

# Semantics of pattern unification

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## Abstract

We propose a notion of syntax with metavariables that generalises Miller’s decidable *pattern* fragment of second-order unification for simply-typed  $\lambda$ -calculus. Using categorical semantics, we show that, under some conditions, a generalisation of Miller’s unification algorithm applies. To illustrate our semantic analysis, we implemented our generic unification algorithm implemented in Agda. The syntax with metavariables given as input of the algorithm is specified by a notion of signature generalising binding signatures, covering a wide range of examples, including ordered  $\lambda$ -calculus and (intrinsic) polymorphic syntax such as System F. Although we do not explicitly handle equations, we also tackle simply-typed  $\lambda$ -calculus modulo  $\beta$ - and  $\eta$ -equations (Miller’s original setting) by working on the syntax of normal forms.

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## 1 Introduction

Unification deals with languages with *metavariables*. Let us assume that a language with metavariables comes with a well-formedness judgement of the shape  $\Gamma; a \vdash t$ , meaning that the term  $t$  is well-formed in the *metavariable context*  $\Gamma$  and the *scope*  $a$ . What we call a scope depends on the language of interest: for a De Bruijn-encoded untyped syntax, it would be a mere natural number; for a simply-typed syntax, it would be a pair of a list of types  $\vec{\sigma}$  and a type  $\tau$  to mean that  $t$  has type  $a$  in the base context  $\vec{\sigma}$ . A *metavariable context*, or *metacontext*, is typically a list of metavariable symbols with their associated *arities*. Metacontexts should form a category whose morphisms are called *metavariable substitutions* or *metasubstitution*. A metasubstitution  $\sigma$  between  $\Gamma$  and  $\Delta$  should also induce a mapping  $t \mapsto t[\sigma]$  sending terms well-formed in the metacontext  $\Gamma$  and scope  $a$  to terms well-formed in the metacontext  $\Delta$  and same scope  $a$ .

In this situation, a unification problem is specified by a pair of terms  $(t_1, t_2)$  such that  $\Gamma; a \vdash t_i$  for  $i \in \{1, 2\}$ . A unifier for this pair is a metasubstitution  $\sigma : \Gamma \rightarrow \Delta$  such that  $t_1[\sigma] = t_2[\sigma]$ , and a most general unifier (abbreviated as mgu) is a unifier  $\sigma$  such that given any other unifier  $\delta$ , there exists a unique  $\sigma'$  such that  $\delta = \sigma' \circ \sigma$ .

**Example: first-order/second-order/pattern unification for an untyped syntax.** Let us illustrate different standard versions of unification, starting from the example of a de Bruijn-encoded untyped syntax specified by a binding signature (Aczel, 1978). We take scopes and

also metavariable arities to be natural numbers. We can define three variants of unification by adding one of the following introduction rules for metavariables.

$$\begin{array}{c}
 \text{First-order} \qquad \text{Second-order} \qquad \text{Pattern} \\
 \qquad \qquad \qquad (t_1, \dots, t_m) = \text{list of distinct variables} \\
 \forall (M : m) \in \Gamma \quad \frac{n = m}{\Gamma; n \vdash M} \text{Fo} \quad \frac{\Gamma; n \vdash t_1 \ \dots \ \Gamma; n \vdash t_m}{\Gamma; n \vdash M(\vec{t})} \text{So} \quad \frac{\overbrace{\Gamma; n \vdash t_1 \ \dots \ \Gamma; n \vdash t_m}^{\text{Pattern}}}{\Gamma; n \vdash M(\vec{t})} \text{PAT}
 \end{array}$$

Note that first-order unification is enough to solve unification problems where metavariables are introduced according to the rule Fo, even without the restriction that  $n = 0$ . Let us take the example of (untyped) pure lambda-calculus: through it is the typical example of a mono-sorted syntax with binders, it can alternatively be presented as a multisorted first-order syntax, where the sorts are the natural numbers. The syntax is generated by the following operations, for each sort  $n$ :

- $n$  constants of that sort (the variables);
- a binary operation  $n \times n \rightarrow n$  (application);
- a unary operation  $n + 1 \rightarrow n$  (lambda-abstraction).

The third *pattern* variant in the rules above was introduced by Miller (1991) as a decidable fragment of second-order unification (for simply-typed  $\lambda$ -calculus modulo  $\beta$ - and  $\eta$ -equations): contrary to the latter case, a metavariable can only be applied to a *pattern*, that is, to a list of distinct variables.

In all of these situations, a *metasubstitution*  $\sigma$  between two metacontexts  $\Gamma$  and  $\Delta$  is defined the same way: it maps each metavariable declaration  $M : m$  in  $\Gamma$  to a term  $\Delta; m \vdash \sigma_M$ . Given a term  $\Gamma; n \vdash t$  we define by recursion the substituted term  $\Delta; n \vdash t[\sigma]$ . Then, composition of metasubstitutions is defined by  $(\sigma \circ \delta)_M = \delta_M[\sigma]$ .

### First contribution: a class of languages with metavariables

Our first contribution is a class of languages with metavariables. Such a language is specified by the following data:

- a small category  $\mathcal{A}$  of *scopes* (or *metavariable arities*)<sup>1</sup>, and *renamings* between them,
- an endofunctor  $F$  on  $[\mathcal{A}, \text{Set}]$  of the shape  $F(X)_a = \coprod_{n \in \mathbb{N}} \coprod_{o \in O_n(a)} X_{\bar{o}_1} \times \dots \times X_{\bar{o}_n}$ , where  $O_n(a)$  is intuitively the set of  $n$ -ary available operation symbols in the scope  $a$ .

The base syntax (in the empty metacontext) is generated by the following single rule.

$$\forall o \in O_n(a) \frac{\bar{o}_1 \vdash t_1 \quad \dots \quad \bar{o}_n \vdash t_n}{a \vdash o(t_1, \dots, t_n)}$$

<sup>1</sup> The fact that the notions of scopes and metavariable arities coincide (as in the previous example) allows us to see terms as substitutions and mgus as coequalisers, as we will see. This is not the case in Vezzosi-Abel's presentation of Miller's original setting (Vezzosi and Abel, 2014).

This rule accounts for (possibly simply-typed) binding arities (Aczel, 1978; Fiore and Hur, 2010) but not only. In particular, in Section §7.3 we handle the syntax of normalised  $\lambda$ -terms, which cannot be specified by a binding signature.

We now present the full syntax with metavariables. Again, a metacontext is a list of metavariable symbols with their associated arities (or scopes). The syntax is generated by two rules, one for operations, and one for metavariables.

$$\forall \Gamma \forall o \in O_n(a) \frac{\Gamma; \bar{o}_1 \vdash t_1 \quad \dots \quad \Gamma; \bar{o}_n \vdash t_n}{\Gamma; a \vdash o(t_1, \dots, t_n)} \quad \frac{M : m \in \Gamma \quad x \in \text{hom}_{\mathcal{A}}(m, n)}{\Gamma; n \vdash M(x)}$$

Let us explain how the right rule instantiates to the above metavariable introduction rule **PAT** for pattern unification. A list of distinct variables  $(x_1, \dots, x_m)$  in the scope  $n$  is equivalently given by an injective map from  $\{1, \dots, n\}$  to  $\{1, \dots, m\}$ . Therefore, by taking for  $\mathcal{A}$  the category  $\mathbb{F}_m$  whose objects are natural numbers and whose morphisms from  $n$  to  $m$  consist of injective maps as above, we recover the above **PAT**. Note that contrary to the traditional definition of pattern unification, where the notion of *pattern* is derived from the notion of variable, in our setting, patterns are built-in (they are morphisms in  $\mathcal{A}$ ) and there is no built-in notion of “variables”.

We can also recover the above metavariable rule **FO** by taking for  $\mathcal{A}$  the discrete category  $\mathbb{N}$  whose objects are natural numbers, because a morphism from  $m$  to  $n$  is nothing but the assertion that  $m = n$ . More generally, our setting allows us to see first-order unification as the special case of pattern unification where  $\mathcal{A}$  is a discrete category. Let us finally mention that the metavariable introduction rule **SO** for second-order unification does not fit into our format<sup>2</sup>.

Following the path sketched for the introductory example, we can define metasubstitutions, their action on terms, and their compositions: unification problems can then be stated.

**Scope of our class of languages.** We account for any syntax specified by a multi-sorted binding signature (Fiore and Hur, 2010): we detail the example of simply-typed  $\lambda$ -calculus (without  $\beta$ - and  $\eta$ -equations) in Section §7.2. Note that our framework handles typed settings in such a way that knowing that  $M(\vec{x})$  and  $M(\vec{y})$  are well-formed in the same metacontext and scope is enough to conclude that the types of  $\vec{x}$  and  $\vec{y}$  are the same.

As already said, our notion of language is more expressive than binding signatures: we mentioned in particular the syntax of normal forms for simply-typed  $\lambda$ -calculus (see Section §7.3), which allows us to cover Miller’s original setting. Our class also includes languages where terms bind type variables such as system F (Section §7.5.1): the scopes then include information about the available type variables. In another direction, we can handle certain kind of constraints on the variables in the context: in Section §7.4, we treat the calculus for ordered linear logic described by Polakow and Pfenning (2000): their notion of context consists of two components, one of which includes variables that must occur exactly once and in the same order as they occur in that context.

<sup>2</sup> Essentially, this is because our languages come from free monads on presheaf categories (Lemma 30), while this is not the case of second-order unification (see (Hamana, 2004) for a description of the corresponding monad).

All the examples are summarised in Tables 1 and 2 in Section §7, where the traditional presentation of each calculus is translated into our notion of specification.

Let us finally mention that fully dependently typed languages, where types can depend on terms, are not supported. Indeed, intuitively, in our notion of specification, types are specified through the set of scopes, which must be given independently and prior to the endofunctor of terms: this sequential splitting is not possible with dependent types.

### *Second contribution: a unification algorithm for pattern-friendly languages*

Our second key contribution consists of working out some conditions ensuring that the main contributions of Miller’s work generalise: given two terms  $\Gamma; a \vdash t, u$ , either their mgu exists, or there is no unifier, and the proof of this statement consists in a recursive procedure (much similar to Miller’s original algorithm) which computes a mgu or detects the absence of any unifier.

Those conditions are essentially that renamings are monomorphic, and  $\mathcal{A}$  has equalisers and pullbacks, and some additional properties about the functor  $F$  related to those limits (see Definition 25). We call one of our languages *pattern-friendly* when it satisfies those properties. All the examples that we already mentioned are pattern-friendly, see Section §7 more details.

**Agda implementation.** We implemented our generic unification algorithm (without mechanisation of the correctness proof) in Agda. We show the most important parts; the interested reader can find the full implementation in the supplemental material. We used Agda as a programming language rather than a theorem prover. In particular, we did not enforce all the invariants in the definition of the data structures (e.g., associativity of composition in the category of scopes): the user has to check by himself that the input data is valid for the algorithm to produce valid outputs. Furthermore, we disable the termination checker and provide instead a termination proof on paper in Section §6.1.

Let us mention that we use a small trick to avoid the traditional presentation of unification as a partial algorithm computing mgus: we add a formal error metacontext  $\perp$  and a single formal error term  $\perp; a \vdash !$  for all scopes  $a$ , so that we get a unique metasubstitution  $!_\Gamma$  from any metacontext  $\Gamma$  to  $\perp$ . This substitution obviously unifies any pair of terms. If two terms are not unifiable in the traditional sense,  $!$  is the mgu. If  $\sigma : \Gamma \rightarrow \Delta$  is the mgu in the traditional sense, then it is still the mgu in this extended setting, because  $!_\Gamma$  uniquely factors as  $!_\Delta \circ \sigma$ . In this way, unification can be seen as a total algorithm that always computes the mgu.

### *Most general unifiers as coequalisers*

It is well-known that unification can be formulated categorically (Goguen, 1989). Let us make this formulation explicit in our setting. The set of terms in the metacontext  $\Gamma$  and scope  $a$  is recovered as the set of morphisms from the singleton metacontext  $(M : a)$  to  $\Gamma$ . With this in mind, a unifier of two terms  $\Gamma; a \vdash t, u$  can be interpreted as a cocone, that is, as a morphism  $\Gamma \rightarrow \Delta$  such that its composition with either of the two terms (interpreted as

morphisms) are equal. A mgu is then a coequaliser: this is the characterisation that we use to prove correctness of our unification algorithm.

Let us finally mention that given a specification, we provide in Proposition 32 a direct characterisation of the category of metacontexts and substitutions as a full subcategory of the Kleisli category of the monad  $T$  freely generated by the endofunctor  $F$ .

### *Motivation*

Let us explain where this work originates from. Pattern unification is used in the implementation of various PLs. As a concrete example, consider Dunfield-Krishnaswami's type inference algorithm for a variant of system F (Dunfield and Krishnaswami, 2019). It only involves first-order unification, but simply adding a monomorphic type with a binder (for example, a recursive type  $\mu a.A[a]$ ) would require pattern unification.

In order to avoid reproving everything for each new type system, pattern unification needs to be formulated generically so that it can be used in a variety of contexts without modification. This is our original motivation for this work. To the best of our knowledge, we are the first to give a general definition of pattern unification that works for a wide class of languages, in the vein of Rydeheard-Burstall's first-order analysis (Rydeheard and Burstall, 1988), see the related work in Section §8 for more details.

### *Plan of the paper*

In section §2, we present our generic pattern unification algorithm, parameterised by our notion of specification. We introduce categorical semantics of pattern unification in Section §3. We show correctness of the two phases of the unification algorithm in Section §4 and Section §5. Termination and completeness are justified in Sections §6. Examples of specifications are given in Section §7, and related work is finally discussed in Section §8. The appendices can be found in the supplemental material.

### *General notations*

Given a list  $\vec{x} = (x_1, \dots, x_n)$  and a list of positions  $\vec{p} = (p_1, \dots, p_m)$  taken in  $\{1, \dots, n\}$ , we denote  $(x_{p_1}, \dots, x_{p_m})$  by  $x_{\vec{p}}$ .

