Commutators for Stochastic Rewriting Systems: Theory and Implementation in Z3

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Abstract. In the semantics of stochastic rewriting systems (SRSs) based on rule algebras, the evolution equations for average expected pattern counts are computed via so-called commutators counting the distinct sequential compositions of rules and observable patterns regarded as identity rules. In this paper, we consider the commutators for conditional SRS in the Sesqui-Pushout (SqPO) approach. However, graphs are often subject to constraints. To minimise the construction of spurious compositions prohibited by such constraints, we develop strategies for computing rule composition, both theoretically and using the SMT solver Z3 with its Python interface. Our two equivalent solutions for checking constraints include a straightforward generate-and-test approach based on forbidden graph patterns and a modular solution, where the patterns are decomposed as pushouts of monic spans into forbidden relation patterns. The implementation is based on a framework that allows a direct and modular representation of the categorical and logical theory in Python/Z3. For an example of SqPO rewriting of rigid multigraphs modelling polymer formation in organic chemistry, we assess and compare the performance of the two strategies.

Keywords: Sesqui-Pushout rewriting · rule algebra · applications of SMT solvers · stochastic mechanics

1 Introduction

Stochastic rewrite systems (SRS) [6,1,3] are categorical generalisations of stochastic graph rewrite systems such as kappa [9] deriving an algebraic structure on rewrite steps to support stochastic analyses of biological systems. Instead of stochastic simulation and model checking with their well-known scalability issues, SRS aim at the derivation of a system of evolution equations which, for a set of graph patterns as observables, predict their number of occurrences over time. For example in models of biochemistry, a pattern could represent a type
of molecule and the number of occurrences of the pattern in a given graph the number of molecules of this type in a given cell. Beyond expressing expected values of such pattern counts over time, we may be interested in equations for higher moments, such as variances expressing how closely the values are spread about the mean. These are important to understand the quality of an approximation of a rule-based system by a set of equations and can be used to derive confidence intervals for error margins in predictions of the model.

In the semantics of SRS based on rule algebras [6,1,3], the evolution equations for average expected pattern counts are derivable via so-called commutators computed by counting the distinct sequential compositions of rules and observable patterns regarded as identity rules. The time-dependent average of the count of a pattern $P$ changes proportionally to the average value of the commutator describing the effect of rules on the number of occurrences of $P$.

Commutators are computed by counting the distinct sequential compositions of rules and patterns regarded as identity rules. However, graphs are often subject to additional constraints, causing the algorithmic challenge of avoiding where possible the construction of spurious rule compositions forbidden by such constraints. In this paper, we consider different strategies for computing rule compositions in the Sesqui-Pushout (SqPO) approach [8], both theoretically and using the SMT solver Z3 with its Python interface. We compare two equivalent options for implementing the checking of constraints. The straightforward generate-and-test strategy is based on forbidden graph patterns, where we first compose rules based on spans describing how they overlap and then check that none of the forbidden graph patterns can be embedded into the composition. A more modular strategy is based on a decomposition of graph patterns as pushouts of monic spans representing forbidden relation patterns, which are used in order to curate admissible overlaps of rules before they are composed.

The embedding of a graph pattern into the pushout object of the span relating the first rule’s right-hand side with the second rule’s left-hand side is an injective graph morphism. Instead, the embedding of a relation pattern into that span is by means of a triple of injections forming two pullbacks. We show that both are equivalent, i.e. given a graph pattern $P$ and all its pushout decompositions $S$, for any pushout graph $G$ over a span $s$ there exists a graph embedding from $P$ iff there exists a span in $S$ with a double-pullback embedding into $s$.

We implement both strategies in Z3 and Python in a class architecture following the categorical concepts of the theory, including classes for graphs, morphisms, rules and spans, pushouts, etc. The declarative nature of SMT solving, where models are only determined up to isomorphism, is a good fit for the categorical theory of graph rewriting, allowing a very direct translation. Based on this implementation we evaluate and discuss both the correctness of both strategies and their relative performance in terms of time and space requirements.

As a case study we consider an example of SqPO rewriting of rigid multigraphs representing polymers in organic chemistry. A multigraph is rigid if it does not contain occurrences of patterns with two edges either in parallel, starting or ending in the same node, or as parallel loops. Based on a simple set
of rules for creating and deleting edges we can model polymer formation, such
that the evolution equations derivable via the commutators computed predict
the number of polymers of a particular length and shape for any time of the
reaction. However, the contribution of this paper is to the theory and efficient
implementation of rule compositions subject to graph constraints.

2 Rule algebras for Conditional SqPO Rewriting

We provide some background on the recent extension of Sesqui-Pushout (SqPO)
rewriting [8] to application conditions [4] and describe the additional assump-
tions on the underlying category to admit a rule algebra construction [1]. We
refer the readers to [5] for the extended discussion of the mathematical concepts.

2.1 Categorical setting

Assumption 1 ([4]). We assume that $\mathcal{C} \equiv (\mathcal{C}, \mathcal{M})$ is a finitary $\mathcal{M}$-adhesive
category with $\mathcal{M}$-effective unions, $\mathcal{M}$-initial object, an epi-$\mathcal{M}$-factorisation, ex-
stistence of final pullback complements (FPCs) for all pairs of composable $\mathcal{M}$-
morphisms and with stability of $\mathcal{M}$-morphisms under FPCs.

Example 1. The prototypical category suited for rewriting in the above sense is
the category $\text{FinGraph}$ of finite directed multigraphs. It is well-known [16] that
the category $\text{Graph}$ of all (not necessarily finite) multigraphs is adhesive
(i.e. $\mathcal{M}$-adhesive for $\mathcal{M} = \text{mono} (\text{Graph})$), and thus due to results of [12] so is its
finitary restriction $\text{FinGraph}$. The finitary restriction preserves the epi-mono-
factorisation, the property of mono-effective unions as well as the mono-initial
object $\emptyset$ (the empty graph). Finally, according to [8], FPCs exist for arbitrary
pairs of composable monos, and monos are stable under FPCs.

2.2 Application conditions

While the theory of SqPO-type rewriting for rules with conditions as presented
in [4] has been developed for the general case of nested application conditions,
in the present paper we will only consider the special case of simple (i.e. non-
nested) conditions. For the readers’ convenience, we recall in Appendix A.1 some
of the relevant background material and standard notations. Conceptually, ap-
plication conditions are defined such as to constrain the matches of rewriting
rules. Another important special case are conditions over the $\mathcal{M}$-initial object $\emptyset$. Such global constraints describe properties of all objects, such as invariants.

