by identities in \( \text{Sets} \).

Consequently, the subobjects in all our sample categories consist of sub-objects in their set components. Therefore, in all our sample categories, the subobjects of an object are uniquely represented by monomorphisms the components of which are subset inclusions. In particular, an object is finite if the set components are finite. But the converse holds, too. Consider, for example, \( \Sigma\text{-Graphs} \). A \( \Sigma\text{-graph} \( G \) with an infinite set of vertices \( V \) has every discrete \( \Sigma\text{-graph} \( (U,\emptyset,\emptyset_U,\emptyset) \) as subgraph so that the inclusions defines an infinite set of subobjects. If \( G = (V,E,s,t,l) \) is a \( \Sigma\text{-graph} \) with a finite set \( V \), but an infinite set \( E \). Then there must be an infinite subset \( I \) of \( E \) such that all edges in \( I \) have the same source \( v_1 \) and the same target \( v_2 \). This yields the infinite set of subgraphs \( \{v_1,v_2\}, \{e\}, s|_{\mathcal{I}}, t|_{\mathcal{I}}, l|_{\mathcal{I}} \) for all \( e \in I \), where \( s|_{\mathcal{I}}, t|_{\mathcal{I}}, l|_{\mathcal{I}} \) denote the restrictions of the domain of \( s,t,l \) to \( \mathcal{I} \), respectively. In other words, if \( G \) is a finite object in \( \Sigma\text{-Graphs} \), then its set components are finite sets.

Similar reasoning yields that the set components of finite objects are finite in all example categories.
2.2. Empty subobjects and intersections

A subobject \( p_0 : P_0 \rightarrow B \) is an empty subobject of \( B \) if each monomorphism \( m : X \rightarrow P_0 \) for some object \( X \) is an isomorphism.

This means that \( P_0 \) has only one subobject represented by the identity.

**Example 2.**

1. In the category \( \text{Sets} \), there is an injective mapping \( \emptyset_B : \emptyset \rightarrow B \) from the empty set \( \emptyset \) into each set \( B \). The identity \( 1_\emptyset \) on \( \emptyset \) is the only mapping into \( \emptyset \) so that the inclusion \( \emptyset_B : \emptyset \rightarrow B \) is an empty subobject of each set in \( \text{Sets} \).

2. Let \( (B, B') \) be an object in the category \( \text{Sets} \times \text{Sets} \). Then the respective empty subobject is represented by the pair of empty morphisms \( (\emptyset_B, \emptyset_{B'}) \).

3. The empty mapping \( \emptyset_\Sigma : \emptyset \rightarrow \Sigma \) together with the empty mapping \( \emptyset_B : \emptyset \rightarrow B \) for some \( \Sigma \)-set \( l : B \rightarrow \Sigma \) is the empty subobject of \( l \) in the category \( \Sigma \text{-Sets} \) as \( \emptyset_\Sigma = l \circ \emptyset_B \).

4. Let \( k : A \rightarrow B \) be an object in the category \( \text{Maps} \). Then the empty mapping \( \emptyset_A : \emptyset \rightarrow \emptyset \) together with the pair of empty mappings \( (\emptyset_A, \emptyset_B) \) represents the empty subobject of \( k \) as \( k \circ \emptyset_A = \emptyset_B \circ \emptyset_B \).

5. Let \( G = (V, E, s, t, l) \) be a \( \Sigma \)-graph. Then the empty \( \Sigma \)-graph \( (\emptyset, \emptyset, \emptyset, \emptyset_\Sigma) \) together with the graph morphism \( (\emptyset_V, \emptyset_E) : (\emptyset, \emptyset, \emptyset, \emptyset_\Sigma) \rightarrow G \) represents the empty subobject of \( G \) as \( \emptyset_V \circ \emptyset_B = \emptyset_V = t \circ \emptyset_E \), and \( \emptyset_\Sigma = l \circ \emptyset_E \).

6. Analogously, \( (\emptyset, \emptyset, \emptyset_{B'}, \emptyset_\Sigma) \) together with the hypergraph morphism \( (\emptyset_V, \emptyset_E) : (\emptyset, \emptyset, \emptyset_{B'}, \emptyset_\Sigma) \rightarrow H \) yields the empty subobject of each \( \Sigma \)-hypergraph \( H \).

7. The empty subobjects in the category \( \text{Monoids} \) are given by the 0-monoid \( (\{0\}, +, 0) \) with \( 0 + 0 = 0 \) together with the inclusion of the 0-monoid to each other monoid mapping 0 to 0.

Let \( p_1 : P_1 \rightarrow B \) and \( p_2 : P_2 \rightarrow B \) represent two subobjects of \( B \). Then the intersection of \( p_1 \) and \( p_2 \) is a subobject \( p_1 \cap p_2 : P_1 \cap P_2 \rightarrow B \) together with two monomorphisms, called inclusions, \( p_i' : P_1 \cap P_2 \rightarrow P_i \) for \( i = 1, 2 \) satisfying the following universal property:

1. \( p_1 \cap p_2 = p_i \circ p_i' \) for \( i = 1, 2 \).

2. For each subobject \( p : P \rightarrow B \) and each two monomorphism \( q_i : P \rightarrow P_i \) with \( p = p_i \circ q_i \) for \( i = 1, 2 \), there exists a unique monomorphism \( q : P \rightarrow P_1 \cap P_2 \) with \( q_i = p_i' \circ q \) and \( p = (p_1 \cap p_2) \circ q \).

The situation can be represented in diagrammatic form:

![Diagram](https://via.placeholder.com/150)

for \( i = 1, 2 \).
The dashed arrow indicates that the morphism exists uniquely.

In common categorical terms, the intersection is a pullback of monomorphisms in the category $\textbf{C}_{\text{mono}}$ and a product in the category $\textbf{Sub}(B, \textbf{C})$ of subobjects of $B$. We prefer the term intersection as it stresses its use in this paper and it is given by the intersection of subsets in all our examples.

**Example 3.** In the category $\textbf{Sets}$, two subsets $P_i \subseteq B$ for $i = 1, 2$ of a set $B$ represent subobjects. Their set-theoretic intersection $P_1 \cap P_2 = \{x \mid x \in P_1 \land x \in P_2\}$ represents the categorical intersection. Clearly, property 1 holds for the respective inclusions. Moreover, as the set-theoretic intersection is the largest subset containing $P_1$ and $P_2$, property 2 holds, too.

The intersection $P_1 \cap P_2$ together with the inclusions $p_i': P_1 \cap P_2 \to P_i$ for $i = 1, 2$ are not only the pullback of the inclusion mappings $p_i: P_i \to B$ in the category $\textbf{Sets}_{\text{mono}}$, but also in $\textbf{Sets}$. This means that for each pair of mappings $f_i: X \to P_i$ for some set $X$ with $p_1 \circ f_1 = p_2 \circ f_2$, there is a unique mapping $f: X \to P_1 \cap P_2$ with $p_i \circ f = f_i$ for $i = 1, 2$.

That the componentwise intersections can be extended to objects in the category $\Sigma\text{-}\textbf{Graphs}$, for example, can be seen as follows using the pullback property of intersections of subsets.

Let $P_i = (V_i, E_i, s_i, t_i, l_i)$ for $i = 1, 2$ be sub-$\Sigma$-graphs of a $\Sigma$-graph $G = (V, E, s, t, l)$ with the inclusions $p_i = (p_{V,i}, p_{E,i}): P_i \to G$ for $i = 1, 2$. Let $p_{V,1} \cap p_{V,2}: V_1 \cap V_2 \to V$ and $p'_{V,i}: V_1 \cap V_2 \to V_i$ for $i = 1, 2$ be the inclusions for the vertex component given by the intersection property and $p_{E,1} \cap p_{E,2}: E_1 \cap E_2 \to E$ and $p'_{E,i}: E_1 \cap E_2 \to E_i$ for $i = 1, 2$ be the respective inclusions for the edge component. Then one gets the $\Sigma$-graph $P_1 \cap P_2 = (V_1 \cap V_2, E_1 \cap E_2, s_{\cap}, t_{\cap}, l_{\cap})$ where $l_{\cap} = l \circ (p_{E,1} \cap p_{E,2})$ and $s_{\cap}$ and $t_{\cap}$ are induced by the universal pullback property of $V_1 \cap V_2$ because the following equations hold:

1. $s \circ (p_{E,1} \cap p_{E,2}) = s \circ p_{E,i} \circ p'_{E,i} = p_{V,i} \circ s_i \circ p'_{V,i}$ for $i = 1, 2$ induces a mapping $s_{\cap}: E_1 \cap E_2 \to V_1 \cap V_2$ with $p'_{V,i} \circ s_{\cap} = s_i \circ p'_{V,i}$ for $i = 1, 2$.
2. Replacing $s$ and $s_i$ by $t$ and $t_i$, respectively one gets $t_{\cap}$.

This also proves that the pairs of inclusions $p_1 \cap p_2 = (p_{V,1} \cap p_{V,2}, p_{E,1} \cap p_{E,2}): P_1 \cap P_2 \to B$ and $p'_i = (p'_{V,i}, p'_{E,i}): P_1 \cap P_2 \to P_i$ are graph morphisms.

