Pushouts in Computational Systems Biology

Jonathan Hayman[1] and Tobias Heindel[2]

[1] Computer Laboratory, University of Cambridge, Cambridge, United Kingdom
[2] LIX, École Polytechnique, Palaiseau, France

Abstract. Rule-based formalisms for modelling biochemical pathways such as Kappa, BioNetGen and PySB have emerged as powerful tools for the analysis of biochemical pathways. They allow concise, intuitive models to be developed, and by avoiding through the use of rules the combinatorial explosion in the number of biochemical species that befalls traditional techniques, they make in-silico experimentation and simulation more feasible. However, the growing number of rule-based modelling languages calls for a general, language-independent theory. The present paper describes an abstract categorical approach based on single-pushout rewriting, in which mixtures of biochemical species are modelled as objects in a category of graph-like objects and system evolution corresponds to taking a pushout over a rule and one of its "redexes" or "matchings", both of which are formalized as special forms of partial map. The main theorem establishes a sufficient condition for the existence of pushouts of partial maps in arbitrary categories; the condition is necessary locally, i.e. it is necessary in all slice categories. The relevance of this theoretical result is illustrated by showing that the condition can be lifted to arbitrary full subcategories, yielding a general method to develop categorical accounts of models in a way that has already been applied successfully to Kappa.

Introduction

Techniques and concepts of graph rewriting have proven useful in a wide spectrum of fields, ranging from symbolic quantum computation [1] to model checking [2]. The analysis of molecular biology was envisaged as an early application area of graph rewriting in [3], not long after the introduction of the algebraic approach [4]. Recently, rule-based modelling of cellular biology has brought this back to the fore [5]: rules describe reactions between protein complexes by specifying their local effect only on the affected fragments of the protein complexes, yielding concise and manageable formalizations of biochemical systems. Their application in this area has been supported by powerful new simulation and static analysis techniques, e.g. the Kappa language [6] and BioNetGen [7], and PySB [8].

Rule-based models can be viewed as specialized graph rewriting systems, as demonstrated in [6, 9], which describe the semantics of the Kappa language using single-pushout (SPO) graph transformation [10, 11]. The SPO approach defines rewriting as taking a pushout of a rule and match, which typically are morphisms in a suitable category of partial maps.

In giving the SPO semantics, a good deal of care is needed to ensure that pushouts correspond to rewriting as specified in the Kappa language. The reason is that, despite the striking similarity of structures described in Kappa or BioNetGen and traditional graphs, the former languages contain additional features and constraints that are necessary for the efficient representation of biochemical systems. This makes the pushout construction, which is already complicated in the case of graphs and algebras [10], even more challenging. For example, though the category that has been presented in [6] does have pushouts of *action maps* against *valid matchings*, this is not the case for all spans of partial maps; furthermore, even if pushouts of spans of total maps exist, they may consist of properly partial maps. As such, the models given for Kappa and its encoding [9] cry out for a more abstract analysis on a categorical level. For this we need to extend the family of recent categorical approaches of graph transformation (as surveyed in [12]) since none of its members considers pushouts of arbitrary (total) maps.

In the present paper, we propose a categorical framework for SPO rewriting, i.e. a class of categories that enforces on its members the key properties of the category of graphs (or of any quasi-topos) that provide enough structure to reason about the existence of pushouts of partial maps. The class includes most of the common categories of graph-like structures. To justify the new framework of *categories with inherited partial map pushouts*, which is based on previous work on hereditary pushouts [13] (see also [14]), we provide a theorem of pure category theory on necessary and sufficient conditions for the existence of pushouts of partial maps. Based on this main theorem, we describe how the involved pushout construction of [9] fits in the framework; we will see that the categorical structure of the construction is reasonably easy, mitigating the complexity on the concrete level of a suitable category of *pattern graphs*, which were introduced in [9] to encode the Kappa modelling language and will serve as paradigmatic example category.

Structure of the Paper We begin with a review of preliminary notions of category theory that are used to define categories of partial maps in Section 1, where we also define the category of pattern graphs of [9], which we use as running example to illustrate the most important concepts. In Section 2, we develop and summarize results concerning pushouts of partial maps that will not only be essential to develop our main theorem but also serve to clarify our contribution. The main theorem itself is developed in Section 3; under a mild assumption, namely existence of cocones for spans, it gives a necessary and sufficient condition for the existence of pushouts of partial maps. Section 4 explains how the main theorem applies to the actual encoding of the Kappa language using pattern graphs, and we discuss further related and future work in Section 5 before we conclude.

1 Preliminaries

Assuming familiarity with basic concepts of category theory (listed in Appendix A), we recall categories of partial maps based on admissible classes of monos [15]; we also define inverse and direct image functions. We shall reuse the authors' pattern graphs from [9] as running example category to illustrate the central concepts.

We use $\mathbb{C}, \mathbb{D}, \mathbb{X}$, etc. to range over categories, and $\mathbb{SET}$ is the category of sets and functions. We write $A \in \mathbb{C}$ if A is an object of the category $\mathbb{C}$ and $f \colon A \to B$ in $\mathbb{C}$ or $A \xrightarrow{f} B$ in $\mathbb{C}$ if f is a morphism in $\mathbb{C}$ with domain A and codomain B; finally, the identity on an object $A \in \mathbb{C}$ is denoted by id_A and $g \circ f$ is the composition of morphisms $f\colon A \to B$ and $g\colon B \to C$ in $\mathbb{C}$; we write $A' \stackrel{m}{\rightarrowtail} A$ if m is a mono. As usual, $\mathbb{C}(A, B)$ is the homset of morphisms with domain A and codomain B (assuming that $\mathbb{C}$ is locally small). We fix a category $\mathbb{C}$ to which all objects and morphisms belong, unless stated otherwise.

1.1 Pattern Graphs

A pattern graph is an edge labelled graph in which the targets of edges can be placeholders for nodes that satisfy a certain *specification*, represented by words over the set of edge labels; the idea is that a word $p = \lambda_1 \dots \lambda_n$ of edge labels λ_i ($i = 1, \dots, n$) stands for some node v that is at the start of a path $v = v_0, e_1, v_1 \dots v_{n-1}, e_n, v_n$ where each edge e_i is labelled by λ_i ($i = 1, \dots, n$). Figure 1 shows an example and the formal definition is as follows.

Definition 1 (Pattern Graph (PG)). *Let Λ be a fixed set of* labels*. We denote the set of prefix-closed languages over Λ by $\wp_{\leq}(\Lambda^*) = \{\phi \subseteq \Lambda^* \mid pq \in \phi$ implies $p \in \phi\}$ where Λ^* is the monoid of words over Λ and $\varepsilon \in \Lambda^*$ is the empty word; elements of $\wp_{\leq}(\Lambda^*)$ are* specifications.

A pattern graph (PG) *is a pair $G = (V_G, E_G)$ where V_G is a set of* nodes *such that $V_G \cap \wp_{\leq}(\Lambda^*) = \varnothing$ and $E_G \subseteq V_G \times \Lambda \times (V_G \cup \wp_{\leq}(\Lambda^*))$ is a set of* edges*. A* basic graph *is a pattern graph (V_G, E_G) such that $E_G \subseteq V_G \times \Lambda \times V_G$.*

Example 1 (Pattern Graph). In the middle of Figure 1, we have illustrated a pattern

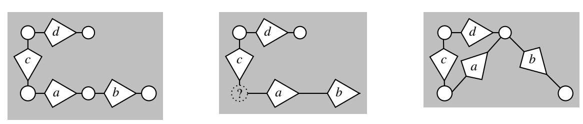


Fig. 1. A pattern graph (centre) between two basic graph "instances"

graph with two nodes (drawn as white circles) and two edges (rendered as labelled kites) with labels c and d; the c-edge has the specification $\{\varepsilon, a, ab\}$ as target, which is drawn as a question mark with two consecutive kites with labels a and b. We can think of this pattern graph as a collection of basic graphs, including the ones shown on the left and the right in Figure 1.

Definition 2 (Semantics of Specifications). *Let $G = (V, E)$ be a pattern graph. A node $v \in V$* satisfies *$p \in \Lambda^*$, written $v \models_G p$, if either p is the empty word ε or $p = \lambda p'$ (for some $\lambda \in \Lambda$ and $p' \in \Lambda^*$) and there exists $(v, \lambda, x) \in E$ such that either*

- *$x \models_G p'$ and $x \in V$ or*
- *$p' \in x$ and $x \in \wp_{\leq}(\Lambda^*)$.*

A node $v \in V$ satisfies *$\phi \in \wp_{\leq}(\Lambda^*)$, written $v \models_G \phi$, if $v \models_G p$ for all $p \in \phi$.*

Pattern graphs congregate into a category where morphisms are functions between node sets that preserve the structure (w.r.t. suitable "instances" of specifications).

Definition 3 (Category of Pattern Graphs). *A* homomorphism *from a pattern graph G to a pattern graph H, denoted by $f\colon G \to H$, is a function $f\colon V_G \to V_H$ such that*

(i) $(f(u), \lambda, f(v)) \in E_H$ *holds whenever* $(u, \lambda, v) \in E_G$ *and* $v \in V_G$*; and*
(ii) *for all edges* $(u, \lambda, \psi) \in E_G$ *with* $\psi \in \wp_{\leq}(\Lambda^*)$*, there exists* $x \in V_H \cup \wp_{\leq}(\Lambda^*)$ *such that* $(f(u), \lambda, x) \in E_H$ *and one of the following hold:*
   (i) $x \in V_H$ *and* $x \models \psi$*;*
   (ii) $x \in \wp_{\leq}(\Lambda^*)$ *and* $\psi \subseteq x$*.*

A homomorphism $f\colon G \to H$ is an inclusion *if $f(v) = v$ holds for all $v \in V_G$, in which case we write $G \subseteq H$ and call G a* subgraph *of H.*

The category of pattern graphs, denoted by $\mathbb{PG}$, has PG*s as objects, homomorphisms as morphisms, the identity on a* PG *G is the function* id_{V_G}*, and composition of morphisms is function composition. Finally, $\mathbb{BG} \subseteq \mathbb{PG}$ is the full subcategory of basic graphs.*

1.2 Categories of Partial Maps

If $\mathbb{C}$ has pullbacks (along monos), we have an associated category of partial maps, which we denote by $\mathbb{C}_*$. It has the same objects as $\mathbb{C}$ and each homset $\mathbb{C}_*(A, B)$ contains partial maps, which are essentially pairs of a mono $A \overset{m}{\leftarrowtail} A'$ in $\mathbb{C}$ and a morphism $A' \xrightarrow{f} B$ in $\mathbb{C}$ (quotiented up to isomorphism at A').

