ABSTRACT

We generalize a pushout complement algorithm from graph rewriting to finitely-presented C-sets and structured cospans, allowing us to perform double pushout rewrites generically over a broad class of combinatorial data structures and open systems thereof. As part of this work, we present a general algorithm for pattern matching in C-sets via the construction of C-set homomorphisms, which generalizes the computation of graph homomorphisms. We demonstrate the utility of this generalization through applications to Petri net model space exploration, rewriting of wiring diagrams with symmetric monoidal structure, and open Petri net rewriting. These applications highlight the important productivity gains due to our implementation of C-set rewriting for arbitrary C, which allows us to easily extend our implementation to new categorical constructions, including slice categories and cospan categories.

Keywords  Double pushout rewriting · category theory · graph rewriting

1 Introduction

Term rewriting is a foundational technique in computer algebra systems, programming language theory, and symbolic reasoning approaches to artificial intelligence. What a symbolic term represents is not determined by its syntax, and likewise the meaning of a syntactic rewrite varies depending on the application. A rewrite can represent an evolution over time, a possible choice, or a replacement with a term that is behaviorally or semantically equivalent.

While term rewriting is concerned with tree-shaped terms in a logical theory, the field of graph rewriting extends these techniques to more general shapes of terms. The primary paradigm for rewriting graphs is double pushout (DPO) rewriting, introduced in 1973 [10] for transforming data structures, most notably graphs. The technique has found many applications in the natural sciences. For example, in chemistry [11], the atoms and bonds of a molecule are modeled as the vertices and edges of a graph, and then chemical reactions become graph transformations. In computer science, specifying computations via graph transformation is a fundamental concept within programming, concurrency, and model transformation [11]. Furthermore, tree-shaped terms can be very space inefficient on a computer due to their requirement of separate copies of shared arguments. Graph terms [22] provide a more efficient representation by allowing argument sharing at a syntactic level.

Considering data structures beyond graphs can also have practical benefits for automated reasoning. As an example, the interchange law of a symmetric monoidal category (SMC) requires that the composition and product operations commute, i.e., $(f; g) \otimes (h; k) = (f \otimes h); (g \otimes k)$ for any compatible morphisms $f, g, h, k$. Due to such equations, the equality of SMC morphisms cannot be determined by structural equality of tree terms. However, by representing SMCs as directed wiring diagrams, the interchange law and other laws are quotiented out [21], which underlines the importance of rewriting for wiring diagrams.

Another mathematical structure of practical value for automated reasoning is the structured cospan, which formalizes open systems that can interact with an external environment [3]. Common examples for these systems include electrical circuits, chemical reaction networks, and internet networks. These are all systems that can be considered in isolation yet can also be reasonably extended or connected to other systems. The structured cospan formalism is compatible with many different structures; however, restricting attention to rewriting open graphs, the data to be rewritten are cospans of graphs. Cicala showed that this is possible by developing a framework relating DPO to structured cospans.

DOUBLE PUSHOUT REWRITING OF C-SETS

Kristopher Brown
Department of Computer Science
University of Florida
kristopher.brown@ufl.edu

Evan Patterson
Topos Institute
evan@topos.institute

James Fairbanks
Department of Computer Science
University of Florida
fairbanksj@ufl.edu
We lastly consider open systems by extending the earlier example of epidemiological Petri net models to the case where

\[ \{ \text{with the set} \} \]

rewriting that lies between the previous two limits, i.e. the application of tactics, which automate the process of

\[ \text{in this setting, one would use rewriting as a “hands-off” or automated system that} \]

We review \( C \)-world, but furthermore yields a means of decomposing complex, closed systems into simpler components as well as a structurally inductive viewpoint on rewriting these systems.

This paper begins by reviewing the double pushout algorithm in the context of graphs, which is the most common setting for DPO. As each of the preceding abstract data structures can be modeled with category-theoretic notion of a \( C \)-set, we review \( C \)-sets before generalizing DPO to arbitrary \( C \)-sets. We lastly study three applications of rewriting, which have been implemented in Catlab.jl \[12\], a core package of the AlgebraicJulia ecosystem. Each of these applications is naturally connected to a different style of user interaction with rewriting systems.

First, the exploration of a scientific or engineering model space is an iterative process that requires close connection between empirical and computational science: one postulates a model, evaluates its fit with the world, and then seeks to incrementally improve the underlying model. With whole-grain Petri net epidemicological models as a case study, this is a paradigm of rewriting as a “hands-on” user interface for direct manipulation of data structures (e.g. Quantomatic \[15\], Cartographer \[25\], the explicit rewrite tactics of proof assistants \[14,13\]). In this scenario, there is a specific rewrite the tool helps the user apply to a target term.

In computer science applications such as functional programming, database queries, and numerical linear algebra, the programming language is modeled as a category whose morphisms are programs, and a compiler can use equational reasoning to analyze, verify, or optimize programs. These systems can be implemented with rewriting wiring diagrams with symmetric monoidal structure. In this setting, one would use rewriting as a “hands-off” or automated system that computes a canonical form. In this case, we seek to apply all possible rewrites indiscriminately until some termination criteria are met.