Given a category  $\mathcal{B}$ , we denote its opposite category by  $\mathcal{B}^{op}$ . If  $a$  and  $b$  are two objects of  $\mathcal{B}$ , we denote the set of morphisms between  $a$  and  $b$  by  $\text{hom}_{\mathcal{B}}(a, b)$ . We denote the identity morphism at an object  $x$  by  $1_x$ . We denote the coproduct of two objects  $A$  and  $B$  by  $A + B$ , the coproduct of a family of objects  $(A_i)_{i \in I}$  by  $\coprod_{i \in I} A_i$ , and similarly for morphisms. If  $f : A \rightarrow B$  and  $g : A' \rightarrow B$ , we denote the induced morphism  $A + A' \rightarrow B$  by  $f, g$ . Coproduct injections  $A_j \rightarrow \coprod_{i \in I} A_i$  are typically denoted by  $\text{in}_j$ . Let  $T$  be a monad on a category  $\mathcal{B}$ . We denote its unit by  $\eta$ , and its Kleisli category by  $Kl_T$ : the objects are the same as those of  $\mathcal{B}$ , and a Kleisli morphism from  $A$  to  $B$  is a morphism  $A \rightarrow TB$  in  $\mathcal{B}$ . We denote the Kleisli composition of  $f : A \rightarrow TB$  and  $g : B \rightarrow TC$  by  $f[g] : A \rightarrow TC$ .

Fig. 1: Syntax of  $\lambda$ -calculus (Section §2.1)

MetaContext = List  $\mathbb{N}$

MetaContext = Maybe MetaContext

data Tm : MetaContext  $\rightarrow \mathbb{N} \rightarrow \text{Set}$

Tm  $\Gamma\ n = \text{Tm } [\Gamma]\ n$

data Tm where

App :  $\forall \{\Gamma\ n\} \rightarrow \text{Tm } \Gamma\ n \rightarrow \text{Tm } \Gamma\ n$

$\rightarrow \text{Tm } \Gamma\ n$

Lam :  $\forall \{\Gamma\ n\} \rightarrow \text{Tm } \Gamma\ (1 + n)$

$\rightarrow \text{Tm } \Gamma\ n$

Var :  $\forall \{\Gamma\ n\} \rightarrow \text{Fin } n \rightarrow \text{Tm } \Gamma\ n$

$\_ (\_) : \forall \{\Gamma\ n\ m\} \rightarrow m \in \Gamma \rightarrow \text{hom } m\ n$

$\rightarrow \text{Tm } \Gamma\ n$

! :  $\forall \{n\} \rightarrow \text{Tm } \perp\ n$

hom :  $\mathbb{N} \rightarrow \mathbb{N} \rightarrow \text{Set}$

hom  $m\ n = \text{Vec } (\text{Fin } n)\ m$

$$\frac{1 \leq i \leq n}{\Gamma; n \vdash \underline{i}} \quad \frac{\Gamma; n \vdash t \quad \Gamma; n \vdash u}{\Gamma; n \vdash t\ u} \quad \frac{\Gamma; n+1 \vdash t}{\Gamma; n \vdash \lambda t}$$
  

$$\frac{M : m \in \Gamma \quad \overbrace{x \in \text{hom}(m, n)}^{x_1, \dots, x_m \in \{1, \dots, n\} \text{ distinct}}}{\Gamma; n \vdash M(x_1, \dots, x_m)}$$
  

$$\frac{}{\perp; a \vdash !}$$

App :  $\forall \{\Gamma\ n\} \rightarrow \text{Tm } \Gamma\ n \rightarrow$

$\text{Tm } \Gamma\ n \rightarrow \text{Tm } \Gamma\ n$

App { $\perp$ } !! = !

App {[ $\Gamma$ ]} t u = App t u

Lam :  $\forall \{\Gamma\ n\} \rightarrow \text{Tm } \Gamma\ (1 + n)$

$\rightarrow \text{Tm } \Gamma\ n$

Lam { $\perp$ } ! = !

Lam {[ $\Gamma$ ]} t = Lam t

Var :  $\forall \{\Gamma\ n\} \rightarrow \text{Fin } n$

$\rightarrow \text{Tm } \Gamma\ n$

Var { $\perp$ } i = !

Var {[ $\Gamma$ ]} i = Var i

$\frac{1 \leq i \leq n}{\Gamma; n \vdash \underline{i}}$	$\frac{\Gamma; n \vdash t \quad \Gamma; n \vdash u}{\Gamma; n \vdash t\ u}$	$\frac{\Gamma; n + 1 \vdash t}{\Gamma; n \vdash \lambda t}$
$x_1, \dots, x_m \in \{1, \dots, n\} \text{ distinct}$		
$\frac{M : m \in \Gamma \quad \overbrace{x \in \text{hom}(m, n)}}{\Gamma; n \vdash M(x_1, \dots, x_m)}$		
$\frac{}{\perp; a \vdash !}$		

## 2 Presentation of the algorithm

In Section §2.1, we start by describing a pattern unification algorithm for pure  $\lambda$ -calculus, summarised in Figure 4. We claim no originality here; minor variants of the algorithm can be found in the literature: it serves mainly as an introduction to the generic algorithm presented in Section §2.2 and summarised in Figure 5.

### 2.1 An example: pure $\lambda$ -calculus.

Consider the syntax of pure  $\lambda$ -calculus extended with pattern metavariables. We list the Agda code in Figure 1, together with a corresponding presentation as inductive rules generating the syntax. We write  $\Gamma; n \vdash t$  to mean  $t$  is a well-formed  $\lambda$ -term in the context  $\Gamma; n$ , consisting of two parts:

1. a metavariable context (or *metacontext*)  $\Gamma$ , which is either a formal error context  $\perp$ , or a *proper* context, as a list  $(M_1 : m_1, \dots, M_p : m_p)$ , of metavariable declarations specifying metavariable symbols  $M_i$  together with their arities, i.e., their number of arguments  $m_i$ ;
2. a scope, which is a mere natural number indicating the highest possible free variable.

Free variables are indexed from 1 and we use the De Bruijn level convention: the variable bound in  $\Gamma; n \vdash \lambda t$  is  $n + 1$ , not 0, as it would be using De Bruijn indices (De Bruijn, 1972).

In Agda, variables in the scope  $n$  consist of elements of `Fin n`, the type of natural numbers between<sup>3</sup> 1 and  $n$ .

In the inductive rules, we use the bold face  $\Gamma$  for any proper metacontext. In the Agda code, we adopt a nameless encoding of proper metacontexts: they are mere lists of metavariable arities, and metavariables are referred to by their index in the list. The type of metacontexts `MetaContext` is formally defined as `Maybe (List ℕ)`, where `Maybe X` is an inductive type with an error constructor  $\perp$  and a *proper* constructor  $[-]$  taking as argument an element of type  $X$ . Therefore,  $\Gamma$  typically translates into  $[\Gamma]$  in the implementation. To alleviate notations, we also adopt a dotted convention in Agda to mean that a proper metacontext is involved. For example, `MetaContext·` and `Tm·`  $\Gamma n$  are respectively defined as `List ℕ` and `Tm [Γ] n`.

The last term constructor `!` builds a well-formed term in any error context  $\perp; n$ . We call it an *error* term: it is the only one available in such contexts. *Proper* terms, i.e., terms well-formed in a proper metacontext, are built from application,  $\lambda$ -abstraction and variables: they generate the (proper) syntax of  $\lambda$ -calculus. Note that `!` cannot occur as a sub-term of a proper term.

**Remark 1.** *The names of constructors of  $\lambda$ -calculus for application,  $\lambda$ -abstraction, and variables, are dotted to indicate that they are only available in a proper metacontext. “Improper” versions of those, defined in any metacontext, are also implemented in the obvious way, coinciding with the constructors in a proper context, or returning `!` in the error context.*

Let us focus on the penultimate constructor, building a metavariable application in the context  $\Gamma; n$ . The argument of type  $m \in \Gamma$  is an index of any element  $m$  in the list  $\Gamma$ . In the pattern fragment, a metavariable of arity  $m$  can be applied to a list of size  $m$  consisting of distinct variables in the scope  $n$ , that is, natural numbers between 1 and  $n$ . We denote by  $\text{hom}(m, n)$  this set of lists. To make the Agda implementation easier, we did not enforce the uniqueness restriction in the definition of `hom m n`. However, our unification algorithm is guaranteed to produce correct outputs only if this constraint is satisfied in the inputs.

The Agda implementation of metavariable substitutions for  $\lambda$ -calculus is listed in the first box of Figure 2. We call a substitution *successful* if it targets a proper metacontext, *proper* if the domain is proper. Note that any successful substitution is proper because there is only one metavariable substitution  $1_\perp$  from the error context: it is a formal identity substitution, targeting itself. A *metavariable substitution*  $\sigma : \Gamma \rightarrow \Delta$  from a proper context assigns to each metavariable  $M$  of arity  $m$  in  $\Gamma$  a term  $\Delta; m \vdash \sigma_M$ .

This assignment extends (through a recursive definition) to any term  $\Gamma; n \vdash t$ , yielding a term  $\Delta; n \vdash t[\sigma]$ . Note that the congruence cases involve improper versions of the operations (Remark 1), as the target metacontext may not be proper. The base case is  $M(x_1, \dots, x_m)[\sigma] = \sigma_M\{x\}$ , where  $-\{x\}$  is variable renaming, defined by recursion. Renaming a  $\lambda$ -abstraction requires extending the renaming  $x : \text{hom } p \ q$  to  $x \uparrow : \text{hom } (p + 1) \ (q + 1)$  to take into account the additional bound variable  $\underline{p + 1}$ , which is

<sup>3</sup> `Fin n` is actually defined in the standard library as an inductive type designed to be (canonically) isomorphic with  $\{0, \dots, n - 1\}$ .

Fig. 2: Metavariable substitution

- Proper substitutions  $\Gamma \cdot \longrightarrow \Delta = [\Gamma] \longrightarrow \Delta$   
 - Successful substitutions  $\Gamma \cdot \longrightarrow^* \Delta = [\Gamma] \longrightarrow [\Delta]$   
 data  $\_ \longrightarrow \_$  where  
 $[\_] : \forall \{\Delta\} \rightarrow ([\_] \cdot \longrightarrow \Delta)$   
 $\_,\_ : \forall \{\Gamma \Delta m\} \rightarrow \text{Tm } \Delta m \rightarrow (\Gamma \cdot \longrightarrow \Delta) \rightarrow (m :: \Gamma \cdot \longrightarrow \Delta)$   
 $1\bot : \bot \longrightarrow \bot$

$\lambda$ -calculus (Section §2.1)

$[\_]t : \forall \{\Gamma n\} \rightarrow \text{Tm } \Gamma n \rightarrow \forall \{\Delta\} \rightarrow (\Gamma \longrightarrow \Delta) \rightarrow \text{Tm } \Delta n$   
 $(\text{App} \cdot tu) [\sigma]t = \text{App } (t [\sigma]t) (u [\sigma]t)$   
 $\text{Lam} \cdot t [\sigma]t = \text{Lam } (t [\sigma]t)$   
 $\text{Var} \cdot i [\sigma]t = \text{Var } i$   
 -  $\_ \{ \_ \} : \text{Tm } \Gamma n \rightarrow \text{hom } n p \rightarrow \text{Tm } \Gamma p$   
 - is renaming (code omitted)  
 $\frac{\Gamma; n \vdash t \quad \sigma : \Gamma \rightarrow \Delta}{\Delta; n \vdash t[\sigma]}$   
 $M(x) [\sigma]t = \text{nth } \sigma M \{x\}$   
 $! [1\bot]t = !$   
 $[\_]s : \forall \{\Gamma \Delta E\} \rightarrow (\Gamma \longrightarrow \Delta) \rightarrow (\Delta \longrightarrow E) \rightarrow (\Gamma \longrightarrow E)$   
 $[\sigma]s = []$   
 $(t, \delta) [\sigma]s = t [\sigma]t, \delta [\sigma]s$   
 $1\bot [1\bot]s = 1\bot$   
 $\frac{\delta : \Gamma \rightarrow \Delta \quad \sigma : \Delta \rightarrow E}{\delta[\sigma] : \Gamma \rightarrow E}$   
 $M \mapsto \delta_M[\sigma]$

Generic syntax (Section §2.2)

$[\_]t : \forall \{\Gamma a\} \rightarrow \text{Tm } \Gamma a \rightarrow \forall \{\Delta\} \rightarrow (\Gamma \longrightarrow \Delta) \rightarrow \text{Tm } \Delta a$   
 $[\_]s : \forall \{\Gamma \Delta E\} \rightarrow (\Gamma \longrightarrow \Delta) \rightarrow (\Delta \longrightarrow E) \rightarrow (\Gamma \longrightarrow E)$   
 $(\text{Rigid} \cdot o \delta) [\sigma]t = \text{Rigid } o (\delta [\sigma]s)$   
 $M(x) [\sigma]t = \text{nth } \sigma M \{x\}$   
 $! [1\bot]t = !$   
 $[\sigma]s = []$   
 $(t, \delta) [\sigma]s = t [\sigma]t, \delta [\sigma]s$   
 $1\bot [1\bot]s = 1\bot$   
 $\frac{\delta : \Gamma \rightarrow \Delta \quad \sigma : \Delta \rightarrow E}{\delta[\sigma] : \Gamma \rightarrow E}$   
 $M \mapsto \delta_M[\sigma]$

renamed to  $q + 1$ . Then,  $(\lambda t)\{x\}$  is defined as  $\lambda(t\{x \uparrow\})$ . While metavariable substitutions change the metacontext of the substituted term, renamings change the scope.

The identity substitution  $1_\Gamma : \Gamma \rightarrow \Gamma$  is defined by the term  $M(1, \dots, m)$  for each metavariable declaration  $M : m \in \Gamma$ . The composition  $\delta[\sigma] : \Gamma_1 \rightarrow \Gamma_3$  of two substitutions  $\delta : \Gamma_1 \rightarrow \Gamma_2$  and  $\sigma : \Gamma_2 \rightarrow \Gamma_3$  is defined as  $M \mapsto \delta_M[\sigma]$ .



