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Companions and an Essential Motion of a Reaction System

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Abstract. For a family of sets we consider elements that belong to the same sets within the family as companions. The global dynamics of a reactions system (as introduced by Ehrenfeucht and Rozenberg) can be represented by a directed graph, called a transition graph, which is uniquely determined by a one-out subgraph, called the 0-context graph. We consider the companion classes of the outsets of a transition graph and introduce a directed multigraph, called an essential motion, whose vertices are such companion classes. We show that all one-out graphs obtained from an essential motion represent 0-context graphs of reactions systems with isomorphic transition graphs. All such 0-context graphs are obtained from one another by swapping the outgoing edges of companion vertices.

Keywords: directed graphs, graph isomorphism, graphs on posets, dynamics of reaction systems, equivalence of reaction systems

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1. Introduction

A formal model of a system of reactions that depends on reactants and inhibitors, introduced by Ehrenfeucht and Rozenberg, can be considered, both with and without environmental interference [3, 1]. The dynamics of the system can be described by a directed graph. In the case when the states of the system change without considering the environmental context, the directed graph is a one-out graph, also called 0-context graph. The full dynamics of the system also includes changes introduced by the environment, and this is represented by a so called transition graph. The transition graph of a reaction system is of a specific form. The collection of all subsets of the background set (the set that provides the environment) S forms the vertex set. The sets that are targets of edges starting at a vertex consist of an element in 2^S and all its supersets. The 0-context graph is a subgraph of the transition graph, and due to the specific form of the transition graph, the 0-context graph uniquely determines the transition graph. In order to better understand the dynamics of a reactions system, properties of the 0-context graphs have been of interest [2, 5] and its relationship to the transition graph has been studied [4]. It turned out that drastically different 0-context graphs can define isomorphic transition graphs [4].

An isomorphism condition for directed graphs using outsets of the graph was introduced in [4]. The result is based on the notion of companion classes defined by a family of sets: two elements are companions if they belong to the same sets of the family. The isomorphism condition was also applied to characterize the 0-context graphs that correspond to reaction systems with isomorphic transition graphs.

With this paper we present the central concept of companions tailored directly to the outsets of transition graphs of reaction systems. We show a natural way to obtain the companion classes in a family of subsets of 2^S. A 0-context graph of a reaction system defines a family of subsets of 2^S and hence it has associated classes of companions. These companion classes can be taken as vertices of a multigraph, called here an *essential motion*. The essential motion has an edge from a class to another if an edge of the 0-context graph has a source and a target in the corresponding companion classes. We observe that any reaction system whose 0-context graph is associated to a given essential motion has a global dynamics with, up to isomorphism, unique transition graph.Therefore, the essential motion captures the global dynamics of a class of reaction systems whose 0-context graphs can be obtained from one another by swapping the targets of outgoing edges from companion vertices.

2. Companions for sets and subsets

For a family $\mathcal{O}$ of sets over a finite set V, two elements x, y of V are companions (with respect to $\mathcal{O}$) if they belong to the same region in the Venn diagram of $\mathcal{O}$, i.e., if they belong to the same sets in $\mathcal{O}$. More precisely:

Definition 2.1. Let V be a finite set and $\mathcal{O} \subseteq 2^V$ be a family of subsets of V and let $x, y \in V$. Then, x, y are *companions* (*with respect to* $\mathcal{O}$) if and only if for each $Z \in \mathcal{O}$ it holds that $x \in Z$ if and only if $y \in Z$.

Observe that the companion relation does not change if we change a family $\mathcal{O}$ to its intersection closure, the smallest family containing $\mathcal{O}$ and closed under intersection. Although this does not change the companion classes, assuming the family to be intersection-closed will later simplify the construction and representation of these classes.

In the context of reaction systems, our main application in this paper, the elements of V that make up the states of the system are sets, i.e., elements of 2^S, for a finite (background context) set S. Thus, $\mathcal{O} \subseteq 2^{2^S}$. In addition, the sets in the family $\mathcal{O}$ are of a special form: an upset of $A \subseteq S$, or the *cone* of A defined with $\mathrm{Up}(A) = \{X \subseteq S \mid A \subseteq X\}$. The minimal (by set inclusion) element A of the cone $\mathrm{Up}(A)$ is called the *apex* of the cone.

Clearly, a cone is unequivocally represented by its apex, and more generally, a family of cones by its family of apexes[1]. Thus, let $\mathcal{A} \subseteq 2^S$ be a collection of apexes. This defines the family $\mathrm{Up}(\mathcal{A}) = \{\mathrm{Up}(A) \mid A \in \mathcal{A}\}$.

If the family of sets is of the form $\mathcal{O} = \mathrm{Up}(\mathcal{A})$ over 2^S, then companionship can be rephrased as follows.