We lastly consider open systems by extending the earlier example of epidemiological Petri net models to the case where models can be both combined and decomposed into subcomponents. This offers opportunities for combining automated reasoning with domain knowledge: for example, a rule which is only applicable in certain contexts can still benefit from the simplicity of “hands-off” rewriting like above, as a domain expert may be able to restrict this rewriting to relevant subcomponents where the rule is known to be valid. This is connected to a third possibility for user interaction with rewriting that lies between the previous two limits, i.e. the application of tactics, which automate the process of selecting rewrites in order to achieve a user-specified goal. This is crucial for many computer algebra tasks, such as proving \( \sin^2(x) + \cos^2(x) = 1 \) via a sequence of rewrites. In such settings, indiscriminately applying rewrite rules is non-terminating and infeasible in practice due to the search space size, whereas manually applying rewrite rules can be incredibly challenging and tedious compared to high-level instructions.

2 Preliminaries

2.1 Graph Rewriting

There are many notions of graph in the literature (simple graphs, directed graphs, multigraphs, colored graphs, with or without loops, with or without weights). For our exposition on graph rewriting, we consider finite, directed multigraphs. A graph \( G \) is defined by two finite sets, denoted \( G_E \) and \( G_V \), for edges and vertices, respectively. Furthermore, two functions \( G_{src}, G_{tgt} : G_E \to G_V \) define the source and target vertex for each edge. We can compactly represent sets and functions by working within the skeleton of \( \text{FinSet} \), i.e. a natural number \([n]\) is identified with the set \( \{1, \ldots, n\} \). A function \( f \) from \([n]\) to \([m]\) can be compactly written as a list \([x_1, x_2, \ldots, x_n]\), where \( x_i \) sends the element \( i \in [n] \) to an element of the codomain \([m]\). As an example, consider the graph \( G \) defined by \( G_V = [3] \), \( G_E = [3] \), \( G_{src} = [1, 2, 2] \), \( G_{tgt} = [2, 3, 3] \):

\[
\begin{array}{ccc}
1 & \rightarrow & 2 \\
\downarrow & & \downarrow \\
&& 3
\end{array}
\]

Given two graphs \( G \) and \( H \), a graph homomorphism (or simply morphism) \( h : G \to H \) is defined as a mapping of edges, \( h_E : G_E \to H_E \), and a mapping of vertices, \( h_V : G_V \to H_V \), such that the structure of \( G \) is preserved, i.e., the following diagrams commute:

\footnote{Baez et al. prove that whole-grain Petri nets are a subcategory of \( \Sigma \) nets, which freely generate strict symmetric monoidal categories \[4\]. Traditional Petri nets freely generate commutative monoidal categories. However, for simplicity, whole-grain Petri nets will be referred to simply as Petri nets unless otherwise stated.}
Intuitively, these homomorphisms find a copy of the source graph in the target graph, potentially condensing nodes or edges together (but never splitting connections apart). Alternatively, treating the source graph as a pattern, the homomorphism describes a pattern match in the target. Figure 1 demonstrates an example.

Figure 1: An example graph homomorphism with components \( h_V = [1, 3, 2] \) (represented by squiggly arrows) and \( h_E = [a, c, c] \) (represented by dotted arrows), with the source graph on the left and target graph on the right. Arrow indices are enumerated alphabetically to distinguish arrow labels from vertex labels.

The double pushout algorithm formalizes a notion of rewriting a portion of a graph. This process generally consists in an addition step (a pushout) and a deletion step (a pushout complement). These constructions are defined generally for any category, noting graphs and graph homomorphisms form a category, \( \text{Grph} \). The pushout, if it exists, is defined for a span of morphisms \( B \leftarrow A \rightarrow C \) as an object \( D \) with a pair of morphisms \( B \rightarrow D \leftarrow C \). This is required not just to be a commutative square but to be the universal one. Namely, for all objects \( X \) equipped with maps \( B \rightarrow X \leftarrow C \) such that a commutative square is formed, there must exist a unique map \( D \rightarrow X \) such that the equations \( j_1 = \iota_1; u \) and \( j_2 = \iota_2; u \) hold. One intuition from \( \text{Set} \) is that \( D \) represents the gluing together of \( B \) and \( C \), where \( A \) serves as the overlap between \( B \) and \( C \).

Constructing a pushout complement also constructs a pushout square; however, the initial data is different. We begin with just \( A \rightarrow B \rightarrow D \) and attempt to find \( A \rightarrow C \rightarrow D \) such that the pushout property holds. While pushouts are guaranteed to exist uniquely for a given span in \( \text{Set} \) and \( \text{Grph} \), the pushout complement construction is more subtle because it is not guaranteed to exist or be unique \([7]\). As shown in Figure 2 in \( \text{Set} \), three pushout complements can be generated for the morphisms \( 2 \rightarrow 1 \rightarrow 1 \), where \( ! \) is the unique map to the terminal object.

However, in the setting of DPO rewriting, the pushout complement is guaranteed to be unique when the first morphism is a monomorphism \([18]\). For the rest of this work, we restrict attention to pushout complements where this is the case.

The pushout and pushout complement operations are combined in the DPO approach, which is visualized in Figure 3 with a concrete example in Figure 4. The general problem consists of a graph \( G \) to be rewritten and a rewrite rule, given...
Double pushout rewriting of C-sets

Figure 2: Demonstration of non-uniqueness of pushout complement in \( \text{Set} \). Note that a function \( 1 \to X \) is specified by picking an element of \( X \). The initial data is given in black, and valid pushout complements are found in purple. None of the pushout complements is a initial pushout complement \cite{27}.

as a span \( L \xleftarrow{I} I \xrightarrow{R} R \). We first compute \( K \), the original graph with deletions applied, via pushout complement. We then produce the final, rewritten graph via pushout of \( R \) and \( K \).