Similar arguments hold for the categories $\textbf{Maps}$ and $\Sigma\text{-}\textbf{Hypergraphs}$. In the category $\Sigma\text{-}\textbf{Sets}$, the intersection in the set component yields the intersection, and in $\textbf{Sets} \times \textbf{Sets}$ the componentwise intersection does the job.

Finally, given submonoids $(P_i, +, 0)$ of a monoid $(B, +, 0)$ for $i = 1, 2$, the set-theoretic intersection of $P_1 \cap P_2$ yields a monoid $(P_1 \cap P_2, +, 0)$ where $+$ is the restriction of $+$ in $B$, $P_1$ and $P_2$, and the inclusions $P_1 \cap P_2 \subseteq P_i$ define monoid morphisms. It is easy to see that this monoid has the properties of the categorical intersection.

Empty subobjects and intersections have some useful properties.

**Properties 2.** 1. As the order of the given subobjects in the definition of intersection is not significant, intersections are commutative.
2. Intersections are unique up to isomorphisms. This is a standard result in category theory.

3. The intersection of some subobject \( p: P \to B \) and an empty subobject \( p_0: P_0 \to B \) is empty. This can be seen as follows. Consider

\[
\begin{array}{ccc}
P & \xrightarrow{p_0} & P_0 \\
\downarrow{p} & & \downarrow{p_0} \\
B & & B \\
\end{array}
\]

By definition of empty subobjects, \( p' \) is an isomorphism such that \( p_0 = p \cap p_0 \) as subobjects. Moreover, one gets \( p_0 = p \circ p_0' \circ p'^{-1} \) proving the following point.

4. An empty subobject of \( B \) factors through each other subobject of \( B \). In usual categorical terms this means that an empty subobject is initial in the category \( \text{Sub}(B, C) \) of subobjects of \( B \).

5. If an object \( B \) has an empty subobject, then this is unique. This can be seen as follows. If the given subobject \( p \) in the diagram in Point 3 is an empty subobject, then \( p_0' \) is an isomorphism like \( p' \) such that \( p_0 = p \circ p_0' \circ p'^{-1} \) meaning that \( p_0 = p \) as subobjects.

In the following \( empty_B: EMPTY_B \to B \) denotes the unique empty subobject of \( B \).

2.3. \textit{Union}

Let \( S \) be a set of subobjects of \( B \). Then the union (of the subobjects) of \( S \) is a subobject of \( B \), denoted by \( \text{union}(S): UNION(S) \to B \), with the following universal property:

1. For each \((p: P \to B) \in S\), there is a monomorphism \( p': P \to UNION(S) \) such that \( \text{union}(S) \circ p' = p \).

2. For each subobject \( m: X \to B \) and a monomorphism \( q: P \to X \) for each \((p: P \to B) \in S\) with \( m \circ q = p \), there exists a unique monomorphism \( m: UNION(S) \to X \) with \( m \circ m = \text{union}(S) \).

The union in diagrammatic form:

\[
\begin{array}{ccc}
P & \xrightarrow{p'} & UNION(S) \\
\downarrow{q} & & \downarrow{m} \\
B & \xrightarrow{m} & \text{union}(S) \end{array}
\]

for each \( p \in S \).
We may write $\bigcup_{p \in S} p$ for $\text{union}(S)$ and $\text{union}(\{p_1, p_2\}) = p_1 \cup p_2$.

Note that $\text{union}(\emptyset)$ for the empty set of subobjects of $B$ is an initial object in the category $\text{Sub}(B, C)$ by definition. Therefore, $\text{union}(\emptyset) = \text{empty}_B$. Further, $\text{union}(\{p: P \to B\})$ of a single subobject is the subobject itself: $\text{union}(\{p\}) = p$ by definition, too.

In different categorial terms, the union is the coproduct in the category $\text{Sub}(B, C)$. We prefer the term union as it emphasizes its use in this paper.

The categorial union has some properties that are useful for the further considerations and correspond to properties of set-theoretic unions.

**Properties 3.**

1. As the order of subobjects in the definition of the binary union is not significant, it is commutative, i.e., $p_1 \cup p_2 = p_2 \cup p_1$ for subobjects $p_1, p_2$.
2. A standard argument in category theory based on the universal property yields that objects and corresponding monomorphisms with the union properties are unique up to isomorphism. Therefore, unions are unique as subobjects.
3. Unions can be constructed stepwise. More precisely, let $S$ be a set of subobjects of an object $B$ and $S_1, S_2 \subseteq S$ with $S_1 \cup S_2 = S$. Then $\text{union}(S) = \text{union}(S_1) \cup \text{union}(S_2)$. This can be seen as follows.

Consider the diagram:

\[
\begin{array}{ccc}
P_1 & \xrightarrow{p_1} & \text{union}(S_1) \\
\downarrow{p_i'} & & \downarrow{u_1} \\
\text{union}(S_1) & \xrightarrow{\cup} & \text{union}(S_2) \\
\downarrow{u_2} & & \downarrow{p_2} \\
P_2 & \xrightarrow{p_2'} & \text{union}(S_2) \\
\end{array}
\]

By definition of the binary union, the monomorphisms $u_i$ for $i = 1, 2$ exist so that the diagrams (1) and (2) are commutative. By definition of the union, the monomorphisms $p_i'$ for all $p_i \in S_i, i = 1, 2$ exist so that the diagrams (3) and (4) commute. Then the monomorphisms $u_i \circ p_i'$ have the property:

$\text{union}(S_1) \cup \text{union}(S_2) \circ u_i \circ p_i' = \text{union}(S_i) \circ p_i' = p_i$

for all $p_i \in S_1 \cup S_2 = S$.

Conversely, let $m: X \to B$ be a subobject of $B$ and $q_i: P_i \to X$ be a monomorphism with $p_i = m \circ q_i$ for all $p_i \in S = S_1 \cup S_2$. Using the
universal property of $\text{union}(S_i)$ for $i = 1, 2$, one gets monomorphisms $\overline{m}_i: \text{UNION}(S_i) \to X$ with $m \circ \overline{m}_i = \text{union}(S_i)$ for $i = 1, 2$. Using the universal property of the binary union, one gets a monomorphism $\overline{m}: \text{UNION}(S_1) \cup \text{UNION}(S_2) \to X$ with $m \circ \overline{m} = \text{union}(S_1) \cup \text{union}(S_2)$.

4. In particular, this proves the associativity of the binary union. Let $p_i: P_i \to B$ for $i = 1, 2, 3$ be subobjects of $B$. Then we get $(p_1 \cup p_2) \cup p_3 = \text{union}((p_1, p_2)) \cup \text{union}((p_3)) = \text{union}((\{p_1, p_2, p_3\}) = \text{union}(\{p_1\} \cup \text{union}(\{p_2, p_3\}) = p_1 \cup (p_2 \cup p_3)$.

5. The union of some subobject $p: P \to B$ and the empty subobject $\text{empty}_B$ is $p$. It is easy to see that $p$ together with the monomorphism $1_p$ and $\text{empty}_B$ has the property required for $p \cup \text{empty}_B$ so that $p \cup \text{empty}_B = p$ according to Point 2.

6. Together with Point 3, one gets for an arbitrary set $S$ of subobjects of $B$: $\text{union}(S \cup \{\text{empty}_B\}) = \text{union}(S) \cup \text{union}(\{\text{empty}_B\}) = \text{union}(S) \cup \text{empty}_B = \text{union}(S)$. In other words, it is enough to consider unions of non-empty subobjects.

7. Let $p: P \to B$ and $p_0: P_0 \to B$ be two subobjects with $p_0 \subseteq p$, i.e., there is a monomorphism $\text{in}: P_0 \to P$ with $p \circ \text{in} = p_0$. Then the union of $p$ and $p_0$ is $p$. This can be seen as follows. Consider the diagram

\[
\begin{array}{ccc}
X & \overset{q_0}{\leftarrow} & B \\
\downarrow_{q} & & \downarrow_{1_p} \\
P & \overset{\text{in}}{\leftarrow} & P_0 \\
\downarrow_{m} & & \downarrow_{m} \\
P & \overset{p_0}{\leftarrow} & P \\
\end{array}
\]

(1) commutes by assumption, (2) and (6) by the identity property; $m: X \to B$ with $q_0: P_0 \to X$ and $q: P \to X$ are arbitrarily chosen such that (3) and (4) commute. Then we get $m \circ q \circ \text{in} = p \circ \text{in} = (\text{in}) (p_0) = m \circ q_0$. This implies $q \circ \text{in} = q_0$ as $m$ is a monomorphism. Therefore, (5) commutes. Altogether, $p$ together with $\text{in}$ and $1_p$ has the property of $p \cup p_0$ such that $p \cup p_0 = p$. This property generalizes Point 5. 8. Points 3 and 7 imply $\text{union}(S_0) \subseteq \text{union}(S)$ for some sets of subobjects $S_0 \subseteq S$ because $\text{union}(S_0) \subseteq \text{union}(S_0) \cup \text{union}(S - S_0) = \text{union}(S)$.