Definition 2.2. Let $\mathcal{A} \subseteq 2^S$ and let $X, Y \in 2^S$. Then X, Y are *companions (with respect to* $\mathrm{Up}(\mathcal{A})$*)* if and only if for each $A \in \mathcal{A}$ it holds that $A \subseteq X$ if and only if $A \subseteq Y$.

Observe that the intersection of two cones is again a cone: $\mathrm{Up}(A) \cap \mathrm{Up}(B) = \mathrm{Up}(A \cup B)$. Two sets X and Y are companions (with respect to $\mathrm{Up}(\mathcal{A})$) if and only if they belong to the same collection of cones. Hence if and only if they belong to the same intersection of cones. It is convenient if the intersection also belongs to the same family $\mathrm{Up}(\mathcal{A})$, i.e., $\mathrm{Up}(\mathcal{A})$ is intersection-closed. This does not change the companion classes. Equivalently, we like to consider that $\mathcal{A}$ is union-closed. We also assume that the empty set is an element in the closure under union (being the identity element for that operation).

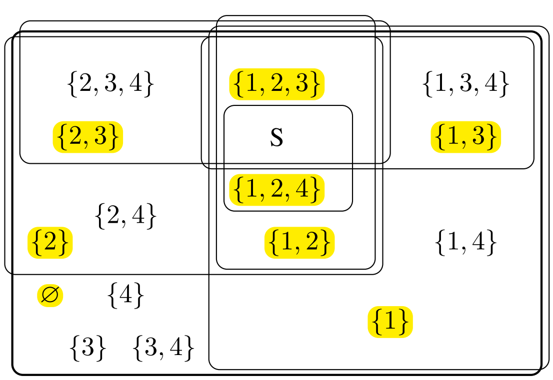


Figure 1. Companion sets, see Example 2.3

Example 2.3. Let $S = \{1,2,3,4\}$ and let $\mathcal{A} = \{\varnothing, \{1\}, \{2\}, \{1,2\}, \{1,3\}, \{2,3\}, \{1,2,3\}, \{1,2,4\}\}$. In Figure 1 (left) we have depicted a Venn diagram for $\mathrm{Up}(\mathcal{A})$, with the elements of $\mathcal{A}$ highlighted. The

[1]That is, *apices* for those appreciating Latin.

regions of the diagram represent the companion sets. This family of sets will return, as the collection of possible results from the reaction system considered in Example 3.2.

Constructing the explicit Venn representation to obtain the companion classes, as done in the example above, may turn out to be a rather tedious process, but more importantly, there is not always a nice "planar" representation in the sense that the companion classes can be represented as non-intersecting regions in the plane. And although one might learn from doing this for small examples, the final representation as a Venn diagram does not take explicitly into account the fact that the sets in $\mathcal{O}$ are cones. In this paper, we present a better method to construct the companion sets using the partial order structure of 2^S. As a teaser to things to come, see Figure 1 (right) where $\mathcal{A}$ is superimposed on the structure of 2^S. The boxed elements belong to $\mathcal{A}$ and the dashed box denotes an element in the closure of $\mathcal{A}$, but not in $\mathcal{A}$. The solid ($\longrightarrow$) arrows represent immediate set inclusions of elements in the closure of $\mathcal{A}$. Dashed (- - -) lines indicate companions in the Hasse diagram. As companionship is an equivalence relation, transitivity is applied.

When the family of cones is intersection-closed, every companion class can be represented by an apex of one of the cones.

Lemma 2.4. Let $\mathcal{A}$ be a union-closed collection in 2^S. Let $X \in 2^S$, and set $U_X = \bigcup_{A \in \mathcal{A}, A \subseteq X} A$. Then $U_X \in \mathcal{A}$ is the only apex companion to X.

Proof:
Since $\mathcal{A}$ is closed under union, the set U_X, as defined, is itself an element of $\mathcal{A}$. Let A be an arbitrary element of $\mathcal{A}$. Then $A \subseteq X$ if and only if $A \subseteq U_X$ (by construction). In other words, X and U_X are companions. The uniqueness of U_X follows from the fact that no two apexes are companions. $\square$

By construction, the set U_X as defined in the lemma above, is the maximal element in $\mathcal{A}$ below X. It is characteristic for the companion class containing X and U_X; it is the minimal element of the class. We will call it the *representative* of the companion set containing X.

This leads to a natural bottom-up way to construct the companion sets, by assigning the representatives to each set.

Construction 2.5. Let $\mathcal{A}$ be a union-closed collection in 2^S. We assign to each element Z in 2^S, the representative of the companion class of Z.

(1) Every set Z in $\mathcal{A}$ is assigned itself as a representative.

Otherwise, let Z in 2^S but not in $\mathcal{A}$. Consider all its predecessors in the Hasse diagram of 2^S, i.e., all sets $Y \subseteq Z$ such that $|Y| = |Z| - 1$.