Fig. 3: Type signatures of the functions implemented in Figure 4 and Figure 5

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369
370 record  $\_ \rightarrow ? \Gamma : \text{Set } k'$  where
371   constructor  $\_ \triangleleft \_$ 
372   field
373      $\Delta : \text{MetaContext}$ 
374      $\sigma : \Gamma \rightarrow \Delta$ 
375
376 record  $[\_] \cup \_ \rightarrow ? m \Gamma : \text{Set } k'$  where
377   constructor  $\_ \triangleleft \_$ 
378   field
379      $\Delta : \text{MetaContext}$ 
380      $u, \sigma : (\text{Tm } \Delta m) \times (\Gamma \rightarrow \Delta)$ 
381
382 record  $\_ \cup \_ \rightarrow ? (\Gamma : \text{MetaContext}) (\Gamma' : \text{MetaContext})$ 
383   :  $\text{Set } (i \sqcup j \sqcup k)$  where
384   constructor  $\_ \triangleleft \_$ 
385   field
386      $\Delta : \text{MetaContext}$ 
387      $\delta, \sigma : (\Gamma \rightarrow \Delta) \times (\Gamma' \rightarrow \Delta)$ 
388
389 prune :  $\forall \{ \Gamma a m \} \rightarrow \text{Tm } \Gamma a \rightarrow \text{hom } m a \rightarrow [\_] \cup \Gamma \rightarrow ?$ 
390 prune- $\sigma$  :  $\forall \{ \Gamma \Gamma' \Gamma'' \} \rightarrow (\Gamma' \rightarrow \Gamma) \rightarrow (\Gamma'' \Rightarrow \Gamma') \rightarrow \Gamma'' \cup \Gamma \rightarrow ?$ 
391
392 unify-flex-* :  $\forall \{ \Gamma m a \} \rightarrow m \in \Gamma \rightarrow \text{hom } m a \rightarrow \text{Tm} \cdot \Gamma a \rightarrow \Gamma \rightarrow ?$ 
393 unify :  $\forall \{ \Gamma a \} \rightarrow \text{Tm } \Gamma a \rightarrow \text{Tm } \Gamma a \rightarrow \Gamma \rightarrow ?$ 
394 unify- $\sigma$  :  $\forall \{ \Gamma \Gamma' \} \rightarrow (\Gamma' \rightarrow \Gamma) \rightarrow (\Gamma' \rightarrow \Gamma) \rightarrow (\Gamma \rightarrow ?)$ 
395
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```

A *unifier* of two terms  $\Gamma; n \vdash t, u$  is a substitution  $\sigma : \Gamma \rightarrow \Delta$  such that  $t[\sigma] = u[\sigma]$ . It is called successful if the underlying substitution is. A *most general unifier* (mgu) of  $t$  and  $u$  is a unifier  $\sigma : \Gamma \rightarrow \Delta$  that uniquely factors any other unifier  $\delta : \Gamma \rightarrow \Delta'$ , in the sense that there exists a unique  $\delta' : \Delta \rightarrow \Delta'$  such that  $\delta = \sigma[\delta']$ . The main property of pattern unification is that any pair of terms has a mgu (although not necessarily successful, as explained in the introduction). Accordingly and as it can be seen in Figure 3, the `unify` function takes two terms  $\Gamma; n \vdash t, u$  as input and returns a record with two fields: a context  $\Delta$ , which is  $\perp$  in case there is no successful unifier, and a substitution  $\sigma : \Gamma \rightarrow \Delta$ , which is the mgu of  $t$  and  $u$  (the latter property is however not explicitly enforced by the type signature). We denote such a situation by  $\Gamma \vdash t = u \Rightarrow \sigma \vdash \Delta$ , leaving the scope  $n$  implicit to alleviate the notation: the symbol  $\Rightarrow$  separates the input and the output of the unification algorithm.

This unification function recursively inspects the structure of the given terms until reaching a metavariable at the top-level, as seen in the second box of Figure 4. The last two cases handle unification of two error terms, and unification of two different *rigid* term constructors (application,  $\lambda$ -abstraction, or variables), resulting in failure.

When reaching a metavariable application  $M(x)$  at the top-level of either term in a metacontext  $\Gamma$ , denoting by  $t$  the other term, three situations must be considered:

1.  $t$  is a metavariable application  $M(y)$ ;
2.  $t$  is not a metavariable application and  $M$  occurs deeply in  $t$ ;
3.  $M$  does not occur in  $t$ .

The `occur-check` function returns `Same-MVar`  $y$  in the first case, `Cycle` in the second case, and `No-Cycle`  $t'$  in the last case, where  $t'$  is  $t$  but considered in the context  $\Gamma$  without  $M$ , denoted by  $\Gamma \setminus M$ .

In the first case, the line `let  $p, z = \text{commonPositions } m \ x \ y$`  computes the *vector of common positions* of  $x$  and  $y$ , that is, the maximal vector of (distinct) positions  $(z_1, \dots, z_p)$  such that  $x_{\bar{z}} = y_{\bar{z}}$ . We denote<sup>4</sup> such a situation by  `$m \vdash x = y \Rightarrow z \vdash p$` . The most general unifier  $\sigma$  coincides with the identity substitution except that  $M : m$  is replaced by a fresh metavariable  $P : p$  in the context  $\Gamma$ , and  $\sigma$  maps  $M$  to  $P(z)$ .

**Example 2.** Let  $x, y, z$  be three distinct variables, and let us consider unification of  $M(x, y)$  and  $M(z, x)$ . Given a unifier  $\sigma$ , since  $M(x, y)[\sigma] = \sigma_M \{ \underline{1} \mapsto x, \underline{2} \mapsto y \}$  and  $M(z, x)[\sigma] = \sigma_M \{ \underline{1} \mapsto z, \underline{2} \mapsto x \}$  must be equal,  $\sigma_M$  cannot depend on the variables  $\underline{1}$  and  $\underline{2}$ . It follows that the most general unifier is  $M \mapsto P$ , replacing  $M$  with a fresh constant metavariable  $P$ . A similar argument shows that the most general unifier of  $M(x, y)$  and  $M(z, y)$  is  $M \mapsto P(\underline{2})$ .

The corresponding rule SAME-MVAR does not stipulate how to generate the fresh metavariable symbol  $P$ , although there is an obvious choice, consisting in taking  $M$  which has just been removed from the context  $\Gamma$ . Accordingly, the implementation keeps  $M$  but changes its arity to  $p$ , resulting in a context denoted by  $\Gamma[M : p]$ .

The second case tackles unification of a metavariable application with a term in which the metavariable occurs deeply. It is handled by the failing rule CYCLE: there is no (successful) unifier because the size of both hand sides can never match after substitution.

The last case described by the rule NO-CYCLE is unification of  $M(x)$  with a term  $t$  in which  $M$  does not occur. This kind of unification problem is handled specifically by a previously defined function `prune`, which we now describe. The intuition is that  $M(x)$  and  $t$  should be unified by replacing  $M$  with  $t[x_i \mapsto i]$ . However, this only makes sense if the free variables of  $t$  are in  $x$ . For example, if  $t$  is a variable that does not occur in  $x$ , then obviously there is no unifier. Nonetheless, it is possible to prune the *outbound* variables in  $t$  as long as they only occur in metavariable arguments, by restricting the arities of those metavariables. As an example, if  $t$  is a metavariable application  $N(x, y)$ , then although the free variables are not all included in  $x$ , the most general unifier still exists, essentially replacing  $N$  with  $M$ , discarding the outbound variable  $y$ .

The pruning phase runs in the metacontext with  $M$  removed. We use the notation  $\Gamma \vdash t : \triangleright x \Rightarrow t'; \sigma \dashv \Delta$ , where  $t$  is a term in the metacontext  $\Gamma$ , while  $x$  is the argument of the metavariable whose arity  $m$  is left implicit, as well as its (irrelevant) name. The output is a metacontext  $\Delta$ , together with a term  $t'$  in context  $\Delta; m$ , and a substitution  $\sigma : \Gamma \rightarrow \Delta$ . If  $\Gamma$  is proper, this is precisely the data for the most general unifier of  $t$  and  $M(x)$ , considered in the extended metacontext  $M : m, \Gamma$ . Following the above pruning intuition,  $t'$  is the term  $t$  where the outbound variables have been pruned, in case of success. This justifies the type signature of the `prune` in Figure 3. This function recursively inspects its argument. The base metavariable case corresponds to unification of  $M(x)$  and  $M'(y)$  where  $M$  and  $M'$  are distinct metavariables. In this case, the line `let  $p, x', y' = \text{commonValues } m \ x \ y$`  computes the vectors of *common value positions*  $(x'_1, \dots, x'_p)$  and  $(y'_1, \dots, y'_p)$  between

<sup>4</sup> The similarity with the above introduced notation is no coincidence: as we will see (Remark 21), both are (co)equalisers.

Fig. 4: Pattern unification for  $\lambda$ -calculus (Section §2.1)

461		
462	$\text{prune } \{ \Gamma \} (M : m(x)) y =$	
463	$\text{let } p, x', y' = \text{commonValues } m x y \text{ in}$	$\frac{m \vdash x :> y \Rightarrow y'; x' \vdash p}{\Gamma[M : m] \vdash M(x) :> y \Rightarrow P(y'); M \mapsto P(x') \vdash \Gamma[P : p]} \text{P-FLEX}$
464	$\Gamma[M : p] \cdot \blacktriangleleft ((M : p)(y'), M \mapsto (x'))$	
465		
466	$\text{prune } !y = \perp \blacktriangleleft (!, !_s)$	$\frac{}{\perp \vdash ! :> x \Rightarrow !; !_s \vdash \perp} \text{P-FAIL}$
467		
468	$\text{prune } (\text{App} \cdot t u) x =$	$\frac{\Gamma \vdash t :> x \Rightarrow t'; \sigma_1 \vdash \Delta_1}{\Delta_1 \vdash u[\sigma_1] :> x \Rightarrow u'; \sigma_2 \vdash \Delta_2} \frac{}{\Gamma \vdash t u :> x \Rightarrow t'[\sigma_2] u'; \sigma_1[\sigma_2] \vdash \Delta_2}$
469	$\text{let } \Delta_1 \blacktriangleleft (t', \sigma_1) = \text{prune } t x$	
470	$\Delta_2 \blacktriangleleft (u', \sigma_2) = \text{prune } (u[\sigma_1] t) x$	
471	$\text{in } \Delta_2 \blacktriangleleft (\text{App } (t'[\sigma_2] t) u', \sigma_1[\sigma_2] s)$	
472		
473	$\text{prune } (\text{Lam} \cdot t) x =$	$\frac{\Gamma \vdash t :> x \uparrow \Rightarrow t'; \sigma \vdash \Delta}{\Gamma \vdash \lambda t :> x \Rightarrow \lambda t'; \sigma \vdash \Delta}$
474	$\text{let } \Delta \blacktriangleleft (t', \sigma) = \text{prune } t(x \uparrow)$	
475	$\text{in } \Delta \blacktriangleleft (\text{Lam } t', \sigma)$	
476		
477	$\text{prune } \{ \Gamma \} (\text{Var} \cdot i) x \text{ with } i \{ x \}^{-1}$	
478	$\dots \mid \perp = \perp \blacktriangleleft (!, !_s)$	$\frac{i \notin x}{\Gamma \vdash \underline{i} :> x \Rightarrow !; !_s \vdash \perp} \quad \frac{i = x_j}{\Gamma \vdash \underline{i} :> x \Rightarrow \underline{j}; 1_\Gamma \vdash \Gamma}$
479	$\dots \mid \lfloor \text{PrelImage } j \rfloor = \Gamma \blacktriangleleft (\text{Var } j, 1_s)$	
480		
481		
482	$\text{unify } t(M(x)) = \text{unify-flex-}^* M x t$	$\frac{m \vdash x = y \Rightarrow z \vdash p}{\Gamma[M : m] \vdash M(x) = M(y) \Rightarrow M \mapsto P(z) \vdash \Gamma[P : p]} \text{SAME-MVAR}$
483	$\text{unify } (M(x)) t = \text{unify-flex-}^* M x t$	
484		
485	$\text{unify-flex-}^* \{ \Gamma \} \{ m \} M x t$	
486	$\text{with occur-check } M t$	
487	$\dots \mid \text{Same-MVar } y =$	$\frac{M \in t \quad t \neq M(\dots)}{\Gamma, M : m \vdash M(x) = t \Rightarrow !_s \vdash \perp} \text{CYCLE}$
488	$\text{let } p, z = \text{commonPositions } m x y$	
489	$\text{in } \Gamma[M : p] \cdot \blacktriangleleft M \mapsto (z)$	
490	$\dots \mid \text{Cycle} = \perp \blacktriangleleft !_s$	$\frac{M \notin t \quad \Gamma \setminus M \vdash t :> x \Rightarrow t'; \sigma \vdash \Delta}{\Gamma \vdash M(x) = t \Rightarrow M \mapsto t', \sigma \vdash \Delta} \text{NO-CYCLE}$
491	$\dots \mid \text{No-Cycle } t' =$	
492	$\text{let } \Delta \blacktriangleleft (u, \sigma) = \text{prune } t' x$	
493	$\text{in } \Delta \blacktriangleleft M \mapsto u, \sigma$	
494		(+ symmetric rules)
495	$\text{unify } (\text{App} \cdot t u) (\text{App} \cdot t' u') =$	$\frac{\Gamma \vdash t = t' \Rightarrow \sigma_1 \vdash \Delta_1}{\Delta_1 \vdash u[\sigma_1] = u'[\sigma_2] \Rightarrow \sigma_2 \vdash \Delta_2} \frac{}{\Gamma \vdash t u = t' u' \Rightarrow \sigma_1[\sigma_2] \vdash \Delta_2}$
496	$\text{let } \Delta_1 \blacktriangleleft \sigma_1 = \text{unify } t t'$	
497	$\Delta_2 \blacktriangleleft \sigma_2 = \text{unify } (u[\sigma_1] t) (u'[\sigma_2] t)$	
498	$\text{in } \Delta_2 \blacktriangleleft \sigma_1[\sigma_2] s$	
499	$\text{unify } (\text{Lam} \cdot t) (\text{Lam} \cdot t') = \text{unify } t t'$	$\frac{\Gamma \vdash t = t' \Rightarrow \sigma \vdash \Delta}{\Gamma \vdash \lambda t = \lambda t' \Rightarrow \sigma \vdash \Delta}$
500	$\text{unify } \{ \Gamma \} (\text{Var} \cdot i) (\text{Var} \cdot j) \text{ with } i \text{ Fin.}^? j$	
501	$\dots \mid \text{no } \_ = \perp \blacktriangleleft !_s$	$\frac{i \neq j}{\Gamma \vdash \underline{i} = \underline{j} \Rightarrow !_s \vdash \perp} \quad \frac{}{\Gamma \vdash \underline{i} = \underline{i} \Rightarrow 1_\Gamma \vdash \Gamma}$
502	$\dots \mid \text{yes } \_ = \Gamma \blacktriangleleft 1_s$	
503		
504	$\text{unify } !! = \perp \blacktriangleleft !_s$	$\frac{}{\perp \vdash !! \Rightarrow !_s \vdash \perp} \text{U-FAIL}$
505		
506	$\text{unify } \_ \_ = \perp \blacktriangleleft !_s$	$\frac{o \neq o' \text{ (rigid term constructors)}}{\Gamma \vdash o(\vec{t}) = o'(\vec{t}') \Rightarrow !_s \vdash \perp}$