Definition 4 (Spans and Partial Maps). *A* span *is a diagram $A \xleftarrow{m} X \xrightarrow{f} B$; such a span is a* partial map span *if m is a mono. A* partial map *from A to B, denoted by $(m, X, f\rangle\colon A \rightharpoonup B$ or just $(m, f\rangle$, is an isomorphism class of a partial map span, i.e.*

$$(m, X, f\rangle = \left\{ A \overset{n}{\leftarrowtail} Y \xrightarrow{g} B \;\middle|\; \begin{array}{l} \text{There exists an isomorphism } i\colon Y \xrightarrow{\cong} X \\ \text{such that } \begin{tikzcd}[row sep=tiny] & X \arrow[dl, tail, "m"'] \arrow[dr, "f"] & \\ A & & B \\ & Y \arrow[ul, tail, "n"] \arrow[uu, "i"] \arrow[ur, "g"'] & \end{tikzcd} \text{ commutes.} \end{array} \right\}$$

for some representative partial map span $A \overset{m}{\leftarrowtail} X \xrightarrow{f} B$. A partial map $(m, f\rangle$ is a total map *if m is an isomorphism.*

Partial maps in $\mathbb{SET}$ are essentially partial functions and a partial map from a PG G to a PG H corresponds to a pair of a subgraph $G' \subseteq G$ and a morphism from G' to H (where G' is the *domain of definition*).

Often one wants to restrict the class of monos that can be used in partial maps. For example, in [9], for the encoding of the Kappa language, it is crucial that the domains of definition in partial maps are *closed*.

Definition 5 (Closed Mono). *An inclusion $i\colon G \overset{\subseteq}{\rightarrow} H$ in $\mathbb{PG}$ is* closed *if $(v, \lambda, x) \in E_H$ and $v \in V_G$ imply $(v, \lambda, x) \in E_G$ for all $v \in V_H$, $\lambda \in \Lambda$, and $x \in V_H \cup \wp_{\leq}(\Lambda^*)$; in this situation G is a* closed subgraph *of H. A mono $m\colon G' \rightarrowtail H$ is* closed *if it is isomorphic to a closed inclusion $i\colon G \overset{\subseteq}{\rightarrow} H$ (in $\mathbb{PG}/H$). The class of closed monos is denoted by $\mathcal{C}\mathcal{l}$.*

Thus, each node v in a closed subgraph $G \subseteq H$ has the same successors as v in H, where a successor of v is any node w for which $(v, \lambda, w) \in E_H$ holds for some $\lambda \in \Lambda$.

To obtain categories of partial maps where the left legs of all partial map spans belong to a certain class $\mathcal{M}$ (as detailed in Definition 7), one has to ensure that $\mathcal{M}$ is *admissible* [15].

Definition 6 (Admissible Classes of Monos). *Let $\mathcal{M}$ be a class of monos in $\mathbb{C}$, the elements of which are called* $\mathcal{M}$-morphisms*, and we write $A' \xhookrightarrow{m} A$ if $m \in \mathcal{M}$. The class $\mathcal{M}$ is* stable (under pullback) *if for each pair of morphisms $B \xrightarrow{f} A \xhookleftarrow{m} C$ with $m \in \mathcal{M}$ and each pullback $B \xleftarrow{m'} D \xrightarrow{f'} C$ of $B \xrightarrow{f} A \xhookleftarrow{m} C$, the mono m' belongs to $\mathcal{M}$.*

The class $\mathcal{M}$ of monos is admissible*, if*

(i) the category $\mathbb{C}$ has pullbacks along $\mathcal{M}$-morphisms;
(ii) the class $\mathcal{M}$ is stable under pullback;
(iii) the class $\mathcal{M}$ contains all identities;
(iv) the class $\mathcal{M}$ is closed under composition: if $(A \xhookrightarrow{m} B), (B \xhookrightarrow{n} C) \in \mathcal{M}$ then $(A \xhookrightarrow{n \circ m} C) \in \mathcal{M}$.

We now fix an admissible class $\mathcal{M}$ in $\mathbb{C}$. Examples of admissible classes (in any category) are regular monos and isomorphisms; open subspaces of topological spaces and downward closed subsets of partial orders induce more interesting examples, insofar as they are nontrivial proper subclasses of all monos, which we shall refer to as $\mathcal{M}ono$. Finally, closed monos are admissible.

Lemma 1 (Closed Monos are Admissible). *The class $\mathcal{C}l$ is an admissible class of monos in $\mathbb{PG}$.*

The definition of admissible classes of monos exactly captures the conditions of a well-defined category of $\mathcal{M}$-partial maps [15].

Definition 7 (Partial Map Categories). *The* category of $\mathcal{M}$-partial maps*, denoted by $\mathbb{C}_{*\mathcal{M}}$, has the same objects as the category $\mathbb{C}$ and the morphisms between two objects $A, B \in \mathbb{C}_{*\mathcal{M}}$ are the elements of*

$$\mathbb{C}_{*\mathcal{M}}(A,B) = \{(m, X, f\rangle \colon A \rightharpoonup B \mid A \xhookleftarrow{m} X \xrightarrow{f} B \ \ \&\ m \in \mathcal{M}\}$$

which contains all $\mathcal{M}$-partial maps *from A to B.*[3]

The identity on an object A is $(\mathrm{id}_A, A, \mathrm{id}_A\rangle$; given two $\mathcal{M}$-partial maps $(m, X, f\rangle \colon A \rightharpoonup B$ and $(k, Z, h\rangle \colon B \rightharpoonup C$, their composition is $(k, Z, h\rangle \circ (m, X, f\rangle = (m \circ p, U, h \circ q\rangle$ where $X \xhookleftarrow{p} U \xrightarrow{q} Z$ is some arbitrary pullback of $X \xrightarrow{f} B \xhookleftarrow{k} Z$.

$$\begin{tikzcd}
 & & U \arrow[dl, hook', "p"'] \arrow[dr, "q"] & & \\
A & X \arrow[l, hook', "m"'] \arrow[dr, "f"'] & & Z \arrow[dl, hook, "k"] \arrow[r, "h"] & C \\
 & & B & &
\end{tikzcd}$$

The covariant embedding *of $\mathbb{C}$, denoted by $\Gamma \colon \mathbb{C} \to \mathbb{C}_{*\mathcal{M}}$, is the unique functor from $\mathbb{C}$ to $\mathbb{C}_{*\mathcal{M}}$ that maps each morphism $f \colon A \to B$ in $\mathbb{C}$ to the total map $\Gamma f = (\mathrm{id}_A, f\rangle \colon A \rightharpoonup B$ in $\mathbb{C}_{*\mathcal{M}}$ (and thus satisfies $\Gamma(A) = A$ for all $A \in \mathbb{C}$).*

We shall call arrows in $\mathbb{C}$ *morphisms* and reserve *'map'* for arrows of $\mathbb{C}_{*\mathcal{M}}$.

We conclude this section with the definition of inverse image functions between meet-semilattices of $\mathcal{M}$-subobjects and a review of direct image functions. For this, recall that each $\mathcal{M}$-morphism $m \colon M \xhookrightarrow{m} A$ is a representative of the subobject $[m]$, i.e. its isomorphism class in the slice category $\mathbb{C}/A$. Note that a $\mathcal{M}ono$-subobject in $\mathbb{SET}$ is essentially a subset and closed subgraphs correspond to $\mathcal{C}l$-subobjects in $\mathbb{PG}$. We denote the poset of $\mathcal{M}$-subobjects over any object $A \in \mathbb{C}$ by $\mathrm{Sub}_{\mathcal{M}}A$; given $\mathcal{M}$-subobjects

[3] This implies that the left leg of each representative partial map span is an $\mathcal{M}$-morphism.

$[m], [n] \in \mathrm{Sub}_{\mathcal{M}}A$, the subobject $[m]$ is *included* in $[n]$, written $m \sqsubseteq n$, if there exists a morphism $i\colon m \to n$ in $\mathbb{C}/A$. For $A \in \mathbb{SET}$, $\mathrm{Sub}_{\mathcal{M}\mathrm{ono}}A$ is isomorphic to the powerset $\wp(A)$ and the relation $\sqsubseteq$ is just the appropriate generalization of inclusions of subsets. The meet $[m] \sqcap [n]$ is given by the diagonal of the pullback of m along n. Finally, inverse images are obtained by pulling back representatives of subobjects along morphisms, and for a partial map $(n, f\rangle$, its *domain of definition* is the subobject $[n]$.

Definition 8 (Inverse Images). *Let $f\colon A \to B$ in $\mathbb{C}$ be a morphism. The* inverse image *function $f^{-1}\colon \mathrm{Sub}_{\mathcal{M}}B \to \mathrm{Sub}_{\mathcal{M}}A$ maps each $[M \xhookrightarrow{m} B] \in \mathrm{Sub}_{\mathcal{M}}B$ to the subobject $f^{-1}([m])$ such that for all pullbacks $A \xhookleftarrow{m'} M' \xrightarrow{f_m} M$ of $A \xrightarrow{f} B \xhookleftarrow{m} M$ we have $f^{-1}([m]) = [m']$.*

For each $\mathcal{M}$-morphism $m\colon Y \hookrightarrow X$, *post-composition with* m, which maps $[y] \in \mathrm{Sub}_{\mathcal{M}}Y$ to $[m \circ y]$, is a monotone function; it is denoted by $\exists_m\colon \mathrm{Sub}_{\mathcal{M}}Y \to \mathrm{Sub}_{\mathcal{M}}X$ (as it is the lower adjoint to m^{-1}).