(2) If one of the predecessors of Z is in $\mathcal{A}$, then we assign that predecessor as a representative of the companion class containing Z.

(3) If none of the predecessors of Z is in $\mathcal{A}$, then each of the predecessors must have the same representative for the companion class containing that predecessor. We assign that set as a representative to the companion class containing Z.

Proof:
First, we show that the procedure is well-defined.

(2) Observe that it is not possible that two predecessors of the set can be in $\mathcal{A}$, as otherwise, the set itself would be in $\mathcal{A}$ since the family is union-closed. Thus, at most one of the predecessors of Z is in $\mathcal{A}$.

(3) The fact that the representatives for all predecessors of Z are equal, can be seen from the following. Let X, X' be two different representatives assigned to predecessors of Z. We may assume these are of maximal size (among the representatives). Due to the union closure, also the union $X \cup X'$ is an element of $\mathcal{A}$ but larger than both X and X'. Thus, either Z equals $X \cup X'$, which means Z belongs to $\mathcal{A}$, a contradiction with our assumption that $Z \notin \mathcal{A}$, or one of the predecessors of Z, say Y, contains $X \cup X'$. Recall that the representative of a set is the maximal set in $\mathcal{A}$ contained in that set. Since one of the predecessors of Z, namely Y, has a representative that contains $X \cup X'$, which is larger than each of X and X', this contradicts our assumption that both X and X' are maximal.

Observe that for each set $Z \in 2^S$, the largest element in $\mathcal{A}$ below that set is defined as the representative of the companion class containing Z. Indeed, the representative is either the set Z itself (Case 1), or the largest set among the representatives of the predecessors Y of Z (Cases 2 and 3). $\square$

Implicitly, the construction yields a representation of the companion classes that is straightforward to obtain. In the Hasse diagram of 2^S mark all elements of (the union closure of) $\mathcal{A}$. Now work bottom up. At each step of the procedure connect a set to the predecessors from which the representative was inherited. This was either (1) none of the predecessors if the set itself belongs to $\mathcal{A}$, (2) a single predecessor if that predecessor is in $\mathcal{A}$, or (3) all predecessors (otherwise).

Example 2.6. Let $S = \{1, 2, 3, 4\}$. We consider two families of sets, and construct their companion classes using the method given above.

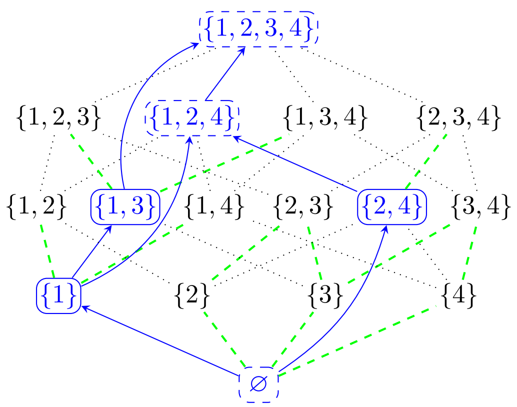


Figure 2. Construction of companions, see Example 2.6. Companion classes are connected by dashed (green) paths. Their representative is the bottom (boxed) element of the class.

First consider the family $\{\{1\}, \{1, 3\}, \{2, 4\}\}$. Closing this family under union, we add $\varnothing$, $\{1, 2, 4\}$, and $\{1, 2, 3, 4\}$ to obtain a set of apexes, depicted in the left diagram of Figure 2. The original sets in the family are boxed and those added by closure are dashed. Their set inclusion relation is depicted by solid (blue) arrows.

The construction adds the dashed (green) lines in the diagram, bottom-up, assigning a companion-representative to the companion class of each set in 2^S by looking at the predecessors for each set, inheriting their companion class representative.

The diagram on the right in Figure 2 shows the result of the construction for the family $\{\{1\},\{3\},\{1,3\},\{2,4\}\}$, where $\{3\}$ is added to the original family depicted on the left.

3. Companions for reaction systems

Reaction systems [3] operate within a finite set of available objects. Starting with a subset of these objects the systems evolves by applying rules called reactions.

Definition 3.1. A *reaction system* is a pair $\mathcal{S} = (S, A)$ where S is a finite set, the *background set*, and $A \subseteq 2^S \times 2^S \times 2^S$ is a set of *reactions* in S. Given a reaction $a = (R, I, P)$ in A, its components are called the *reactant*, *inhibitor*, and *product set of* a, respectively.

Let $X \subseteq S$. We say that the reaction $a = (R, I, P)$ is *enabled* in X if all of its reactants are present in X, while none of its inhibitors is. In that case, the *result* of the reaction equals P. Thus, $\mathrm{res}_a(X) = P$ if and only if $R \subseteq X$ and $I \cap X = \varnothing$. Otherwise, a is not enabled in X and $\mathrm{res}_a(X) = \varnothing$. Different reactions do not compete for resources, thus the result of X in $\mathcal{S}$ equals the union of the individual results for all reactions, that is, $\mathrm{res}_{\mathcal{S}}(X) = \bigcup_{a\in A} \mathrm{res}_a(X)$.