Example 2. Our running example throughout this paper will be the category $\text{rGraph}$ of finite rigid directed multigraphs. Referring to [10] for an extended
discussion of the rigidity phenomenon, suffice it here to introduce this category
as a refinement of the category $\text{FinGraph}$ via imposing the following global constraint formulated via a set $\mathcal{N}$ of forbidden patterns:

$$c_\mathcal{N} := \bigwedge_{N \in \mathcal{N}} \neg \exists (\emptyset \leftrightarrow N), \quad \mathcal{N} := \{ \begin{array}{c}
\begin{array}{c}
\text{\begin{tikzpicture}[baseline=0cm]
\node (A) at (0,0) {$\cdot$};
\node (B) at (0.5,0) {$\cdot$};
\draw (A) -- (B);
\end{tikzpicture}}
\end{array}
, \begin{array}{c}
\begin{tikzpicture}[baseline=0cm]
\node (A) at (0,0) {$\cdot$};
\node (B) at (0.5,0) {$\cdot$};
\draw (A) -- (B);
\end{tikzpicture}
\end{array}, \ldots, \begin{array}{c}
\begin{tikzpicture}[baseline=0cm]
\node (A) at (0,0) {$\cdot$};
\node (B) at (0.5,0) {$\cdot$};
\draw (A) -- (B);
\end{tikzpicture}
\end{array} \end{array} \}.$$ (1)
Graphs in rGraph are thus either “directed paths” of edges, or closed directed loops of edges (possibly with individual loops on vertices, albeit we will only consider loop-less graphs in our applications).

### 2.3 SqPO direct derivations and rule compositions

The theory of “compositional” SqPO rewriting as introduced in [1,4] is an extension of the traditional SqPO theory [8] by concurrency and associativity theorems that hold under suitable assumptions on the underlying categories.

**Remark 1.** Contrary to standard conventions we will read rewriting rules from input to output, i.e. in particular from right to left. This is so as to be compatible with the standard mathematical convention of left-multiplication for matrices (see below in the context of representations).

**Definition 1.** Let $C$ be an $M$-adhesive category satisfying Assumption 1, and let $\text{Lin}(C)$ denote the set of linear rewriting rules with conditions,

$$\text{Lin}(C) := \{(O \leftarrow K \leftarrow I; c_I) \mid (K \leftarrow O), (K \leftarrow I) \in M, c_I \in \text{cond}(C)\}. \quad (2)$$

Let $\text{Lin}(C)_\sim$ be the set of equivalence classes of linear rules with conditions under the equivalence relation $\sim$ defined as follows:

$$(r, c_I) \sim (r', c'_I) :\iff r \equiv r' \land c_I \equiv c'_I. \quad (3)$$

Here, $r \equiv r'$ iff there exist isomorphisms $(\omega : O \rightarrow O'), (\kappa : K \rightarrow K'), (\iota : I \rightarrow I') \in \text{iso}(C)$ such that the evident diagram commutes.

The following definition provides a notion of direct derivations for SqPO rules with conditions.

**Definition 2 ([4], Def. 17; compare [8], Def. 4).** Given an object $X \in \text{obj}(C)$ and a linear rule with condition $R = (r, c_I) \in \text{Lin}(C)$, we define the set of admissible matches $M^\text{sq}_R(X)$ as

$$M^\text{sq}_R(X) := \{ (m : I \rightarrow X) \in M \mid m \models c_I \}. \quad (4)$$

A direct derivation of $X$ along $R$ with match $m \in M^\text{sq}_R(X)$ is defined via constructing the diagram on the right, with final pullback complement marked FPC and pushout marked PO. We write $R_m(X) := X'$ for the object “produced” by the above diagram, and we refer to $m^*$ as the comatch of $m$.

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

The second main definition of SqPO-type “compositional” rewriting theory is given by a notion of sequential composition for rules with application conditions.
Definition 3 ([4]). With notations as above, let \( R_j = (r_j, c_{I_j}) \in \text{Lin}(C)_\sim \) be two equivalence classes of linear rules with conditions \((j = 1, 2)\). Fixing concrete representatives \((O_j \leftarrow K_j \rightarrow I_j; c_{I_j})\), and for monic span \( \mu = (I_2 \leftarrow M_{21} \rightarrow O_1) \), we define \( \mu \) to be an SqPO-admissible match of \( R_2 \) into \( R_1 \), denoted \( \mu \in M_{sq}^{R_2}(R_1) \), if the pushout complement marked PO in the diagram below exists.

\[
\begin{array}{cccccc}
O_2 & \xrightarrow{K_2} & I_2 & \xrightarrow{M_{21}} & O_1 & \xleftarrow{K_1} & I_1 \\
\downarrow \text{PO} & & \downarrow \text{FPC} & & \downarrow \text{PO} & & \downarrow \text{PO} \\
O_{21} & \xleftarrow{K_{21}} & N_{21} & \xrightarrow{K_1'} & K_{21} & \xrightarrow{I_{21}} & I_{21} \\
\end{array}
\]

and if in addition \( c_{I_{21}} \neq \text{false}_{I_{21}} \), where
\[
c_{I_{21}} = \text{Shift}(I_1 \rightarrow I_{21}, c_{I_{21}}) \land \text{Trans}(N_{21} \leftarrow K_1' \rightarrow I_{21}, \text{Shift}(I_2 \leftrightarrow N_{21}), c_{I_2}).
\]

In this case, we define the SqPO-type composition of \( R_2 \) with \( R_1 \) along \( \mu_{21} \) as the following equivalence class:
\[
R_2 \circ_1 R_1 := [(O_{21} \leftarrow K_{21} \rightarrow I_{21}; c_{I_{21}})]_\sim.
\]

2.4 SqPO-type rule algebra construction

Intuitively, an interesting and computationally versatile possibility to encode the non-determinism in the composition of rules with conditions is the following precise implementation of “summing over all possibilities to compose two rules”:

Definition 4 ([5]). Given an \( M \)-adhesive category \( C \) satisfying Assumption 1, let \( \overline{R}_C \) denote the \( \mathbb{R} \)-vector space whose set of basis vectors is in bijection with the set of equivalence classes \( \text{Lin}(C)_\sim \) of rules with conditions (via some bijection \( \delta : \text{Lin}(C)_\sim \rightarrow \text{basis}(\overline{R}_C) \)). Then the SqPO-type rule algebra over \( C \), denoted \( \overline{R}_C^{SqPO} := (\overline{R}_C, \circ_C) \), is defined via equipping the \( \mathbb{R} \)-vector space \( \overline{R}_C \) with a binary operation \( \circ_C \) that is defined via its action on basis vectors,
\[
\forall R_1, R_2 \in \text{Lin}(C)_\sim : \ \delta(R_2) \circ_C \delta(R_1) := \sum_{\mu \in M_{sq}^{R_2}(R_1)} \delta \left( R_2 \overset{\mu}{\circ} R_1 \right).
\]

Theorem 1 ([5]). \( \overline{R}_C^{SqPO} \) is a unital, associative algebra, with unit element \( \delta(R_{\emptyset}) \), for \( R_{\emptyset} = (\emptyset \leftrightarrow \emptyset \rightarrow \emptyset; \text{true}). \)

Crucially, we will be able to utilise a certain device referred to as a representation of a SqPo-type rule algebra in order to “convert” back and forth between applying rules sequentially to objects vs. applying composites of rules to objects (i.e. a form of generalised notion of concurrency theorem).
Definition 5 ([5]). Let \( \mathcal{C} \) be an \( \mathbb{R} \)-vector space whose set of basis vectors is in bijection with the set \( \text{obj}(\mathcal{C})_\simeq \) of isomorphism classes of objects of \( \mathcal{C} \) (via some bijection \( |\cdot| : \text{obj}(\mathcal{C})_\simeq \to \text{basis}(\mathcal{C}) \)). Then the canonical representation \( \overline{\rho}_C \) of \( \overline{\mathcal{R}}_{sqPO} \) is defined via its action on generic \( R \in \overline{\text{Lin}}(\mathcal{C})_{\_\_} \) and \( X \in \text{obj}(\mathcal{C})_\simeq \) as

\[
\overline{\rho}_C : \overline{\mathcal{R}}_{sqPO} \to \text{End}_\mathbb{R}(\overline{\mathcal{C}}), \quad \overline{\rho}_C(\delta(R)|X) := \sum_{m \in M^\alpha_m(X)} |R_m(X)|. \tag{9}
\]

Theorem 2 ([5]). \( \rho_C \) is an algebra homomorphism (and thus indeed a well-defined representation), i.e. we have that (for all \( R_1, R_2 \in \overline{\text{Lin}}(\mathcal{C})_{\_\_} \))

\[
\overline{\rho}_C(\delta(R_2)) = \text{Id}_{\text{End}_{\mathbb{C}}(\mathcal{C})}, \quad \overline{\rho}_C(\delta(R_2)) \overline{\rho}_C(\delta(R_1)) = \overline{\rho}_C(\delta(R_2) \circ C \circ \delta(R_1)). \tag{10}
\]

2.5 Commutators

One of the central computational strategies in rule-algebraic constructions is played by the notion of commutators.

Definition 6. For two rule algebra elements \( A, B \in \overline{\mathcal{R}}_{sqPO}^C \), the commutator of \( A \) and \( B \) is defined as

\[
[A, B]_\circ := A \circ_C B - B \circ_C A. \tag{11}
\]

By standard mathematical convention, we reserve the symbol \( [\cdot, \cdot] \) without the \( \circ \) index for the commutator of the representations of \( A \) and \( B \),

\[
[\overline{\rho}_C(A), \overline{\rho}_C(B)] := \overline{\rho}_C(A) \overline{\rho}_C(B) - \overline{\rho}_C(B) \overline{\rho}_C(A). \tag{12}
\]

Intuitively, given two rule algebra elements \( \delta(R_1) \) and \( \delta(R_2) \) (for \( R_1, R_2 \in \overline{\text{Lin}}(\mathcal{C})_{\_\_} \)) and some \( X \in \text{obj}(\mathcal{C})_\simeq \), the computation encoded in

\[
\overline{\rho}_C(\delta(R_2)) \overline{\rho}_C(\delta(R_1)) |X\rangle = \overline{\rho}_C(\delta(R_2)) \overline{\rho}_C(\delta(R_1)) |X\rangle - \overline{\rho}_C(\delta(R_1)) \overline{\rho}_C(\delta(R_2)) |X\rangle \tag{13}
\]

evaluates to the difference of all ways to apply first \( R_1 \) and then \( R_2 \) to \( X \) minus all outcomes of applying first \( R_2 \) and then \( R_1 \). The rule algebra framework and in particular the computational properties described in Theorem 2 permit to simplify the above computation via

\[
[\overline{\rho}_C(\delta(R_2)), \overline{\rho}_C(\delta(R_1))] = \overline{\rho}_C([\delta(R_2), \delta(R_1)]_\circ). \tag{14}
\]

From a high-level perspective, commutators encode computationally crucial causal information on a given rewriting system. A famous example to illustrate this point is given by the following commutator for \( \mathcal{C} = \text{uGraph} \):

\[
a := \overline{\rho}_C(\delta(\emptyset \leftrightarrow \emptyset \leftrightarrow \bullet)), \quad a^\dagger := \overline{\rho}_C(\delta(\bullet \leftrightarrow \emptyset \leftrightarrow \emptyset))
\]

\[
\Rightarrow [a, a^\dagger] = \text{Id}_{\text{End}_{\mathbb{C}}(\mathcal{C})}. \tag{15}
\]
Here, the annihilation operator $a$ and the creation operator $a^\dagger$ are the representations of the rules of vertex deletion and creation, respectively. Intuitively, the commutator of these operators evaluated against some graph state $|X\rangle$ expresses the fact that if one first applies vertex creation and then vertex deletion to $X$, either the deletion picks a vertex from $X$, or it picks the vertex just created. The latter option just returns $X$ itself. In the reverse order of rule application, the latter option is not present. Thus the difference evaluates precisely to the identical operation on $X$, a result known in the literature as the canonical commutation relation, which is of central importance in the theory of generating functions, mathematical chemistry and quantum physics (cf. e.g. [7] for further details).