Figure 3: DPO application of a rewrite rule to a graph \( G \). The initial data is in black, intermediate computations in grey, and the final result in green. The morphism \( m \) is called the \textit{match} morphism. The meaning of \( L \) is to provide a pattern that \( m \) will match to a subgraph in \( G \). \( R \) represents the graph which will be substituted back in for the matched pattern to yield the rewritten graph, and \( I \) indicates what fragment of \( L \) is preserved in the rewrite and its relation to \( R \).

Figure 4: \textbf{Left:} DPO simultaneous deletion and insertion. Because a vertex and edge are in the \( L \) pattern but not present in the interface \( I \), the elements in \( G \) these map to will be deleted. The presence of an extra reversed arrow in \( R \) that is not found in the interface indicates that this will be inserted into the final result. The match morphism picks where to apply the substitution (deciding which node gets deleted, which edge gets a reverse arrow added). \textbf{Right:} user-exposed interface for performing the same rewrite in Catlab.jl.

For the pushout complement construction to be valid in \( \text{Graph} \), further restrictions are required on the match morphism. These conditions are called the identification condition and the dangling condition, collectively the \textit{gluing conditions}. Formally, the \textit{identification condition} states:

\[
\forall v_1 \in L_V \setminus l_V(I_V), \forall v_2 \in L_V, m_V(v_1) = m_V(v_2) \implies v_1 = v_2 \quad (2)
\]

\[
\forall e_1 \in L_E \setminus l_E(I_E), \forall e_2 \in L_E, m_E(e_1) = m_E(e_2) \implies e_1 = e_2 \quad (3)
\]

\textit{Notational conventions:} \( f(A) \) refers to the image of \( A \) under \( f \). Likewise, \( f^{-1}(A) \) refers to the preimage. \( A \setminus B \) refers to the set difference of \( A \) and \( B \). \( f; g \) is the composition \( g \circ f \). \( A \xrightarrow{f} B \) is the inclusion function given a subset relation \( A \subseteq B \).
This condition forbids \(m\) to map a deleted element and a preserved element in \(L\) to the same element in \(G\), in addition to forbidding two deleted elements in \(L\) to be mapped to the same element in \(G\). For injective match morphisms, this is satisfied trivially.

The **dangling condition** is expressed by the following constraints:

\[
G^{-1}_{\text{src}}(G_V \setminus m_V(L_V \setminus l_V(I_V))) \subseteq G_E \setminus m_E(L_E \setminus l_E(I_E)) \tag{4}
\]

\[
G^{-1}_{\text{tgt}}(G_V \setminus m_V(L_V \setminus l_V(I_V))) \subseteq G_E \setminus m_E(L_E \setminus l_E(I_E)) \tag{5}
\]

This condition requires that the preimage for \(G_{\text{src}}\) and \(G_{\text{tgt}}\) of deleted vertices must only include edges that themselves are deleted. Alternatively, for each deleted vertex, we must also delete all edges incident to that vertex.

The pushout complement \(K \xrightarrow{g} G\) in \textbf{Graph} is specified by the following formulas [5]:

\[
K_V := G_V \setminus m(V(l(I_V))) \tag{6}
\]

\[
K_E := G_E \setminus m(E(l(I_E))) \tag{7}
\]

\[
k := l;m \tag{8}
\]

\[
g := (K_V \hookrightarrow G_V, K_E \hookrightarrow G_E) \tag{9}
\]

This procedure identifies the graph \(K\) with a subgraph of \(G\), making its morphism to \(G\) trivial. By taking the morphism to \(K\) to be the composite of \(l\) and \(m\), we are guaranteed that the square commutes.

### 2.2 C-sets

Lack and Sobociński studied the minimum structure required for DPO rewriting, leading to the identification of *adhesive categories* as a general setting [17]. There are many equivalent specifications of the property of adhesivity, one being that monomorphisms have pushouts and pullbacks, and pushouts are Van Kampen [24]. C-sets generalize graphs while still forming adhesive categories.

The definition of a graph was given in terms of two finite sets \((V, E)\) and two finite functions \((\text{src}, \text{tgt})\). Consider the category freely generated by the graph \(\bullet \xRightarrow{E} \bullet\). A functor from this category to \textbf{FinSet} will assign to each object a finite set and to each arrow a finite function from the source set to the target set. This is equivalent to our definition of graphs, and, moreover, the definition of graph homomorphisms between graphs \(G\) and \(H\) is recovered by the notion of a natural transformation of functors \(G\) and \(H\). For the purposes of our software implementation, C-sets are functors from a finitely-presented category \(C\) to the skeleton of \textbf{FinSet}. The category \(C\) is equivalently referred to as the indexing category or schema and the functor category \([C, \textbf{Set}]\) is referred to as \(C\)-set or the category of instances, models, presheaves, or databases. Given a \(C\)-set \(X\), the finite set that \(X\) sends a component \(c \in \text{Ob} \ C\) to is denoted by \(X_c\) or \(X(c)\). Likewise, the finite function \(X\) sends a morphism \(f \in \text{Hom}_C(a, b)\) is denoted by \(X_f\) or \(X(f)\).