2 Pushouts of Partial Maps: the State of the Art

Pushouts of partial maps are at the heart of single pushout rewriting [11], one of the standard approaches to graph rewriting; rules of rewriting can be arbitrary partial maps and applying rewriting rules amounts to taking pushouts of rules along a class of *matching morphisms*, which often are assumed to be total. Thus, the existence of pushouts of partial maps (along total maps) is pivotal. In this section, we therefore discuss results on the existence of certain pushouts in $\mathbb{C}_{*\mathcal{M}}$ and their corresponding diagrams in our fixed category $\mathbb{C}$ with its admissible class of monos $\mathcal{M}$. We have not found the following results formulated anywhere in the literature (despite closely related work [16, 17, 14]).

2.1 A Necessary Condition for Pushouts of Partial Maps

We begin with a discussion of the crucial role of upper adjoints to inverse image functions, which appears to have been neglected in the literature.

Definition 9 (Upper Adjoints to Inverse Images). *Let $f\colon A \to B$ in $\mathbb{C}$, and let $f^{-1}\colon \mathrm{Sub}_{\mathcal{M}}B \to \mathrm{Sub}_{\mathcal{M}}A$ be its inverse image function. A $\sqsubseteq$-monotone function $\mathcal{U}\colon \mathrm{Sub}_{\mathcal{M}}A \to \mathrm{Sub}_{\mathcal{M}}B$ is an* upper adjoint *of f^{-1} if for all $n \in \mathrm{Sub}_{\mathcal{M}}B$ and all $m \in \mathrm{Sub}_{\mathcal{M}}A$, we have $f^{-1}(n) \sqsubseteq m$ if and only if $n \sqsubseteq \mathcal{U}(m)$; if an upper adjoint of f^{-1} exists, it is denoted by $\forall_f$ and we write $f^{-1} \dashv \forall_f$ or $\forall_f \vdash f^{-1}$.*[4]

An example of how the upper adjoint of a morphism in $\mathbb{PG}$ can act on subobjects is given in Figure 2, which will be discussed in detail in Example 2.

Proposition 1 (Necessity of Upper Adjoints to Inverse Images). *If $\mathbb{C}_{*\mathcal{M}}$ has all pushouts (along total maps), i.e. if for every morphism $f\colon A \to B$ in $\mathbb{C}$ and every map $\phi\colon A \rightharpoonup C$ in $\mathbb{C}_{*\mathcal{M}}$, there is a pushout of $C \overset{\phi}{\leftharpoonup} A \overset{(\mathrm{id},f\rangle}{\rightharpoonup} B$ in $\mathbb{C}_{*\mathcal{M}}$, then the upper adjoint $\forall_f \vdash f^{-1}$ exists for any morphism f in $\mathbb{C}$.*

[4] Recall that upper adjoints are actually unique if they exist.

Proof. The proof is given in Appendix B.

Thus, if we want $\mathbb{C}_{*\mathcal{M}}$ to have pushouts along total maps, we need upper adjoints of inverse image functions of $\mathcal{M}$-subobjects in $\mathbb{C}$. It is typically easy to check whether the latter exist; it suffices to show that for all morphisms $f\colon A \to B$ in $\mathbb{C}$ and every subobject $[m] \in \mathrm{Sub}_{\mathcal{M}}A$, the join $[m'] := \bigsqcup\{[n] \in \mathrm{Sub}_{\mathcal{M}}B \mid f^{-1}([n]) \sqsubseteq m\}$ exists and that setting $\forall_f([m]) := [m']$ yields $\forall_f \vdash f^{-1}$.

Lemma 2 (Upper Adjoint for Inverse Images of Closed Monos). *In $\mathbb{PG}$, for all $f\colon A \to B$, the upper adjoint $\forall_f\colon \mathrm{Sub}_{\mathcal{Cl}}A \to \mathrm{Sub}_{\mathcal{Cl}}B$ exists.*

Example 2 (Implicit Deletion in SPO Rewriting). In Figure 2, we have a closed subgraph $m\colon K \hookrightarrow L$, a morphism $f\colon L \to G$, and $\forall_f([m])$ yields the result of applying the rule $(m, \mathrm{id}_K\rangle$ at f using the SPO approach (cf. Proposition 1, Theorem 2). Roughly, this amounts to removing everything that is in the codomain of m but not in its domain. Due to the choice of closed monos, removal of the node ③ forces the removal of the node ①, which would leave the "dangling edge" $-\langle d\rangle-$②, which is therefore also removed.

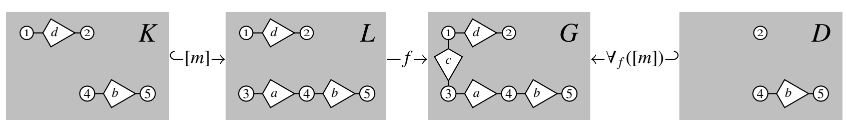


Fig. 2. Implicit deletion with closed monos

We will now turn to our second condition for the existence of pushouts in $\mathbb{C}_*$, which is necessary if $\mathbb{C}$ is a slice category $\mathbb{C} = \mathbb{D}/T$.

2.2 A Locally Necessary Condition

One might expect that taking a pushout of a span of total maps in $\mathbb{C}_{*\mathcal{M}}$ yields a cospan of total maps; however, this is only true if spans in $\mathbb{C}$ have cocones, as (implicitly[5]) assumed in [14]. This assumption implies that all pushouts in $\mathbb{C}$ are hereditary if $\mathbb{C}_{*\mathcal{M}}$ has pushouts.

Definition 10 (Hereditary Pushouts). *A pushout $B \xrightarrow{b} D \xleftarrow{c} C$ of a span $B \xleftarrow{f} A \xrightarrow{g} C$ in $\mathbb{C}$ is* hereditary *if $B \overset{\ulcorner b \urcorner}{\rightharpoonup} D \overset{\ulcorner c \urcorner}{\leftharpoonup} C$ is a pushout of the span $B \overset{\ulcorner f \urcorner}{\leftharpoonup} A \overset{\ulcorner g \urcorner}{\rightharpoonup} C$ in $\mathbb{C}_{*\mathcal{M}}$.*

Proposition 2 (Pushouts of Total Maps). *Suppose the category $\mathbb{C}$ has cocones for spans, i.e. for each span $C \xleftarrow{g} A \xrightarrow{f} B$, there exists a cospan $C \xrightarrow{f'} D \xleftarrow{g'} B$ such that $g' \circ f = f' \circ g$. If $\mathbb{C}_{*\mathcal{M}}$ has pushouts of partial maps (along total maps), then $\mathbb{C}$ has pushouts and the latter are hereditary.*

[5] This assumption is implicitly made in the proof of Theorem 3.2(iii) in [14, p. 6] where Kennaway writes "forming a commutative square in **C** with some arrows $N' \to D'$ and $O' \to D'$".

Proof. Let $C \xleftarrow{g} A \xrightarrow{f} B$ be a span in $\mathbb{C}$ with cocone $C \xrightarrow{f'} D \xleftarrow{g'} B$; moreover let $C \xrightharpoonup{(m,M,h)} E \xleftharpoonup{(k,N,n)} B$ be a pushout of $C \xleftharpoonup{\Gamma g} A \xrightharpoonup{\Gamma f} B$. By the universal property of the pushout in $\mathbb{C}_{*\mathcal{M}}$, there is a unique map $\phi\colon E \rightharpoonup D$ such that $\Gamma(f') = \phi \circ (m, h)$ and $\Gamma(g') = \phi \circ (n, k)$. The latter implies that $\mathrm{id}_C \sqsubseteq m$ and $\mathrm{id}_B \sqsubseteq n$ and thus both of n and m are isomorphisms. Now one can show that $C \xrightarrow{h \circ m^{-1}} E \xleftarrow{k \circ n^{-1}} B$ is a pushout of $C \xleftarrow{g} A \xrightarrow{f} B$ in $\mathbb{C}$ and that it is hereditary follows from $\Gamma(h \circ m^{-1}) = (m, h)$ and $\Gamma(k \circ n^{-1}) = (n, k)$. ◻

Remark 1. Pushouts are not hereditary, in general. For example, $\Gamma\colon \mathbb{PG} \to \mathbb{PG}_{*\mathcal{M}ono}$ does not preserve pushouts. To see why, consider the span ①–a→② $\xleftarrow{\iota}$ ① ② $\xrightarrow{\iota}$ ①–a→② where the morphism ι is the inclusion; this span has the pushout ①–a→② $\xrightarrow{\mathrm{id}}$ ①–a→② $\xleftarrow{\mathrm{id}}$ ①–a→② in $\mathbb{PG}$. However, the embedding of this pushout into $\mathbb{PG}_{*\mathcal{M}ono}$ is not a pushout. To see this, note that ①–a→② $\xrightharpoonup{(\iota,\iota)}$ ①–a→② $\xleftharpoonup{\mathrm{id}}$ ①–a→② is a cocone in $\mathbb{PG}_{*\mathcal{M}ono}$; moreover it is easy to show that there is no mediating morphism, making a case distinction on whether the edge is in the domain of definition or not. Thus, even if all pushouts exist, they need not be hereditary; the class of monos is crucial.

Thus, under mild assumptions on $\mathbb{C}$, having pushouts of partial maps (along total ones) implies that $\mathbb{C}$ has hereditary pushouts. The latter condition is often easy to check using the theorem that left adjoint functors preserve *all* colimits. Thus, to show that all pushouts (that exist) are hereditary, it suffices to establish a right adjoint to the covariant embedding $\Gamma\colon \mathbb{C} \to \mathbb{C}_{*\mathcal{M}}$.