In the setting of continuous-time Markov chain (CTMC) theory for stochastic rewriting systems as developed in [2,6,3,1,7,5], commutator computations are quintessential for deriving the dynamical evolution equations for statistical moments of pattern-count observables. As a prototypical example of such a computation, the evolution equation for the average value $\langle O^P_P(t) \rangle$ of a pattern-count observable $O^P_P := \rho^C(\delta(O_j \leftarrow K_j \rightarrow I_j; c_{I_j}))$ of some CTMC for a rewriting system with infinitesimal generator $H := \sum_{j=1}^{n} \kappa_j \rho^C(\delta(O_j \leftarrow K_j \rightarrow I_j; c_{I_j}))$ (where the parameters $\kappa_j \in \mathbb{R}_{>0}$ are the base rates of the individual rules) reads

$$\frac{d}{dt} \langle O^P_P(t) \rangle = \langle [O^P_P, H](t) \rangle.$$  

(16)

Referring to loc. cit. for further details and background information, it is precisely this application scenario that motivated us to search for an automated algorithmic implementation of commutator calculations.

### 3 Constraint-checking Strategies in Rule Compositions

When computing SqPO-type compositions of conditional rules, an algorithmically expensive step consists in verifying the satisfaction of both the global and application conditions in a given overlap, followed by computing the derived application conditions of the admissible composites. Both in order to experiment with the implementations of such algorithms via Z3 (see next Section) and out of a theoretical interest, we consider different implementation strategies for the steps involved in this rule composition operation. We will present here the “direct” strategy (i.e. following precisely the traditional constructions involving Shift and Trans) as well as an alternative strategy based upon certain span (non-)embedding criteria. From this section onwards, we will fix a category $C$ satisfying Assumption 1, and assume a set of global conditions $c_N$ as in (2) on objects. Let us further assume that all rules are endowed with application conditions that ensure the preservation of $c_N$.

**Definition 7 (direct strategy).** Given two linear rules with conditions $R_j \equiv (r_j, c_{I_j}) \in \text{Lin}(C)$ ($j = 1, 2$) and a candidate match (i.e. monic span) $\mu = (I_2 \leftarrow M_{21} \rightarrow O_1)$, the direct strategy to verify whether $\mu$ is an admissible match is defined as follows:
1. Construct the pushout \((I_2 \leftrightarrow N_{21} \leftrightarrow O_1)\) of \(\mu\). Verify that \(N_{21} \models c_{N_{21}}\), and that \((I_2 \leftrightarrow N_{21}) \models c_{I_2}\).

2. If the pushout complement of \((N_{21} \leftrightarrow O_1, O_1 \leftrightarrow K_1)\) exists, perform the SqPO-type composition of the plain rules. Verify that the composite rule’s application condition satisfies \(c_{I_{21}} \neq false\), with

\[ c_{I_{21}} := \text{Shift}(I_1 \leftrightarrow I_{21}, c_{I_1}) \land \text{Trans}(N_{21} \leftrightarrow I_{21}, \text{Shift}(I_2 \leftrightarrow N_{21}, c_{I_2})). \]  
(17)

If both steps are successful, \(\mu\) is an admissible SqPO-type match of \(R_2\) into \(R_1\).

As an alternative strategy, let us restate the “forbidden” patterns \(N \in \mathcal{N}\) via their pushout decompositions, defined as follows:

**Definition 8.** We define the set of “forbidden relations” \(S_N\) as

\[ S_N := \{ s = (C_1 \leftarrow D \rightarrow C_2) \mid C_1, D, C_2 \models c_{N} \land \exists N \in \mathcal{N} : \text{PO}(s) \cong N \}. \]  
(18)

**Example 3.** For the category \(\text{rGraph}\) as introduced in Ex. 2, one may compute the following set of “forbidden relations” (with colours encoding the respective embeddings):

\[ S_N = \left\{ \begin{array}{c}
\begin{array}{c}
\ast \quad \ast \quad \ast \quad \ast \quad \ast \quad \ast \quad \ast \quad \ast \quad \ast \quad \ast \\
\end{array}
\end{array} \right\}. \]

The pushout decompositions of forbidden patterns allows an modular approach to testing admissibility of rule overlaps that does not require to find embeddings of patterns into the pushout of the overlap, but double-pullback embeddings (DPEs) of forbidden spans into the monic spans representing the overlaps.

**Theorem 3.** With notations as above, given a pushout \(P\) of a monic span \((I_1 \leftrightarrow M_{21} \leftrightarrow O_1)\), the violation of \(c_{N}\) is equivalently verified as follows:

\[ P \not\models c_{N} \iff \exists s = (C_2 \leftarrow D \rightarrow C_1) \in S_N : \exists (C_2 \leftrightarrow I_2), (D \leftrightarrow M_{21}), (C_1 \leftrightarrow O_1) \in \text{mono}(C) : (C_2 \leftrightarrow D \rightarrow M_{21}) = \text{PB}(C_2 \leftrightarrow I_2 \leftrightarrow M_{21}) \land (C_2 \leftrightarrow D \rightarrow M_{21}) = \text{PB}(C_2 \leftrightarrow I_2 \leftrightarrow M_{21}). \]  
(20)
Here, each DPE shown in (20) encodes a commutative diagram of the form

\[ \begin{array}{c}
C_2 & \xleftarrow{D} & C_1 \\
\text{PB} & & \text{PB} \\
I_2 & \xleftarrow{M_{21}} & O_1
\end{array} \]  \hspace{1cm} \text{(21)}

\begin{proof}
See Appendix B.
\end{proof}

The alternative test for constraint satisfaction via DPEs of spans of \( S_N \) according to Theorem 3 permits to formulate the following alternative SqPO-type rule composition strategy:

\textbf{Definition 9 (modular strategy).} Given two linear rules with conditions \( R_j \equiv (r_j, c_{I_j}) \in \text{Lin}(C) \) \((j = 1, 2)\) and a candidate match (i.e. monic span) \( \mu = (I_2 \xleftarrow{M_{21}} O_1) \), the modular strategy to verify whether \( \mu \) is an admissible match is defined as follows:

1. Verify that there does not exist any double-pullback embedding of a span of \( S_N \) into the span \( \mu \).
2. Verify that \((I_2 \xleftarrow{M_{21}} O_1) \models c_{I_2}\).
3. If the pushout complement of \((N_{21} \xleftarrow{O_1} O_1 \xleftarrow{K_1})\) exists, perform the SqPO-type composition of the plain rules. Verify that the application condition \( c_{I_{21}} \) of the composite rule satisfies \( c_{I_{21}} \not\equiv \text{false} \), with

\[ c_{I_{21}} := \text{Shift}(I_1 \xleftarrow{I_{21}} c_{I_1}) \land \text{Trans}(N_{21} \xleftarrow{I_{21}} \text{Shift}(I_2 \xleftarrow{N_{21}} c_{I_2})). \]  \hspace{1cm} \text{(22)}

If all steps are successful, \( \mu \) is an admissible SqPO-type match of \( R_2 \) into \( R_1 \).