This abstraction provides value by unifying the diverse family of graph-like structures mentioned at the start of this section. For example, by modifying \(C\) to add an edge \(\text{refl} : V \rightarrow E\) and equations \(\text{refl} ; \text{src} = \text{refl}; \text{tgt} = \text{id}_V\), we obtain a \(C\) whose \(C\)-set instances are reflexive graphs (graphs with a designated reflexive edge for each vertex, which must be sent by morphisms to a designated reflexive edge in the codomain). By changing the shape of the indexing category, one can drastically change the category of instances. Because each category \(C\)-Set forms a topos [2] Section 8.8], and because all toposes are adhesive categories [19], it is possible to study rewriting of \(C\)-sets.

### 3 Extension from Graphs to C-sets

#### 3.1 Construction

As a particular instance of a colimit, the construction of pushouts in \(C\)-Set is known [2] Section 8.6]. Generalizing DPO, then, requires only extending the pushout complement to \(C\)-Set. We must generalize the identification and dangling conditions as well as the construction itself. When using set-theoretic operations such as subset or set difference in the context of \(C\)-sets, it is implied that these operations are applied pointwise over the objects of \(C\). We will make reference to the named objects and morphisms of the diagram in Figure [5] which should be reinterpreted as living in the category \(C\)-Set rather than \textbf{Graph} specifically.
3.1.1 Gluing conditions

The generalized identification condition can be expressed as a condition holding for each object in the indexing category. Namely, for every object \( c \in C \), deleted element \( x \in L_c \setminus l_c(I_c) \), and arbitrary element \( y \in L_c \),

\[
m_c(x) = m_c(y) \implies x = y.
\]

(10)

The generalized dangling condition can be expressed as a condition holding for each morphism in the indexing category. As a shorthand, let \( G'_c := m_c(L_c \setminus l_c(I_c)) \) represent the portion of \( G_c \) that is to be deleted for each component \( c \in C \).

Then the condition asserts that for every morphism \( f : a \to b \) in \( C \),

\[
G_f^{-1}(G'_b) \subseteq G'_a.
\]

(11)

3.1.2 Generalized pushout complement construction

We now consider the construction of a pushout complement, given \( C \)-set morphisms \( l : I \to L \) and \( m : L \to G \) satisfying the gluing conditions. To do this, we construct \( K \), the intermediate rewrite result that has had deletions made to it, as a subset of \( G \).

\[
K_c := G_c \setminus m(L_c \setminus l(I_c)), \quad c \in C.
\]

(12)

We also verify that the morphisms \( k \) and \( g \) are valid \( C \)-set morphisms, i.e. that they are natural with respect to each \( f \in Hom_C(a, b) \). For example, for \( k \):

\[
\begin{array}{ccc}
G_a & \xrightarrow{k_n} & X_a \\
& G_f \downarrow & \downarrow X_f \\
G_b & \xrightarrow{k_b} & X_b
\end{array}
\]

(15)

The naturality of \( k \) follows from its definition as the composite of \( l \) and \( m \), which each satisfy naturality. As \( g \) is a simple inclusion, it is also natural.

3.2 Correctness

Claim: For a fixed \( C \), the algorithm as described above produces the pushout complement in \( C \)-Set, assuming the identification and dangling conditions hold.

Proof:

We begin by showing that the constructed \( C \)-set \( K \) is well-defined. Explicitly, for each component \( c \in C \), \( K_c \) was defined as a subset of \( G_c \). However, \( K \) must also map each morphism \( f \in Hom_C(a, b) \) to a function \( K_a \xrightarrow{K_f} K_b \) in \( \text{FinSet} \). Because \( K_c \subseteq G_c \) for all components, we take the function \( K_f \) to be the restriction of \( G_f \). A function restriction is unremarkable when the domain is being restricted; however, we must also restrict the codomain. For this to be well-defined, \( x \in K_b \) being removed must imply that the preimage \( K_f^{-1}(x) \) was removed from \( K_a \). This is what the dangling condition asserts.

We also verify that the morphisms \( k \) and \( g \) are valid \( C \)-set morphisms, i.e. that they are natural with respect to each \( f \in Hom_C(a, b) \). For example, for \( k \):

\[
\begin{array}{ccc}
G_a & \xrightarrow{k_n} & X_a \\
& G_f \downarrow & \downarrow X_f \\
G_b & \xrightarrow{k_b} & X_b
\end{array}
\]

(15)

The naturality of \( k \) follows from its definition as the composite of \( l \) and \( m \), which each satisfy naturality. As \( g \) is a simple inclusion, it is also natural.

With \( K, k, \) and \( g \) well-defined, we demonstrate that the pushout property holds. As colimits are computed pointwise in \( C \)-Set [2 Section 8.6], this means we must verify for each component \( c \in C \) that the following universal property holds for all sets \( X_c \) such that the outer square commutes:

\[
\begin{array}{ccc}
I_c & \xrightarrow{l_c} & L_c \\
& k_c \downarrow & \downarrow m_c \\
K_c & \xrightarrow{g_c} & G_c \\
& x \downarrow u_c & \downarrow x \downarrow
\end{array}
\]

(16)
We construct the function $G_c \xrightarrow{u_c} X_c$ as follows:

$$u_c(g) = \begin{cases} x_{2c}(g) & \text{if } g \in K_c \\ x_{1c}(m_c^{-1}(g)) & \text{otherwise} \end{cases}$$

We show this is well-defined, makes the diagram commute, and is the only function from $G_c$ to $X_c$ with this property. The first case is itself well-defined, as $K_c$ is defined as a subset of $G_c$. For the second case to be well-defined, any two elements of $L_c$ (say, $a$ and $b$) mapping to the same element in $G_c$ by $m_c$ must be mapped to the same element of $X_c$ by $x_{1c}$. Suppose $a$ and $b$ are both in the image of $l_c$: they are mapped to the same element of $K_c$ (and, therefore, the same element of $X_c$ by $x_{2c}$). The commutivity of the outer square then forces $x_{1c}$ to map $a$ and $b$ to the same element of $X_c$. Conversely, suppose either $a$ or $b$ is not in the image of $l_c$: then the inverse map is unique due to the identification condition.