9. Let $S$ be a set of subobjects of $B$ and $p_1, p_2 \in S$. Then $p_1 \cap p_2 \subseteq \text{union}(S)$. This can be seen as follows. Consider subobjects $p_i: P_i \to B$ for $i = 1, 2$. By definition of union and intersection, there are, for $i = 1, 2$, monomorphisms $p'_i: P_i \to \text{UNION}(S)$ and $p''_i: P_i \cap P_i \to P_i$ with $p_i = \text{union}(S) \circ p'_i$ and $p_1 \cap p_2 = p_1 \circ p''_i$ such that $p_1 \cap p_2 = \text{union}(S) \circ p'_i \circ p''_i$. This proves
the statement. The following diagram illustrates the situation.

$$
\begin{array}{c}
P_i \\ \coprod P \subset \coprod S \\ \coprod S \\
\end{array}
$$

10. If the empty subobject, the intersections and the binary unions exist in $\text{Sub}(B, C)$, then $\text{Sub}(B, C)$ is not only a preorder with respect to subobject inclusion, but a (bounded) lattice with intersection as join, and union as meet, the empty subobject as top and $1_B$ as bottom.

**Example 4.** In the category $\text{Sets}$, a set $S$ of subsets of a set $B$ represents a set of subobjects of $B$ by means of the respective inclusions. Then the set-theoretic union $\bigcup_{P \in S} P = \{ x \in P \mid P \in S \}$ represents the categorical union of $S$ because $\bigcup_{P \in S} P$ is the smallest subset of $B$ that includes all $P \in S$.

As the two set components of objects of $\text{Sets} \times \text{Sets}$ do not interfere with each other, the componentwise union yields the union in $\text{Sets} \times \text{Sets}$.

Consider now the category $\Sigma$-Graphs. Let $S$ be a set of sub-$\Sigma$-graphs of a $\Sigma$-graph $B$, and let $\bigcup_{P \in S} V_P$ and $\bigcup_{P \in S} E_P$ be the union of the set of vertices and the set of edges of all $P \in S$ respectively. Then the two sets induce a sub-$\Sigma$-graph of $B$, $U(S) = (\bigcup_{P \in S} V_P, \bigcup_{P \in S} E_P, s_U, t_U, l_U)$ with $s_U(e) = s_P(e)$, $t_U(e) = t_P(e)$, and $l_U(e) = l_P(e)$ for all $e \in E_P, P \in S$. This means, in particular, that all $P \in S$ are sub-$\Sigma$-graphs of $U(S)$ if $s_U, t_U$ and $l_U$ are mappings which can be seen as follows. Let $e \in E_P$ and $e \in E_{P'}$ for $P, P' \in S$, $P \neq P'$. We must show that $s_P(e) = s_{P'}(e)$. But this holds as $P$ and $P'$ are sub-$\Sigma$-graphs of $B$ so that $s_P(e) = s_B(e) = s_{P'}(e)$. The same arguments works for $t_U$ and $l_U$. If there is now another sub-$\Sigma$-graph $X$ that includes all $P \in S$, then $X$ includes also $U(S)$ because this holds for the set of vertices and edges separately and $s_X, t_X$ and $l_X$ must be equal to $s_U, t_U$, and $l_U$ on $\bigcup_{P \in S} E_P$ respectively, as sub-$\Sigma$-graphs of $B$.

The same argumentation works for $\Sigma$-Sets, Maps, and $\Sigma$-Hypergraphs.

In the category Monoids, the situation is a bit more complicated. It is easy to see that the union of the base sets of submonoids of a monoid are usually not closed under the inner composition so that the set-theoretic union does not induce a submonoid directly. But one can close the union under inner composition yielding a submonoid that is obviously the smallest one that contains all the pre-given submonoids and, therefore, the categorical union.
3. Reaction systems and interactive processes over a category

In this section, reaction systems over a category are introduced. While the original notion of reaction systems is purely set-theoretic and generalized to a graph-based variant in [8, 9], the concept is carried over to a categorical framework.

If one assumes a category with empty subobjects, intersections and unions, then reaction systems over this category can be defined in a straightforward way by replacing every occurrence of “(sub)set/(sub)graph” in the definition of set/graph-based reaction systems by “(sub)object” with one exception: the enabledness with respect to the inhibitor. In the set case, it is required that the intersection of an inhibitor set and the state set is empty. This could be easily formulated for an inhibitor object and a state object. But in the graph case, various examples show that an inhibitor graph that is required to be disjoint from a state graph is too restrictive. Therefore, a reaction of a graph-based reaction system has a pair of a set of vertices and a set of edges as inhibitor and enabledness requires that none of the vertices and edges belong to the considered state graph. This allows to forbid edges without forbidding their sources and targets. Unfortunately, categorical objects do not provide any internal information like vertices and edges. Categorical inhibitors must be defined in terms of objects with certain properties. We choose the categorical inhibitor of a reaction as a pair of a subobject of the underlying background object and a subsubobject, i.e., a subobject of the subobject. Then a reaction is enabled on a state object with respect to the inhibitor if the intersection of the subobject and the state is included in the subsubobject. This means that not the whole subobject is forbidden, but only the “complement” of the subobject and the subsubobject. Nicely enough, this covers the graph-based case if one chooses the subsubgraph as a discrete graph with an empty set of edges.

3.1. General assumption

Let $C$ be a category which satisfies the following conditions for every finite object $B$:

1. There is an empty subobject $\text{empty}_B$.
2. For every two subobjects $p_1$ and $p_2$ of $B$, $p_1 \cap p_2$ exists.
3. For every set $S$ of subobjects of $B$, $\text{union}(S)$ exists.

All the examples discussed in Section 2 meet the general assumptions.

3.2. Reaction systems over $C$

The general assumption allows us to define reaction systems over $C$ in a way analogous to set-based and graph-based reaction systems.

**Definition 1.** Let $B$ be a finite object in $C$. A reaction over $B$ is a triple $a = (r: R \to B, (i: I \to B, i_0: I_0 \to I), p: P \to B)$ where $r$ and $p$ are non-empty subobjects of $B$, $i$ is a subobject of $B$ and $i_0$ is a subobject of $I$. The subobject $r$ is called reactant, the pair $(i, i_0)$ is called inhibitor, and
is called product. \( r, (i, i_0) \) and \( p \) may also be denoted by \( r_\alpha, (i_\alpha, (i_0)_\alpha) \) and \( p_\alpha \), respectively.

2. A state is a subobject of \( B \).

3. A reaction \( a = (r: R \to B, (i: I \to B, i_0: I_0 \to I), p: P \to B) \) is enabled on a state \( t: T \to B \), denoted by \( \text{en}_a(t) \), if \( r \subseteq t \) and \( t \cap i \subseteq i \circ i_0 \), i.e., there is a monomorphism \( s: R \to T \) with \( r = t \circ s \) and, for the intersection \( (T \cap I, i', t') \) of \( t \) and \( i \), there is a monomorphism \( s': T \cap I \to I_0 \) with \( t \cap i = i \circ i_0 \circ s' \).

4. The result of a reaction \( a \) on a state \( t \) is \( \text{res}_a(t) = p_\alpha \) for \( \text{en}_a(t) \) and \( \text{res}_a(t) = \text{empty}_B \) otherwise.

5. Given a state \( t: T \to B \), the result of a set of reactions \( A \) on \( t \) is \( \text{res}_A(t) = \bigcup_{a \in A} \text{res}_a(t) \).

6. A reaction system over \( C \) is a pair \( A = (B, A) \) consisting of some finite object \( B \), called background, and a finite set \( A \) of reactions over \( B \).

7. Given a state \( t: T \to B \), the result of \( A \) on \( t \) is the result of \( A \) on \( t \).

Remark 1. Some basic properties of enabledness and results which are known for set- and graph-based reaction systems carry over to reaction systems over a category.

1. A current state vanishes completely. But it or some subobject of it may be reproduced by the products of enabled reactions.

2. \( \text{res}_A(t) \) is uniquely defined for every state \( t \) so that \( \text{res}_A(t) \) is a function on the set of states of \( B \).

3. All reactions contribute to \( \text{res}_A(t) \) in a maximally parallel and cumulative way. There is never any conflict.

4. As the addition of the empty subobject to a subobject by union does not change the subobject, \( \text{res}_A(t) = \text{res}_{\{a \in A | \text{en}_a(t)\}}(t) \) holds for all states \( t \).

5. As the intersection of a subobject and the empty subobject is empty, a reaction with an empty inhibitor, i.e., \( a = (r, (\text{empty}_B, 1_{\text{EMPTY}_B}), p) \) is enabled on a state \( t \) if \( r \subseteq t \). The empty inhibitor has no effect. Therefore, the reaction is called uninhibited.

3.3 Sample reaction systems over \( \Sigma \)-Hypergraphs

To illustrate how reaction systems over the category \( \Sigma \)-Hypergraphs look like, we model a colorability test (cf., e.g., [14, 15]) by a family of reaction systems.
A Σ-hypergraph $H = (V, E, att, l)$ with $l(e) = *$ for some label $* \in \Sigma$ for all $e \in E$ (this means that all hyperedges are equally labeled and, hence, can be considered as unlabeled) where all hyperedges have types greater than 1 is k-colorable for some $k \in \mathbb{N}$ if there is a mapping $col: V \to [k]$, called coloring, where $[k] = \{1, \ldots, k\}$, such that each $e \in E$ has at least two attachment vertices $v, v'$ with $col(v) \neq col(v')$, i.e., no attachment is monochromatic.