Finally, a useful corollary of Theorem 3 is the following alternative algorithm for minimal constraint-preserving application conditions for SqPO-type rules:

\textbf{Corollary 1.} With notations as above, given a “plain” linear rule \( r = (O \xleftarrow{K} I) \in \text{Lin}(C) \), perform the following steps:

1. For each \((C_2 \xleftarrow{D} C_1) \in S_N\),
   \( (a) \) Find all pullback embeddings of \((C_2 \xleftarrow{D})\) into \((O \xleftarrow{K})\), i.e. pairs of \( M \)-morphisms \((C_2 \xleftarrow{O}) \) and \((D \xleftarrow{K})\) s.t. \( D = \text{PB}(C_2 \xleftarrow{D} \xleftarrow{K}) \).
   \( (b) \) For each pullback embedding, construct \((C_1 \xleftarrow{P} I)\) by taking the pushout of the span \((C_1 \xleftarrow{D} K \xleftarrow{I})\); if \( P \models c_N \), then this pullback embedding contributes a negative condition of the form \( \neg \exists(I \xleftarrow{P}, \text{true}) \).

Then the (minimal) constraint-preserving application condition \( c_I \) is given by the conjunction over all individual contributions computed above.

\begin{proof}
See Appendix C.
\end{proof}

A heuristic solution for this problem has been proposed in [17]. For the case of forbidden graph patterns and negative conditions, our result makes it easy to satisfy our assumption that all rules should preserve the constraints in \( S_N \) while avoiding the expensive \text{Shift} and \text{Trans} constructions and subsequent minimisation, \cite{13,11}.
4 Rule Composition with Graph vs. Relation Patterns

This section discusses the implementation of the theory presented above using the SMT solver Z3. SMT solvers are well suited to encode categorical constructions [15] since they are declarative by nature and models are determined only up to isomorphism. Using Z3 through its Python API allows an object-oriented design where classes represent concepts of the problem domain (i.e., category theory and graph transformation) to generate assertions in Z3.

4.1 The category of directed multigraphs in Z3/Python

Every Python class in the below diagram corresponds to a categorical structure in the theory. For example, `Graph` and `GraphMorph` correspond to graph and graph morphism respectively.

![Diagram showing the relationship between classes and methods](image)

Each class has a constructor that initialises any objects created and generates the Z3 structures to keep their data and constraints. Objects can either be given as input or constructed by Z3. To facilitate both cases, the constructors declare (rather than defines by enumerating elements and mappings) any sorts and functions required. For example, when an object of class `Graph` is created, if no vertices or edges are given, two `Set` objects only declare a sort for the vertex and edge sets but do not assert any other distinct elements. If an object is fixed, the `closeRange` method is called. The source and target functions in a `Graph` object are declared but the mapping is not fixed in the constructor. Its definition can be added to the solver by calling the method `initFs`.

Two classes are not shown in the diagram: 1) `ForbiddenGraph`, and 2) `ForbiddenRelation`. These are designed to read the forbidden graphs/relations from GraphML files, encode them logically and add them to the solver. Based on our experiments, the checking of logically encoded constraints is more efficient than the direct approach where forbidden graphs/relations are categorical structures and the solver checks the existence of morphisms into the graphs/spans.
4.2 Curating rule compositions

Given two graphs $X$ and $Y$ and a set $S$ of forbidden graphs, the aim is to test if there is a pushout graph $P$ of $X$ and $Y$ such that none of the forbidden graphs in $N$ has an embedding in $P$.

1. **Direct strategy:** find all spans $sp: X \leftarrow I \rightarrow Y$ between $X$ and $Y$ whose pushout graph $P$ has no embedding of any of the forbidden graphs in $N$.

2. **DPE strategy:** with $S$ the set of all spans obtained as pushout decompositions of graphs in $N$, find all spans $sp: X \leftarrow I \rightarrow Y$ such that none of the spans in $S$ can be embedded into $sp$ by a double pullback.

As an example, consider input $X = \xymatrix{f & x_1 \ar[l] 
\ar[r] & x_2} \quad Y = \xymatrix{h & y_1 \ar[l] 
\ar[r] & y_2}$, and the forbidden graph $N = \xymatrix{e_1 & u_1 \ar[l] 
\ar[r] & u_2 \ar[r] & u_3 \ar[l] & e_2}$. In the direct approach, a pushout graph $P$ is calculated and the assertion preventing an embedding of $N$ into $P$ is as follows:

```plaintext
# for all nodes u1, u2, u3, and edges e1 and e2 in P,
ForAll([u1, u3, u2, e1, e2],
  # it is not True that
  Not(And(
    # u1, u2, u3 and null are all distinct, and
    Distinct(u1, u2, u3, null),
    # e1, e2, and null are distinct, and
    Distinct(e1, e2, null),
    po-src(e1) == u2, # the source of e1 in P is u2, and
    po-tar(e1) == u1, # the target of e1 in P is u1, and
    po-src(e2) == u2, # the source of e2 in P is u2, and
    po-tar(e2) == u3))) # and the target of e2 in P is u3
```

In the DPE approach, the first step is to generate all decompositions $s$ of $N$, i.e., all proper sub-graphs whose union is $N$, see Table 1. Then, for each of these forbidden relation patterns we derive an assertion and add it to the solver. For example for the first one we have the Python code shown below the table.