The triangles commute, being of the form $\phi; \phi^{-1}; \psi = \psi$ (the inverse $g_c^{-1}$ has been left implicit due to $K_c \subseteq G_c$). $u_c$ determines a value for each $g \in G_c$, via the first case or second case, solely by considering the satisfaction of the lower or upper triangles, respectively. Therefore, it is the unique function the satisfies the commutivity constraints.

### 3.3 Computation of homomorphisms and isomorphisms of C-sets

For the DPO rewriting algorithm to be of practical use, a match morphism must be supplied. The specification of a $C$-set morphism requires a nontrivial amount of data as well as satisfying the naturality condition. Furthermore, in confluent rewriting systems, manually finding matches is an unreasonable request to make of the end user, as the goal is to apply all rewrites possible until the term reaches a normal form. For this reason, DPO rewriting of $C$-sets benefits from a generic algorithm to find homomorphisms, analogous to structural pattern matching in the tree term rewriting case.

The problem of finding a $C$-set homomorphism $X \rightarrow Y$, given a finitely presented category $C$ and two finite $C$-sets $X$ and $Y$, is at least as hard as the graph homomorphism problem, which is NP-complete. On the other hand, the $C$-set homomorphism problem can be framed as a constraint satisfaction problem (CSP), a classic problem in computer science for which many algorithms are known [23, Chapter 6]. Since $C$-sets are a mathematical model of relational databases [26], the connection between $C$-set homomorphisms and constraint satisfaction is a facet of the better-known connection between databases and CSPs [28].

To make this connection precise, we introduce the slightly nonstandard notion of a typed CSP. Given a finite set $T$ of types, the slice category $\text{FinSet}/T$ is the category of $T$-typed finite sets. A typed CSP then consists of $T$-typed finite sets $V$ and $D$, called the variables and the domain, and a finite set of constraints of form $(x, R)$, where $x = (x_1, \ldots, x_k)$ is a list of variables and $R \subseteq D^{-1}(V(x_1)) \times \cdots \times D^{-1}(V(x_k))$ is a compatibly typed $k$-ary relation. An assignment is a map $\phi : V \rightarrow D$ in $\text{FinSet}/T$. The goal is to find a solution to the CSP, namely an assignment $\phi$ such that $(\phi(x_1), \ldots, \phi(x_k)) \in R$ for every constraint $(x, R)$.

The problem of finding a $C$-set morphism $X \rightarrow Y$ translates to a typed CSP by taking the elements of $X$ and $Y$ to be the variables and the domain of the CSP, respectively. To be precise, let the types $T$ be the objects of $C$. The variables $V : \{(c, x) : c \in C, x \in X(c)\} \rightarrow \text{Ob} C$ are given by applying the objects functor $\text{Ob} : \text{Cat} \rightarrow \text{Set}$ to $\int X \rightarrow C$, the category of elements of $X$ with its canonical projection. Similarly, the domain is $D := \text{Ob}(\int Y \rightarrow C)$. Finally, for every generating morphism $f : c \rightarrow c'$ of $C$ and every element $x \in X(c)$, introduce a constraint $\{(x, x'), R\}$ where $x' := X(f)(x)$ and $R := \{(y, y') \in X(c) \times X(c') : Y(f)(y) = y'\}$ is the graph of $Y(f)$. By construction, an assignment $\phi : V \rightarrow D$ is the data of a $C$-set transformation and $\phi$ is a solution if and only if the transformation is natural. Thus, the solutions of the typed CSP are exactly the $C$-set homomorphisms $X \rightarrow Y$.

With this reduction, CSP algorithms are straightforwardly ported to algorithms for finding $C$-set morphisms, where the types and special structure may permit optimizations. We have adapted backtracking search [23, Section 6.3], a simple but fundamental CSP algorithm, to find $C$-set homomorphisms. By also maintaining a partial inverse assignment, this algorithm is easily extended to finding $C$-set monomorphisms, an important constraint when matching for rewriting. Since a monomorphism between finite $C$-sets $X$ and $Y$ is an isomorphism if and only if $X(c)$ and $Y(c)$ have the same cardinality for all $c \in C$, this extension also yields an algorithm for isomorphism testing, which is useful for checking the correctness of rewrites.