Proposition 3 (Hereditary Pushouts of Pattern Graphs). *Pushouts of the category $\mathbb{PG}$ are hereditary w.r.t. $\Gamma\colon \mathbb{PG} \to \mathbb{PG}_{*\mathcal{C}l}$.*

Proof. Spelling out the definition of a right adjoint to Γ leads to the fact that it is enough to give for each PG G a closed inclusion $\tilde{g}\colon G \hookrightarrow G'$ such that for each partial map $(n, H', f)\colon H \rightharpoonup G$ there is a unique morphism $f'\colon H \to G'$ satisfying $[n] = f'^{-1}([\tilde{g}])$. In fact, defining $G' = (V_G \cup \{\bot\}, E_G \cup \{\bot\} \times \Lambda \times (V_G \cup \{\bot\} \cup \wp_{\leq}(\Lambda^*)))$ yields the desired. ◻

Our main result will show that the discussed two conditions for the existence of pushouts of partial maps (which are necessary in the presence of cocones of spans) are in fact sufficient. To understand the main difficulty of this result, we discuss a peculiar fact about pushouts in $\mathbb{C}_{*\mathcal{M}}$ in terms of the underlying diagrams in $\mathbb{C}$.

2.3 Challenge for a Sufficient Condition

Our main theorem will establish that upper adjoints of inverse image functions and hereditary pushouts together are in fact sufficient to obtain pushouts of all spans of partial maps. The crucial point in the proof is the construction of the domain of definition of the diagonal of a pushout candidate. The main difficulty is to show the existence of the join of subobjects that is illustrated in Figure 3 below. More precisely, we have the following proposition (using the proof idea of Theorem 3.2 of [14]).

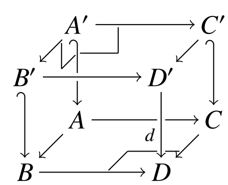
Proposition 4 (Pushout Diagonal). *Assuming that $\mathbb{C}$ has cocones for all spans, let $C \xleftharpoonup{(g,N,n)} A \xrightharpoonup{(m,M,f)} B$ be a span with pushout $C \xrightharpoonup{(m',M',f')} X \xleftharpoonup{(g',N',n')} B$ in $\mathbb{C}_{*\mathcal{M}}$, and, let $(k, h) = (n', g') \circ (m, f)$ be the diagonal of the resulting pushout square. Then there is a diagram as in Figure 3 in $\mathbb{C}$ (where the marked squares are pullbacks in $\mathbb{C}$).*

$$
\begin{tikzcd}
A & M \arrow[l, hook', "m"'] \arrow[r, "f"] & B \\
N \arrow[u, hook, "n"] \arrow[d, "g"'] & K \arrow[l, hook'] \arrow[r] \arrow[u, hook] \arrow[d] \arrow[ul, "k"] & N' \arrow[u, hook', "n'"'] \arrow[d, "g'"] \\
C & M' \arrow[l, hook', "m'"] \arrow[r, "f'"'] & X
\end{tikzcd}
\qquad
[\boldsymbol{k}] = \bigsqcup \left\{ x \in \mathrm{Sub}_{\mathcal{M}} A \;\middle|\; \begin{array}{l} \exists b \in \mathrm{Sub}_{\mathcal{M}} B.\, \exists c \in \mathrm{Sub}_{\mathcal{M}} C. \\ \exists_m(f^{-1}(b)) = x = \exists_n(g^{-1}(c)) \end{array} \right\}
$$

Fig. 3. The domain of definition of the diagonal of a pushout of partial maps

In previous work, the existence of the join $[\boldsymbol{k}]$ in Figure 3 was either trivial [10] or assumed implicitly [14]; related assumptions are used for span-based rewriting, namely limits of small diagrams in [17] and the rather unwieldy final *triple diagrams* in [16]. In contrast, we shall *show* how existence of $[\boldsymbol{k}]$ follows from upper adjoints to inverse image functions and hereditary pushouts. Interestingly, this will involve the following characterization of hereditary pushouts from [13] (see also Theorem B.4 of [18]).

Theorem 1 (Hereditary Pushout Characterization [13]). *Let $\mathbb{C}$ be a category with pushouts and let $\mathcal{M}$ be an admissible class of monos in $\mathbb{C}$; let $B \leftarrow A \rightarrow C$ be a span with pushout $B \rightarrow D \leftarrow C$.*
The pushout is hereditary if and only if for every completion to a commutative cube as shown to the right, where the morphisms $B' \hookrightarrow B$ and $C' \hookrightarrow C$ are $\mathcal{M}$-morphisms and the back faces are pullback squares, the top face is a pushout if and only if the front faces are pullbacks and $d\colon D' \rightarrow D$ is an $\mathcal{M}$-morphism.



In the proof of our main theorem, we also shall use the following consequence from [13], generalizing Lemma 2.3 of [19].

Lemma 3 (Pushouts along $\mathcal{M}$-morphisms [19, 13]). *Let $C \xleftarrow{m} A \xrightarrow{f} B$ be a span with $m \in \mathcal{M}$ and let $C \xrightarrow{g} D \xleftarrow{n} B$ be a pushout that is hereditary and assume $\mathbb{C}$ has pushouts. Then n is an $\mathcal{M}$-morphism, $[m] = f^{-1}[n]$, and $[n] = \forall_f([m])$.*

In particular, $\mathcal{M}$ is pushout stable and pushouts along $\mathcal{M}$ yield pullback squares.

3 Partial Map Pushouts by Inheritance

We now present our main contribution: a construction of pushouts of partial maps that uses only hereditary pushouts and upper adjoints of inverse image functions. Thus, the conditions from the previous section, which are necessary locally, turn out to be sufficient. As a direct consequence, our construction of partial map pushouts directly transfers to slice categories, which turns out to be surprisingly useful in practice [9].

Theorem 2 (Existence of Pushouts of Partial Maps). *Let $\mathbb{C}$ be a category with cocones for spans with an admissible class of monos $\mathcal{M}$. The partial map category $\mathbb{C}_{*\mathcal{M}}$ has pushouts if and only if $\mathbb{C}$ has hereditary pushouts and inverse image functions between $\mathcal{M}$-subobject posets have upper adjoints.*

Proof. The *only if*-part follows from Proposition 1 and Proposition 2.

For the converse, let $C \leftharpoonup\!\!\!(g,N,n)\!- A -\!(m,M,f)\!\rightharpoonup B$ be a span in $\mathbb{C}_{*\mathcal{M}}$, assume that $\mathbb{C}$ has hereditary pushouts, and that for any morphism $h\colon Y \to Z$ in $\mathbb{C}$, the upper adjoint $\forall_h$ of the inverse image function $h^{-1}\colon \mathrm{Sub}_{\mathcal{M}}Z \to \mathrm{Sub}_{\mathcal{M}}Y$ exists. We shall first construct a suitable subobject $[k] \in \mathrm{Sub}_{\mathcal{M}}A$ (cf. Figure 3).

The Domain of Definition of the Diagonal Working in $\mathbb{C}$, we start by constructing the diagram on the left in Figure 4. Thus, $C \xhookrightarrow{\bar{n}} G \xleftarrow{\bar{g}} A$ is the pushout of $C \xleftarrow{g} N \xhookrightarrow{n} A$

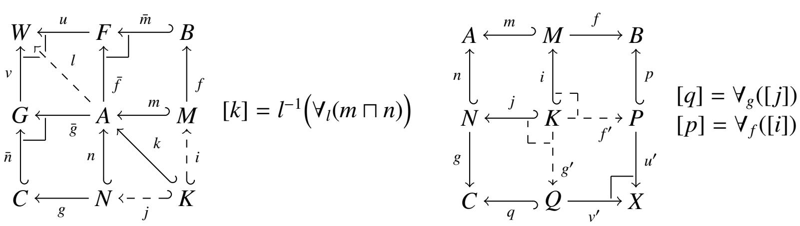


Fig. 4. Construction of pushouts of partial maps

and $A \xrightarrow{\bar{f}} F \xhookleftarrow{\bar{m}} B$ is the pushout of $A \xhookleftarrow{m} M \xrightarrow{f} B$; moreover, $G \xrightarrow{v} W \xleftarrow{u} F$ is the pushout of $G \xleftarrow{\bar{g}} A \xrightarrow{\bar{f}} F$ and $l = v \circ \bar{g} = u \circ \bar{f}$, which is the diagonal of the latter pushout in $\mathbb{C}$. Finally, we put $[k] := l^{-1}(\forall_l(m \sqcap n))$.

Note that $[k] = l^{-1}(\forall_l(m \sqcap n)) \sqsubseteq (n \sqcap m)$ (by Lemma 8). Hence, there are unique morphisms $j\colon k \to n$ and $i\colon k \to m$ (in $\mathbb{C}/A$), witnessing the respective inclusions $k \sqsubseteq n$ and $k \sqsubseteq m$ (which follow from $k \sqsubseteq (m \sqcap n) \sqsubseteq n$ and $k \sqsubseteq (m \sqcap n) \sqsubseteq m$).

The Construction of a Pushout Candidate Let $[q] = \forall_g([j])$ and $[p] = \forall_f([i])$. As illustrated in Figure 4 on the right, we claim that there exist arrows $g'\colon (g \circ j) \to q$ in $\mathbb{C}/C$ and $f'\colon (f \circ i) \to p$ in $\mathbb{C}/B$, which then let us construct a pushout $Q \xrightarrow{v'} X \xleftarrow{u'} P$ of $Q \xleftarrow{g'} K \xrightarrow{f'} P$ (in $\mathbb{C}$) to obtain $C -\!(q,v')\!\rightharpoonup X \leftharpoonup\!(u',p)\!- B$ as a pushout candidate, i.e. $(q, v') \circ (n, g) = (p, u') \circ (m, f)$ in $\mathbb{C}_{*\mathcal{M}}$. Thus, we first have to prove the following claim.

Claim. The equations $g^{-1} \circ \forall_g([j]) = [j]$ and $f^{-1} \circ \forall_f([i]) = [i]$ hold.