Example 3.2. We return to the example of [1]. Consider the following six reactions on background set $S = \{1, 2, 3, 4\}$:

$$a_1 = (\{1\},\{3\},\{2\}) \qquad a_2 = (\{2\},\{1\},\{1\}) \qquad a_3 = (\{2\},\{3\},\{3\})$$
$$a_4 = (\{3\},\{1,2\},\{1,2,4\}) \quad a_5 = (\{4\},\{3\},\{1,2\}) \quad a_6 = (\{1,3\},\{2,4\},\{2,3\})$$

In $X = \{1, 3\}$, reactions a_1, a_2, a_3, a_4 and a_5 are not enabled because one of their inhibitors is present in X. Consequently only a_6 is enabled, and $\mathrm{res}_{\mathcal{S}}(X) = \{2, 3\}$. In $X = \{2\}$ both a_2 and a_3 are enabled and $\mathrm{res}_{\mathcal{S}}(X) = \{1, 3\}$.

As an isolated system, the result function $\mathrm{res}_{\mathcal{S}}$ describes the step-by-step evaluation of the system $\mathcal{S}$ from state X to its successor state $\mathrm{res}_{\mathcal{S}}(X)$. In general, however, the system operates within an environment. At each step, this environment may add new elements to the state, and thus, the system may evolve from state X to any state that includes $\mathrm{res}_{\mathcal{S}}(X)$ as a subset.

These two viewpoints, the isolated system and the system in context, lead to two graphs representing the step-wise behaviour of a reaction system. Recall that a one-out graph is a (directed) graph where each vertex has a unique outgoing edge.

Definition 3.3. The 0-*context graph* of a reaction system $\mathcal{S} = (S, A)$ is the one-out graph $G^0_{\mathcal{S}} = (2^S, E)$ with edge set $E = \{\, (v, \mathrm{res}_{\mathcal{S}}(v)) \mid v \in 2^S \,\}$.

The *(global) transition graph* of $\mathcal{S}$ is the graph $G_{\mathcal{S}} = (2^S, E)$ with edge set $E = \{\, (v, w) \mid v \in 2^S, \mathrm{res}_{\mathcal{S}}(v) \subseteq w \,\}$.

In these two graphs the nodes are sets, and as such, they have a clear identity. Using this identity the transition graph of a system can be obtained directly from its 0-context graph: $G_\mathcal{S} = \upharpoonleft G^0_\mathcal{S}$, where for a one-out graph G with node set 2^S, its *extension* $\upharpoonleft G$ contains all edges (u, w) with $v \subseteq w$ for which (u, v) is an edge in G.

Two transition graphs can be isomorphic, even when the 0-context graphs for their reaction systems are non-isomorphic. A critical tool to describe this is the collection of all possible sets that are the result of the system for some subset of S, i.e, the range of the result function $\mathrm{res}_\mathcal{S}$. We denote this collection by $\mathrm{RES}_\mathcal{S}$.

Example 3.4. The 0-context graph $G^0_\mathcal{S}$ of the system $\mathcal{S}$ from Example 3.2 is depicted in Figure 3.

In this example, $\mathrm{RES}_\mathcal{S} = \{\varnothing, \{1\}, \{2\}, \{1, 2\}, \{1, 3\}, \{2, 3\}, \{1, 2, 3\}, \{1, 2, 4\}\}$. These are the nodes of $G^0_\mathcal{S}$ with incoming edges.

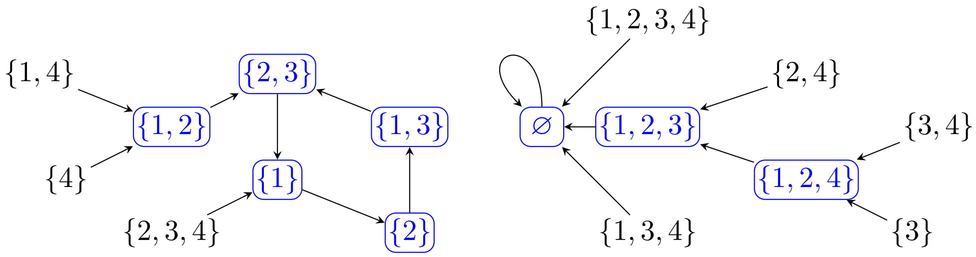


Figure 3. The zero-context graph $G^0_\mathcal{S}$ for the reaction system from Example 3.2

Note that in most papers on reaction systems, the reactant and inhibitor sets are postulated to be non-empty. In our paper, this technical requirement is not essential.