### 3.4 Extension from closed systems to open systems

The forms of rewriting discussed up to this point have concerned rewriting closed systems. Structured cospans are a general model for open systems, consisting of cospans of form $La \rightarrow x \leftarrow Lb$, where the apex $x$ represents the system.
itself and the feet \( L_a \) and \( L_b \) represent the inputs and outputs. Here, \( L : A \to X \) is a functor that maps from the system interface category \( A \) to the system category \( X \). Larger systems are built up from smaller systems via pushouts in \( X \), which glue systems together along a shared interface:

\[
(L_a \to x \leftarrow L_b \to y \leftarrow L_c) \mapsto (L_a \to x \leftarrow L_b y \leftarrow L_c).
\]

When \( L, I, \) and \( R \) are each structured cospans, there is extra data to consider when rewriting, as shown in Figure 5. In ordinary DPO rewriting, if the \( R \) of one rewrite rule equals the \( L \) of another, a composite rewrite rule can be constructed, giving rewrite rules a composition structure referred to as vertical composition. In the case of structured cospans, another form of composition (call this horizontal composition) emerges from composing the pairs of \( L, I, \) and \( R \) structured cospans of two rewrite rules. These two forms of composition together yield a double category of structured cospan rewrites, where horizontal arrows are in correspondence with structured cospans and squares are in correspondence with all possible rewrites \[8\]. These squares are constructed inductively from vertical and horizontal compositions of open rewrite rules.

When searching for a match in a large \( C \)-set, the search space grows as \( O(n^k) \) where \( k \) is the size of the pattern \( L \) and \( n \) is the size of the \( G \). However, after decomposing \( G \) into a composite of multiple substructures and restricting matches to those homomorphisms into a specific substructure, the search space is limited by \( O(m^k) \) where \( m < n \) is the size of the substructure. Not only does this accelerate the computation, but it can be semantically meaningful to restrict matches to certain pieces of the original \( C \)-set.

A goal of AlgebraicJulia software interfaces is to allow scientific computing practitioners to specify models hierarchically so that techniques like \( C \)-set rewriting can leverage that hierarchical structure to accelerate computations on those models. In this case, hierarchically decomposed graphs can support faster pattern matching for rewrite application, and

---

\[3\]The \( L \) of structured cospans should not be confused with the \( L \) of the rewrite rule \( L \leftarrow I \to R \).

---

Figure 5: Applying a structured cospan rewrite rule. \( C \)-sets and morphisms in black are the initial data: the upper face represents the open rewrite rule, the upper left edge represents the open pattern to be matched, and the left face represents the matching. Green morphisms are computed by pushout complement in \( C \)-Set. The purple morphisms are computed by the rewriting pushouts and red morphisms are computed by the structured cospan pushouts. Figure adapted from \[8\] Section 4.2.

When searching for a match in a large \( C \)-set, the search space grows as \( O(n^k) \) where \( k \) is the size of the pattern \( L \) and \( n \) is the size of the \( G \). However, after decomposing \( G \) into a composite of multiple substructures and restricting matches to those homomorphisms into a specific substructure, the search space is limited by \( O(m^k) \) where \( m < n \) is the size of the substructure. Not only does this accelerate the computation, but it can be semantically meaningful to restrict matches to certain pieces of the original \( C \)-set.

A goal of AlgebraicJulia software interfaces is to allow scientific computing practitioners to specify models hierarchically so that techniques like \( C \)-set rewriting can leverage that hierarchical structure to accelerate computations on those models. In this case, hierarchically decomposed graphs can support faster pattern matching for rewrite application, and

---

\[3\]The \( L \) of structured cospans should not be confused with the \( L \) of the rewrite rule \( L \leftarrow I \to R \).

---

Figure 6: Pattern matching and the decomposition of a \( C \)-set via structured cospans. \textbf{Left}: a graph pattern is sought in a relatively complex graph. \textbf{Right}: the target graph is decomposed into four subgraphs composed with structured cospans. Such a decomposition can restrict the set of matches to those localized to the target subgraph.
a thoughtfully structured model may allow a scientist more freedom to use automated match finding, even for sensitive rewrites that are not globally appropriate.

4 Example applications

4.1 Model exploration

A common scientific and engineering task is to analyze measurements of a complex system and build a model that faithfully reproduces the measurements. Examples of this are common in chemistry, where chemical reaction networks serve as models to capture the dynamics of chemical species concentrations changing over time. These networks can be represented as bipartite graphs, with the first vertex set representing chemical species and the second representing the set of reactions (see Figure 7a).

This stepwise development of models has been explored in the context of Petri Nets, where versions of the pushout complement construction and gluing conditions were crafted for this special case. We can model this data structure with a C-set (modulo quotienting by permutations of the set of states on a transition) and recover the same gluing conditions and pushout complement constructions from the general C-set formula.

An example of this iterative approach to the development of models occurs in the context of epidemiology. The SIR model developed by Kermack and McKendrick forms the basis for many different compartmental models of infectious disease. Mathematical modelers of disease will start with an existing model in this family known to have mechanics similar to their disease of interest such as having an incubation period or being carried by mosquitoes. From this model they will manually develop variants of the model to address some phenomena specific to their disease. The modeler will analyze the new models analytically or through numerical simulation, then estimate their parameters from data and make predictions of disease dynamics. This process can be partially automated through the use of C-set rewriting. As an example, we present the results of rewriting of epidemiological models (SIR, SEIR, SEIRS, SEIRD) in AlgebraicJulia in Figure 7b.