The relevant steps are two: first, we verify that $(\bar{g})^{-1}(\forall_{\bar{g}}([k])) = [k]$, and thus $\forall_{\bar{g}}([k]) \sqsubseteq [\bar{n}]$ (using Lemma 3); second, we show that $\forall_{\bar{g}}([k]) = [\bar{n} \circ q]$, whence the desired follows (using Lemma 6). The details of the proof, including the universal property of the candidate, are given in Appendix C. □

Corollary 1. *If a category has cocones for spans of morphisms and pushouts of partial maps, the same is true for all of its slice categories.*

We give a name to categories that "inherit" partial map pushouts.

Definition 11 (Inherited Partial Map Pushouts). *A category $\mathbb{C}$ with an admissible class of monos $\mathcal{M}$ has* inherited $\mathcal{M}$-partial map pushouts *or is a* $\mathcal{M}$IPMAP category *if $\mathbb{C}$ has hereditary pushouts and upper adjoints to inverse image functions.*

Note that Mipmap categories are in particular vertical weak adhesive High Level Replacement Categories (cf. [12]) and partial map adhesive [13]. The category $\mathbb{PG}$ belongs to this class as does every (quasi-)topos (which directly follows from the definition of quasi-topos given in [20]).

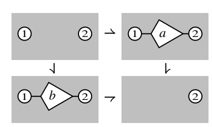
4 On Pushouts in Full Subcategories

Mipmap categories share many properties with adhesive categories [19], are a further development of recent generalizations [18, 13], and fit well with the theory of categorical frameworks for rewriting (as surveyed in [12]). In particular, they allow the development of standard results of graph rewriting [11] that can be applied to a wide range of graph-like structures. However, the structure of fragments of biochemical species, as modelled by the Kappa language, imposes additional constraints that add an extra level of complication to the picture [9]; the fundamental reason is that the seemingly natural condition that all spans have cocones is not satisfied. We resolve this by working with broader categories that do satisfy the constraints to be a Mipmap category, and then consider reflective subcategories to obtain a characterization of pushouts. We use a simplified example to illustrate the additional details that are involved in a faithful model of Kappa.

Example 3 (Branching-Free Graphs I). Let $\mathbb{B} \subseteq \mathbb{BG}$ be the full subcategory of all basic graphs that have at most one outgoing edge per node, i.e. in every graph $G \in \mathbb{B}$, any two edges (v, λ, u) and (v, λ', u') that share the same source node v are identical, i.e., $\lambda = \lambda'$ and $u = u'$. In this full subcategory $\mathbb{B} \subseteq \mathbb{BG}$, we have the following example of a span without cocone.

Note that if a cocone for this span would exist in $\mathbb{B}$, the image of node ① in the "tip" of the cocone would be the source of two different edges, namely one labelled a and one labelled b – a contradiction to branching-freeness.

In contrast, the embedding of this span into $\mathbb{B}_{*el}$ has not only a cocone but we even have the pushout that is shown to the right. Note that both partial maps of the pushout cocone have {②} as domain of definition and thus are properly partial (cf. Proposition 2). To see that this square actually is a pushout square, we first observe that the maps of any cocone cannot have node ① in the domain of definition as then both maps would also have the outgoing edge in the domain of definition, which in turn would imply that the "tip" of the cocone is not branching-free. The only remaining choice for a cocone is to either not contain node ② in the domains of definition or that it is mapped to the same node by both morphisms. There is an obvious unique mediating morphism for both cases.



This example shows that pushouts in partial map categories are even more intricate if the category of total maps is not a Mipmap-category. The concrete details of conditions for spans of partial maps that ensure the existence of a pushout can be rather complex; the prime example is the situation of [9]. However, non-constructively, we can show that all pushouts that do exist in a full subcategory $\mathbb{D} \subseteq \mathbb{C}_{*\mathcal{M}}$ can be *lifted* from a canonical subcategory $\mathbb{X} \subseteq \mathbb{C}_{*\mathcal{M}}$.

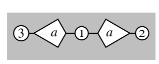
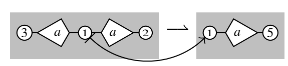
Lemma 4 (Pushout via Reflection). *Let $\mathbb{D} \subseteq \mathbb{E}$ be a full subcategory of an arbitrary category $\mathbb{E}$. There exists a greatest full subcategory $\mathbb{X} \subseteq \mathbb{E}$ such that $\mathbb{D} \subseteq \mathbb{X}$ is a reflective subcategory.*

Proof. Clearly, $\mathbb{D}$ is a reflective subcategory of itself. Moreover, a subcategory $\mathbb{X} \subseteq \mathbb{E}$ contains $\mathbb{D}$ as reflective subcategory if and only if for each object $X \in \mathbb{X}$ there exists a morphism $\eta_X : X \to \bar{X}$ in $\mathbb{E}$ with $\bar{X} \in \mathbb{D}$ such that for every other morphism $f : X \to D$ in $\mathbb{E}$ with $D \in \mathbb{D}$, there is a unique arrow $f^\sharp : \bar{X} \to D$ in $\mathbb{E}$ satisfying $f = f^\sharp \circ \eta_X$. Now, $\mathbb{X}$ is just the category that contains all objects $X \in \mathbb{X}$ for which there exist η_X as above, because these η_X define the unit of the reflection $\mathbb{D} \subseteq \mathbb{X}$. $\square$

This result allows to characterize when pushouts in $\mathbb{D}$ exist: a span $B \xleftarrow{f} A \xrightarrow{g} C$ in $\mathbb{D}$ has a pushout in $\mathbb{D}$ if, and only if, it has a pushout $B \xrightarrow{g'} X \xleftarrow{f'} C$ in $\mathbb{E}$ such that $X \in \mathbb{X}$. If such a pushout exists, then it can be lifted from $\mathbb{X}$ to $\mathbb{D}$, using the left adjoint $\mathcal{L}$ to the inclusion $\mathbb{D} \subseteq \mathbb{X}$, namely $B \xrightarrow{\mathcal{L}(g')} \mathcal{L}(X) \xleftarrow{\mathcal{L}(f')} C$ is the pushout of $B \xleftarrow{f} A \xrightarrow{g} C$; finally we have $\mathcal{L}(g') = \eta_X \circ g$ and $\mathcal{L}(f') = \eta_X \circ f$.

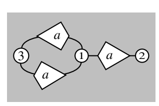
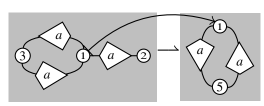
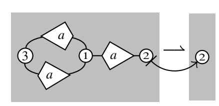
The category $\mathbb{X}$ of Lemma 4 can be non-trivial, i.e. $\mathbb{D} \neq \mathbb{X} \neq \mathbb{E}$, as in the example of branching-free graphs.

Example 4 (Branching-Free Graphs II). The greatest subcategory of $\mathbb{X} \subseteq \mathbb{BG}$ that contains the category of branching-free graphs $\mathbb{B}$ as reflective category is non-trivial. To see this, we first consider the *fork* graph F, below on the left.

$F =$  $\eta_F :$ 

While F is clearly branching and $F \notin \mathbb{B}$, it is easy to verify that the map η_F above on the right is the universal way to make F branching-free, i.e. for any other $f : F \rightharpoonup F'$ such that F' is branching-free, there exists a unique $f^\sharp : \bar{F} \rightharpoonup F'$ such that $f = f^\sharp \circ \eta_F$.

In contrast, consider the situation in the *lollipop* L, below one the left.

$L =$  $g_1 :$  $g_2 :$ 

There are essentially two ways to remedy the branching at node ①: either ① is in the domain of definition, or not; the above partial maps g_1 and g_2 are examples for the respective cases. Now, suppose there was a universal arrow $\eta_L : L \to \bar{L}$ with $L \in \mathbb{B}$. If ① is in the domain of definition, then $\eta_L(②) = \eta_L(③)$ by branching-freeness and closure of domains of definition; as a consequence, there does not exist any $g_2^\sharp$ such that $g_2 = g_2^\sharp \circ \eta_L$. Thus, the only possibility would be that ① is not in the domain of definition. However, in the latter case, there is no $g_1^\sharp$ such that $g_1 = g_1^\sharp \circ \eta_L$. In the end, we see that also $L \notin \mathbb{X}$, and thus $\mathbb{B} \neq \mathbb{X} \neq \mathbb{BG}$.

The encoding of the Kappa calculus into pattern graphs from [9] fits the situation of Lemma 4, using a full subcategory of a suitable slice category of pattern graphs (as discussed further in the next section). We expect that a similar approach is suitable to encode BioNetGen and future extensions of Kappa without major complications.

5 Related and Future Work

The reference article for single pushout rewriting using the algebraic approach is [10], which gives set-theoretic characterizations of pushouts; the idea of a categorical characterization of pushouts of partial maps was first given in [14]. The present article gives a streamlined and rigorous account of (consequences of) results from [14], fixing minor omissions of the latter (see Footnote 5). Most importantly, our pushout construction in Figure 4 does not involve any assumptions about existence of joins in subobject lattices (which again are assumed implicitly in [14]), and it only uses pushouts, pullbacks, and upper adjoints of inverse images in $\mathbb{C}$. This can be useful for applications as we can develop algorithms to construct pushouts in $\mathbb{C}_{*\mathcal{M}}$ using well-understood constructions in $\mathbb{C}$. Even for the case of algebras over a signature [10], our main results sheds new light on pushouts of partial maps.

The restriction to full subcategories in applications has an elegant theoretical solution (Lemma 4), even if the complexity of the details of the encoding of Kappa [9] as a full subcategory of $(\mathbb{PG}/T_\kappa)_{*\mathcal{M}}$ for a suitable type graph T_κ is daunting. Another example of a subcategory of an adhesive category has been used in [21] in combination with the double pushout approach (DPO) [4], which is a special case of SPO in the presence of hereditary pushouts (by Lemma 3).

For DPO rewriting, the literature contains a variety of categorical frameworks and here we comment only on those of the last decade that are surveyed in [12]. In proposing $\mathcal{M}$IPMAP-categories as a framework for SPO rewriting, we do not intend to replace any of these; $\mathcal{M}$IPMAP-categories are also not the most modest strengthening, as partial map adhesive categories with relatively pseudo-complemented subobject posets have already pushouts along monos in $\Gamma(\mathcal{M})$ (cf. [22]). $\mathcal{M}$IPMAP-categories are based on our main theorem, can be instantiated to many examples (including all quasi-topoi), and have additional properties that are relevant for double pushout rewriting, e.g. the so-called Twisted-Triple-Pushout property (reusing the proof of Lemma 8.5 of [19]) without additional assumptions.