| Table 1. Decompositions of forbidden relation $N$ |
|--------------------------------------------------|
| $(\xymatrix{e_1 & u_1 \ar[l] \ar[r] & u_2 \ar[r] & u_3 \ar[l] & e_2})$ | $(\xymatrix{e_1 & u_1 \ar[l] \ar[r] & u_3 \ar[l] & u_2 \ar[r] & e_2})$ |
| $(\xymatrix{e_1 & u_1 \ar[l] \ar[r] & u_2 \ar[r] & u_3 \ar[l] & e_2})$ | $(\xymatrix{e_1 & u_1 \ar[l] \ar[r] & u_2 \ar[r] & u_3 \ar[l] & e_2})$ |

```plaintext
# there do not exist nodes u1X, u2X, u3X and
# edge e1X in X and nodes u2I, u3I in I and
# nodes u2Y and u3Y and edge e2Y in Y s.t.
Not(Exists([u1X, u2X, u3X, e1X, u2I, u3I, u2Y, u3Y, e2Y],
  # u2I and u3I and null are distinct, and
  And(Distinct(u2I, u3I, null),
  # u1X, u2X, u3X, and null are distinct, and
```
Distinct(u1X, u2X, u3X, null),
e1X != null, \# e1X is not null, and
X-src(e1X) == u2X \# source of e1X in X is u2X, and
X-tar(e1X) == u1X \# target of e1X in X is u1X, and
\# u2Y and u3Y and null are distinct, and
Distinct(u2Y, u3Y, null),
e2Y != null, \# e2Y is not null, and
Y-src(e2Y) == u2Y \# source of e2Y in Y is u2Y, and
Y-tar(e2Y) == u3Y, \# target of e2Y in Y is u3Y, and
IXV(u2I) == u2X, \# morphism of u2I in I to X is u2X, and
IXV(u3I) == u3X, \# morphism of u3I in I to X is u3X, and
IYV(u2I) == u2Y, \# morphism of u2I in I to Y is u2Y, and
IYV(u3I) == u3Y)) \# morphism of u3I in I to Y is u3Y

The number of variables and quantifications is clearly higher in the DPE strategy. Next we discuss correctness and compare the performance of the two approaches.

4.3 Correctness

For the running example, both strategies produce the same set of solutions. Table 2 shows the number of distinct solutions for each ordered pair of rules. The diagonal elements are disregarded because the order of \((r, r)\) is irrelevant and so in the computation of commutators the number of solutions for \((r, r)\) is both added and subtracted, rendering it inconsequential.

|                | delete-edge | create-edge | delete-node | create-node |
|----------------|-------------|-------------|-------------|-------------|
| delete-edge    | -           | 6           | 2           | unsat       |
| create-edge    | 4           | -           | 2           | unsat       |
| delete-node    | unsat       | unsat       | -           | unsat       |
| create-node    | 2           | 2           | 1           | -           |

For the right-hand side of create-edge and the left-hand side of delete-node, the solutions are:

In more complex examples, the solver (which employs a randomised search strategy) sometimes returns unknown rather than sat (when a solution is found or unsat (when there are no further solutions). To ensure that we get all solutions, a naive implementation of either strategy runs the algorithm repeatedly until it returns unsat. However, it would be wasteful to discard solutions found in runs ending in unknown. Therefore we save such solutions and in subsequent iterations ask the solver to find solutions that are distinct from all previous ones. Because for complex formulae it can be inherently difficult to find even a single solution, we introduce additional optimisation below.
4.4 Evaluation

For selected indicators, average measurements over 10 runs are given for each strategy in Table 3. The mean execution time is measured only for the satisfiability check with a single solution once all assertions are added to the solver.

Table 3. Running Example

| Indicator        | Direct Strategy | DPE Strategy |
|------------------|-----------------|--------------|
| exe time         | 0.2             | 0.63         |
| memory           | 119.8           | 216.04       |
| mk bool var      | 5063.87         | 32314.07     |
| quant instantiations | 1890.03     | 17993.04     |

Here the direct strategy outperforms DPE. However, for more complex graphs DPE performs better. Consider two rules, break-chain and create-chain, in a polymer model. Both rules have a path of length \( n \) in their left-hand side. In the RHS, the former deletes an edge whereas the latter connects the ending node to the starting node forming a cycle of length \( n + 1 \). Table 4 shows results for \( n = 2 \) and \( n = 5 \) averaged over 5 runs for each permutation of the rules.

Table 4. Naive Implementations ran on Polymer Model with 2 and 5 edges

| Indicator        | Polymer model with 2 edges | Polymer model with 5 edges |
|------------------|-----------------------------|-----------------------------|
|                  | Direct Strategy | DPE Strategy | Direct Strategy | DPE Strategy |
| exe time         | 4.91            | 11.17         | 45.53           | 36.85         |
| memory           | 173.55          | 136.60        | 196.22          | 256.49        |
| mk bool var      | 44993.8         | 40270.45      | 490215.5        | 48485.7       |
| quant instantiations | 19109.4      | 22138.1       | 209256.0        | 26435.9       |

This shows that DPE is more scalable than the direct strategy. However, it still struggles to give a definite answer (either \( sat \) or \( unsat \)) when the input graphs get more complex (e.g. the polymer model with 7 edges). We have implemented several optimisations for both strategies. One is based on the observation that quantification is one of the most expensive operations and so performance can be enhanced by factoring out quantifiers where possible. For example given the two formulae \( \exists [x, y]. \text{Condition1} \) and \( \exists [x, y, z]. \text{Condition2} \), one can factor out the shared quantification over \( x \) and \( y \) and obtain \( \exists [x, y]. (\text{Condition1} \land \exists [z]. \text{Condition2}) \). Table 5 shows the impact of this optimisation on the performance of the two strategies in the polymer model with 2 and 5 edges:

The preliminary results show that the advantage of optimisation by factoring out quantifiers scales with the DPE strategy whereas for the direct one the improvement is not as significant and is gradually lost as the size of the problem increases. In fact the optimised DPE also finds a solution for the polymer model with 7 edges in average time of 1.89 but even the optimised direct strategy remains unresponsive for too long.
Table 5. Optimised Implementations ran on Polymer Model with 2 and 5 edges

| Indicator        | Polymer model with 2 edges | Polymer model with 5 edges |
|------------------|---------------------------|---------------------------|
|                  | Direct Strategy | DPE Strategy | Direct Strategy | DPE Strategy |
| exe time         | 2.97            | 0.2           | 28.11           | 0.64         |
| memory           | 172.57          | 20.97         | 192.66          | 73.94        |
| mk bool var      | 38009.7         | 3199.55       | 344336.0        | 6129.4       |
| quant instantiations | 13945.9     | 1552.3        | 167608.1        | 3064.15      |

4.5 Discussion

Our experiments showed that the DPE strategy substantially outperforms the direct one and that, moreover, it is amenable to optimisation of quantifiers. We believe this is down to two factors. First, the DPE strategy avoids constructing pushouts for spans where the pushout object would violate the constraints. More significant, we suspect, is the fact that we match several smaller sub-graphs rather than their unions. This decomposition of graphs leads to a reduction in complexity, which is exponential in the size of the graphs matched.

The quantifier optimisation is more effective in the case of DPE because it addresses a specific weakness of that approach. When we replace a forbidden sub-graph check by a check for all forbidden spans arising from its decompositions (4 on average in our example), in the naive implementation every one of those spans gives rise to a constraint that is quantified separately. By joining these constraints we therefore avoid this replication of quantifiers.