![Indexing schema for bipartite directed graphs, which model Petri Nets. S refers to places/states, T refers to transitions, I and O are inputs and outputs of transitions, respectively. A series of compartmental models with simulations of their dynamics under the law of mass action. Depending on the mechanism of action for a particular disease, an epidemiologist will use a different model. These models can be derived from the original SIR model by the application of C-set rewriting. Petri net visualizations and dynamics are computed by AlgebraicPetri.jl.](image)

4.2 Wiring diagram rewriting with symmetric monoidal structure

When implementing a computer algebra system or theorem prover for SMCs, one immediately finds that the axioms of the generalized algebraic theory of SMCs cannot be directed so as to apply traditional term rewriting techniques. The interchange law \((f \otimes g) \cdot (f' \otimes g') = (f \cdot f') \otimes (g \cdot g')\) of an SMC does not prefer one expression over the other; neither possible orientation is preferred when building a set of term rewriting rules for classical term rewriting. Another problem in implementing rewriting for SMCs comes from the fact that the braiding morphisms \(\sigma_{X,Y} \colon X \otimes Y \to Y \otimes X\) allow one to swap the order of any monoidal product. This high degree of symmetry would require large number of
term rewrites just to compute permutations of such products. In order to avoid these problems, SMC morphisms are represented by wiring diagrams, which normalize the interchange law and braiding symmetries such that two morphisms have isomorphic wiring diagrams if and only if some sequence of these rewrite rules connects them [21]. This allows computational and user focus to be directed at more interesting rewrites, such as the associativity of addition as in Figure 8 encoded as a rewrite of objects in a slice category [6].

\[
\phi = \text{CSetTransformation}(H, H\Sigma, \\
V=\text{ones}(\text{Int}, 9), \\
E_{11} = [1,2,1,2], \\
E_{21} = \text{ones}(\text{Int},2))
\]

![Wiring Diagram](image)

Figure 8: a.) An element of the slice category Hyp ↓ HΣ, i.e. a wiring diagram the category presented by the monoidal signature Σ. The hypergraph H and monoidal signature HΣ (which captures facts such as plus taking two inputs and producing one output) are each encoded as hypergraphs, and the Catlab declaration of a C-set homomorphism φ is shown in between. We then can internalize this morphism data itself as a C-set, visualized below by coloring the nodes of H using φ. b.) A DPO rewrite in the category of Hyp ↓ HΣ in the style of Figure 3 (interfaces I and K not shown). By rewriting in this category rather than Hyp, we guarantee any rewrite relation will satisfy the signature Σ. That the extension from rewriting in Hyp to Hyp ↓ Σ follows seamlessly from defining the C-Set of C-set homomorphisms demonstrates the generality of our approach, a generalization that would require much greater implementation effort if starting from an implementation of hypergraph rewriting specifically.

### 4.3 Open systems: structured cospan rewrites

The example of rewriting Petri nets for epidemiological models can be extended to rewriting open Petri nets. The ability to rewrite locally becomes important as the overall model complexity increases. Models in practice must capture heterogeneous dynamics by, for example, segmenting populations by age and geographic location [20].

Structured cospan rewriting is demonstrated in Figure 9. In this example, we consider the SIR model and perform a rewrite to add exposure dynamics. We separately consider a model of infected populations that quarantine and eventually recover (IQR). This model can be made more realistic by adding a transition for quarantine violations. Note
Double pushout rewriting of C-sets

Figure 9: Horizontal composition of structured cospan rewrite rules. The $L$ and $R$ structured cospans are positioned on the top and bottom, respectively. For clarity, $I$ cospans are omitted, and the only cospan legs shown are those relevant for composition.

This IQR rewrite rule can be applied to local subcomponents specified by open Petri nets, independent of a larger context. In closed system rewriting, to apply this we have to identify which nodes and transitions the IQR pattern corresponds to within the possibly massive overall model. We then use the cospan structure to compute an open rewrite rule that applies both transformations.

5 Conclusions and Future Work

DPO rewriting can be performed on arbitrary C-sets, and we have presented the first known algorithm and implementation for this. This result allows generic rewrite operations to be used in a variety of contexts, when it would be otherwise time-consuming and error-prone to develop custom rewrite algorithms for such a multitude of data structures. By developing this class of rewrite algorithms, we enable domain experts to implement a wide range of symbolic computation algorithms. We have demonstrated this capability via examples in model structure exploration, term rewriting in symmetric monoidal categories, and structured cospan rewriting. By implementing structured cospan rewriting for the first time, we combine the compositionality of open systems with the computational expressivity of DPO rewriting.

Our future work is guided by the goal of implementing practical scientific software that leverages rewriting and theorem proving via Catlab.jl. Challenging theoretical and implementation questions remain to be investigated including many subtleties in implementing C-set rewriting for theorem proving. Another key area of work is the design of interfaces, data structures, and algorithms for scaling up rewriting to practical software applications. As a tactic to automatically find proofs of reasonable complexity, the E-graphs \cite{e} algorithm could be fit into our framework by generalizing it from term rewriting to C-set rewriting. Since structured cospans are such a new approach to the specification and analysis of complex systems, future work should explore the design space of such inductive rewriting systems.

References

[1] Jakob L Andersen, Christoph Flamm, Daniel Merkle, and Peter F Studler. Inferring chemical reaction patterns using rule composition in graph grammars. *Journal of Systems Chemistry*, 4(1):1–14, 2013.

[2] Steve Awodey. *Category theory*. Oxford university press, 2010.

[3] John C Baez and Kenny Courser. Structured cospans. *arXiv preprint arXiv:1911.04630*, 2019.

[4] John C Baez, Fabrizio Genovese, Jade Master, and Michael Shulman. Categories of nets. *arXiv preprint arXiv:2101.04238*, 2021.

[5] Richard Banach. The contractum in algebraic graph rewriting. In *International Workshop on Graph Grammars and Their Application to Computer Science*, pages 16–26. Springer, 1994.