As future work, we plan to extend the category of pattern graphs in the spirit of graphs with constraints [23] and to incorporate negative application conditions. This will also involve translations of SPO-rewriting rules into families of DPO-rules, including a detailed study of the implicit application conditions of DPO rewriting.

Conclusion

The main result is a theorem of category theory that shows that upper adjoints of inverse images are a necessary and sufficient condition for the existence of pushouts of partial maps, provided that spans have cocones. Based on this theorem, we propose $\mathcal{M}$IPMAP-categories as a uniform framework for SPO and DPO rewriting. They are a natural strengthening of partial map adhesive categories [13], and even though they are not most general, $\mathcal{M}$IPMAP-categories are the first categorical framework that is relevant to both single and double pushout rewriting. A subtle point is the restriction to full subcategories of partial maps. While it does not pose any theoretical problems (cf. Lemma 4), it adds an extra level of complexity to the pushout construction, which can require substantial additional work in practice [9].

We have chosen the category of pattern graphs from [9] as example for $\mathcal{M}$IPMAP-categories, as the latter have been used to encode the rule-based modelling language Kappa [5, 6]. Pattern graphs bear obvious similarities with graphs from traditional graph transformation, and $\mathcal{M}$IPMAP-categories yield a formal connection to categorical frameworks [12]. The “missing link” to rule-based modelling in computational systems biology is given by Lemma 4, which also explains why the existing literature on graph transformation [11] was not of direct use as a semantic foundation for rule-based modelling.

In summary, our central results of category theory, Theorem 2 and Lemma 4, allow us to pinpoint the problems that had to be solved to give a formal SPO semantics to the Kappa modelling language [6]. Future work will further explore the use of graph-based formalisms in computational systems biology, symbolic quantum computation and traditional applications of graph rewriting.

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A Basic Category Theory

Here, we give definitions of selected notions that are used in the paper and can be found in virtually any textbook on category theory.

Definition 12 (Full Subcategory). *Let* $\mathbb{C}, \mathbb{D}$ *be categories. The category* $\mathbb{D}$ *is a* subcategory *of* $\mathbb{C}$ *if each object* $D \in \mathbb{D}$ *is also an object of* $\mathbb{C}$*, i.e.* $D \in \mathbb{C}$*, and we have inclusions of homsets* $\mathbb{D}(A, B) \subseteq \mathbb{C}(A, B)$ *for all objects* $A, B \in \mathbb{D}$*; it is a* full subcategory *if moreover we have equalities of homsets* $\mathbb{D}(A, B) = \mathbb{C}(A, B)$ *for all objects* $A, B \in \mathbb{D}$*.*

Definition 13 (Slice Category). *Let* $\mathbb{C}$ *be a category and let* $T \in \mathbb{C}$ *be an object. The* category of objects over T *or the* slice category over T*, denoted by* $\mathbb{C}/T$*, has* $\mathbb{C}$*-morphisms with codomain* T *as objects, and for two objects* $(A \xrightarrow{t_A} T), (B \xrightarrow{t_B} T) \in \mathbb{C}/T$*, a morphism from* t_A *to* t_B *is an arrow* $f \colon A \to B$ *in* $\mathbb{C}$ *such that* $t_B \circ f = t_A$*. Identities and composition are taken from* $\mathbb{C}$*.*

Recall that a functor between categories $\mathcal{F} \colon \mathbb{C} \to \mathbb{D}$ maps each object $A \in \mathbb{C}$ to an object $\mathcal{F}(A) \in \mathbb{D}$ and preserves identities and composition, i.e. $\mathcal{F}(\mathrm{id}_A) = \mathrm{id}_{\mathcal{F}(A)}$ and $\mathcal{F}(f \circ g) = \mathcal{F}(f) \circ \mathcal{F}(g)$.

We shall use the following definition of an adjunction.

Definition 14 (Adjoint Functors). *Let* $\mathcal{F} \colon \mathbb{C} \to \mathbb{D}$ *and* $\mathcal{G} \colon \mathbb{D} \to \mathbb{C}$ *be functors. The functor* $\mathcal{G}$ *is* right adjoint *to* $\mathcal{F}$ *or* $\mathcal{F}$ *is* left adjoint *to* $\mathcal{G}$ *if for each* $X \in \mathbb{C}$*, there exists an arrow* $\eta_X \colon X \to \mathcal{G} \circ \mathcal{F}(X)$ *such that for each object* $Y \in \mathbb{D}$ *and each arrow* $f \colon X \to \mathcal{G}(Y)$*, there is a unique arrow* $f^\sharp \colon \mathcal{F}(X) \to Y$ *such that* $f = \mathcal{G}(f^\sharp) \circ \eta_X$*.*

Recall that left adjoints preserve all colimits in a category. As a special case of adjunctions, we have reflective subcategories.

Definition 15 (Reflective Subcategory). *Let* $\mathbb{C}, \mathbb{D}$ *be categories and let* $\mathbb{D}$ *be a subcategory of* $\mathbb{C}$*. It is* reflective *if the inclusion functor* $\mathbb{D} \subseteq \mathbb{C}$ *has a left adjoint.*

Another special case of adjuctions are adjoints between posets, as the latter can be seen as categories with at most one morphism in each homset. The definition in terms of posets is as follows.

Definition 16 (Upper and Lower Adjoints). *Let* $(X, \sqsubseteq)$ *and* $(Y, \preceq)$ *be posets; let* $f \colon X \to Y$ *be a monotone function, i.e.* $x \sqsubseteq x'$ *implies* $f(x) \preceq f(x')$ *for all* $x, x' \in X$*. A monotone function* $g \colon Y \to X$ *is an* upper *adjoint of* f *if for all* $x \in X$ *and* $y \in Y$ *we have* $f(x) \preceq y$ *if and only if* $x \sqsubseteq g(y)$*; it is a* lower *adjoint of* f *if for all* $x \in X$ *and* $y \in Y$ *we have* $g(y) \sqsubseteq x$ *if and only if* $y \preceq f(x)$*.*

Note that each monotone function has at most one upper or lower adjoint, which then is referred to as *the* respective adjoint.

B On Necessary Conditions

We now show that upper adjoints of inverse image functions are a necessary condition for pushouts of partial maps (along total ones) and thus provide the proof for Proposition 1.

Let $f\colon A \to B$ be a morphism in $\mathbb{C}$, and we want to show that the upper adjoint to f^{-1} exists provided that $\mathbb{C}_{*\mathcal{M}}$ has pushouts (along total morphisms). It suffices to show that for each $\mathcal{M}$-morphism $m\colon A' \hookrightarrow A$, there is an $\mathcal{M}$-subobject $[n] \in \mathrm{Sub}_{\mathcal{M}} B$ such that for every $[p] \in \mathrm{Sub}_{\mathcal{M}} B$, $f^{-1}([p]) \sqsubseteq m$ if and only if $p \sqsubseteq n$, because putting $\forall_f([m]) := [n]$ yields the upper adjoint.

Thus, to show that a suitable $[n] \in \mathrm{Sub}_{\mathcal{M}} B$ exists, let $B \xrightharpoonup{(n,i)} D \xleftharpoondown{(g,j)} A'$ be the pushout of $B \xleftharpoondown{\Gamma f} A \xrightharpoonup{(m,\mathrm{id})} A'$ in $\mathbb{C}_{*\mathcal{M}}$. Thus, in $\mathbb{C}$, we have a diagram as shown on the left in (1).

$$
\begin{tikzcd}
A & A' \arrow[l, hook', "m"'] \arrow[r, "\mathrm{id}"] & A' \\
A \arrow[u, hook, "\mathrm{id}"] \arrow[d, "f"'] & X \arrow[l, hook', "n'"'] \arrow[u, hook] \arrow[r] \arrow[d] \arrow[ul, phantom, "\lrcorner", very near start] \arrow[ur, phantom, "\lrcorner", very near start] & Y \arrow[u, hook, "j"'] \arrow[d, "g"] \\
B & B' \arrow[l, hook', "n"] \arrow[r, "i"'] & D
\end{tikzcd}
\quad [n'] = f^{-1}([n])
\qquad
\begin{tikzcd}
A & A' \arrow[l, hook', "m"'] \\
A \arrow[u, hook, "\mathrm{id}"] \arrow[d, "f"'] & \\
 & Q \arrow[ul, hook', "p'"'] \arrow[uu, "q"'] \arrow[d, "h"] \\
B & B' \arrow[l, hook', "n"'] \\
 & P \arrow[ul, hook', "p"]
\end{tikzcd}
\quad [p'] = f^{-1}([p]) \tag{1}
$$

Let $[p] \in \mathrm{Sub}_{\mathcal{M}} B$ be a subobject satisfying $p \sqsubseteq n$; we directly have the inclusion $f^{-1}([p]) \sqsubseteq f^{-1}([n]) = [n'] \sqsubseteq m$ using commutativity of the left hand diagram in (1) and that f^{-1} is monotone.

It remains to show that for each $[p] \in \mathrm{Sub}_{\mathcal{M}} B$ that satisfies $f^{-1}([p]) \sqsubseteq m$, we also have $p \sqsubseteq n$. Thus let $[p] \in \mathrm{Sub}_{\mathcal{M}} B$ be a subobject with $f^{-1}([p]) \sqsubseteq m$. There exist $h\colon Q \to P$ and $q\colon Q \to A'$ that yields the situation of the right diagram in (1), i.e. $A \xhookleftarrow{p'} Q \xrightarrow{h} P$ is a pullback of $A \xrightarrow{f} B \xhookleftarrow{p} P$ and also $p' = m \circ q$. This implies that $(p, \mathrm{id}) \circ \Gamma f = (q, h) \circ (m, \mathrm{id})$. Since $B \xrightharpoonup{(n,i)} D \xleftharpoondown{(g,j)} A'$ is a pushout, there exists a map $(k, r)\colon D \rightharpoonup P$ such that $(k, r) \circ (n, i) = (p, \mathrm{id})$. Hence, $p \sqsubseteq n$, and the proof is complete.