The evaluation currently only gives limited insights into the scalability of the solution to real examples, especially to larger rules with many more potential embeddings. However, more complex models are usually also typed, reducing the number of matches. While our categorical theory applies to typed graphs directly, the implementation following categorical principles is easy to adapt to different graph models. There are further opportunities for optimisation, e.g. using pattern-based quantification in Z3 or breaking down large problems into smaller, more manageable ones to address scalability bottlenecks.

5 Conclusion, Related Work and Outlook

We have presented results of both theoretical and experimental nature on the efficient construction of overlap spans with constraints for the computation of commutators for stochastic rewrite systems. On the theoretical side we showed how commutators are constructed for SqPO rules with application conditions, how the constraint checking step in this construction can be modularised, avoiding the direct generate-and-test strategy (of first composing rules and then validating them) by replacing checks for forbidden graph patterns by checks for forbidden relation patterns, and how the same technique can be used to efficiently derive minimal negative conditions preserving forbidden graph constraints. On the experimental side, we have provided an implementation of both strategies in
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Z3 based on the categorical concepts and constructions of the theory, evaluated the correctness of both implementations by testing them against each other and compared their performance through a series of experiments, which showed that with increasing problem size the modular strategy outperforms the direct one and, moreover, is amenable to quantifier optimisation.

Apart from the references already discussed, there is related work on the derivation of systems of differential equations from rewrite rules, all in the context of or inspired by kappa [9]. Such approaches are generalised by the rule algebra construction [3]. The computation of relations between rules subject to constraints is also an element of critical pair analysis [14]. A detailed comparison of the different implementation approaches ad their applicability to more substantial examples is a subject of future work.

We also plan to implement the complete commutator computation, including constructing rules with conditions and counting their isomorphism classes, and explore applications in rule-based models of biochemistry and adaptive networks to derive their evolution equations.

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A Background material on SqPO-rewriting for rules with conditions

A.1 Application conditions

Definition 10 (cf. e.g. [13,11]). Given an \( \mathcal{M} \)-adhesive category \( \mathcal{C} \) satisfying Assumption 1, the conditions \( \text{cond}(\mathcal{C}) \) over \( \mathcal{C} \) are recursively defined as follows:

1. For all objects \( X \in \text{obj}(\mathcal{C}) \), \( \text{true}_X \) is a condition.
2. For every \( \mathcal{M} \)-morphism \( (f : X \leftrightarrow Y) \in \mathcal{M} \) and for every condition \( c_Y \in \text{cond}(\mathcal{C}) \) over \( Y \), \( \exists (f, c_Y) \) is a condition.
3. If \( c_X \in \text{cond}(\mathcal{C}) \) is a condition over \( X \), so is \( \neg c_X \).
4. If \( c_X^{(1)}, c_X^{(2)} \in \text{cond}(\mathcal{C}) \) are conditions over \( X \), so is \( c_X^{(1)} \land c_X^{(2)} \).

The satisfaction of a condition \( c_X \) by an \( \mathcal{M} \)-morphism \( (h : X \leftrightarrow Z) \in \mathcal{M} \) is recursively defined as follows:

1. \( h \models \text{true}_X \).
2. \( h \models \exists (f : X \leftrightarrow Y, c_Y) \) iff there exists \( (g : X \leftrightarrow Y) \in \mathcal{M} \) such that \( h = g \circ f \) and \( g \models c_Y \).
3. \( h \models \neg c_X \) iff \( h \not\models c_X \).
4. \( h \models c_X^{(1)} \land c_X^{(2)} \) iff \( h \models c_X^{(1)} \) and \( h \models c_X^{(2)} \).

Two conditions \( c_X, c_X' \in \text{cond}(\mathcal{C}) \) are equivalent, denoted \( c_X \equiv c_X' \), iff for every \( (h : X \leftrightarrow Z) \in \mathcal{M} \) we find that \( f \models c_X \) implies \( f \models c_X' \) and vice versa.

We will employ the following standard shorthand notations:

\[ \exists (f : X \leftrightarrow Y) := \exists (f : X \leftrightarrow Y, \text{true}_Y), \forall (f : X \leftrightarrow Y, c_Y) := \neg \exists (f : X \leftrightarrow Y, \neg c_Y). \]

An auxiliary construction [13] embeds conditions into a larger context.

Theorem 4. With notations as above and for \( (f : X \leftrightarrow Y) \in \mathcal{M} \), there exists a shift construction \( \text{Shift} \) such that

\[ \forall c_X \in \text{cond}(\mathcal{C}), \forall (h : X \leftrightarrow Z) \in \mathcal{M} : \exists (g : Y \leftrightarrow Z) \in \mathcal{M} : h = g \circ f \]

\[ \Rightarrow (h \models c_X \iff g \models \text{Shift}(f, c_X)). \tag{23} \]

Proof. See e.g. [4] for a concrete construction and further details.

For the computation of SqPO rule compositions for rules with conditions, we need an additional auxiliary construction for the calculus of conditions:

Theorem 5 ([4], Thm. 7). Given a linear rule \( r = (O \leftrightarrow K \leftrightarrow I) \in \text{Lin}(\mathcal{C}) \) and a condition \( c_O \in \text{cond}(\mathcal{C}) \) over \( O \), there exists a transport construction \( \text{Trans} \) such that for any object \( X \in \text{obj}(\mathcal{C}) \) and for any SqPO-admissible match \( m \in \text{M}^*_r(X) \) of \( r \) into \( X \), if \( (m^* : O \leftrightarrow r_m(X)) \in \mathcal{M} \) denotes the comatch of \( m \), the following holds:

\[ m^* \models c_O \iff m \models \text{Trans}(r, c_O). \tag{24} \]

B Proof of Theorem 4

The statement of the theorem follows from the \( \mathcal{M} \)-vanKampen property of the category \( \mathcal{C} \).
For the $\Rightarrow$ direction, suppose that $P \not\models c_N$, which entails that there exists an $N \in \mathcal{N}$ and an embedding $(N \hookrightarrow P)$. Construct the commutative cube on the left via (1) taking pullbacks in order to obtain objects $C_2$ and $C_1$ and (2) letting $D$ be defined as the pullback of $(C_2 \hookrightarrow N \hookleftarrow C_1)$. By stability of $\mathcal{M}$-morphisms and by their decomposition properties, all arrows in the top square and all vertical arrows are $\mathcal{M}$-morphisms. Since the bottom square is a pushout along $\mathcal{M}$-morphisms and thus a pullback, and since the front and top squares are pullbacks, by pullback-pullback decomposition the back square is a pullback, and analogously so is the right square. Thus by the $\mathcal{M}$-vanKampen property, the top square is a pushout, and we have proved that $(C_2 \hookleftarrow D \hookrightarrow C_1)$ is in $\mathcal{S}_N$.