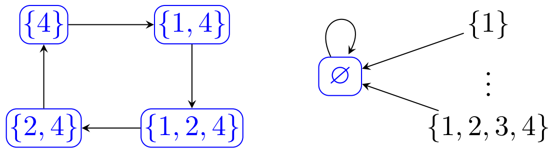
If we allow ourselves this generality, *every* suitable one-out graph is a 0-context graph: for each one-out graph G on 2^S there is a reaction system $\mathcal{S}$ such that G is the 0-context graph of $\mathcal{S}$. The reason is that we can 'program' the edges of G by choosing a single reaction for each edge, cf. [1]. For edge (X, Y) we set the reaction $(X, S \setminus X, Y)$ that is only enabled in X, and hence $\mathrm{res}(X) = Y$. Such systems are called maximally inhibited reaction systems in [6]. The only difference with reaction systems in the restricted sense is that $(\varnothing, \varnothing)$ and $(S, \varnothing)$ are edges in G_S, as no reactions are enabled in either the empty set or the full background set, when we assume that each reaction needs both a reactant and an inhibitor.

Reaction systems can be designed such that their behaviour exhibits certain properties. One of the examples is the design of a Gray code by Kleijn et al. [5]. We use these systems as a case study.

Example 3.5. The two element Gray code $00 \to 01 \to 11 \to 10 \to 00$ is implemented in a reaction system (see Example 2.1 in [5]) with background set $\{1, 2, 3, 4\}$ and the three reactions:

$$a = (\{4\}, \{3\}, \{4\}) \quad b = (\{1, 4\}, \{3\}, \{2\}) \quad c = (\{4\}, \{2, 3\}, \{1\})$$

The symbols $3, 4$ act as a universal inhibitor and universal reactant respectively. They are 'dummy' symbols added to satisfy the requirement that the first two components are nonempty. The four sets that contain 4 but not 3 form the required Gray code, with 1 and 2 representing the two bits of the code. In all twelve remaining sets, none of the reactions is enabled, so each will yield the empty set. The resulting 0-context graph is depicted below.



Computing the companion classes, see Figure 4 (left), we observe that all sets without 4 form a large companion class with a representative $\varnothing$. Each of the four sets with 4 but without 3 is companion to its copy with 3 added.

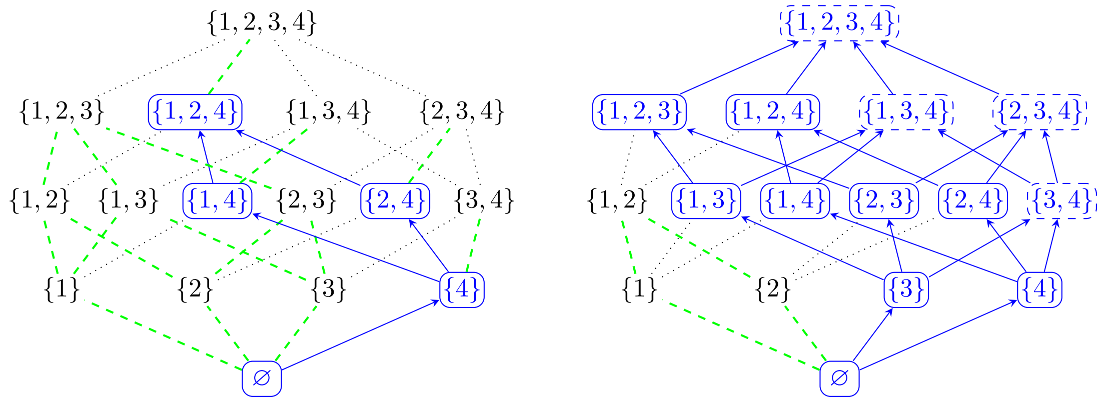
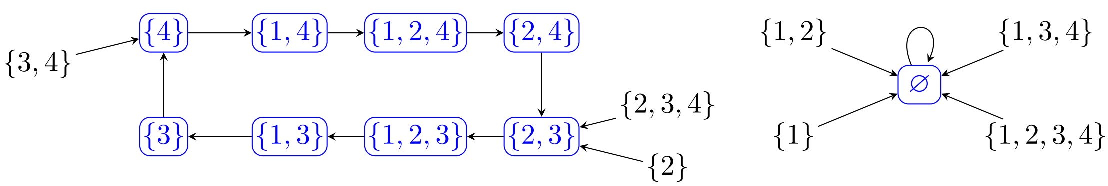


Figure 4. Companion classes for Example 3.5 and Example 3.6.