C Proving the Main Theorem

In this section, we complete the proof of Theorem 2. For this, we first give auxiliary results of inverse image functions and their upper adjoints that we shall use to finish the proof. Also recall the folklore Pullback Lemma.

Lemma 5 (Pullback Lemma). *Let the squares below on the left be commutative squares in an arbitrary category $\mathbb{C}$.*

$$
\begin{tikzcd}
Q \arrow[r, "q"] & C \arrow[r, "\bar{n}"] & G \\
K \arrow[u, "g'"] \arrow[r, "j"'] & N \arrow[u, "g"] \arrow[r, "n"'] & A \arrow[u, "\bar{g}"']
\end{tikzcd}
\Rightarrow
\left(
\begin{tikzcd}
Q \arrow[r, "q"] & C \arrow[r, "\bar{n}"] & G \\
K \arrow[u, "g'"] \arrow[r, "j"'] & N \arrow[u, "g"] \arrow[r, "n"'] & A \arrow[u, "\bar{g}"']
\end{tikzcd}
\Leftrightarrow
\begin{tikzcd}
Q \arrow[r, "q"] & C \arrow[r, "\bar{n}"] & G \\
K \arrow[u, "g'"] \arrow[r, "j"'] & N \arrow[r, "n"'] & A \arrow[u, "\bar{g}"']
\end{tikzcd}
\right)
$$

If $C \xleftarrow{g} N \xrightarrow{n} A$ is a pullback of $C \xhookrightarrow{\bar{n}} G \xleftarrow{\bar{g}} A$, then $Q \xleftarrow{g'} K \xrightarrow{j} N$ is a pullback of $Q \xrightarrow{q} C \xleftarrow{g} N$ if and only if $Q \xleftarrow{g'} K \xrightarrow{n \circ j} A$ is a pullback of $Q \xrightarrow{\bar{n} \circ q} G \xleftarrow{\bar{g}} A$.

C.1 Basic Properties of Upper Adjoints to Inverse Image Functions

Lemma 6 (Splitting Upper Adjoints). *Let $C \xhookrightarrow{\bar{n}} G \xleftarrow{\bar{g}} A$ be a cospan in $\mathbb{C}$ with pullback $C \xleftarrow{g} N \xhookrightarrow{n} A$ such that $\bar{n} \in \mathcal{M}$ and $[\bar{n}] = \forall_{\bar{g}}([n])$; moreover, let $q\colon Q \hookrightarrow C$ be an $\mathcal{M}$-morphism, let $Q \xleftarrow{g'} K \xhookrightarrow{j} N$ be the pullback of $Q \xhookrightarrow{q} C \xleftarrow{g} N$, and assume that $[\bar{n} \circ q] = \forall_{\bar{g}}([n \circ j])$.*

$$
\begin{tikzcd}
Q \arrow[r, hook, "q"] & C \arrow[r, hook, "\bar{n}"] & G \\
K \arrow[u, "g'"] \arrow[r, hook, "j"'] & N \arrow[u, "g"] \arrow[r, hook, "n"'] & A \arrow[u, "\bar{g}"']
\end{tikzcd}
\qquad [\bar{n}] = \forall_{\bar{g}}([n]) \quad [\bar{n} \circ q] = \forall_{\bar{g}}([n \circ j])
$$

Then $[q] = \forall_g[j]$.

Proof. Let $q'\colon Q' \hookrightarrow C$ be an $\mathcal{M}$-morphism. If $[q'] \sqsubseteq [q]$ holds then we derive $g^{-1}([q']) \sqsubseteq g^{-1}([q]) = [j]$, using that g^{-1} is monotone; conversely, assume that $g^{-1}([q']) \sqsubseteq [j]$. Using the Pullback Lemma, we obtain $\bar{g}^{-1}([\bar{n} \circ q']) \sqsubseteq [n \circ j]$, which in turn implies that $[\bar{n} \circ q'] \sqsubseteq \forall_{\bar{g}}([n \circ j]) = [\bar{n} \circ q]$ (where the latter equality is part of the assumptions). Finally, $[q'] \sqsubseteq [q]$ follows since $\bar{n}$ is a mono. $\square$

Lemma 7 (Composition of Inverse Image Functions). *For any pair of composable morphisms $f\colon A \to B$ and $g\colon B \to C$ we have*

$$(g \circ f)^{-1} = f^{-1} \circ g^{-1}.$$

Proof. This is a direct consequence of the Pullback Lemma (Lemma 5). $\square$

Lemma 8 (Counit of Upper Adjoints). *Let $h\colon Y \to Z$ be an arrow in $\mathbb{C}$ such that the upper adjoint $\forall_h \vdash h^{-1}$ exists; then, for all $y \in \mathrm{Sub}_{\mathcal{M}} Y$, we have*

$$h^{-1}(\forall_h(y)) \sqsubseteq y.$$

Proof. Given $y \in \mathrm{Sub}_{\mathcal{M}} Y$, we use the defining property of $\forall_h$ on the subobjects y and $\forall_h(y) \in \mathrm{Sub}_{\mathcal{M}} Z$, i.e. $h^{-1}(\forall_h(y)) \sqsubseteq y$ if and only if $\forall_h(y) \sqsubseteq \forall_h(y)$; now the desired follows, as the latter is trivially true. $\square$

C.2 Completing the Proof of the Main Theorem

We continue the proof of the Theorem 2. The proposed construction of a pushout candidate for a given span $C \overset{(g,N,n)}{\leftharpoondown} A \overset{(m,M,f)}{\rightharpoonup} B$ in $\mathbb{C}_{*\mathcal{M}}$ is shown in Figure 5. We first

$$
\begin{tikzcd}
W & F \arrow[l, "u"'] & B \arrow[l, hook', "\bar{m}"'] \\
G \arrow[u, "v"] & A \arrow[l, "\bar{g}"] \arrow[u, "\bar{f}"] \arrow[ul, dashed, "l"] \arrow[ur, phantom, "(ʒ)"] & M \arrow[l, hook', "m"'] \arrow[u, "f"'] \\
C \arrow[u, hook, "\bar{n}"] \arrow[ur, phantom, "(ꝺ)"] & N \arrow[l, "g"] \arrow[u, hook, "n"'] & K \arrow[l, dashed, hook', "j"] \arrow[ul, hook', "k"'] \arrow[u, dashed, hook, "i"']
\end{tikzcd}
\quad [k] = l^{-1}\big(\forall_l(m \sqcap n)\big)
\qquad
\begin{tikzcd}
A & M \arrow[l, hook', "m"'] \arrow[r, "f"] & B \\
N \arrow[u, hook, "n"] \arrow[d, "g"'] & K \arrow[l, hook', "j"'] \arrow[u, hook, "i"'] \arrow[r, dashed, "f'"'] \arrow[d, dashed, "g'"] & P \arrow[u, hook, "p"'] \arrow[d, "u'"] \\
C & Q \arrow[l, hook', "q"] \arrow[r, "v'"'] & X
\end{tikzcd}
\quad
\begin{array}{l} [q] = \forall_g([j]) \\ [p] = \forall_f([i]) \end{array}
$$

Fig. 5. Construction of pushouts of partial maps

prove Claim 3, and we start with the equation $g^{-1} \circ \forall_g([j]) = [j]$. By definition, we have $[k] = l^{-1}(\forall_l([m] \sqcap [n]))$ and thus $[k] = (\bar{g})^{-1}(v^{-1}(\forall_l([m] \sqcap [n])))$ (using Lemma 7). Now, let $\bar{k}\colon Q \hookrightarrow G$ be a representative $\mathcal{M}$-morphism of $[\bar{k}] = v^{-1}(\forall_l([m] \sqcap [n]))$; moreover, let $g'\colon K \to Q$ be the unique morphism that makes $Q \xleftarrow{g'} K \xhookrightarrow{k} A$ a pullback of $Q \xhookrightarrow{\bar{k}} G \xleftarrow{\bar{g}} A$, leading to the situation of the left one of the below diagrams.

$$
\begin{tikzcd}
Q \arrow[rr, hook, bend left, "\bar{k}"] & C \arrow[r, hook, "\bar{n}"'] & G \\
K \arrow[u, "g'"] \arrow[r, hook, "j"'] & N \arrow[u, "g"] \arrow[r, hook, "n"'] & A \arrow[u, "\bar{g}"']
\end{tikzcd}
\qquad\qquad
\begin{tikzcd}
Q \arrow[rr, hook, bend left, "\bar{k}"] \arrow[r, dashed, hook, "q"] & C \arrow[r, hook, "\bar{n}"'] & G \\
K \arrow[u, "g'"] \arrow[r, hook, "j"'] & N \arrow[u, "g"] \arrow[r, hook, "n"'] & A \arrow[u, "\bar{g}"']
\end{tikzcd}
$$

Thus, as $(\bar{g})^{-1}([\bar{k}]) = [k] \sqsubseteq [n]$, we have $[\bar{k}] \sqsubseteq \forall_{\bar{g}}([n]) = [\bar{n}]$ (where the last equation follows from Lemma 3 and (ꝺ) from Figure 5 being a pushout square); hence, there is a unique morphism $q\colon \bar{k} \to \bar{n}$ in $\mathbb{C}/G$. Now, we derive $[j] = g^{-1}([q])$ using the Pullback Lemma, and Lemma 6 implies $[q] = \forall_g([j])$; thus $[j] = g^{-1}([q]) = g^{-1} \circ \forall_g([j])$. This yields the first equation of Claim 3 and, *mutatis mutandis*, we derive $f^{-1} \circ \forall_f([i]) = [i]$. Thus, we have established

$$g^{-1} \circ \forall_g([j]) = [j] \text{ and } f^{-1} \circ \forall_f([i]) = [i], \tag{2}$$

and can in fact construct our candidate for a pushout as on the right in Figure 5, where $Q \xrightarrow{v'} X \xleftarrow{u'} P$ is the pushout of $Q \xleftarrow{g'} K \xrightarrow{f'} P$.