Assuming $[k] \subseteq \Sigma$, a mapping $col: V \to [k]$ induces an extension $(H, col)$ of $H$ by a $col(v)$-flag (type-1 hyperedge) at each $v \in V$. Obviously, a collection of such flags defines a mapping $col: V \to [k]$ such that coloring hypergraphs can be handled by attaching flags.

The k-colorability test employs the reaction system $A_{n,m,k} = (B_{n,m,k}, A_{n,m,k})$ for some $n, m, k \in \mathbb{N}$ with $2 \leq m \leq n$ defined as follows. Let $[[n]]$ be the set of all strings over $[n]$ of length between 2 and $m$ without repetitions, i.e., none of these strings has a decomposition $uxvxw$ with $x \in [n]$. Then the complete hypergraph $CH_{n,m}$ is defined by $CH_{n,m} = ([[n]], [[n]] \times [[m]])$, with $att$ and the label.

The background hypergraph $B_{n,m,k}$ consists of $CH_{n,m}$ extended by an extra vertex with a failed-flag as well as by the set $[[n]] \times [k]$ of flags where the first component is the attachment vertex and the second component is the label. $A_{n,m,k}$ contains the following reactions, where, due to the one-to-one correspondence of categorial subobjects of a Σ-hypergraph and sub-Σ-hypergraphs, the subobjects are represented by the domain objects of the inclusion morphisms. All reactions are uninhibited. The symbol “−” is a shortcut for the inhibitor ($empty_{B_{n,m,k}}, 1_{EMPTY_{B_{n,m,k}}}$).

1. $([j], −, [j])$ for all $j \in [n]$.
2. $(u^*, −, u^*)$ for all $u \in [n]$, where $u^*$ is the hyperedge $u$ with itself as attachment, i.e., $u^* = ([x_1, \ldots, x_l], [u], att_{u^*}, lab_{u^*})$ with $att_{u^*}(u) = x_1 \cdots x_l, x_j \in [n]$ for $j = 1, \ldots, l$.
3. $([j], 1_{\mathcal{C}} - [y], [j], 1_{\mathcal{C}})$ for all $j \in [n]$ and $y \in [k]$.
4. $([\mathcal{C} failed], −, [\mathcal{C} failed])$.
5. $((u, y)^*, −, [\mathcal{C} failed])$ for all $u \in [n]$ and $y \in [k]$ where $(u, y)^*$ is $u^*$ extended by a flag at each vertex.

The first four types of reactions applied to a state make sure that the state is sustained. The only changing reactions are of the fifth type. They add the extra vertex with the failed-flag provided that there is a hyperedge and all its attachment vertices carry a flag with the same label. In the drawings, a circle represents a vertex and a box a flag. The label is inside the box, and a line from a box to a circle represents the attachment.

The modeling of a colorability test is continued in Section 3.6.
3.4. Sample reaction systems over Monoid

As a second illustration, we model – similar to the Sieve of Eratosthenes – an algorithm for finding all prime numbers up to given limits by means of a family of reaction systems \( A_n = (B_n, A_n) \) for \( n > 1 \) over the category of monoids.

The background monoid \( B_n = (S_n, \ast, 1) \) is the monoid of marked positive integers up to \( n > 1 \) with an adapted integer multiplication. The underlying set is \( S_n = \{1\} \cup \{(2, \ldots, n) \times \{p, c, ?\}\} \cup \{\infty\} \) for some \( n \geq 2 \) where \( p, c, ? \) are shortcuts for “prime”, “composite” and “unknown”, respectively and \( \infty \) refers to all numbers beyond \( n \). A marked integer \((x, m)\) is also denoted by \( x_m \). The operation \( \ast \) is given by:

1. \( 1 \ast x = x = x \ast 1 \) for all \( x \in S_n \),
2. \( v_m \ast v'_m = (v \cdot v')_c \) if \( v \cdot v' \leq n \) and \( \infty \) otherwise for all \( v, v' \in \{2, \ldots, n\} \) and \( m, m' \in \{p, c, ?\} \), and
3. \( x \ast \infty = \infty = \infty \ast x \) for all \( x \in S_n \).

It is easy to see that the operation \( \ast \) is associative using the associativity of the multiplication of integers.

Each subset \( S \subseteq S_n \) generates a submonoid \( \langle S \rangle \) of \( B_n \) by adding \( 1 \) and closing \( S \) under the operation. To simplify the notation, we omit the set braces for singleton sets. Some sample submonoids of \( B_9 \) are:

- \( \langle \emptyset \rangle = \langle 1 \rangle = (\{1\}, \ast, 1) \),
- \( \langle \infty \rangle = (\{1, \infty\}, \ast, 1) \),
- \( \langle 2_p \rangle = (\{1, 2_p, 4_c, 8_c, \infty\}, \ast, 1) \),
- \( \langle 3_c \rangle = (\{1, 3_c, 9_c, \infty\}, \ast, 1) \).

The set \( A_n \) of reactions contains two types of reactions:

1. \( (\langle x_m \rangle, (\langle \emptyset \rangle, \langle \emptyset \rangle), (\langle x_m \rangle)) \) for \( x \in \{2, \ldots, n\} \) and \( m \in \{p, c\} \),
2. \( (\langle x_c \rangle, (\langle x_c \rangle, \langle \infty \rangle), (\langle x_p \rangle)) \) for \( x \in \{2, \ldots, n\} \).

The first type of reactions is used to sustain the submonoid generated by some positive integer marked by \( p \) or \( c \). Integers marked by \( ? \) are never sustained. The second type of reactions is applicable if a submonoid generated by some marked positive integer with unknown marking is present and the corresponding submonoid but with composite marking is not present up to \( 1 \) and \( \infty \). The product is the submonoid generated by the corresponding submonoid but with prime marking.

The algorithm is continued in Section 3.7.

3.5. Interactive processes

The definition of reaction systems over a category is chosen in such a way that the semantic notion of interactive processes can be carried over directly from the set-based and graph-based cases.
Definition 2. 1. Let $A = (B, A)$ be a reaction system over $C$. An interactive process $\pi = (\gamma, \delta)$ on $A$ consists of two sequences of subobjects of $B$ $\gamma = c_0, \ldots, c_n$ and $\delta = d_0, \ldots, d_n$ for some $n \geq 1$ such that $d_i = \text{res}_A(c_{i-1} \cup d_{i-1})$ for $i = 1, \ldots, n$. The sequence $\gamma$ is called context sequence, the sequence $\delta$ is called result sequence, and the sequence $\tau = t_0, \ldots, t_n$ with $t_i = c_i \cup d_i$ for $i = 0, \ldots, n$ is called state sequence.

2. $\pi$ is called context-independent if $c_i \subseteq d_i$ for $i = 0, \ldots, n$.

Remark 2. Consider a context-independent process $\pi = (c_0, \ldots, c_n, d_0, \ldots, d_n)$.

1. Using point [4] of Properties [3] in the previous section, $c_i \subseteq d_i$ for $i = 0, \ldots, n$ implies $t_i = c_i \cup d_i = d_i$ meaning that the result sequence and state sequence coincide and that the state sequence describes the whole process determined by its initial state $t_0 = d_0$. Therefore, whenever context-independent processes are considered, one can focus on their state sequences.

2. Let $\tau = t_0, \ldots, t_n$ for some $n \geq 1$ be a state sequence. Then $\tau$ is either repetition-free, i.e., $t_i \neq t_j$ for all $i, j$ with $0 \leq i < j \leq n$, or there is a smallest pair $t_{i_0}, t_{j_0}$ with $0 \leq i_0 < j_0 \leq n$ and $t_{i_0} = t_{j_0}$ such that $\tau = t_0, \ldots, t_{i_0}, (t_{i_0+1}, \ldots, t_{j_0})^m t_k, \ldots, t_n$ for some $m \in \mathbb{N}$ where $k = i_0 + 1 + m(j_0 - i_0) + 1$ and $t_k, \ldots, t_n$ is an initial section of $t_{i_0+1}, \ldots, t_{j_0}$. According to the choice of $i_0$ and $j_0$, the section $t_{i_0}, \ldots, t_{j_0-1}$ is repetition-free.

3. Using the pigeonhole principle, the pair $i_0, j_0$ exists if $n - 1$ is greater than the number of states. Therefore, every state sequence runs into a unique cycle eventually.

It is beyond the scope of this paper to go further into the theory of (set-based) reaction systems. There are various concepts and results concerning time, functions, sequences, fixed points, and attractors which rely on the principles of interactive processes rather than on set-theoretical properties (cf., e.g., [3, 5, 6, 7]). Therefore, we assume that there is a good chance to lift such concepts and results to the categorical level.

3.6. Interactive processes for $\Sigma$-Hypergraphs

Interactive processes over the reaction system $A_{n,m,k}$ of Section 3.3 with certain context sequences can be used as a colorability test.