[6] Filippo Bonchi, Fabio Gadducci, Aleks Kissinger, Pawel Sobocinski, and Fabio Zanasi. String diagram rewrite theory i: Rewriting with frobenius structure. *arXiv preprint arXiv:2012.01847*, 2020.
Double pushout rewriting of C-sets

[7] Benjamin Braatz, Ulrike Golas, and Thomas Soboll. How to delete categorically—two pushout complement constructions. *Journal of Symbolic Computation*, 46(3):246–271, 2011.

[8] Daniel Cicala. Rewriting structured cospans: A syntax for open systems. *arXiv preprint arXiv:1906.05443*, 2019.

[9] Hartmut Ehrig, Kathrin Hoffmann, Julia Padberg, Claudia Ermel, Ulrike Prange, Enrico Biermann, and Tony Modica. Petri net transformations. In *Petri Net, Theory and Applications*. IntechOpen, 2008.

[10] Hartmut Ehrig, Michael Pfender, and Hans Jürgen Schneider. Graph-grammars: An algebraic approach. In *14th Annual Symposium on Switching and Automata Theory (swat 1973)*, pages 167–180. IEEE, 1973.

[11] Hartmut Ehrig and Ulrike Prange. Modeling with graph transformations. In *Advances in Multiagent Systems, Robotics and Cybernetics: Theory and Practice. Proceedings of Intern. Conf. on Systems Research, Informatics and Cybernetics*, volume 57, 2005.

[12] Micah Halter, Evan Patterson, Andrew Baas, and James Fairbanks. Compositional scientific computing with catlab and semanticmodels. *arXiv preprint arXiv:2005.04831*, 2020.

[13] Jieh Hsiang, Hélène Kirchner, Pierre Lescanne, and Michaël Rusinowitch. The term rewriting approach to automated theorem proving. *The Journal of Logic Programming*, 14(1-2):71–99, 1992.

[14] Gérard Huet, Gilles Kahn, and Christine Paulin-Mohring. The coq proof assistant a tutorial. *Rapport Technique*, 178, 1997.

[15] Aleks Kissinger and Vladimir Zamdzhiev. Quantomatic: A proof assistant for diagrammatic reasoning. In *International Conference on Automated Deduction*, pages 326–336. Springer, 2015.

[16] Joachim Kock. Elements of petri nets and processes. *arXiv preprint arXiv:2005.05108*, 2020.

[17] Stephen Lack and Paweł Sobociński. Adhesive categories. In *International Conference on Foundations of Software Science and Computation Structures*, pages 273–288. Springer, 2004.

[18] Stephen Lack and Paweł Sobociński. Adhesive and quasiadhesive categories. *RAIRO-Theoretical Informatics and Applications*, 39(3):511–545, 2005.

[19] Stephen Lack and Paweł Sobociński. Toposes are adhesive. In *International Conference on Graph Transformation*, pages 184–198. Springer, 2006.

[20] Mélodie Monod, Alexandra Blenkinsop, Xiaoyue Xi, Daniel Hebert, Sivan Bershak, Simon Tietze, Marc Baguelin, Valerie C Bradley, Yu Chen, Helen Coupland, et al. Age groups that sustain resurging covid-19 epidemics in the united states. *Science*, 371(6536), 2021.

[21] Evan Patterson, David I Spivak, and Dmitry Vagner. Wiring diagrams as normal forms for computing in symmetric monoidal categories. *arXiv preprint arXiv:2101.12046*, 2021.

[22] Detlef Plump. Essentials of term graph rewriting. *Electronic Notes in Theoretical Computer Science*, 51:277–289, 2002.

[23] Stuart Russell and Peter Norvig. *Artificial intelligence: a modern approach*. Prentice Hall, 3 edition, 2010.

[24] Paweł Sobociński and Tobias Heindel. Being van kampen is a universal property. *arXiv preprint arXiv:1101.4594*, 2011.

[25] Paweł Sobociński, Paul W. Wilson, and Fabio Zanasi. CARTOGRAPHER: A Tool for String Diagrammatic Reasoning (Tool Paper). In Markus Roggenbach and Ana Sokolova, editors, *8th Conference on Algebra and Coalgebra in Computer Science (CALCO 2019)*, volume 139 of *Leibniz International Proceedings in Informatics (LIPIcs)*, pages 20:1–20:7, Dagstuhl, Germany, 2019. Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik. URL: http://drops.dagstuhl.de/opus/volltexte/2019/11448 doi:10.4230/LIPIcs.CALCO.2019.20

[26] David I. Spivak. Functorial data migration. *Information and Computation*, 217:31–51, 2012. doi:10.1016/j.ic.2012.05.001

[27] Gabriele Taentzer. Distributed graphs and graph transformation. *Applied Categorical Structures*, 7(4):431–462, 1999.

[28] Moshe Y. Vardi. Constraint satisfaction and database theory: a tutorial. In *Proceedings of the nineteenth ACM SIGMOD-SIGACT-SIGART symposium on Principles of database systems*, pages 76–85, 2000. doi:10.1145/335168.335209

[29] Max Willsey, Chandrakana Nandi, Yisu Remy Wang, Oliver Flatt, Zachary Tatlock, and Pavel Panchekha. egg: fast and extensible equality saturation. *Proceedings of the ACM on Programming Languages*, 5(POPL):1–29, 2021.