Fig. 5: Our generic pattern unification algorithm

<pre> 507 508 <b>prune</b> { [ <math>\Gamma</math> ] } ( <math>M : m(x)</math> ) <math>y =</math> 509   <b>let</b> <math>p, x', y' = \text{pullback } m x y</math> <b>in</b> 510   <math>\Gamma [ M : p ] \triangleleft ((M : p)(y'), M \mapsto (x'))</math> 511 512 513   Same as the rule P-FLEX in Figure 4. </pre>	<pre> <b>prune</b> ! <math>y = \perp \triangleleft (!, !_s)</math> </pre> <p>Same as the rule P-FAIL in Figure 4.</p>
<pre> 515 516 <b>prune</b> (Rigid <math>\cdot o \delta</math>) <math>x</math> <b>with</b> <math>o \{x\}^{-1}</math> 517 ...   <math>\perp = \perp \triangleleft (!, !_s)</math> 518 ...   [ <b>PrelImage</b> <math>o'</math> ] = 519   <b>let</b> <math>\Delta \triangleleft (\delta', \sigma) = \text{prune-}\sigma \delta (x \wedge o')</math> 520   <b>in</b> <math>\Delta \triangleleft (\text{Rigid } o' \delta', \sigma)</math> </pre>	$\frac{o \neq \dots \{x\}}{\Gamma \vdash o(\delta) :> x \Rightarrow !; !_s \vdash \perp} \text{P-RIG-FAIL}$ $\frac{\Gamma \vdash \delta :> x^{o'} \Rightarrow \delta'; \sigma \vdash \Delta \quad o = o' \{x\}}{\Gamma \vdash o(\delta) :> x \Rightarrow o'(\delta'); \sigma \vdash \Delta} \text{P-RIG}$
<pre> 521 522 <b>prune-}\sigma</b> { <math>\Gamma</math> } [ ] [ ] = <math>\Gamma \triangleleft ([ ], 1_s)</math> 523 <b>prune-}\sigma</b> ( <math>t, \delta</math> ) ( <math>x_0 :: xs</math> ) = 524   <b>let</b> <math>\Delta_1 \triangleleft (t', \sigma_1) = \text{prune } t x_0</math> 525   <math>\Delta_2 \triangleleft (\delta', \sigma_2) = \text{prune-}\sigma (\delta [ \sigma_1 ]_s) xs</math> 526   <b>in</b> <math>\Delta_2 \triangleleft ((t' [ \sigma_2 ]_t, \delta'), (\sigma_1 [ \sigma_2 ]_s))</math> </pre>	$\frac{}{\Gamma \vdash () :> () \Rightarrow (); 1_\Gamma \vdash \Gamma} \text{P-EMPTY}$ $\frac{\Gamma \vdash t :> x_0 \Rightarrow t'; \sigma_1 \vdash \Delta_1 \quad \Delta_1 \vdash \delta[\sigma_1] :> x \Rightarrow \delta'; \sigma_2 \vdash \Delta_2}{\Gamma \vdash t, \delta :> x_0, x \Rightarrow t'[\sigma_2], \delta'; \sigma_1[\sigma_2] \vdash \Delta_2} \text{P-SPLIT}$
<p><b>unify-flex-*</b> is defined as in Figure 4, replacing <b>commonPositions</b> with <b>equaliser</b>, but note that it now calls the above <b>prune</b> function instead of the one for <math>\lambda</math>-calculus.</p>	
<pre> 530 531 532 533 <b>unify</b> <math>t (M(x)) = \text{unify-flex-}^* M x t</math> 534 <b>unify</b> ( <math>M(x)</math> ) <math>t = \text{unify-flex-}^* M x t</math> </pre>	<p>See the rules SAME-MVAR, CYCLE, and NO-CYCLE in Figure 4.</p>
<pre> 535 536 537 <b>unify</b> (Rigid <math>\cdot o \delta</math>) (Rigid <math>\cdot o' \delta'</math>) <b>with</b> <math>o \stackrel{?}{=} o'</math> 538 ...   <b>no</b> <math>\_ = \perp \triangleleft !_s</math> 539 ...   <b>yes</b> <math>\equiv \text{refl} = \text{unify-}\sigma \delta \delta'</math> </pre>	$\frac{o \neq o'}{\Gamma \vdash o(\delta) = o'(\delta') \Rightarrow !_s \vdash \perp} \text{CLASH}$ $\frac{\Gamma \vdash \delta = \delta' \Rightarrow \sigma \vdash \Delta}{\Gamma \vdash o(\delta) = o(\delta') \Rightarrow \sigma \vdash \Delta} \text{U-RIG}$
<pre> 540 541 542 <b>unify</b> ! <math>! = \perp \triangleleft !_s</math> </pre>	<p>Same as the rule U-FAIL in Figure 4.</p>
<pre> 543 544 545 <b>unify-}\sigma</b> { <math>\Gamma</math> } [ ] [ ] = <math>\Gamma \triangleleft 1_s</math> 546 <b>unify-}\sigma</b> ( <math>t_1, \delta_1</math> ) ( <math>t_2, \delta_2</math> ) = 547   <b>let</b> <math>\Delta \triangleleft \sigma = \text{unify } t_1 t_2</math> 548   <math>\Delta' \triangleleft \sigma' = \text{unify-}\sigma (\delta_1 [ \sigma ]_s) (\delta_2 [ \sigma ]_s)</math> 549   <b>in</b> <math>\Delta' \triangleleft \sigma [ \sigma' ]_s</math> </pre>	$\frac{}{\Gamma \vdash () = () \Rightarrow 1_\Gamma \vdash \Gamma} \text{U-EMPTY}$ $\frac{\Gamma \vdash t_1 = t_2 \Rightarrow \sigma \vdash \Delta \quad \Delta \vdash \delta_1[\sigma] = \delta_2[\sigma] \Rightarrow \sigma' \vdash \Delta'}{\Gamma \vdash t_1, \delta_1 = t_2, \delta_2 \Rightarrow \sigma[\sigma'] \vdash \Delta'} \text{U-SPLIT}$
<pre> 550 <b>unify-}\sigma</b> <math>1 \perp 1 \perp = \perp \triangleleft !_s</math> </pre>	$\frac{}{\perp \vdash 1 \perp = 1 \perp \Rightarrow !_s \vdash \perp} \text{U-ID-FAIL}$

Fig. 6: Generalised binding signatures in Agda

```

553
554 record Signature i j k : Set (lsuc (i ⊔ j ⊔ k)) where
555   field
556     A : Set i
557     hom : A → A → Set j
558     id : ∀ {a} → hom a a
559     _◦_ : ∀ {a b c} → hom b c → hom a b → hom a c
560     O : A → Set k
561     α : ∀ {a} → O a → List A
562
563   - Functoriality components
564     _{ } : ∀ {a b} → O a → hom a b → O b
565     _^_ : ∀ {a b} (x : hom a b) (o : O a) → α o ⇒ α (o { x } )
566
567

```

$x_1, \dots, x_m$  and  $y_1, \dots, y_{m'}$ , i.e., the pair of maximal lists  $(\vec{x'}, \vec{y'})$  of distinct positions such that  $x_{\vec{x'}} = y_{\vec{y'}}$ . We denote<sup>5</sup> such a situation by  $m \vdash x \text{ :> } y \Rightarrow y'; x' \dashv p$ . The most general unifier  $\sigma$  coincides with the identity substitution except that the metavariables  $M$  and  $M'$  are removed from the context and replaced by a single metavariable declaration  $P : p$ . Then,  $\sigma$  maps  $M$  to  $P(x')$  and  $M'$  to  $P(y')$ .

**Example 3.** Let  $x, y, z$  be three distinct variables. The most general unifier of  $M(x, y)$  and  $N(z, x)$  is  $M \mapsto N'(1), N \mapsto N'(2)$ . The most general unifier of  $M(x, y)$  and  $N(z)$  is  $M \mapsto N', N \mapsto N'$ .

As for the rule SAME-VAR, the corresponding rule P-FLEX does not stipulate how to generate the fresh metavariable symbol  $P$ , although the implementation makes an obvious choice, reusing the name  $M$ .

The intuition for the application case is that if we want to unify  $M(x)$  with  $t u$ , we can refine  $M(x)$  to be  $M_1(x) M_2(x)$ , where  $M_1$  and  $M_2$  are two fresh metavariables to be unified with  $t$  and  $u$ . Assume that those two unification problems yield  $t'$  and  $u'$  as replacements for  $t$  and  $u$ , as well as substitution  $\sigma_1$  and  $\sigma_2$ , then  $M$  should be replaced accordingly with  $t'[\sigma_2] u'$ . Note that this really involves improper application, taking into account the following three subcases at once.

$$\frac{\Gamma \vdash t \text{ :> } x \Rightarrow t'; \sigma_1 \dashv \Delta_1 \quad \Delta_1 \vdash u[\sigma_1] \text{ :> } x \Rightarrow u'; \sigma_2 \dashv \Delta_2}{\Gamma \vdash t u \text{ :> } x \Rightarrow t'[\sigma_2] u'; \sigma_1[\sigma_2] \dashv \Delta_2}$$

$$\frac{\Gamma \vdash t \text{ :> } x \Rightarrow t'; \sigma_1 \dashv \Delta_1 \quad \Delta_1 \vdash u[\sigma_1] \text{ :> } x \Rightarrow !; !_s \dashv \perp}{\Gamma \vdash t u \text{ :> } x \Rightarrow !; !_s \dashv \perp} \quad \frac{\Gamma \vdash t \text{ :> } x \Rightarrow !; !_s \dashv \perp \quad \perp \vdash ! \text{ :> } x \Rightarrow !; !_s \dashv \perp}{\Gamma \vdash t u \text{ :> } x \Rightarrow !; !_s \dashv \perp}$$

<sup>5</sup> The similarity with the notation for the pruning phase is no coincidence: both can be interpreted as pullbacks (or pushouts), as we will see in Remark 49.

Fig. 7: Syntax generated by a GB-signature

```

MetaContext $\cdot$  = List A
MetaContext = Maybe MetaContext $\cdot$ 

data Tm : MetaContext  $\rightarrow$  A
       $\rightarrow$  Set (i  $\sqcup$  j  $\sqcup$  k)
Tm $\cdot$   $\Gamma$  a = Tm [  $\Gamma$  ] a

data Tm where
  Rigid $\cdot$  :  $\forall \{\Gamma a\} (o : \text{O } a) \rightarrow (\alpha o \cdot \rightarrow \Gamma)$ 
            $\rightarrow$  Tm $\cdot$   $\Gamma$  a
  _( $\_$ ) :  $\forall \{\Gamma a m\} \rightarrow m \in \Gamma \rightarrow \text{hom } m a$ 
         $\rightarrow$  Tm $\cdot$   $\Gamma$  a
  ! :  $\forall \{a\} \rightarrow \text{Tm } \perp a$ 

```

The same intuition applies for  $\lambda$ -abstraction, but here we apply the fresh metavariable corresponding to the body of the  $\lambda$ -abstraction to the bound variable  $n + 1$ , which needs not be pruned. In the variable case,  $i\{x\}^{-1}$  returns the index  $j$  such that  $i = x_j$ , or fails if no such  $j$  exist.

This ends our description of the unification algorithm, in the specific case of pure  $\lambda$ -calculus.

## 2.2 Generalisation

In this section, we show how to abstract over  $\lambda$ -calculus to get a generic algorithm for pattern unification, parameterised by our new notion of specification to account for syntax with metavariables. We split this notion in two parts:

1. a notion of generalised binding signature, or GB-signature (formally introduced in Definition 23), specifying a syntax with metavariables, for which unification problems can be stated;
2. some additional structures used in the algorithm to solve those unification problems, as well as properties ensuring its correctness, making the GB-signature *pattern-friendly* (see Definition 25).

This separation is motivated by the fact that in the case of  $\lambda$ -calculus, the vectors of common (value) positions are involved in the algorithm, but not in the definition of the syntax and associated operations (renaming, metavariable substitution).

A GB-signature consists in a tuple  $(\mathcal{A}, O, \alpha)$  consisting of

- a small category  $\mathcal{A}$  whose objects are called *arities* or *scopes*, and whose morphisms are called *patterns* or *renamings*;
- for each variable context  $a$ , a set of operation symbols  $O(a)$ ;
- for each operation symbol  $o \in O(a)$ , a list of scopes  $\alpha_o = (\bar{o}_1, \dots, \bar{o}_n)$ .

such that  $O$  and  $\alpha$  are functorial in a suitable sense (see Remark 8 below).

Fig. 8: Implementation of the signature of pure  $\lambda$ -calculus

```

645
646 data O n : Set where
647   Var : Fin n → O n
648   App : O n
649   Lam : O n
650
651  $\alpha : \{n : \mathbb{N}\} \rightarrow O n \rightarrow \text{List } \mathbb{N}$ 
652  $\alpha (\text{Var } x) = []$ 
653  $\alpha \{n\} \text{ App} = n :: n :: []$ 
654  $\alpha \{n\} \text{ Lam} = 1 + n :: []$ 
655
656  $\_ \{ \_ \} : \forall \{a b : \mathbb{N}\} \rightarrow O a \rightarrow \text{hom } a b \rightarrow O b$ 
657  $\text{Var } x \{ s \} = \text{Var } (\text{Vec.lookup } s x)$ 
658  $\text{App } \{ s \} = \text{App}$ 
659  $\text{Lam } \{ s \} = \text{Lam}$ 
660
661 - Pointwise hom  $[a_1, \dots, a_n] [b_1, \dots, b_n]$  is the type of the
662 - lists of the shape  $[c_1, \dots, c_n]$  with  $c_i : \text{hom } a_i b_i$ 
663  $\_ \wedge \_ : \{a b : \mathbb{N}\} (x : \text{hom } a b) (o : O a) \rightarrow \text{Pointwise hom } (\alpha o) (\alpha (o \{ x \}))$ 
664  $x \wedge \text{Var } y = []$ 
665  $x \wedge \text{App} = x :: x :: []$ 
666  $x \wedge \text{Lam} = (x \uparrow) :: []$ 

```

**Remark 4.** This definition of GB-signatures superficially differs from the notion of specification that we mention in the introduction, in the sense that here the endofunctor is implicit. Moreover, the set of operation symbols  $O(a)$  in a scope  $a$  is not indexed by natural numbers. The two descriptions are equivalent:  $O_n(a)$  is recovered as the subset of  $n$ -ary operation symbols in  $O(a)$ , and conversely,  $O(a)$  is recovered as the union of all the  $O_n(a)$  for every natural number  $n$ .