Let $H \subseteq CH_{n,m}$ be a sub-$\Sigma$-hypergraph with $l$ vertices, and let $\text{col} = y_1 \cdots y_l \in [k]^*$ be a sequence of $l$ labels. Then one can consider the interactive process $\pi(H, \text{col}) = (\gamma(H, \text{col}), \delta(H, \text{col}))$ given by $\gamma(H, \text{col}) = \bigcup_{i_1} \bigcup_{y_2} \cdots, \bigcup_{i_l} \bigcup_{y_l}, \text{EMPTY}_{B_{n,m,k}}$ and $H$ as first result. The mapping $\text{col}_{\text{col}}: V_H \to [k]$ with $\text{col}_{\text{col}}(i_j) = y_j$ for $j = 1, \ldots, l$ is a $k$-coloring of $H$ if and only if the final result does not contain the failed-flag. This means that the $k$-colorability of $H$ can be tested by running all interactive processes $\pi(H, \text{col})$ for all $\text{col} \in [k]^*$ of length $l$. 

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Example 5. Let $\gamma(H, \text{col}) = c_0, c_1, c_2, c_3, c_4, \text{EMPTY}_{B_{5,3,3}}$, where $H$ is the
hypergraph depicted in Figure 1a, $c_0 = 1^1 \text{red}$, $c_1 = 2^1 \text{red}$, $c_2 = 3^1 \text{blue}$,
$c_3 = 4^1 \text{red}$, $c_4 = 5^1 \text{blue}$, and let $d_0 = H$. Then the successor results $d_1, \ldots, d_5$
are depicted in Figure 1b–1f, respectively. In the drawings of the hypergraphs, the bullets represent hyperedges of type 3 in
addition to the vertex circles and flag boxes. The lines connecting a bullet with
vertex circles provide the attachment where the numbering establishes its order.
The label $*$ is invisible (as it is without any significance).

If one chooses $c_2 = 3^1 \text{red}$, then $d_3$ is the hypergraph depicted in Figure 1g. Because the hyperedge connecting 1, 2, 3 is monochromic, the reaction
$((123, \text{red})^*, -, \circ \text{failed})$ becomes enabled. Its application adds $\circ \text{failed}$.
Everything else is sustained.

Note that it is also possible to choose several colors in parallel, e.g., choose $c'_0$ to be $\bigcup_{i=0}^4 c_i$ using the $c_i$ defined above and $c'_1 = \text{EMPTY}_{B_{5,3,3}}$ meaning that the test can be done in one step.

3.7. Interactive processes for Monoid
Interactive processes over the reaction system $A_n$ of Section 3.4 with certain context sequences can be used for finding prime numbers.
Consider the interactive process with start $H = \langle \emptyset \rangle$ and context sequence $\langle 2 \rangle, \ldots, \langle n \rangle$. Then the final result contains – besides 1 and $\infty$ – the integers 2, $\ldots$, $n$ marked either by $p$ or by $c$. An integer is marked by $p$ if and only if it is a prime number. This can be proved by a simple induction on $n$.

**Example 6.** Let $n = 9$, i.e., $c_0 = \langle 2 \rangle, \ldots, c_7 = \langle 9 \rangle, c_8 = \langle \emptyset \rangle$. Then we get results of the result sequence $d_0, \ldots, d_8$ as follows.

- $d_0 = H = \langle \emptyset \rangle$
- $d_1 = \text{res}_{A_0}(\langle \emptyset \rangle \cup \langle 2 \rangle) = \langle 2p \rangle$,
- $d_2 = \text{res}_{A_0}(d_1 \cup \langle 3 \rangle) = \langle \{1, 2p, 3p, 4c, 6c, 8c, 9c, \infty\}, *, 1 \rangle$. Note that the operation closure after the union adds $\langle 6, c \rangle$ to the set.
- $d_3 = \text{res}_{A_0}(d_2 \cup \langle 4 \rangle) = d_2$ because $\langle 4c \rangle$ is present. Hence, the reaction of the second type is inhibited.
- $d_4 = \text{res}_{A_0}(d_3 \cup \langle 5 \rangle) = \langle \{1, 2p, 3p, 4c, 5p, 6c, 8c, 9c, \infty\}, *, 1 \rangle$.
- $d_5 = \text{res}_{A_0}(d_4 \cup \langle 6 \rangle) = d_4$ because $\langle 6c \rangle$ is present.
- $d_6 = \text{res}_{A_0}(d_5 \cup \langle 7 \rangle) = \langle \{1, 2p, 3p, 4c, 5p, 6c, 7p, 8c, 9c, \infty\}, *, 1 \rangle$.
- $d_7 = \text{res}_{A_0}(d_6 \cup \langle 8 \rangle) = d_6$ because $\langle 8c \rangle$ is present.
- $d_8 = \text{res}_{A_0}(d_7 \cup \langle 9 \rangle) = d_7$ because $\langle 9c \rangle$ is present.

4. **Reaction systems over Sets**

In this section, we show that the classical set-based reaction systems can be transformed into reaction systems over the category **Sets** in such a way that enabledness of reactions on states and the respective results are preserved. The reaction systems resulting from this transformation are those where the inhibitor of each reaction has the special form $(i : I \to B, \emptyset I)$. It turns out that these reaction systems over **Sets** are normal forms in the class of all reaction systems over **Sets**. Altogether, set-based reaction systems and reaction systems over **Sets** have the same expressive power. The only difference is that the categorical framework is slightly more general on the syntactic level.

**Definition 3.**

1. A **set-based reaction system** $A = (B, A)$ consists of a finite set $B$, called **background set**, and a set $A$ of reactions where a **reaction** over $B$ is a triple $a = (R, I, P)$ of three subsets of $B$ with $R \neq \emptyset \neq P$.
2. A **state** of $A$ is a subset of $B$.
3. A reaction $a = (R, I, P)$ is **enabled** on a state $T$ if $R \subseteq T$ and $I \cap T = \emptyset$.
4. The **result** of $a$ on $T$, denoted by $\text{res}_a(T)$, is $P$ if $a$ is enabled on $T$, and $\emptyset$ otherwise.
5. The **result** of $A$ on $T$ is the union of the results of all reactions in $A$ on $T$, i.e., $\text{res}_A(T) = \bigcup_{a \in A} \text{res}_a(T)$.

Our definition of set-based reaction systems is a bit more liberal than the original one as we allow an empty inhibitor and we do not require that the intersection of reactant set and inhibitor set of a reaction is empty (although such reactions are void because they are never enabled).
A set-based reaction system $\mathcal{A} = (B, A)$ induces a transformed reaction system over $\textbf{Sets}$ $\text{trans}(\mathcal{A}) = (B, \text{trans}(A))$ with $\text{trans}(A) = \{\text{trans}(a) \mid a \in A\}$ and $\text{trans}(a) = (r: R \to B, (i: I \to B, \emptyset_I), p: P \to B)$ for $a = (R, I, P) \in A$ where $r, i, p$ are the inclusions of $R, I, P$ into $B$, respectively.

Given this transformation, the following holds.

**Proposition 1.** 1. $a \in A$ is enabled on $T \subseteq B$ if and only if $\text{trans}(a)$ is enabled on $t: T \to B$ where $t$ is the inclusion of $T$ into $B$.

2. $\text{res}_{\text{trans}(a)}(t) = \text{in}_a \cdot \text{res}_a(T) \to B$ where $\text{in}_a$ is the inclusion of $\text{res}_a(T)$ into $B$.

3. $\text{res}_{\text{trans}(A)}(t) = \text{in}_A \cdot \text{res}_A(T) \to B$ where $\text{in}_A$ is the inclusion of $\text{res}_A(T)$ into $B$.

**Proof.** 1. Let $a = (R, I, P) \in A$ and $\text{trans}(a) = (r, (i, \emptyset_I), p)$. Then $a$ is enabled on $T \subseteq B$ if $R \subseteq T$ and $I \cap T = \emptyset$. This is equivalent to $r \subseteq t$ and $i \cap t = \emptyset_B$ meaning that $\text{trans}(a)$ is enabled on $t$ because $i \cap t = \emptyset_B = i \circ \emptyset_I$.

2. Because of Point 1, there are two cases to consider.
   (a) $a$ is enabled on $T$ and $\text{trans}(a)$ on $t$: Then $(\text{in}_a: \text{res}_a(T) \to B) = (p: P \to B) = \text{res}_{\text{trans}(a)}(t)$.
   (b) Otherwise, $a$ is not enabled on $T$ and $\text{trans}(a)$ not on $t$: Then $(\text{in}_a: \text{res}_a(T) \to B) = \emptyset_B = \text{res}_{\text{trans}(a)}(t)$.

3. Using Point 2 and the construction of the categorical union in $\textbf{Sets}$ one gets: $(\text{in}_A: \text{res}_A(T) \to B) = (\text{in}_A: \bigcup_{a \in A} \text{res}_a(T) \to B) = \bigcup_{a \in A} (\text{res}_a(T) \to B) = \bigcup_{a \in A} (\text{res}_{\text{trans}(a)}(t)) = \text{res}_{\text{trans}(A)}(t)$.

\[ \square \]

It is obvious that a reaction system over $\textbf{Sets}$ is an image of the transformation $\text{trans}$ if and only if each inhibitor has the form $(i: I \to B, \emptyset_I)$. A reaction system over $\textbf{Sets}$ with this property is said to be in normal form as the following holds.