Example 3.6. Example 2.3 from [5] implements a reaction system that mimics the forward and backward generation of Gray code. Its six reactions are as follows.

$$
\begin{array}{lll}
a = (\{4\}, \{2,3\}, \{1,4\}) & b = (\{1,4\}, \{3\}, \{2,4\}) & c = (\{2,3\}, \{4\}, \{1\}) \\
d = (\{2\}, \{1\}, \{2,3\}) & e = (\{1,3\}, \{4\}, \{3\}) & f = (\{3\}, \{1,2\}, \{4\})
\end{array}
$$

We depict its 0-context graph below. The central eight node loop is the desired feature. It consists of all sets that contain exactly one of 4 ('forward') or 3 ('backward').



We again compute the companion classes, see Figure 4 (right). Unlike in the previous example, several sets have to be added to the resulting sets of the reaction system to make the family union-closed (dashed boxes in the diagram). Since the number of out-sets (and their closure) is rather large, there is only a single non-singleton companion class, consisting of all sets containing neither 3 nor 4.

4. Essential motion

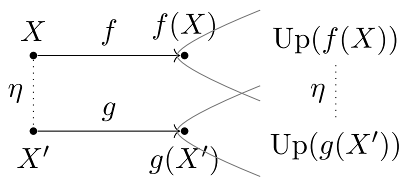
In this section, we associate the notion of companion sets with the notion of companion one-out graphs. In [4], it was shown that the companions of the one-out graph G_S^0 uniquely determine the isomorphism class of G_S. Here, we present how a graph structure obtained from the equivalence classes of companion sets can intrinsically contain all companion one-out zero context graphs. We call this structure the essential motion of a reaction system.

Edges of a one-out graph define a function from vertices to vertices. We identify a function $f : V \to V$ with the one-out graph G_f that has edges $(x, f(x))$ for all $x \in V$.

Above we have introduced the 0-context graph $G_{\mathcal{S}}^0$ of a reaction system $\mathcal{S}$ as the one-out graph representing the function $\mathrm{res}_{\mathcal{S}}$. If, as in this case, the nodes of the graph are, in fact, sets ($V = 2^S$), then we can use the set structure to extend the graph G_f to $\upharpoonleft G_f$, and study when G_f and G_g define isomorphic graphs $\upharpoonleft G_f$ and $\upharpoonleft G_g$.

The following concept is central to our considerations cf. [4].

Definition 4.1. We say that two functions $f, g : 2^S \to 2^S$ are *companions* if there is a bijection η on 2^S such that, if $\eta(X) = X'$, then $\eta(\mathrm{Up}(f(X))) = \mathrm{Up}(g(X'))$ for each $X \subseteq S$.



We call one-out graphs G_f and G_g *companions* whenever their functions f and g are. The following theorem is a direct consequence of Theorem 3.6 in [4].

Theorem 4.2. Let $f, g : 2^S \to 2^S$. Then $\upharpoonleft G_f$ and $\upharpoonleft G_g$ are isomorphic if and only if f and g are companions.

This has an immediate implication for reaction systems and the graphs representing their behaviour, without and with context.

Corollary 4.3. (Theorem 5.6 in [4])
For reaction systems $\mathcal{S}$ and $\mathcal{S}'$, their transition graphs $G_{\mathcal{S}}$ and $G_{\mathcal{S}'}$ are isomorphic if and only if the 0-context graphs $G_{\mathcal{S}}^0$ and $G_{\mathcal{S}'}^0$ are companions (if and only if the functions $\mathrm{res}_{\mathcal{S}}$ and $\mathrm{res}_{\mathcal{S}'}$ are companions).

A generic way of obtaining pairs of functions that are companions is by swapping the targets of the outgoing edges of a pair of companion nodes.

Definition 4.4. Let $f : 2^S \to 2^S$ be a function, and let $X, Y \in 2^S$ be companions with respect to $\mathrm{range}(f)$. The X, Y-*swap* of f, denoted $f_{X,Y}$, is the function that equals f, except that $f_{X,Y}(X) = f(Y)$ and $f_{X,Y}(Y) = f(X)$.

Lemma 4.5. Let $f : 2^S \to 2^S$ be a function, and let X, Y in 2^S be companions with respect to range(f). Then f and $f_{X,Y}$ are companions.

Proof:
Consider the bijection on 2^S that is the identity on 2^S, except that the elements X and Y are swapped: $\eta(X) = Y$ and $\eta(Y) = X$. We will show that the upsets of f and $f_{X,Y}$ are related via η.

First, see Lemma 3.1 in [4], observe that X and Y are elements of the same upsets of f: $X \in \mathrm{Up}(f(U))$ if and only if $f(U) \subseteq X$, but this is equivalent to $f(U) \subseteq Y$, as X and Y are companions for $\mathrm{range}(f)$, hence $Y \in \mathrm{Up}(f(U))$. Let $U \in 2^S$. If U differs from X, Y, then $\eta(U) = U$, and $f(U) = f_{X,Y}(U)$. Now η is a bijection on $f(U)$ as it is the identity on 2^S except that X, Y are swapped. However, whenever one of X, Y is in $f(U)$, they both are.