To establish the universal property of $C \overset{(q,v')}{\rightharpoonup} X \overset{(u',p)}{\leftharpoondown} B$, it will be appropriate to first characterize $[k]$ as a certain join (cf. Figure 3).

On the Domain of Definition of the Diagonal The crucial part of the proof is to show that $[k]$ can be characterized as the join $[k] = \bigsqcup \mathcal{A}$ where

$$\mathcal{A} = \left\{ x \in \mathrm{Sub}_{\mathcal{M}} A \;\middle|\; \begin{array}{l} \exists c \in \mathrm{Sub}_{\mathcal{M}} C.\, \exists b \in \mathrm{Sub}_{\mathcal{M}} B. \\ \exists_m(f^{-1}(b)) = x = \exists_n(g^{-1}(c)) \end{array} \right\}.$$

For this, we shall use that $G \xrightarrow{v} W \xleftarrow{u} F$ is a hereditary pushout of the span $G \xleftarrow{\bar{g}} A \xrightarrow{\bar{f}} F$ (as defined on the left in Figure 5).

It suffices to show that $[k]$ is a greatest element of $\mathcal{A}$. As $[k] \in \mathcal{A}$ follows from Equation (2) and $k = n \circ j = m \circ i$, it remains to show that it is an upper bound of $\mathcal{A}$. Thus let $[a\colon A' \hookrightarrow A] \in \mathcal{A}$; this means that there are $\mathcal{M}$-morphisms $b\colon B' \hookrightarrow B$, $c\colon C' \hookrightarrow C$ and pullbacks $M \xleftarrow{i'} A' \xrightarrow{f''} B'$, $N \xleftarrow{j'} A' \xrightarrow{g''} C'$ (of $M \xrightarrow{f} B \xleftarrow{b} B'$ and $N \xrightarrow{g} C \xleftarrow{c} C'$, respectively) such that $i'\colon a \to m$ and $j'\colon a \to n$ (as illustrated on the left in (3) where (♌) and (♉) are pullback squares).

$$\begin{tikzcd}
C' \arrow[d, hook, "c"'] \arrow[r, phantom, near end, "(\text{♌})"'] & A' \arrow[l, "g''"'] \arrow[r, equal] \arrow[d, hook, "j'"] & A' \arrow[r, equal] \arrow[d, hook, "a"] & A' \arrow[r, "f''"] \arrow[d, hook, "i'"'] \arrow[r, phantom, near end, "(\text{♉})"'] & B' \arrow[d, hook, "b"] \\
C & N \arrow[l, "g"] \arrow[r, hook, "n"'] & A & M \arrow[l, hook', "m"] \arrow[r, "f"'] & B
\end{tikzcd}
\quad
\begin{tikzcd}
C' \arrow[d, hook, "c"'] \arrow[r, phantom, near end, "(\text{♌})"'] & A' \arrow[l, "\bar{g}''"'] \arrow[r, "\bar{f}''"] \arrow[dd, "a"] \arrow[r, phantom, near end, "(\text{♉})"'] & B' \arrow[d, hook, "b"] \\
C \arrow[d, hook, "\bar{n}"'] \arrow[r, phantom, near end, "(\text{♁})"'] & & B \arrow[d, hook, "\bar{m}"] \\
G & A \arrow[l, "\bar{g}"] \arrow[r, "\bar{f}"'] \arrow[u, phantom, near start, "(\text{♃})"] & F
\end{tikzcd}
\quad
\begin{tikzcd}
& A' \arrow[rr, "f''"] \arrow[dl, "g''"'] \arrow[dd, hook] & & B' \arrow[dl] \arrow[dd, hook, "\bar{m}\circ b"] \\
C' \arrow[rr] \arrow[dd, hook, "\bar{n}\circ c"'] & & W' \arrow[dd, dashed, near start, "w"] & \\
& A \arrow[rr] \arrow[dl] & & F \arrow[dl, "u"] \\
G \arrow[rr, "v"'] & & W &
\end{tikzcd}
\tag{3}$$

Next, we paste pullback squares as illustrated in the middle of (3): by combining (♌) with (♁) and (♉) with (♃) (where (♁) and (♃) are taken from Figure 5), we obtain $C' \xleftarrow{g''} A' \xhookrightarrow{a} A$ and $A \xhookleftarrow{a} A' \xrightarrow{f''} B'$ as pullbacks of $C' \xhookrightarrow{\bar{n}\circ c} G \xleftarrow{\bar{g}} A$ and $A \xrightarrow{\bar{f}} F \xhookleftarrow{\bar{m}\circ b} B'$, respectively. Taking the pushout $C' \xrightarrow{\bar{f}''} W' \xleftarrow{\bar{g}''} B'$ of $C' \xleftarrow{g''} A' \xrightarrow{f''} B'$ yields a unique morphism $w\colon W' \to W$ such that $w \circ \bar{g}'' = u \circ \bar{m} \circ b$ and $w \circ \bar{f}'' = v \circ \bar{n} \circ c$ (as illustrated on the right in (3)). Using that pushouts are hereditary and Theorem 1, the spans $W' \xleftarrow{\bar{g}''} B' \xhookrightarrow{\bar{m}\circ b} F$ and $G \xhookleftarrow{\bar{n}\circ c} C' \xrightarrow{\bar{f}''} W'$ are pullbacks (of $W' \xrightarrow{w} W \xleftarrow{u} F$ and $G \xrightarrow{v} W \xleftarrow{w} W'$, respectively), and moreover w is an $\mathcal{M}$-morphism. This implies that $[a] = l^{-1}([w])$ as the "diagonal" of the right hand cube in (3) is a pullback square by the Pullback Lemma; clearly, $l^{-1}([w]) = [a] \sqsubseteq m \sqcap n$ and thus $[w] \sqsubseteq \forall_l(m \sqcap n)$, whence $[a] = l^{-1}([w]) \sqsubseteq l^{-1}(\forall_l(m \sqcap n)) = [k]$, using monotonicity of l^{-1}.

Existence and Uniqueness of Mediating Morphisms Existence and uniqueness of mediating morphisms are now a relatively easy consequence. Roughly, having the equation $[k] = \bigsqcup \mathcal{A}$, the mediating maps from our pushout candidate and their uniqueness are also "inherited" from the hereditary pushout $Q \xrightarrow{v'} X \xleftarrow{u'} P$ of the span $Q \xleftarrow{g'} K \xrightarrow{f'} P$ in Figure 5. The details are as follows.

Let $C \xrightarrow{(r,d\rangle} X' \xleftarrow{(e,s)} B$ be a cospan with $(r,d\rangle \circ (n,g\rangle = (s,e\rangle \circ (m,f\rangle =: (k',h'\rangle$ in $\mathbb{C}_{*\mathcal{M}}$. Spelling out commutativity of the corresponding square in $\mathbb{C}_{*\mathcal{M}}$, we see that $\exists_n(g^{-1}([r])) = [k'] = \exists_m(f^{-1}([s]))$ and thus $[k'] \in \mathcal{A}$ and $[k'] \sqsubseteq [k] = [n \circ j] = [m \circ i]$ (cf. Figure 5). Hence, we have $g^{-1}([r]) \sqsubseteq [j]$ and $f^{-1}[s] \sqsubseteq [i]$ as n and m are monos. Next, using that $[q] = \forall_g([j])$ and $[p] = \forall_f([i])$, we obtain $[r] \sqsubseteq [q]$ and $[s] \sqsubseteq [p]$ with respective inclusion morphisms $r' \colon r \to q$ and $s' \colon s \to p$.

$$\begin{tikzcd}
C & Q \arrow[l, hook', "q"'] \arrow[r, "v'"] & X & P \arrow[l, "u'"'] \arrow[r, hook, "p"] & B \\
& R \arrow[ul, hook, "r"] \arrow[u, hook, "r'"'] \arrow[r, "d"'] & X' & S \arrow[l, "e"] \arrow[u, hook', "s'"] \arrow[ur, hook', "s"']
\end{tikzcd}
\qquad\qquad
\begin{tikzcd}
K \arrow[r, "f'"] \arrow[d, "g'"'] & P \arrow[d, "u'"] \\
Q \arrow[r, "v'"'] & X \arrow[ul, phantom, "\ulcorner", very near start]
\end{tikzcd}$$

In fact, $Q \xrightharpoonup{(r',d)} X' \xleftharpoondown{(e,s')} P$ is a cospan for $Q \xleftharpoondown{\Gamma(g')} K \xrightharpoonup{\Gamma(f')} P$ in $\mathbb{C}_{*\mathcal{M}}$ as $g'^{-1}([r']) = f'^{-1}([s'])$ (using that $[k'] \sqsubseteq [k]$ and the Pullback Lemma).

As $Q \xrightarrow{v'} X \xleftarrow{u'} P$ is a hereditary pushout of $Q \xleftarrow{g'} K \xrightarrow{f'} P$, there is a unique map $\phi \colon X \rightharpoonup X'$ such that

$$(r', d) = \phi \circ \Gamma(v') \text{ and } (s', e) = \phi \circ \Gamma(u'),$$

which implies $(r, d) = \phi \circ (q, v')$ and $(s, e) = \phi \circ (p, u')$, and thus ϕ is a mediating map. Any other map $\psi \colon X \to X'$ such that $(r, d) = \psi \circ (q, v')$ and $(s, e) = \psi \circ (p, u')$ satisfies

$$(r', d) = \psi \circ \Gamma(v') \text{ and } (s', e) = \psi \circ \Gamma(u')$$

(as the morphisms $r' \colon r \to q$ and $s' \colon s \to p$ are unique). Thus, using that $Q \xrightharpoonup{\Gamma v'} X$ and $X \xleftharpoondown{\Gamma u'} P$ are jointly epi (as they form a pushout), we derive $\psi = \phi$.