Let $\overline{\mathcal{A}} = (B, \overline{A})$ be a reaction system over $\textbf{Sets}$ that is not in normal form.

Then it can be transformed into one in normal form by $\text{nf}(\overline{\mathcal{A}}) = (B, \text{nf}(\overline{A}))$ with $\text{nf}(\overline{A}) = \{\text{nf}(\overline{a}) \mid \overline{a} \in \overline{A}\}$ and $\text{nf}(\overline{a}) = (r, (i - i_0: (I - I_0) \to B, \emptyset_I), p)$ for $\overline{a} = (r, (i: I \to B, i_0: I_0 \to I), p) \in \overline{A}$ where $I - I_0$ is the set-theoretic difference and $i - i_0$ the inclusion of $I - I_0$ into $B$.

Given this construction, the following holds.

**Proposition 2.** 1. $\overline{a} \in \overline{A}$ is enabled on $t: T \to B$ if and only if $\text{nf}(\overline{a})$ is enabled on $t$.

2. $\text{res}_{\text{nf}(\overline{a})}(t) = \text{res}_{\overline{a}}(t)$ for all $\overline{a} \in \overline{A}$.

3. $\text{res}_{\text{nf}(\overline{A})}(t) = \text{res}_{\overline{A}}(t)$.

**Proof.** 1. Enabledness requires $r \subseteq t$ in both cases with respect to the reactant part of enabledness. With respect to the inhibitor part of enabledness, one can use the set-theoretic property $I \cap T \subseteq I_0$ if and only if
\[(I - I_0) \cap T = (I \cap T) - I_0 \subseteq I_0 - I_0 = \emptyset\] because this implies for the corresponding inclusions \((i \cap t: I \cap T \to B) \subseteq i \circ (i_0: I_0 \to I)\) if and only if \(((i - i_0) \cap t: (I - I_0) \cap T \to B) \subseteq \emptyset\). The latter inclusion must be the equality because \(\emptyset\) has only itself as subset. Consequently, \(\bar{\pi}\) and \(\text{nf}(\bar{\pi})\) are both enabled on \(t\) or both not.

2. and 3. Point 1 together with the fact that \(\bar{\pi}\) and \(\text{nf}(\bar{\pi})\) have the same product for each \(\bar{\pi} \in A\) yields that the results are equal.

\[\square\]

5. Reaction systems over \(\Sigma\)-Graphs

In this section, we show that the graph-based reaction systems introduced in [8, 9] can be transformed into reaction systems over the category \(\Sigma\)-Graphs in such a way that enabledness of reactions on states and the respective results are preserved. The reaction systems resulting from this transformation are those where (1) the background \(\Sigma\)-graph \(G = (V, E, s, t, l)\) is simple, i.e., for each triple \((v, v', x) \in V \times V \times \Sigma\), there is at most one \(e \in E\) with \(s(e) = v, t(e) = v'\) and \(l(e) = x\), and (2) the inhibitor has the form \((i: I \to B, i_0: I_0 \to I)\) with a discrete graph \(I_0\), i.e., \(E_{I_0} = \emptyset\). In this way, graph-based reaction system can be seen as special cases of reaction systems over \(\Sigma\)-Graphs where the latter allows graphs with multiple edges.

**Definition 4.** 1. A graph-based reaction system \(A = (B, A)\) consists of a finite simple \(\Sigma\)-graph \(B\) and a set \(A\) of (graph-based) reactions of the form \(a = (R, I, P)\) where \(R\) and \(P\) are non-empty sub-\(\Sigma\)-graphs of \(B\) and \(I = (X, Y)\) is a pair of sets with \(X \subseteq V_B\) and \(Y \subseteq E_B\).

2. A state of \(A\) is a sub-\(\Sigma\)-graph of \(B\).

3. A reaction \(a = (R, (X, Y), P)\) is enabled on a state \(T\) if \(R \subseteq T\) and \(X \cap V_T = \emptyset = Y \cap E_T\).

4. The result of \(a\) on \(T\), denoted by \(\text{res}_a(T)\), is \(P\) if \(a\) is enabled on \(T\) and the empty graph \((\emptyset, \emptyset, 1_\emptyset, 1_\emptyset, 0_\Sigma)\) otherwise.

5. The result of \(A\) on \(T\), denoted by \(\text{res}_A(T)\), is the union \(\bigcup_{a \in A} \text{res}_a(T)\) of sub-\(\Sigma\)-graphs of all reactions in \(A\) on \(T\).

Note that, the definition of enabledness allows to forbid edges without forbidding all their sources and targets. More precisely, \(X\) and \(Y\) are independent of each other, i.e., \(X\) may contain vertices which are neither sources nor targets of edges in \(Y\) and \(Y\) may contain edges whose sources or targets are not in \(X\). To provide this option, the inhibitor of a reaction is not required to be a sub-\(\Sigma\)-graph. To construct the transformation, we use two sub-\(\Sigma\)-graphs of a \(\Sigma\)-graph \(B\) that are induced by \(I = (X, Y)\) with \(X \subseteq V_B\) and \(Y \subseteq E_B\):

1. \(\text{gr}(I) = (X \cup \{s_B(e), t_B(e) \mid e \in Y\}, Y, s_I, t_I, l_I)\) with \(s_I(e) = s_B(e), t_I(e) = t_B(e),\) and \(l_I(e) = l_B(e)\) for \(e \in Y\), and

2. \(\text{comp}(I) = (V_0 = \{s_B(e), t_B(e) \mid e \in Y\} \setminus X, \emptyset, \emptyset, \emptyset, \emptyset, \emptyset)\).
$gr(I)$ is the smallest sub-$\Sigma$-graph of $B$ that contains $I$, and $comp(I)$ is the discrete sub-$\Sigma$-graph of $B$ with the vertices one must add to $I$ to get $gr(I)$.

Now, let $A = (B, A)$ be a graph-based reaction system. Then one can construct the transformed reaction system over the category $\Sigma$-Graphs as follows. $trans(A) = (B, trans(A))$ with $trans(A) = \{ trans(a) \mid a \in A \}$ and $trans(a) = (r: R \rightarrow B, (i: gr(I) \rightarrow B, i_0: comp(I) \rightarrow gr(I)), p: P \rightarrow B)$ for $a = (R, I, P) \in A$ where $r, i$, and $p$ are the inclusions of $R, gr(I), P$ into $B$, respectively, and $i_0$ is the inclusion of $comp(I)$ into $gr(I)$.

For this transformation, the following holds for each graph-based reaction system $A = (B, A)$.

**Proposition 3.** 1. Let $a \in A$ and $T \subseteq B$. Then $a$ is enabled on $T$ if and only if $trans(a)$ is enabled on $t: T \rightarrow B$ where $t$ is the inclusion of $T$ into $B$.

2. $res_{trans(a)}(t) = in_a: res_a(T) \rightarrow B$ where $in_a$ is the inclusion of $res_a(T)$ into $B$.

3. $res_{trans(A)}(t) = in_A: res_A(T) \rightarrow B$ where $in_A$ is the inclusion of $res_A(T)$ into $B$.

**Proof.** Let $a = (R, I = (X, Y), P) \in A$ be enabled on $T \subseteq B$ meaning that

(a) $R \subseteq T$ and (b) $X \cap V_T = \emptyset = Y \cap E_T$. Consider, on the other hand, that $trans(a)$ is enabled on $t$ meaning that (c) $r \subseteq t$ and (d) $i \cap t \subseteq i \circ i_0$. As all morphisms are inclusions, (a) and (c) are equivalent, and (d) is equivalent to (e) $gr(I) \cap T \subseteq comp(I)$. As both graphs in (e) are sub-$\Sigma$-graphs of $B$, it is enough to consider the sets of vertices and edges separately. Therefore, (e) is equivalent to (f) $V_{gr(I) \cap T} \subseteq V_0$ and $E_{gr(I) \cap T} = \emptyset$. (f) turns out be equivalent to (b) as the following holds by the definition of intersection and $gr(I)$ as well as $X \cap V_0 = \emptyset$:

$$V_0 \supseteq V_{gr(I) \cap T} = (X \cup V_0) \cap V_T = (X \cap V_T) \cup (V_0 \cap V_T)$$

$$\emptyset = E_{gr(I) \cap T} = E_{gr(I)} \cap E_T = Y \cap E_T.$$

Altogether, this proves the first statement. The second and third statement follow from the first one and the fact that there is a one-to-one correspondence between sub-$\Sigma$-graphs and inclusions.

6. A further look at the categorial framework

In Section 3 one can see that reaction systems over a category can be smoothly defined if the underlying category provides empty subobjects, intersections, and unions. Moreover, seven example categories are discussed that meet these requirements. In this section, we want to point out two further significant aspects. First, the examples $Sets \times Sets, \Sigma-Sets, Maps$, and $\Sigma$-Graphs follow a common building principle, called diagram categories, that provides a reservoir of further potential example categories over which reaction systems are defined. Second, we have shown that the example categories meet the requirement for each category separately. It would be much more convenient if
one would get this for free – at least for certain types of categories. Actually, there is a chance with respect to diagram categories, but only if one strengthens the requirements.