Now consider $U = X$. Then $\eta(X) = Y$, and $f_{X,Y}(Y) = f(X)$. Again η is a bijection on $\mathrm{Up}(f(X))$. The case $U = Y$ is symmetric. □

Swaps can be composed. Given a sequence of (distinct) sets $X_1, \ldots X_n$, all in the same companion class, and a sequence $Z_1, \ldots, Z_n$ such that $f(X_i) = Z_i$, successive swaps can implement any permutation $\pi = (\pi(i), \ldots, \pi(n))$ of $1, \ldots, n$ and define a new function with $f_\pi(X_i) = Z_{\pi(i)}$ (and $f(X) = f_\pi(X)$ unchanged for other values). The resulting function is companion to the original, by successive application of Lemma 4.5.

Example 4.6. Consider the reaction system from Example 3.2, the 0-context graph of which was given in Figure 3. The relevant companion classes are depicted in Figure 1.

The pair $\{1,3\}, \{1,3,4\}$ are companions and we may swap their out-edges. Moreover, the triple $\varnothing, \{4\}, \{3,4\}$ consists of companions, so again, we can cyclically shift their outgoing edges. In this way, we obtain a new one-out graph, the 0-context graph of a new reaction system, see Figure 5.

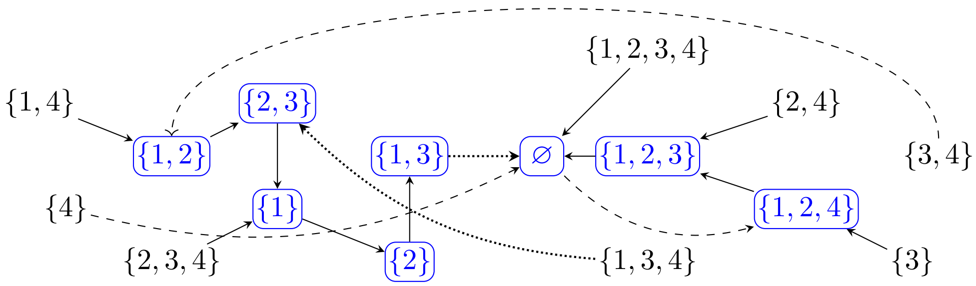
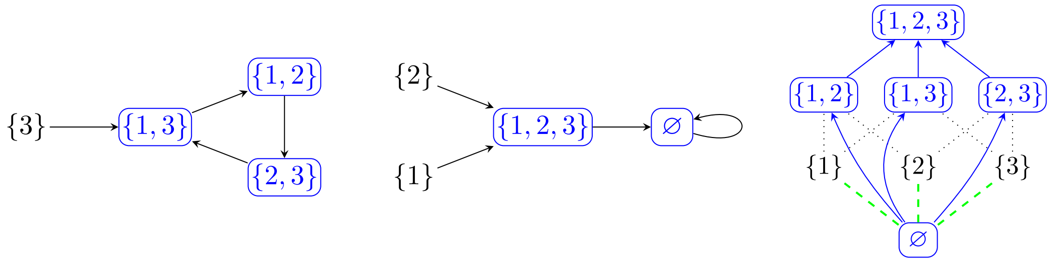


Figure 5. Zero context graph $G^0_{\mathcal{S}}$ for the reaction system from Example 3.2 with swaps

Note that a bijection $\eta : 2^S \to 2^S$ as in the definition of companion functions is a set to set mapping. It is not necessarily an extension of a bijection $\xi : S \to S$, i.e., an element to element mapping.

Example 4.7. In the diagram illustrated below, $\{2\}$ and $\{3\}$ are companions, so when we switch their outgoing edge targets, $\{2\} \to \{1,3\}$ and $\{3\} \to \{1,2,3\}$. Thus, $\eta(\{2\}) = \{3\}$ and $\eta(\{3\}) = \{2\}$, whereas $\eta(X) = X$ for all $X \not\in \{\{2\}, \{3\}\}$. Now, $f(\{2\}) = \{1,2,3\}$ and $g(\eta(\{2\})) = g(\{3\}) = \{1,2,3\}$.

Thus, $\eta(\mathrm{Up}(\{1,2,3\}) = \eta(\{\{1,2,3\}\}) = \{\{1,2,3\}\} = \mathrm{Up}(\{1,2,3\}) = \mathrm{Up}(g(\{3\})$. However, if $\xi(2) = 3$ and $\xi(3) = 2$, this would lead to $\{1,3\} \to \{1,2\}$, which is clearly not the case as $\{1,3\}$ has two incoming edges and $\{1,2\}$ has one.