For the $\Leftarrow$ direction, suppose the bottom pushout square as well as the back and left pullback squares were given (with all involved morphisms in $\mathcal{M}$), and such that $(C_2 \hookleftarrow D \hookrightarrow C_1) \in \mathcal{S}_N$. Then letting $N$ be the pushout of $(C_2 \hookrightarrow D \hookrightarrow C_1)$ (which by definition of $\mathcal{S}_N$ entails that $N \in \mathcal{N}$), there exists by universal property of the pushout a morphism $(N \twoheadrightarrow P)$. It remains to demonstrate that $(N \twoheadrightarrow P)$ is in $\mathcal{M}$. To this end, let us assemble the auxiliary above right. By assumption, squares (1) and (4) are pullbacks, square (3) a pushout along $\mathcal{M}$-morphisms (and thus a pullback), while squares of the form (2) are pullbacks by universal category theory. Consequently, we find by composition of pullbacks that $D$ is the pullback of $(C_2 \hookrightarrow P \hookleftarrow C_1)$. Thus finally by virtue of the assumption of $\mathcal{M}$-effective unions, we can confirm that $(N \twoheadrightarrow P)$ is in $\mathcal{M}$.

C Proof of Corollary 1

$\Rightarrow$ direction: Let us assume that a given SqPO-type direct derivation along rule $(O \leftarrow K \leftarrow I)$ with candidate match $(m : I \leftarrow X_0) \in \mathcal{M}$ results in an object $X_1$ with $X_1 \not\models c_N$. By definition of satisfiability and of $c_N$, this entails that there exists an $N \in \mathcal{N}$ and an $\mathcal{M}$-morphism $(N \hookrightarrow X_1) \in \mathcal{M}$. In complete analogy to the proof of Theorem 3 as given in the previous section, construct
Here, $C_1$ and $C_2$ are constructed by taking pullbacks, which by stability of $\mathcal{M}$-morphisms under pullbacks entails that the newly constructed morphism are also in $\mathcal{M}$. $D$ is constructed as a pullback of $(C_2 \leftarrow N \leftarrow C_1)$ (with $\mathcal{M}$-morphisms in the resulting span), while the morphism $(D \rightarrow K)$ is an $\mathcal{M}$-morphism by the decomposition property of $\mathcal{M}$-morphisms. Since the bottom left square is a pushout along $\mathcal{M}$-morphisms and thus a pullback, we find via pullback-pullback decomposition that also the squares $\Box_{D, C_2, O, K}$ (back left) and $\Box_{D, C_1, X_0, K}$ (middle vertical) are pullbacks, and thus by the $\mathcal{M}$-VK property the top left square is a pushout. Next, construct the following three pushouts:

$\overline{D} := \text{PO}(C_1 \leftarrow D \leftarrow K)$, $\overline{C}_2 := \text{PO}(O \leftarrow K \leftarrow \overline{D})$, $P := \text{PO}(\overline{D} \leftarrow K \leftarrow I)$.

As depicted in the diagram below, by the universal properties of the relevant pushouts and via $\mathcal{M}$-effective unions, there exist morphisms (drawn below with dotted lines) that are in fact $\mathcal{M}$-morphisms:

Finally, there are two cases to consider: if $P \models c_N$, we have exhibited a $\mathcal{M}$-morphism $(I \leftrightarrow P)$ through which $(I \leftrightarrow X_0)$ factors, and which thus by the
above construction proves that the rewrite will lead to an $X_1$ with at least one embedding of a “forbidden pattern” $N \in N$. If on the other hand $P \not\models c_N$, we have proved that $X_0 \not\models c_N$; consequently, the $\mathcal{M}$-morphism $(I \mapsto P)$ would in this case not contribute to a constraint-preserving application condition for $(O \mapsto K \mapsto I)$.

⇐ direction: Let us assume we were given the data of the diagram below (i.e. a SqPO-type direct derivation of $X_0$ along candidate match $(I \mapsto X_0) \in \mathcal{M}$ as well as a pattern $P$ such that $(I \mapsto X_0)$ factors through some $(I \mapsto P)$ constructed according to the statement of the Corollary):

Here, in order to demonstrate the existence of the morphism $(\mathcal{D} \mapsto X_0)$, let us first introduce a useful auxiliary formula: given a commutative diagram of $\mathcal{M}$-morphisms as below left,

this data yields the diagram above right. Since the right square is a pullback and the left square a pushout along $\mathcal{M}$-morphisms and thus also a pullback, we find by composition of pullbacks that $\square_{A,C,E,B}$ is a pullback.

Back to the diagram in (27), since $\square_{K,X_0,X_0,I}$ is by assumption a final pullback complement and $\square_{K,P,X_0,I}$ is a pullback by virtue of the auxiliary formula, the universal property of FPCs entails the existence of $(\mathcal{D} \mapsto X_0)$, which by the decomposition property of $\mathcal{M}$-morphisms is an $\mathcal{M}$-morphism. Moreover, by FPC-pushout decomposition [4], $\square_{\mathcal{D},X_0,X_0,P}$ is an FPC.

It then suffices to construct the pushout $C_2 := \text{PO}(O \mapsto K \mapsto \mathcal{D})$, which through the universal properties of the various pushouts involved yields the existence of morphisms $(N \mapsto \mathcal{C})$ and $(\mathcal{C} \mapsto X_1)$ (resulting in a diagram of the form
in (26). Utilising pushout-pushout decompositions (yielding that $\square_{C_2,N,C_2,O}$ and $\square_{D,C_2,X_1,X_0}$ are pushouts), stability of $M$-morphisms under pushouts, the above auxiliary formula (i.e. to demonstrate that $\square_{C_2,N,X_1,O}$ and $\square_{D,C_1,X_0,K}$ are pullbacks) and the property of $M$-effective unions, we find that $(N \rightarrow C_2) \in M$ and $(C_2 \rightarrow X_1) \in M$, such that we have in summary exhibited a $M$-morphism $(N \hookrightarrow X_1) \in M$, which verifies that $X_1 \not\in \mathcal{N}$. 