**Example 5.** We give the signature for pure  $\lambda$ -calculus. As explained in the introduction, we take  $\mathcal{A} = \mathbb{F}_m$ . In the scope  $n$  we have  $n$  nullary available operation symbols (one for each variable), one unary operation  $\text{abs}^n$ , and one binary operation  $\text{app}^n$ , so that  $O(n) = \{1, \dots, n, \text{abs}^n, \text{app}^n\}$ , with associated arities  $\alpha_i = ()$ ,  $\alpha_{\text{abs}^n} = (n + 1)$  and  $\alpha_{\text{app}^n} = (n, n)$ . The corresponding Agda implementation can be found in Figure 8.

The Agda implementation in Figure 6 does not include properties such as associativity of morphism composition, although they are assumed in the proof of correctness. For example, the latter associativity property ensures that composition of metavariable substitutions is associative.

The syntax specified by a GB-signature  $(\mathcal{A}, O, \alpha)$  is inductively defined in Figure 7, where a context  $\Gamma; a$  is defined as in Section §2.1 for  $\lambda$ -calculus, except that scopes and metavariable types are objects of  $\mathcal{A}$  instead of natural numbers.

We call a term *rigid* if it is of the shape  $o(\dots)$ , *flexible* if it is some metavariable application  $M(\dots)$ .

**Remark 6.** Recall that the Agda code uses a nameless convention for metacontexts: they are just lists of scopes. Therefore, the arity  $\alpha_o$  of an operation  $o$  can be considered as a metacontext. It follows that the argument of an operation  $o$  in the context  $\Gamma; a$  can be specified either as a metavariable substitution (defined in Figure 2) from  $\alpha_o = (\bar{o}_1, \dots, \bar{o}_n)$  to  $\Gamma$ , as in the Agda code, or explicitly as a list of terms  $(t_1, \dots, t_n)$  such that  $\Gamma; \bar{o}_i \vdash t_i$ , as in the rule  $\text{RIG}$ . In the following, we will use either interpretation.

**Remark 7.** The syntax in the empty metacontext does not depend on the morphisms in  $\mathcal{A}$ . In fact, by restricting the morphisms in  $\mathcal{A}$  to identity morphisms, any GB-signature induces an indexed container (Altenkirch and Morris, 2009) generating the same syntax without metavariables.

**Remark 8.** In the notion of GB-signature, functoriality ensures that the generated syntax supports renaming: given a morphism  $x : a \rightarrow b$  in  $\mathcal{A}$  and a term  $\Gamma; a \vdash t$ , we can recursively define a term  $\Gamma; b \vdash t\{x\}$ . The metavariable base case is the same as in Section §2.1:  $M(y)\{x\} = M(x \circ y)$ . For an operation  $o(t_1, \dots, t_n)$ , functoriality provides the following components:

1. a  $n$ -ary operation symbol  $o\{x\} \in O(b)$ ;
2. a list of morphisms  $(x_1^o, \dots, x_n^o)$  in  $\mathcal{A}$  such that  $x_i^o : \bar{o}_i \rightarrow \overline{o\{x\}}_i$  for each  $i \in \{1, \dots, n\}$ .

Then,  $o(t_1, \dots, t_n)\{x\}$  is defined as  $o\{x\}(t_1\{x_1^o\}, \dots, t_n\{x_n^o\})$ .

**Notation 9.** If  $\Gamma$  and  $\Delta$  are two metacontexts  $M_1 : m_1, \dots, M_p : m_p$  and  $N_1 : n_1, \dots, N_p : n_p$  of the same length, we write  $\delta : \Gamma \Longrightarrow \Delta$  to mean that  $\delta$  is a vector of renamings  $(\delta_1, \dots, \delta_n)$  between  $\Gamma$  and  $\Delta$ , in the sense that each  $\delta_i$  is a morphism between  $m_i$  and  $n_i$ . The second functoriality component in Remark 8 is accordingly specified as a vector of renamings  $x^o : \alpha_o \Longrightarrow \alpha_{o\{f\}}$  in Figure 7, considering operation arities as nameless metacontexts (Remark 6). We extend the renaming notation to substitutions: given  $\delta : \Gamma \rightarrow \Delta$  and  $x : \Delta' \Longrightarrow \Delta$ , we define  $\delta\{x\} : \Gamma \rightarrow \Delta'$  as  $(\delta_1\{x_1\}, \dots, \delta_n\{x_n\})$  where  $n$  is the length of  $\Delta$ , so that  $o(\delta)\{x\}$  can be equivalently defined as  $o\{x\}(\delta\{x^o\})$ . Note that a vector of renamings  $\delta : \Gamma \Longrightarrow \Delta$  canonically induces a metavariable substitution  $\bar{\delta} : \Delta \rightarrow \Gamma$ , mapping  $N_i$  to  $M_i(\delta_i)$ .

The Agda code adapting the definitions of Section §2.1 to a syntax generated by a generic signature is usually shorter because the application,  $\lambda$ -abstraction, and variable cases are replaced with a single rigid case. Because of Remark 6, it is more convenient to define operations on terms mutually with the corresponding operations on substitutions. For example, composition of substitutions is defined mutually with substitution of terms in the second box of Figure 2. The same applies for renaming of terms and substitution as in Notation 9.

We are similarly led to generalise unification of terms to unification of proper substitutions, and we extend accordingly the notation. Given two substitutions  $\delta_1, \delta_2 : \Gamma' \rightarrow \Gamma$ , we write  $\Gamma \vdash \delta_1 = \delta_2 \Rightarrow \sigma \vdash \Delta$  to mean that  $\sigma : \Gamma \rightarrow \Delta$  unifies  $\delta_1$  and  $\delta_2$ , in the sense that



$\delta_1[\sigma] = \delta_2[\sigma]$ , and is the most general one, i.e., it uniquely factors any other unifier of  $\delta_1$  and  $\delta_2$ . The main unification function is thus split in two functions, **unify** for single terms, and **unify- $\sigma$**  for substitutions. Similarly, we define pruning of terms mutually with pruning of proper substitutions. We thus also extend the pruning notation: given a substitution  $\delta : \Gamma' \rightarrow \Gamma$  and a vector  $x : \Gamma'' \Rightarrow \Gamma'$  of renamings, the judgement  $\Gamma \vdash \delta :> x \Rightarrow \delta'; \sigma \vdash \Delta$  means that the substitution  $\sigma : \Gamma \rightarrow \Delta$  extended with  $\delta' : \Gamma'' \rightarrow \Delta$  is the most general unifier of  $\delta$  and  $\bar{x}$  as substitutions from  $\Gamma, \Gamma'$  to  $\Delta$ . The outputs of **unify** and **unify- $\sigma$**  are gathered as fields of record types (see Figure 3).

In the  $\lambda$ -calculus implementation (Figure 4), unification of two metavariable applications requires computing the vector of common positions or value positions of their arguments, depending on whether the involved metavariables are identical. Both vectors are characterised as equalisers or pullbacks in the category of natural numbers and injective renamings between them, thus providing a canonical replacement in the generic algorithm, along with new interpretations of the notations  $m \vdash x = y \Rightarrow z \vdash p$  and  $m \vdash x :> y \Rightarrow y'; x' \vdash p$  as equalisers and pullbacks.

**Notation 10.** We denote an equaliser  $p \xrightarrow{z} m \xrightleftharpoons[y]{x} \dots$  in  $\mathcal{A}$  by  $m \vdash x = y \Rightarrow z \vdash p$ .

Similarly,  $m \vdash x :> y \Rightarrow y'; x' \vdash p$  denotes a pullback in  $\mathcal{A}$  of the shape

$$\begin{array}{ccc} p & \xrightarrow{x'} & m \\ y' \downarrow & & \downarrow x \\ \dots & \xrightarrow{y} & \dots \end{array}.$$

Let us now comment on pruning rigid terms, when we want to unify an operation  $o(\delta)$  with a fresh metavariable application  $M(x)$ . Any unifier must replace  $M$  with an operation  $o'(\delta')$ , such that  $o'\{x\}(\delta'\{x^{o'}\}) = o(\delta)$ , so that, in particular,  $o'\{x\} = o$ . In other words,  $o$  must have a preimage  $o'$  for renaming by  $x$ . This is precisely the point of the inverse renaming  $o\{x\}^{-1}$  in the Agda code: it returns a preimage  $o'$  if it exists, or fails. In the  $\lambda$ -calculus case, this check is only explicit for variables, since there is a single version of application and  $\lambda$ -abstraction symbols in any variable context. Uniqueness of the preimage is guaranteed for *pattern-friendly* GB-signatures, which are GB-signatures with additional components listed in Figure 9 on which the algorithm relies. To sum up,

- equalisers and pullbacks are used when unifying two metavariable applications;
- equality of operation symbols is used when unifying two rigid terms;
- inverse renaming is used when pruning a rigid term.

The formal notion of pattern-friendly signatures (Definition 25) includes additional properties ensuring correctness of the algorithm.

Fig. 9: Friendly GB-signatures in Agda

```

record isFriendly {i j k} (S : Signature i j k) : Set (i ⊔ j ⊔ k) where
  open Signature S
  field
    equaliser : ∀ {a} m → (x y : hom m a) → Σ A (λ p → hom p m)
    pullback   : ∀ m {m' a} → (x : hom m a) → (y : hom m' a)
                  → Σ A (λ p → hom p m × hom p m')
    _≡_        : ∀ {a} (o o' : O a) → Dec (o ≡ o')
    _{ }-1      : ∀ {a} (o : O a) → ∀ {b} (x : hom b a)
                  → Maybe (pre-image _{ x } ) o

```

### 3 Categorical semantics

To prove that the algorithm is correct, we show in the next sections that the inductive rules describing the implementation are sound. For instance, the rule U-SPLIT is sound on the condition that the output of the conclusion is a most general unifier whenever the output of the premises are most general unifiers. We rely on the categorical semantics of pattern unification that we introduce in this section. In Section §3.1, we relate pattern unification to a coequaliser construction, and in Section §3.2, we provide a formal definition of GB-signatures with Initial Algebra Semantics for the generated syntax.

#### 3.1 Pattern unification as a coequaliser construction

In this section, we assume given a GB-signature  $S$  and explain how most general unifiers can be thought of as equalisers in a multi-sorted Lawvere theory, as is well-known in the first-order case (Rydeheard and Burstall, 1988; Barr and Wells, 1990). We furthermore provide a formal justification for the error metacontext  $\perp$ .

**Lemma 11.** *Proper metacontexts and substitutions (with their composition) between them define a category  $\mathbf{MCon}(S)$ .*

This relies on functoriality of GB-signatures that we will spell out formally in the next section. There, we will see in Proposition 32 that this category fully faithfully embeds in a Kleisli category for a monad generated by  $S$  on  $[\mathcal{A}, \mathbf{Set}]$ .

**Remark 12.** *The opposite category of  $\mathbf{MCon}(S)$  is equivalent to a multi-sorted Lawvere theory whose sorts are the objects of  $\mathcal{A}$ . In general, this theory is not freely generated by operations unless  $\mathcal{A}$  is discrete, in which case we recover (multi-sorted) first-order unification.*

**Lemma 13.** *The most general unifier of two parallel substitutions  $\Gamma' \xrightarrow[\delta_2]{\delta_1} \Gamma$  is characterised as their coequaliser.*

This motivates a new interpretation of the unification notation, that we introduce later in Notation 20, after explaining how failure is categorically handled. Indeed, pattern unification is typically stated as the existence of a coequaliser on the condition that there is a unifier in this category  $\mathbf{MCon}(S)$ . But we can get rid of this condition by considering the category  $\mathbf{MCon}(S)$  freely extended with a terminal object  $\perp$ , resulting in the full category of metacontexts and substitutions.

**Definition 14.** *Given a category  $\mathcal{B}$ , let  $\mathcal{B}_\perp$  denote the category  $\mathcal{B}$  extended freely with a terminal object  $\perp$ .*

**Notation 15.** *We denote by  $!_s$  any terminal morphism to  $\perp$  in  $\mathcal{B}_\perp$ .*

**Lemma 16.** *Metacontexts and substitutions between them define a category which is isomorphic to  $\mathbf{MCon}(S)_\perp$ .*

In Section §2.1, we already made sense of this extension. Let us rephrase our explanations from a categorical perspective. Adding a terminal object results in adding a terminal cocone to all diagrams. As a consequence, we have the following lemma.

**Lemma 17.** *Let  $J$  be a diagram in a category  $\mathcal{B}$ . The following are equivalent:*

1.  *$J$  has a colimit as long as there exists a cocone;*
2.  *$J$  has a colimit in  $\mathcal{B}_\perp$ .*

The following results are also useful.

**Lemma 18.** *Let  $\mathcal{B}$  be a category.*

- (i) *The canonical embedding functor  $\mathcal{B} \rightarrow \mathcal{B}_\perp$  creates colimits.*
- (ii) *Any diagram  $J$  in  $\mathcal{B}_\perp$  such that  $\perp$  is in its image has a colimit given by the terminal cocone on  $\perp$ .*

This ensures in particular that coproducts in  $\mathbf{MCon}(S)$ , which are computed as union of metacontexts, are also coproducts in  $\mathbf{MCon}(S)_\perp$ . It also justifies defining the union of a proper metacontext with  $\perp$  as  $\perp$ .

The main property of this extension for our purposes is the following corollary.

**Corollary 19.** *Any coequaliser in  $\mathbf{MCon}(S)$  is also a coequaliser in  $\mathbf{MCon}(S)_\perp$ . Moreover, whenever there is no unifier of two lists of terms, then the coequaliser of the corresponding parallel arrows in  $\mathbf{MCon}(S)_\perp$  exists: it is the terminal cocone on  $\perp$ .*

This justifies the following interpretation to the unification notation.