The importance of the swap operation is indicated by the following result, which shows that the swap of function values at companion sets (with respect to the range of the function) leads to isomorphic graph extensions. The result below is a special case of Theorem 4.2.

Corollary 4.8. Let $f : 2^S \to 2^S$ be a function, and let X, Y in 2^S be two companions with respect to $\mathrm{range}(f)$. Then $\upharpoonleft f$ and $\upharpoonleft f_{X,Y}$ are isomorphic.

We introduce a convenient abstraction of one-out graphs on 2^S, such that all graphs obtained by edge swaps on companion nodes are represented by the same object. This is done by defining a multigraph, where nodes represent the companion classes, and every edge from a set in one companion class to a set in another is represented by a separate edge from the first companion class to the second.

For a family of sets $\mathcal{A}$ over 2^S we use $\mathcal{A}(X)$ to denote the companion class of $X \in 2^S$ with respect to $\mathcal{A}$.

Definition 4.9. Let $f : 2^S \to 2^S$, and let $\mathcal{A}$ be the union closure of $\mathrm{range}(f)$. The *essential motion* of f is the multigraph with vertices $\{\mathcal{A}(X) \mid X \in \mathcal{A}\}$ and edges $(\mathcal{A}(X), \mathcal{A}(f(X)))$ for all $X \in 2^S$.

Example 4.10. Consider the reaction system $\mathcal{S}$ from Example 3.2, the 0-context graph of which was depicted in Figure 3. Its companion sets are given in Figure 1.

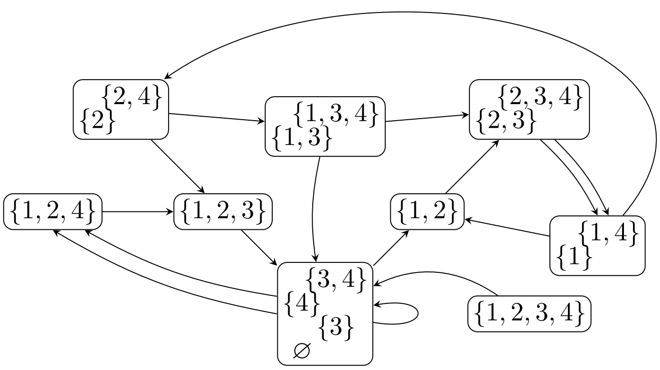


Figure 6. The essential motion of the reaction system from Figure 3.

The vertices of the essential motion for $\mathcal{S}$, or rather $\mathrm{res}_{\mathcal{S}}$, are the nine companion classes of $\mathrm{res}_{\mathcal{S}}$.

The companion class containing $\varnothing$ contains four elements: $\varnothing$, $\{3\}$, $\{4\}$ and $\{3,4\}$. The result function $\mathrm{res}_{\mathcal{S}}$ maps these sets to $\varnothing$, $\{1,2,4\}$, $\{1,2\}$, and $\{1,2,4\}$, respectively. This implies that the vertex representing this class has four outgoing edges, to the vertices representing the respective classes of these four sets. Among these edges, there is one loop and a pair of parallel edges. For the final multigraph, see Figure 6.

Corollary 4.11. If g is obtained by a finite sequence of edge swaps from a function $f : 2^S \to 2^S$ then f and g define the same essential motion.

Proof:
Consider the swaps at each companion class C separately. Assume that $C = \{X_1, \dots, X_n\}$ is a companion class of $\mathrm{range}(f)$ and let $f(X_i) = Z_i$ for $i = 1, \dots, n$. All edges (X_i, Z_i) in the one-out graph G_f representing f, are mapped to edges starting at C in the essential motion. Permuting the order of the Z_i does not change the resulting multi-graph. □

We can reverse the process and obtain any function g that results from swapping companion edges given function $g : 2^S \to 2^S$ starting at the essential motion graph and for each companion class C associate the outgoing edges to the elements of C.

Example 4.12. In Figure 6, consider the vertex corresponding to the companion class of the set $\{1,3\}$, which also contains the set $\{1,3,4\}$. Since this class contains two sets, the vertex corresponding to this class has two outgoing edges, namely, to the classes of $\varnothing$ and $\{2,3\}$. Thus, we have two possibilities for the function g that defines this essential motion. Either $g(\{1,3\}) = \varnothing$ and $g(\{1,3,4\}) = \{2,3\}$, as done in Figure 5, or $g(\{1,3\}) = \{2,3\}$ and $g(\{1,3,4\}) = \varnothing$, as in Figure 3. Similar choices apply to the other classes.

Note that the only two outgoing edges from the vertex with companions $\{2,3\}$ and $\{2,3,4\}$ are parallel. Hence, swapping those two edges will not change the function at all.

Any two reaction systems that have 0-context graphs that can be derived from an essential motion are related by a series of swaps and by Corollary 4.8 have isomorphic transition graphs.

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