6.1. Diagram categories

It may be noted that the category $\Sigma$-Graphs combines the category $\Sigma$-Sets for the labeling and two copies of Maps providing sources and targets. Moreover, the categories $\text{Sets} \times \text{Sets}$, $\Sigma$-Sets, Maps, and $\Sigma$-Graphs are built according to a common principle. They are diagram categories in the following sense.

Let $\text{Scm} = (C, A, s \colon A \to C, t \colon A \to C)$ be a directed graph (without labeling), called scheme, where the vertices are also called components and the edges arrows. Then $\text{Scm}$ induces the diagram category $C^{\text{Scm}}$ over $C$. Its objects are graph morphisms $\delta \colon \text{Scm} \to \text{gr}(C)$, where the domain is the scheme $\text{Scm}$ and the codomain is the category $C$ considered as a (very large) graph, i.e., $\text{gr}(C) = (\text{Ob}_C, \sum_{X,Y \in \text{Ob}_C} \text{Mor}_C(X,Y), \hat{s}, \hat{t})$ with objects of $C$ as vertices and the disjoint union of all sets of morphisms as set of edges, and $\hat{s}(f \colon X \to Y) = X$ and $\hat{t}(f \colon X \to Y) = Y$ for all $f \in \text{Mor}_C(X,Y)$ and all $X,Y \in \text{Ob}_C$. The objects of $C^{\text{Scm}}$ are called diagrams. Given two diagrams $\delta, \delta' \colon \text{Scm} \to \text{gr}(C)$, a morphism $g \colon \delta \to \delta'$ is given by a family of morphisms in $C$ such that $g_{(a)} \circ \delta_E(a) = \delta'_E(a) \circ g_{s(a)}$ for all $a \in A$. This means that the following diagram commutes:

$$
\begin{array}{ccc}
\delta_V(s(a)) & \xrightarrow{\delta_E(a)} & \delta_V(t(a)) \\
\downarrow{g_{s(a)}} & = & \downarrow{g_{t(a)}} \\
\delta'_V(s(a)) & \xrightarrow{\delta'_E(a)} & \delta'_V(t(a))
\end{array}
$$

The composition and the identities are defined componentwise in the category $C$. The components of $\text{Scm}$ are placeholders for objects, the arrows for morphisms. We also allow fixed components meaning that such a component is instantiated by some fixed object in each diagram.

Schemes may be drawn in the usual way: Bullets represent components connected by arrows from source bullet to target bullet each. In the case of a fixed object, the bullet is replaced by this object.

Four of our sample categories turn out to be diagram categories:

1. $\text{Sets} \times \text{Sets} = \text{Sets}^{\ast \ast}$,
2. $\Sigma$-Sets = $\text{Sets}^{\ast \to \Sigma}$,
3. Maps = $\text{Sets}^{\ast \to \ast}$,
4. $\Sigma$-Graphs = $\text{Sets}^{\Sigma \leftarrow \ast \to \ast}$.

If one allows to replace a bullet in a scheme $\text{Scm}$ by a $\ast$ and uses it in $\text{Sets}^{\text{Scm}}$ in such a way that the $\ast$ is not replaced by a set $X$, but by the set of strings $X^*$ over $X$, then even the category of $\Sigma$-Hypergraphs can be obtained as a diagram category: $\Sigma$-Hypergraphs = $\text{Sets}^{\Sigma \leftarrow \ast \to \ast}$. 

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Using the diagram concept, many categories like \( \Sigma\text{-Graphs} \) can be defined. Examples are the following.

1. The category \( \text{Graphs} = \text{Sets} \xrightarrow{\cdot \to \cdot} \) of directed (unlabeled) graphs.

2. The category \((\Sigma_V, \Sigma_E)\text{-Graphs} = \text{Sets} \xrightarrow{\Sigma_E \to \Sigma_V} \) of directed vertex- and edge-labeled graphs.

3. The category \( \text{BipartiteGraphs} = \text{Sets} \xrightarrow{\cdot \to \cdot} \) of bipartite directed graphs.

Let \( G = (V_1, V_2, E_1, E_2, s_1 : E_1 \to V_1, s_2 : E_2 \to V_2, t_1 : E_1 \to V_2, t_2 : E_2 \to V_1) \) be an object. There are two sets of vertices and two sets of edges. Edges have sources in \( V_1 \) and targets in \( V_2 \) or the other way round.

4. The category \( 3\text{-Hypergraphs} = \text{Sets} \xrightarrow{\cdot \to \cdot \to \cdot \to \cdot} \) of hypergraphs with hyper-edges of type 3. Let the three arrows be \( l, r, t \) respectively, and let \( H = (V, E, l_H, r_H, t_H) \) be an object. Then each \( e \in E \) is attached to a “left”, a “right”, and a “top” vertex so that \( e \) can be seen as a triangle.

5. The category \( 4\text{-Hypergraphs} = \text{Sets} \xrightarrow{\cdot \to \cdot \to \cdot \to \cdot} \) of hypergraphs with hyper-edges of type 4. Let the four arrows be \( \text{north}, \text{east}, \text{south}, \text{west} \), then the hyperedges are of type 4 and can be seen as “cells” with “tentacles” to the respective directions.

6. An interesting example where the underlying category is not \( \text{Sets} \) is the category \( \text{Graphs} \xrightarrow{\cdot \to \cdot} TG \) of \( TG \)-typed graphs for some type graph \( TG \). They are often used in the area of graph transformation as a well-working generalization of labeled graphs. A \( TG \)-typed graph is represented by a pair \((G, t)\), where \( G \) is a directed (unlabeled) graph and \( t : G \to TG \) is a graph morphism specifying the structure of \( G \). A \( TG \)-type-graph morphism \( f : (G_1, t_1) \to (G_2, t_2) \) is a graph morphism \( f_G : G_1 \to G_2 \) such that \( t_2 \circ f_G = t_1 \).

Indeed, \( \Sigma\text{-Graphs} \) is in a one-to-one correspondence to \( \text{Graphs} \xrightarrow{\cdot \to \cdot} TG(\Sigma) \) where \( TG(\Sigma) \) has a single vertex and, for each \( x \in \Sigma \), an \( x \)-labeled loop at the vertex. Similarly, \((\Sigma_V, \Sigma_E)\text{-Graphs} \) is in a one-to-one correspondence to \( \text{Graphs} \xrightarrow{\cdot \to \cdot} TG(\Sigma_V, \Sigma_E) \) where \( TG(\Sigma_V, \Sigma_E) = (\Sigma_V, \Sigma_V \times \Sigma_E \times \Sigma_V, pr_1, pr_3) \) with the first and third projections \( pr_1 \) and \( pr_3 \) as source and target mappings respectively.

Concerning diagram categories, it may be noted that categories of the form \( C \xrightarrow{\cdot \to \cdot} X \) for some fixed object \( X \) are called slice categories. Two of our examples, \( \Sigma\text{-Sets} = \text{Sets} \xrightarrow{\cdot \to \cdot \Sigma} \) and \( \text{TypedGraphs} = \text{Graphs} \xrightarrow{\cdot \to \cdot TG} \) are slice categories. Moreover, there is an alternative way to define diagrams that is often preferred in category theory. Instead of considering categories as graphs so that a diagram can be defined as a graph morphism, one may consider schemes as categories and a diagram as a functor. In this paper, we prefer the graph version to avoid the introduction of functors.

### 6.2. Strengthening of assumptions

If a diagram category \( C^{Scm} \) would inherit all needed properties from the underlying category \( C \) to define reaction systems over \( C^{Scm} \), then plenty of base
categories would be available for free. Unfortunately, this works only for a quite restricted, less interesting kind of schemes as long as one requires the properties of the general assumption in Section 3.1. To see this, let $C$ be a category meeting the general assumption, and $Scm = (C, A, s, t)$ be a scheme such that fixed components have only incoming arrows. One may try to construct empty subobjects, intersections, and unions by choosing the respective constructs componentwise for the free components. Consider, for example, the situation for the empty subobjects. Let $\beta : Scm \to gr(C)$ be a diagram of $C^{Scm}$. Then we want to construct $empty_\beta : \epsilon \to \beta$ for some $\epsilon : Scm \to gr(C)$ by $\epsilon(c) = EMPTY_{\beta_\epsilon(c)}$ for the free components $c$ and $\epsilon(\Sigma) = \Sigma$ for the fixed components $\Sigma$. But how can arrows be instantiated? If the arrow $ar$ has the source $c$ and the target $\Sigma$ for some fixed object $\Sigma$, then $\epsilon(ar)$ can be chosen as $\beta_E(ar) \circ empty_\beta_\epsilon(c)$ meaning that $empty_\beta_\epsilon(c)$ and $1_\Sigma$ satisfy the condition required for morphisms from $\epsilon$ to $\beta$ with respect to $ar$. But for an arrow $ar'$ with free source $c$ and free target $c'$, one fails to find a morphism $\epsilon(ar') : EMPTY_{\beta_\epsilon(c')} \to EMPTY_{\beta_\epsilon(c)}$, in general, because there are only morphisms from $EMPTY_{\beta_\epsilon(c)}$ to subobjects of $\beta_\epsilon(c)$ according to the property of empty subobjects. An exception is the case that $\beta_E(ar') \circ empty_\beta_\epsilon(c)$ is a monomorphism because then $\beta_E(ar') \circ empty_\beta_\epsilon(c)$ has the property required for $empty_\beta_\epsilon(c)$ so that both are equal as subobjects and the isomorphism from $EMPTY_{\beta_\epsilon(c)}$ to $EMPTY_{\beta_\epsilon(c')}$ can be chosen as $\epsilon(ar')$. Concerning intersection and union, one is faced with the same problem. Therefore, $C^{Scm}$ has componentwise constructed empty subobjects, intersections, and unions provided that the scheme consists of isolated components and arrows from free components to fixed components. It works also for objects $\beta$ where $\beta_E(ar')$ is a monomorphism for each $ar'$ with a free target. Both cases are rarely interesting. Of our example categories, only $\text{Sets} \times \text{Sets}$ and $\Sigma\text{-Sets}$ are of the first case. And the second case means, for example, for graphs, that source and target mapping need to be injective. Such a graph is a disjoint union of simple paths.