**Notation 20.**  $\Gamma \vdash \delta_1 = \delta_2 \Rightarrow \sigma \vdash \Delta$  denotes a coequaliser  $\dots \xrightarrow[\delta_2]{\delta_1} \Gamma \xrightarrow{\sigma} \Delta$  in  $\mathbf{MCon}(S)_\perp$ .

**Remark 21.** This is the same interpretation as in Notation 10 for equaliser, taking  $\mathcal{A}$  to be the opposite category of  $\text{MCon}(S)_\perp$ .

Categorically speaking, our pattern-unification algorithm provides an explicit proof of the following statement, where the conditions for a signature to be *pattern-friendly* are introduced in the next section (Definition 25).

**Theorem 22.** Given any pattern-friendly signature  $S$ , the category  $\text{MCon}(S)_\perp$  has coequalisers.

### 3.2 Initial Algebra Semantics for GB-signatures

The proofs of various statements presented in this section are detailed in the appendices found in the supplemental material.

**Definition 23.** A generalised binding signature, or GB-signature, is a tuple  $(\mathcal{A}, O, \alpha)$  consisting of

- a small category  $\mathcal{A}$  of arities and renamings between them;
- a functor  $O_-(-) : \mathbb{N} \times \mathcal{A} \rightarrow \text{Set}$  of operation symbols;
- a family of functors  $(\alpha_{n,i} : \int O_n \rightarrow \mathcal{A})_{n,i \leq n}$  indexed by natural numbers  $i, n$  such that  $i \leq n$ ,

where  $\int O_n$  denotes the category of elements of  $O_n : \mathcal{A} \rightarrow \text{Set}$ , defined as follows:

- objects are pairs  $(a, o)$  such that  $o \in O_n(a)$
- a morphism between  $(a, o)$  and  $(a', o')$  is a morphism  $f : a \rightarrow a'$  such that  $o\{f\} = o'$  where  $o\{f\}$  denotes the image of  $o$  by the function  $O_n(f) : O_n(a) \rightarrow O_n(a')$ .

**Notation 24.** Given a GB-signature  $(\mathcal{A}, O, \alpha)$  and  $o \in O_n(a)$ , we write  $\bar{o}_j$  for  $\alpha_{n,j}(o)$  and  $\alpha_o$  for the tuple  $(\bar{o}_1, \dots, \bar{o}_n)$ .

We now introduce our conditions for the generic unification algorithm to be correct.

**Definition 25.** A GB-signature  $S = (\mathcal{A}, O, \alpha)$  is said to be pattern-friendly if

1.  $\mathcal{A}$  has finite connected limits (or equivalently,  $\mathcal{A}$  has pullbacks and equalisers);
2. all morphisms in  $\mathcal{A}$  are monomorphic;
3. each  $O_n(-) : \mathcal{A} \rightarrow \text{Set}$  preserves finite connected limits;
4. each  $\alpha_{n,i}$  preserves finite connected limits.

**Remark 26.** As a counter-example, take  $\mathcal{A}$  to be the category  $a \xrightarrow{f} b$  consisting of two objects and one non-identity morphism between them, and consider the syntax generated by two nullary operations in environment  $a$  and one nullary operation  $*$  in scope  $b$ . Then,  $M(f) \stackrel{?}{=} *$  has two unifiers but no most general unifier.

These conditions ensure the following two properties.

**Property 27** (proved in §3.3.1). *The following properties hold for pattern-friendly signatures.*

- (i) *The action of  $O_n : \mathcal{A} \rightarrow \text{Set}$  on any renaming is an injection: given any  $o \in O_n(b)$  and renaming  $f : a \rightarrow b$ , there is at most one  $o' \in O_n(a)$  such that  $o = o' \{f\}$ .*
- (ii) *Let  $\mathcal{L}$  be the functor  $\mathcal{A}^{OP} \rightarrow \text{MCon}(S)_\perp$  mapping a morphism  $x \in \text{hom}_{\mathcal{A}}(b, a)$  to the substitution  $(X : a) \rightarrow (X : b)$  selecting (by the Yoneda Lemma) the term  $X(x)$ . Then,  $\mathcal{L}$  preserves finite connected colimits: it maps pullbacks and equalisers in  $\mathcal{A}$  to pushouts and coequalisers in  $\text{MCon}(S)_\perp$ .*

The first property is used for soundness of the rules P-RIG and P-RIG-FAIL. The second one is used to justify unification of two metavariable applications as pullbacks and equalisers in  $\mathcal{A}$ , in the rules SAME-MVAR and P-FLEX.

**Remark 28.** *A metavariable application  $\Gamma; a \vdash M(x)$  corresponds to the composition  $\mathcal{L}x[in_M]$  as a substitution from  $X : a$  to  $\Gamma$ , where  $in_M$  is the coproduct injection  $(X : m) \cong (M : m) \hookrightarrow \Gamma$  mapping  $M$  to  $M(1_m)$ .*

In the rest of this section, we provide Initial Algebra Semantics for the generated syntax (this is used in the proof of Property 27.(ii)).

Any GB-signature  $S = (\mathcal{A}, O, \alpha)$ , generates an endofunctor  $F_S$  on  $[\mathcal{A}, \text{Set}]$ , that we denote by just  $F$  when the context is clear, defined by

$$F_S(X)_a = \coprod_{n \in \mathbb{N}} \coprod_{o \in O_n(a)} X_{\bar{o}_1} \times \cdots \times X_{\bar{o}_n}.$$

**Lemma 29** (proved in §3.3.2).  *$F$  is finitary and generates a free monad  $T$ . Moreover,  $TX$  is the initial algebra of  $Z \mapsto X + FZ$ .*

**Lemma 30.** *The proper syntax generated by a GB-signature (see Figure 7) is recovered as free algebras for  $F$ . More precisely, given a metacontext  $\Gamma = (M_1 : m_1, \dots, M_p : m_p)$ ,*

$$T(\underline{\Gamma})_a \cong \{t \mid \Gamma; a \vdash t\}$$

*where  $\underline{\Gamma} : \mathcal{A} \rightarrow \text{Set}$  is defined as the coproduct of representable functors  $\coprod_i ym_i$ , mapping  $a$  to  $\coprod_i \text{hom}_{\mathcal{A}}(m_i, a)$ . Moreover, the action of  $T(\underline{\Gamma})$  on morphisms of  $\mathcal{A}$  correspond to renaming.*

**Notation 31.** *Given a proper metacontext  $\Gamma$ . We sometimes denote  $\underline{\Gamma}$  just by  $\Gamma$ .*

If  $\Gamma = (M_1 : m_1, \dots, M_p : m_p)$  and  $\Delta$  are metacontexts, a Kleisli morphism  $\sigma : \Gamma \rightarrow T\Delta$  is equivalently given (by combining the above lemma, the Yoneda Lemma, and the universal property of coproducts) by a metavariable substitution from  $\Gamma$  to  $\Delta$ . Moreover, Kleisli composition corresponds to composition of substitutions. This provides a formal link between the category of metacontexts  $\text{MCon}(S)$  and the Kleisli category of  $T$ .

**Proposition 32.** *The category  $\mathbf{MCon}(S)$  is equivalent to the full subcategory of  $\mathbf{Kl}_T$  spanned by coproducts of representable functors.*

**Remark 33.** *It follows from Proposition 32 and (Exercise VI.5.1 Mac Lane, 1998) that  $\mathbf{MCon}(S)$  fully faithfully embeds in the category of algebras of  $T$ , by mapping a metacontext  $\Gamma$  to the free algebra  $T\Gamma$ . In fact,  $\mathbf{MCon}(S)_\perp$  also fully faithfully embeds in the category of algebras by mapping  $\perp$  to the terminal algebra, whose underlying functor maps any object of  $\mathcal{A}$  to a singleton set.*

We exploit this characterisation to prove various properties of this category when the signature is *pattern-friendly*.

**Notation 34.** *Given a GB-signature  $S = (\mathcal{A}, O, \alpha)$ , we denote the full subcategory of  $[\mathcal{A}, \mathbf{Set}]$  consisting of functors preserving finite connected limits by  $\mathcal{C}_S$ , or sometimes by  $\mathcal{C}$ , leaving  $S$  implicit.*

**Lemma 35** (proved in §3.3.3). *Given a GB-signature  $S = (\mathcal{A}, O, \alpha)$  such that  $\mathcal{A}$  has finite connected limits,  $F_S$  restricts as an endofunctor on  $\mathcal{C}_S$  if and only if the last two conditions of Definition 25 hold.*

We now assume given a pattern-friendly signature  $S = (\mathcal{A}, O, \alpha)$ .

**Lemma 36** (proved in §3.3.4).  *$\mathcal{C}$  is closed under limits, coproducts, and filtered colimits. Moreover, it is cocomplete.*

**Corollary 37** (proved in §3.3.5).  *$T$  restricts as a monad on  $\mathcal{C}$  freely generated by the restriction of  $F$  as an endofunctor on  $\mathcal{C}$  (Lemma 35).*

### 3.3 Proofs of statements in Section 3.2

#### 3.3.1 Property 27

We use the notations and definitions of Section §3.2.

Let us first prove the first item.

#### Proof of Property 27.(i)

We show that given any  $o \in O_n(b)$  and renaming  $f : a \rightarrow b$ , there is at most one  $o' \in O_n(a)$  such that  $o = o' \{f\}$ .

Since  $O_n$  preserves finite connected limits, it preserves monomorphisms because a morphism  $f : a \rightarrow b$  is monomorphic if and only if the following square is a pullback (see (Mac Lane, 1998, Exercise III.4.4)).

$$\begin{array}{ccc} A & \xlongequal{\quad} & A \\ \parallel & & \downarrow f \\ A & \xrightarrow{f} & B \end{array}$$

■

The rest of this section is devoted to the proof of Property 27.(ii).

By right continuity of the homset bifunctor, any representable functor is in  $\mathcal{C}$  and thus the embedding  $\mathcal{C} \rightarrow [\mathcal{A}, \text{Set}]$  factors the Yoneda embedding  $\mathcal{A}^{op} \rightarrow [\mathcal{A}, \text{Set}]$ .

**Lemma 38.** *Let  $\mathcal{D}$  denote the opposite category of  $\mathcal{A}$  and  $K : \mathcal{D} \rightarrow \mathcal{C}$  the factorisation of  $\mathcal{C} \rightarrow [\mathcal{A}, \text{Set}]$  by the Yoneda embedding. Then,  $K : \mathcal{D} \rightarrow \mathcal{C}$  preserves finite connected colimits.*

**Proof** This essentially follows from the fact functors in  $\mathcal{C}$  preserves finite connected limits. Let us detail the argument: let  $y : \mathcal{A}^{op} \rightarrow [\mathcal{A}, \text{Set}]$  denote the Yoneda embedding and  $J : \mathcal{C} \rightarrow [\mathcal{A}, \text{Set}]$  denote the canonical embedding, so that

$$y = J \circ K. \quad (3.1)$$

Now consider a finite connected limit  $\lim F$  in  $\mathcal{A}$ . Then,

$$\begin{aligned} \mathcal{C}(K \lim F, X) &\cong [\mathcal{A}, \text{Set}](JK \lim F, JX) && (J \text{ is fully faithful}) \\ &\cong [\mathcal{A}, \text{Set}](y \lim F, JX) && (\text{By Equation (3.1)}) \\ &\cong JX(\lim F) && (\text{By the Yoneda Lemma.}) \\ &\cong \lim(JX \circ F) && (X \text{ preserves finite connected limits}) \\ &\cong \lim([\mathcal{A}, \text{Set}](yF-, JX)) && (\text{By the Yoneda Lemma}) \\ &\cong \lim([\mathcal{A}, \text{Set}](JKF-, JX)) && (\text{By Equation (3.1)}) \\ &\cong \lim \mathcal{C}(KF-, X) && (J \text{ is full and faithful}) \\ &\cong \mathcal{C}(\text{colim } KF, X) && (\text{By left continuity of the hom-set bifunctor}) \end{aligned}$$

These isomorphisms are natural in  $X$  and thus  $K \lim F \cong \text{colim } KF$ . ■

**Proof of Property 27.(ii)** Note that  $\mathcal{L}$  factors as

$$\mathcal{D} \xrightarrow{\mathcal{L}^\bullet} \text{MCon}(S) \hookrightarrow \text{MCon}(S)_\perp,$$

where the right embedding preserves colimits by Lemma 18.(i), so it is enough to show that  $\mathcal{L}^\bullet$  preserves finite connected colimits. Let  $T|_{\mathcal{C}}$  be the monad  $T$  restricted to  $\mathcal{C}$ , following Corollary 37. Since  $K : \mathcal{D} \rightarrow \mathcal{C}$  preserves finite connected colimits (Lemma 38), composing it with the left adjoint  $\mathcal{C} \rightarrow Kl_{T|_{\mathcal{C}}}$  yields a functor  $\mathcal{D} \rightarrow Kl_{T|_{\mathcal{C}}}$  also preserving those colimits. Since it factors as  $\mathcal{D} \xrightarrow{\mathcal{L}^\bullet} \text{MCon}(S) \hookrightarrow Kl_{T|_{\mathcal{C}}}$ , where the right functor is full and faithful,  $\mathcal{L}^\bullet$  also preserves finite connected colimits. ■

### 3.3.2 Lemma 29

$F$  is finitary because filtered colimits commute with finite limits (Mac Lane, 1998, Theorem IX.2.1) and colimits. The free monad construction is due to Reiterman (1977).

### 3.3.3 Lemma 35

**Notation 39.** *Given a functor  $F : I \rightarrow \mathcal{B}$ , we denote the limit (resp. colimit) of  $F$  by  $\int_{i:I} F(i)$  or  $\lim F$  (resp.  $\int^{i:I} F(i)$  or  $\text{colim } F$ ) and the canonical projection  $\lim F \rightarrow Fi$  by  $p_i$  for any object  $i$  of  $I$ .*

This section is dedicated to the proof of the following lemma.

**Lemma 40.** *Given a GB-signature  $S = (\mathcal{A}, O, \alpha)$  such that  $\mathcal{A}$  has finite connected limits,  $F_S$  restricts as an endofunctor on the full subcategory  $\mathcal{C}$  of  $[\mathcal{A}, \text{Set}]$  consisting of functors preserving finite connected limits if and only if each  $O_n \in \mathcal{C}$ , and  $\alpha_{n,i} : \int O_n \rightarrow \mathcal{A}$  preserves finite connected limits.*

We first introduce a bunch of intermediate lemmas.

**Lemma 41.** *Let  $F : \mathcal{B} \rightarrow \text{Set}$  be a functor. For any functor  $G : I \rightarrow \int F$ , denoting by  $H$  the composite functor  $I \xrightarrow{G} \int F \rightarrow \mathcal{B}$ , there exists a unique  $x \in \lim(F \circ H)$  such that  $Gi = (Hi, p_i(x))$ .*

**Proof**  $\int F$  is isomorphic to the opposite of the comma category  $y/F$ , where  $y : \mathcal{B}^{op} \rightarrow [\mathcal{B}, \text{Set}]$  is the Yoneda embedding. The statement follows from the universal property of a comma category. ■

**Lemma 42.** *Let  $F : \mathcal{B} \rightarrow \text{Set}$  and  $G : I \rightarrow \int F$  such that  $F$  preserves the limit of  $H : I \xrightarrow{G} \int F \rightarrow \mathcal{B}$ . Then, there exists a unique  $x \in F \lim H$  such that  $Gi = (Hi, Fp_i(x))$  and moreover,  $(\lim H, x)$  is the limit of  $G$ .*

**Proof** The unique existence of  $x \in F \lim H$  such that  $Gi = (Hi, Fp_i(x))$  follows from Lemma 41 and the fact that  $F$  preserves  $\lim H$ . Let  $\mathcal{C}$  denote the full subcategory of  $[\mathcal{B}, \text{Set}]$  of functors preserving  $\lim G$ . Note that  $\int F$  is isomorphic to the opposite of the comma category  $K/F$ , where  $K : \mathcal{B}^{op} \rightarrow \mathcal{C}$  is the Yoneda embedding, which preserves colim  $G$ , by an argument similar to the proof of Lemma 38. We conclude from the fact that the forgetful functor from a comma category  $L/R$  to the product of the categories creates colimits that  $L$  preserve. ■

**Corollary 43.** *Let  $I$  be a small category,  $\mathcal{B}$  and  $\mathcal{B}'$  be categories with  $I$ -limits (i.e., limits of any diagram over  $I$ ). Let  $F : \mathcal{B} \rightarrow \text{Set}$  be a functor preserving those colimits. Then,  $\int F$  has  $I$ -limits, preserved by the projection  $\int F \rightarrow \mathcal{B}$ . Moreover, a functor  $G : \int F \rightarrow \mathcal{B}'$  preserves them if and only if for any  $d : I \rightarrow \mathcal{B}$  and  $x \in F \lim d$ , the canonical morphism  $G(\lim d, x) \rightarrow \int_{i:I} G(d_i, Fp_i(x))$  is an isomorphism.*

**Proof** By Lemma 42, a diagram  $d' : I \rightarrow \int F$  is equivalently given by  $d : I \rightarrow \mathcal{B}$  and  $x \in F \lim d$ , recovering  $d'$  as  $d'_i = (d_i, Fp_i(x))$ , and moreover  $\lim d' = (\lim d, x)$ . ■

**Corollary 44.** *Assuming that  $\mathcal{A}$  has finite connected limits and each  $O_n$  preserves finite connected limits, the finite limit preservation on  $\alpha : \int J \rightarrow \mathcal{A}$  of Lemma 40 can be reformulated as follows: given a finite connected diagram  $d : D \rightarrow \mathcal{A}$  and element  $o \in O_n(\lim d)$ , the following canonical morphism is an isomorphism*

$$\bar{o}_j \rightarrow \int_{i:D} \overline{o\{p_i\}}_j$$



for any  $j \in \{1, \dots, n\}$ .

**Proof** Note that, by definition,  $\bar{o}_j = \alpha_{n,j}(\lim d, o)$ , and  $\overline{o\{p_i\}}_j = \alpha_{n,j}(d_i, o\{p_i\})$ . This is a direct application of Corollary 43. ■

**Lemma 45** (Limits commute with dependent pairs). *Given functors  $K : I \rightarrow \text{Set}$  and  $G : \int K \rightarrow \text{Set}$ , the following canonical morphism is an isomorphism*

$$\coprod_{\alpha \in \lim K} \int_{i:I} G(i, p_i(\alpha)) \rightarrow \int_{i:I} \coprod_{x \in Ki} G(i, x)$$

**Proof** The domain consists of a family  $(\alpha_i)_{i \in I}$  where  $\alpha_i \in K_i$  together with a family  $(g_i)_{i \in I}$  where  $g_i \in G(i, \alpha_i)$ , such that that for each morphism  $i \xrightarrow{u} j$  in  $I$ , we have  $Ku(\alpha_i) = \alpha_j$  and  $(Gu)(g_i) = g_j$ .

The codomain consists of a family  $(x_i, g_i)_{i \in I}$  where  $x_i \in K_i$  and  $g_i \in G(i, x_i)$ , such that for each morphism  $i \xrightarrow{u} j$  in  $I$ , we have  $Ku(x_i) = x_j$  and  $(Gu)(g_i) = g_j$ .

The canonical morphism maps  $((x_i)_{i \in I}, (g_i)_{i \in I})$  to the family  $(x_i, g_i)_{i \in I}$ . It is clearly a bijection. ■

**Lemma 46.** *A coproduct  $\coprod_i G_i$  of functors from a small category  $\mathcal{B}$  with finite connected limits to  $\text{Set}$  preserves those limits if and only if each  $G_i$  does.*

**Proof** This is a consequence of the following statement, which is a direct application of Adámek et al. (2002, Theorem 2.4 and Example 2.3.(iii)): if  $\mathcal{B}$  is a small category with finite connected limits, then a functor  $G : \mathcal{B} \rightarrow \text{Set}$  preserves those limits if and only if  $\int G$  is a coproduct of filtered categories. ■

**Proof of Lemma 40** Let  $d : I \rightarrow \mathcal{A}$  be a finite connected diagram and  $X$  be a functor preserving finite connected limits. Then,

$$\begin{aligned} \int_{i:I} F(X)_{d_i} &= \int_{i:I} \coprod_n \coprod_{o \in O_n(d_i)} X_{\bar{o}_1} \times \cdots \times X_{\bar{o}_n} \\ &\cong \coprod_n \int_{i:I} \coprod_{o \in O_n(d_i)} X_{\bar{o}_1} \times \cdots \times X_{\bar{o}_n} && \text{(Coproducts commute with connected limits)} \\ &\cong \coprod_n \coprod_{o \in \int_i O_n(d_i)} \int_{i:I} X_{\overline{p_i(o)}_1} \times \cdots \times X_{\overline{p_i(o)}_n} && \text{(By Lemma 45)} \\ &\cong \coprod_n \coprod_{o \in \int_i O_n(d_i)} \int_{i:I} X_{\overline{p_i(o)}_1} \times \cdots \times \int_{i:I} X_{\overline{p_i(o)}_n} && \text{(By commutation of limits)} \end{aligned}$$

Thus, since  $X$  preserves finite connected limits by assumption,

$$\int_i F(X)_{d_i} = \coprod_n \coprod_{o \in \int_i O_n(d_i)} X_{\int_{i:I} \overline{p_i(o)}_1} \times \cdots \times X_{\int_{i:I} \overline{p_i(o)}_n} \quad (3.2)$$

Now, let us prove the only if statement first. Assume that each  $O_n$  and  $\alpha_{n,i} : \int O_n \rightarrow \mathcal{A}$  preserve finite connected limits. Then,

$$\begin{aligned}
 \int_i F(X)_{d_i} &\cong \coprod_n \coprod_{o \in \int_i O_n(d_i)} X_{\int_{i:I} \overline{p_i(o)}_1} \times \cdots \times X_{\int_{i:I} \overline{p_i(o)}_n} && \text{(By Equation (3.2))} \\
 &\cong \coprod_n \coprod_{o \in O_n(\lim d)} X_{\int_{i:I} \overline{o\{p_i\}}_1} \times \cdots \times X_{\int_{i:I} \overline{o\{p_i\}}_n} && \text{(By assumption on } O_n) \\
 &\cong \coprod_n \coprod_{o \in O_n(\lim d)} X_{\overline{o}_1} \times \cdots \times X_{\overline{o}_n} && \text{(By Corollary 44)} \\
 &= F(X)_{\lim d}
 \end{aligned}$$

Conversely, let us assume that  $F$  restricts to an endofunctor on  $\mathcal{C}$ . Then,  $F(1) = \coprod_n O_n$  preserves finite connected limits. By Lemma 46, each  $O_n$  preserves finite connected limits. By Corollary 44, it is enough to prove that given a finite connected diagram  $d : D \rightarrow \mathcal{A}$  and element  $o \in O_n(\lim d)$ , the following canonical morphism is an isomorphism

$$\overline{o}_j \rightarrow \int_{i:D} \overline{o\{p_i\}}_j$$

Now, we have

$$\begin{aligned}
 \int_{i:I} F(X)_{d_i} &\cong F(X)_{\lim d} && \text{(By assumption)} \\
 &= \coprod_n \coprod_{o \in O_n(\lim d)} X_{\overline{o}_1} \times \cdots \times X_{\overline{o}_n}
 \end{aligned}$$

On the other hand,

$$\begin{aligned}
 \int_{i:I} F(X)_{d_i} &\cong \coprod_n \coprod_{o \in \int_i O_n(d_i)} X_{\int_{i:I} \overline{p_i(o)}_1} \times \cdots \times X_{\int_{i:I} \overline{p_i(o)}_n} && \text{(By Equation (3.2))} \\
 &= \coprod_n \coprod_{o \in O_n(\lim d)} X_{\int_{i:I} \overline{o\{p_i\}}_1} \times \cdots \times X_{\int_{i:I} \overline{o\{p_i\}}_n} \\
 &&& (O_n \text{ preserves finite connected limits})
 \end{aligned}$$

It follows from those two chains of isomorphisms that each function  $X_{\overline{o}_j} \rightarrow X_{\int_{i:I} \overline{o\{p_i\}}_j}$  is a bijection, or equivalently (by the Yoneda Lemma), that  $\mathcal{C}(K\overline{o}_j, X) \rightarrow \mathcal{C}(K \int_{i:I} \overline{o\{p_i\}}_j, X)$  is an isomorphism. Since the Yoneda embedding is fully faithful,  $\overline{o}_j \rightarrow \int_{i:D} \overline{o\{p_i\}}_j$  is an isomorphism. ■

### 3.3.4 Lemma 36

Cocompleteness follows from Adámek and Rosický (1994, Remark 1.56), since  $\mathcal{C}$  is the category of models of a limit sketch, and is thus locally presentable, by Adámek and Rosický (1994, Proposition 1.51).

For the claimed closure property, all we have to check is that limits, coproducts, and filtered colimits of functors preserving finite connected limits still preserve finite connected limits. The case of limits is clear, since limits commute with limits. Coproducts and filtered colimits also commute with finite connected limits (Adámek et al., 2002, Example 1.3.(vi)).

## 3.3.5 Corollary 37

The result follows from the construction of  $T$  using colimits of initial chains, thanks to the closure properties of  $\mathcal{C}$ . More specifically,  $TX$  can be constructed as the colimit of the chain  $\emptyset \rightarrow H\emptyset \rightarrow HH\emptyset \rightarrow \dots$ , where  $\emptyset$  denotes the constant functor mapping anything to the empty set, and  $HZ = FZ + X$ .

## 4 Soundness of the pruning phase

In this section, we assume a pattern-friendly GB-signature  $S$  and discuss soundness of the main rules of the two mutually recursive functions `prune` and `prune- $\sigma$`  listed in Figure 5, which handles unification of two substitutions  $\delta : \Gamma'_1 \rightarrow \Gamma$  and  $\bar{x} : \Gamma'_1 \rightarrow \Gamma'_2$  where  $\bar{x}$  is induced by a vector of renamings  $x : \Gamma'_2 \Rightarrow \Gamma'_1$ . Strictly speaking, this is not unification as we introduced it because  $\delta$  and  $\bar{x}$  do not target the same context, but it is straightforward to adapt the definition: a unifier is given by two substitutions  $\sigma : \Gamma \rightarrow \Delta$  and  $\sigma' : \Gamma'_2 \rightarrow \Delta$  such that the following equation holds

$$\delta[\sigma] = \bar{x}[\sigma'] \quad (4.1)$$

As usual, the mgu is defined as the unifier uniquely factoring any other unifier.

**Remark 47.** The right hand-side  $\bar{x}[\sigma']$  in (4.1) is actually equal to  $\sigma'\{x\}$ . Indeed,  $\bar{x} = (\dots, M_i(x_i), \dots)$  and  $M_i(x_i)[\sigma'] = \sigma'_i\{x_i\}$ .

From a categorical point of view, such a mgu is characterised as a pushout.

**Notation 48.** Given

- $\delta : \Gamma'_1 \rightarrow \Gamma$ ,
- $x : \Gamma'_2 \Rightarrow \Gamma'_1$ ,
- $\sigma : \Gamma \rightarrow \Delta$ ,
- $\sigma' : \Gamma'_2 \rightarrow \Delta$ ,

the notation  $\Gamma \vdash \delta :> x \Rightarrow \sigma'; \sigma \dashv \Delta$  means that the square

$$\begin{array}{ccc} \Gamma'_1 & \xrightarrow{\bar{x}} & \Gamma'_2 \\ \delta \downarrow & & \downarrow \sigma' \\ \Gamma & \xrightarrow{\sigma} & \Delta \end{array} \quad \text{is a pushout}$$

in  $\text{MCon}(S)_\perp$ .

**Remark 49.** This justifies the similarity between the pruning notation  $- \vdash - :> - \Rightarrow -$ ;  $-$  and the pullback notation of Notation 10, since pushouts in a category are nothing but pullbacks in the opposite category.

In the following subsections, we detail soundness of the rules for the rigid case (Section §4.1) and then for the flex case (Section §4.2).

The rules P-EMPTY and P-SPLIT are straightforward adaptations specialised to those specific unification problems of the rules U-EMPTY and U-SPLIT described later in Section §5.1. The failing rule P-FAIL is justified by Lemma 18.(ii).