To do better, one can strengthen the requirements of the general assumption.

1. If a category $C$ has an initial object INIT meaning that there is a unique morphism $init_B : INIT \to B$ for each object $B \in Ob_C$, then $init_B$ is the empty subobject of $B$ provided that $init_B$ is a monomorphism and $init_B$ has only itself as subobject, i.e., each monomorphism $m : X \to INIT$ is an isomorphism. This allows to construct an initial object $\nu init$ in $C^{Scm}$ by $\nu init_\epsilon(c) = INIT$ for each free component $c$, $\nu init_\epsilon(\Sigma) = \Sigma$ for each fixed component $\Sigma$, $\nu init_\epsilon(ar) = init_\Sigma$ for each arrow $ar$ from component $c$ to a fixed component $\Sigma$, and $\nu init_\epsilon(ar') = 1_{INIT}$ for each arrow between free components. Let $\beta$ be an object of $C^{Scm}$. Then the family of monomorphism $init_\beta(c)$ for free components $c$ and $1_\Sigma$ for fixed components is obviously a monomorphism from $\nu init$ to $\beta$. Altogether, the situation can be seen as follows.
Concerning unions, the situation is more complicated. Nevertheless, there is a way to get the desired results if one combines the definition of union with the property \( \beta \) in Section 2.3 and strengthens them. To be precise, the pullback property makes sure that \( \beta \) is a monomorphism as all the component morphisms are monomorphisms. And \( \omega \iota \tau \) has only itself as subobject because all the free components have these properties. Altogether, \( \omega \iota \tau \) behaves in \( \mathbf{C}^{Scm} \) as \( \text{INIT} \) in \( \mathbf{C} \). The empty set \( \emptyset \) is such an initial object in the category \( \mathbf{Sets} \). This property is used in Section 2.2 to get the empty subobjects of the discussed examples.

If one changes the definition of an intersection in Section 2.2 in such a way that the three monomorphisms \( q_1, q_2 \) and \( q \) are replaced by arbitrary monomorphisms, then one has the definition of a pullback of two monomorphisms. The pullback property makes sure that \( p_1' \) and \( p_2' \) are monomorphisms so that \( p_1 \cap p_2 = p_i \circ p_i', i = 1, 2, \) is a monomorphism, too. In other words, a pullback of two monomorphisms is an intersection of the subobjects represented by the two monomorphisms. It is a well-known result in category theory that a pullback in \( \mathbf{C}^{Scm} \) can be constructed by the componentwise pullbacks into \( \mathbf{C} \). This means that \( \mathbf{C}^{Scm} \) provides intersection by pullbacks of monomorphisms if \( \mathbf{C} \) does. This is the case for the category \( \mathbf{Sets} \). We used the extendability of pullbacks in \( \mathbf{Sets} \) to pullbacks in \( \mathbf{Sets}^{Scm} \) for the examples in Section 2.2.

Concerning unions, the situation is more complicated. Nevertheless, there is a way to get the desired results if one combines the definition of union with the property \( \beta \) in Section 2.3 and strengthens them. To be precise, let \( S \) be a set of subobjects of an object \( B \). Let \( PB(S) \) be the set of all triples \( (p_1 \cap p_2): P_1 \cap P_2 \rightarrow B, p_1': P_1 \cap P_2 \rightarrow P_1, p_2': P_1 \cap P_2 \rightarrow P_2 \) being the intersections of \( p_1, p_2 \) for each pair \((p_1: P_1 \rightarrow B, p_2: P_2 \rightarrow B) \in S\). Then an object \( \text{COLIMIT}(PB(S)) \) together with a morphism \( p': P \rightarrow \text{COLIMIT}(PB(S)) \) for each \((p: P \rightarrow B) \in S\) is the colimit of \( PB(S) \) if the following holds.

(a) \( p'' \circ p_1' = p'' \circ p_2' \) for each triple \((p_1 \cap p_2, p_1', p_2') \in PB(S)\).

(b) For each object \( X \) together with a monomorphism \( \hat{p}: P \rightarrow X \) for each \((p: P \rightarrow B) \in S\) satisfying \( \hat{p} \circ p_1' = \hat{p} \circ p_2' \) for each triple \((p_1 \cap p_2, p_1', p_2') \in PB(S)\), there exists a unique morphism \( m: \text{COLIMIT}(PB(S)) \rightarrow X \) such that \( m \circ p'' = \hat{p} \) for each \( p \in S\).

The morphisms \( p \in S \) induce a morphism \( m_B: \text{COLIMIT}(PB(S)) \rightarrow B \). If this morphisms is a monomorphism and all the morphisms \( p'' \) are monomorphisms, then the
colimit of $PB(S)$ has the property required for $union(S)$ so that both coincide as subobjects.

Similarly to the intersection given by the pullback, the union given by the colimit can be extended from a category $C$ to each diagram category $C^{{Scm}}$. There is a further interesting aspect. The colimit of two subobjects as defined above is also called pushout – the pushout of a pullback. Moreover, the colimit of more than two subobjects can be constructed stepwise by iterated pushouts.

The considerations in this subsection indicate that it is meaningful to strengthen the general assumptions by requiring initial objects, pullbacks and colimits so that they provide empty subobjects, intersections, and unions, respectively, in the way described above. Categories satisfying these strengthened assumptions are closely related to the various variants of adhesive categories [16, 17, 10, 18, 12] which are successfully applied in the area of graph transformation. In adhesive categories, very strong relations - stronger than in our case - between pullbacks and pushouts of monomorphisms are required making intersections and unions of subobjects available for the definition of the application of graph transformation rules. Therefore, it may be interesting to relate our framework with adhesive categories. To work this out in detail is beyond the scope of this paper.

7. Conclusion

In this paper, we have proposed a categorical framework for the modeling of reaction systems. We have provided appropriate categorical notions including finite objects, subobjects, subobject inclusions, empty subobjects, intersections and unions of subobjects that allow the definition of reaction systems over a category and their interactive-process semantics in a quite similar way to the known set- and graph-based reactions systems. Moreover, we have shown that many categories meet the categorical requirements so that many structures become available on which reaction systems may be based on. This includes, in particular, quite a variety of graphs, hypergraphs, and other graph-like structures. But we have only done the very first steps into a categorical approach. To shine more light on the significance of the framework, the investigation should be continued including the following topics beside the issues raised at the end of the previous section.

1. Another way to find appropriate categories is the restriction of categories with the desired properties to subcategories. For example, if one restricts the category $\Sigma$-Graphs to simple graphs, then this category is closed under empty subobjects, intersections and unions so that this category inherits all reaction systems over $\Sigma$-Graphs if the background graph is simple. How do general restriction principles look like that yield such subcategories?
2. Most of the example categories in this paper have graph-like structures as objects. But we have pointed out that also monoids fit into the framework. Hence, one may like to know which kinds of algebraic structures form proper categories and how interesting reaction systems over such algebraic structures look like besides the prime number test in Section 3.

3. As pointed out at the end of Section 3.5 we expect that a good part of the theory of (set-based) reaction systems can be carried over to reaction systems over categories. Clearly, this needs to be worked out.

4. So far, everything we have discussed concerns reactions systems over categories. But there are more ways to bring reaction systems and category theory together. An example is the following. Whenever one has a class of entities, one may try to use them as objects of a category by choosing suitable morphisms. Therefore, one may ask how reaction systems over a category may be provided with a meaningful notion of morphisms. For example, given a reaction system $A = (B, A)$, a monomorphism $m: B \to B'$ induces a reaction system $m(A)$ by composing all the components of reactions with $m$. This is a candidate of a morphism on reaction systems. But we expect that there is much more to it.

5. Another direction of research of this kind may be to consider functors. A functor relates two categories by mapping the objects and morphisms of one category to the objects and morphisms of the other category respectively in such a way that compositions and identities are preserved. For instance, the usual embedding of $\Sigma$-graphs into $\Sigma$-hypergraphs induces such a functor. The other way round, the usual transformation of a hypergraph into a graph can be extended to morphisms. The question is which properties of a functor $F: C \to C'$ are sufficient such that a reaction system $A$ over $C$ is translated into a reaction system $F(A)$ over $C'$ by applying $F$ to all objects and morphisms of $A$. Whenever this works, one can compare reaction systems over different categories.

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