#### 4.1 Rigid (rules P-RIG and P-RIG-FAIL)

The rules P-RIG and P-RIG-FAIL handle non-cyclic unification of  $M(x)$  with  $\Gamma; a \vdash o(\delta)$  for some  $o \in O_n(a)$ , where  $M \notin \Gamma$ . By Remark 47, a unifier is given by a substitution  $\sigma : \Gamma \rightarrow \Delta$  and a term  $u$  such that

$$o(\delta[\sigma]) = u\{x\}. \quad (4.2)$$

Now,  $u$  is either some  $M(y)$  or  $o'(\vec{v})$ . But in the first case,  $u\{x\} = M(y)\{x\} = M(x \circ y)$ , contradicting Equation (4.2). Therefore,  $u = o'(\delta')$  for some  $o' \in O_n(m)$  and  $\delta'$  is a substitution from  $\alpha_{o'}$  to  $\Delta$ . Then,  $u\{x\} = o'\{x\}(\delta\{x^{o'}\})$ . It follows from Equation (4.2) that  $o = o'\{x\}$ , and  $\delta[\sigma] = \delta'\{x^{o'}\}$ .

Note that there is at most one  $o'$  such that  $o = o'\{x\}$ , by Property 27.(i). In this case, a unifier is equivalently given by substitutions  $\sigma : \Gamma \rightarrow \Delta$  and  $\sigma' : \alpha_{o'} \rightarrow \Delta$  such that  $\delta[\sigma] = \sigma'\{x^{o'}\}$ . But, by Remark 47, this is precisely the data for a unifier of  $\delta$  and  $x^{o'}$ . This actually induces an isomorphism between the two categories of unifiers, thus justifying the rules P-RIG and P-RIG-FAIL.

#### 4.2 Flex (rule P-FLEX)

The rule P-FLEX handles unification of  $M(x)$  with  $N(y)$  where  $M \neq N$  in a scope  $a$ . More explicitly, this is about computing the pushout of  $(X : a) \xrightarrow{\mathcal{L}x} (X : m) \cong (M : m) \xrightarrow{in_M} \Gamma$  and  $(X : a) \xrightarrow{\mathcal{L}y} (X : n) \cong (N : n)$ .

Thanks to the following lemma, it is actually enough to compute the pushout of  $\mathcal{L}x$  and  $\mathcal{L}y$ , taking  $A = (X : a)$ ,  $B = (X : m)$ ,  $C = (X : n)$ ,  $Y = \Gamma \setminus M$ , so that  $B + Y \cong \Gamma$ .

**Lemma 50.** *In any category, if the square below left is a pushout, then so is the square below right.*

$$\begin{array}{ccc} A & \xrightarrow{f} & B \\ g \downarrow & & \downarrow \sigma \\ C & \xrightarrow{u} & Z \end{array} \quad \begin{array}{ccccc} A & \xrightarrow{f} & B & \xrightarrow{in_1} & B + Y \\ g \downarrow & & \downarrow & & \downarrow \sigma + Y \\ C & \xrightarrow{u} & Z & \xrightarrow{in_1} & Z + Y \end{array}.$$

By Property 27.(ii), the pushout of  $\mathcal{L}x$  and  $\mathcal{L}y$  is the image by  $\mathcal{L}$  of the pullback of  $x$  and  $y$  in  $\mathcal{A}$ , thus justifying the rule P-FLEX.

### 5 Soundness of the unification phase

In this section, we assume a pattern-friendly GB-signature  $S$  and discuss soundness of the main rules of the two mutually recursive functions `unify` and `unify- $\sigma$`  listed in Figure 5, which compute coequalisers in  $\text{MCon}(S)_\perp$ .

The failing rules U-FAIL and U-ID-FAIL are justified by Lemma 18.(ii). Both rules CLASH and U-RIG handle unification of two rigid terms  $o(\delta)$  and  $o'(\delta')$ . If  $o \neq o'$ , they do not have any unifier: this is the rule CLASH. If  $o = o'$ , then a substitution is a unifier if and only if it unifies  $\delta$  and  $\delta'$ , thus justifying the U-RIG rule.

In the next subsections, we discuss the rule sequential rules U-EMPTY and U-SPLIT (Section §5.1), the rule NO-CYCLE transitioning to the pruning phase (Section §5.2), the rule SAME-MVAR unifying metavariable with itself (Section §5.3), and the failing rule CYCLE for cyclic unification of a metavariable with a term which includes it deeply (Section §5.4).

### 5.1 Sequential unification (rules U-EMPTY and U-SPLIT)

The rule U-EMPTY is a direct application of the following general lemma.

**Lemma 51.** *If  $A$  is initial in a category, then any diagram of the shape  $A \rightrightarrows B \xrightarrow{1_B} B$  is a coequaliser.*

The rule U-SPLIT is a direct application of a stepwise construction of coequalisers valid in any category, as noted by (Rydeheard and Burstall, 1988, Theorem 9): if the first two diagrams below are coequalisers, then the last one as well.

$$\begin{array}{ccc}
 \Gamma'_1 & \xrightleftharpoons[u_1]{t_1} & \Gamma \xrightarrow{\sigma_1} \Delta_1 \\
 & & \Gamma'_2 \xrightarrow{t_2} \Gamma \xrightarrow{\sigma_1} \Delta_1 \xrightarrow{\sigma_2} \Delta_2 \\
 & & \Gamma'_2 \xrightarrow{u_2} \Gamma \xrightarrow{\sigma_1} \Delta_1 \xrightarrow{\sigma_2} \Delta_2 \\
 & & \Gamma'_1 + \Gamma'_2 \xrightleftharpoons[u_1, u_2]{t_1, t_2} \Gamma \xrightarrow{\sigma_2 \circ \sigma_1} \Delta_2
 \end{array}$$

### 5.2 Flex-Flex, no cycle (rule NO-CYCLE)

The rule NO-CYCLE transitions from unification to pruning. While unification is a coequaliser construction, in Section §4, we explained that pruning is a pushout construction. The rule is justified by the following well-known connection between those two notions, taking  $B$  to be  $\Gamma \setminus M$  and  $C$  to be the singleton context  $M : m$ , so that the coproduct of those two contexts in  $\text{MCon}(S)_\perp$  is their disjoint union  $\Gamma$ .

**Lemma 52.** *Consider a commuting square*

$$\begin{array}{ccc}
 A & \xrightarrow{u} & B \\
 v \downarrow & & \downarrow f \\
 C & \xrightarrow{g} & D
 \end{array}$$

*if the coproduct  $B + C$  of  $B$  and  $C$  exists, then this is a pushout if and only if  $B + C \xrightarrow{f, g} D$  is the coequaliser of  $\text{in}_1 \circ u$  and  $\text{in}_2 \circ v$ .*

### 5.3 Flex-Flex, same metavariable (rule SAME-MVAR)

Here we detail unification of  $M(x)$  and  $M(y)$ , for  $x, y \in \text{hom}_{\mathcal{A}}(m, a)$ . By Remark 28,  $M(x) = \mathcal{L}x[in_M]$  and  $M(y) = \mathcal{L}y[in_M]$ . We exploit the following lemma with  $u = \mathcal{L}x$  and  $v = \mathcal{L}y$ .

**Lemma 53.** *In any category, if the below left diagram is a coequaliser, then so is the below right diagram.*

$$A \xrightarrow[u]{u} B \xrightarrow[h]{h} C \qquad A \begin{array}{c} \xrightarrow{u} B \\ \xrightarrow{v} B \end{array} \begin{array}{c} \xrightarrow{in_B} B + D \\ \xrightarrow{in_B} B + D \end{array} \xrightarrow[h+1_D]{h+1_D} C + D$$

It follows that it is enough to compute the coequaliser of  $\mathcal{L}x$  and  $\mathcal{L}y$ . Furthermore, by Property 27.(ii), it is the image by  $\mathcal{L}$  of the equaliser of  $x$  and  $y$ , thus justifying the rule SAME-MVAR.

### 5.4 Flex-rigid, cyclic (rule CYCLE)

The rule CYCLE handles unification of  $M(x)$  and a term  $t$  such that  $t$  is rigid and  $M$  occurs in  $t$ . In this section, we show that indeed there is no successful unifier. More precisely, we prove Corollary 58 below, stating that if there is a unifier of a term  $t$  and a metavariable application  $M(x)$ , then either  $M$  occurs at top-level in  $t$ , or it does not occur at all. The argument follows the basic intuition that  $\sigma_M = t[M \mapsto \sigma_M]$  is impossible if  $M$  occurs deeply in  $u$  because the sizes of both hand sides can never match. To make this statement precise, we need some recursive definitions and properties of size.

**Definition 54.** *The size  $|t| \in \mathbb{N}$  of a proper term  $t$  is recursively defined by  $|M(x)| = 0$ , and  $|o(\vec{t})| = 1 + |\vec{t}|$ , with  $|\vec{t}| = \sum_i t_i$ .*

We will also need to count the occurrences of a metavariables in a term.

**Definition 55.** *For any term  $t$  we define  $|t|_M$  recursively by  $|M(x)|_M = 1$ ,  $|N(x)|_M = 0$  if  $N \neq M$ , and  $|o(\vec{t})|_M = |\vec{t}|_M$  with the sum convention as above for  $|\vec{t}|_M$ .*

**Lemma 56.** *For any term  $\Gamma; a \vdash t$ , if  $|t|_M = 0$ , then  $\Gamma \setminus M; a \vdash t$ . Moreover, for any  $\Gamma = (M_1 : m_1, \dots, M_n : m_n)$ , well-formed term  $t$  in context  $\Gamma; a$ , and successful substitution  $\sigma : \Gamma \rightarrow \Delta$ , we have  $|t[\sigma]| = |t| + \sum_i |t|_{M_i} \times |\sigma_i|$ .*

**Corollary 57.** *For any term  $t$  in context  $\Gamma; a$  with  $(M : m) \in \Gamma$ , successful substitution  $\sigma : \Gamma \rightarrow \Delta$ , morphism  $x \in \text{hom}_{\mathcal{A}}(m, a)$  and  $u$  in context  $\Delta; u$ , we have  $|t[\sigma, M \mapsto u]| \geq |t| + |u| \times |t|_M$  and  $|M(x)[u]| = |u|$ .*

**Corollary 58.** *Let  $t$  be a term in context  $\Gamma; a$  with  $(M : m) \in \Gamma$  and  $x \in \text{hom}_{\mathcal{A}}(m, a)$  such that  $(M \mapsto u, \sigma) : \Gamma \rightarrow \Delta$  unifies  $t$  and  $M(x)$ . Then, either  $t = M(y)$  for some  $y \in \text{hom}_{\mathcal{A}}(m, a)$ , or  $\Gamma; a \vdash t$ .*

**Proof** Since  $t[\sigma, M \mapsto u] = M(x)[u]$ , we have  $|t[\sigma, M \mapsto u]| = |M(x)[u]|$ . Corollary 57 implies  $|u| \geq |t| + |u| \times |t|_M$ . Therefore, either  $|t|_M = 0$  and we conclude by Lemma 56, or  $|t|_M > 0$  and  $|t| = 0$ , so that  $t$  is  $M(y)$  for some  $y$ . ■

## 6 Termination and completeness

### 6.1 Termination

In this section, we sketch an explicit argument to justify termination of our algorithm described in Figure 5. Note that the pruning and the unification phases are not mutually recursive: the latter depends on the former, but not conversely. Therefore, we can show first that the pruning phase terminates, and then that the unification does. Both phases involve three recursive calls (cf. the rules P-RIG, P-SPLIT, U-RIG and U-SPLIT). In each phase, the second recursive call for splitting is not structurally recursive, making Agda unable to check termination. However, we can devise an adequate notion of input size so that for each recursive call, the inputs are strictly smaller than the inputs of the calling site. First, we define the size  $|\Gamma|$  of a proper metacontext  $\Gamma$  as its length, while  $|\perp| = 0$  by definition. We also recursively define the size<sup>6</sup>  $||t||$  of a proper term  $t$  by  $||M(x)|| = 1$  and  $||o(\vec{t})|| = 1 + ||\vec{t}||$ , with  $||\vec{t}|| = \sum_i ||t_i||$ . We also define the size of the error term  $||!||$  as 1. Note that no term is of size 0.

**Definition 59.** We say that a substitution  $\sigma : \Gamma \rightarrow \Delta$  is monotone if  $||t[\sigma]|| \leq ||t||$  for any term well-formed in the metacontext  $\Gamma$ .

**Example 60.** The error substitution  $!$  is monotone since there is no term of size 0. A substitution  $\sigma : \Gamma \rightarrow \Delta$  such that  $\sigma_M$  is a metavariable application for any  $(M : m) \in \Gamma$  is monotone (as in the output of the rules P-FLEX and SAME-MVAR).

Let us first quickly justify termination of the pruning phase.

**Lemma 61.** If there is a finite derivation tree of  $\Gamma \vdash \vec{t} :> x \Rightarrow \vec{w}; \sigma \vdash \Delta$  then  $\sigma$  is monotone.

**Corollary 62.** The pruning phase always terminates.

**Proof** Consider the above defined size of the input, which is a term  $t$  for **prune**, or a list of terms  $\vec{t}$  for **prune- $\sigma$** . It is straightforward to check that the sizes of the inputs of recursive calls are strictly smaller thanks to the previous lemma. Let us detail the case of the rule P-SPLIT. We show that the input  $\delta[\sigma_1]$  of the second recursive call is smaller than the original input  $t, \delta$ . By Lemma 61, we know that  $\sigma_1$  is either a metavariable renaming or the

<sup>6</sup> The difference with the notion of size introduced in Definition 54 is that metavariable applications are now of size 1 instead of 0.

error substitution !. Then,

$$\begin{aligned}
 ||\delta[\sigma_1]|| &\leq ||\delta|| && \text{(By Lemma 61)} \\
 &< ||\delta|| + ||t|| && \text{(No term is of size 0)} \\
 &= ||t, \delta||
 \end{aligned}$$

■

For termination of the main unification phase, we consider the size of the input to be the (lexicographic) pair  $(|\Gamma|, ||t||)$  for **unify** or  $(|\Gamma|, ||\vec{t}||)$  for **unify- $\sigma$** , given as input a pair of terms  $(t, t')$  or lists of terms  $(\vec{t}, \vec{t}')$  in the metacontext  $\Gamma$ .

**Lemma 63.** *If there is a finite derivation tree of  $\Gamma \vdash \vec{t} :> x \Rightarrow \vec{w}; \sigma \vdash \Delta$  or  $\Gamma \vdash \vec{t} = \vec{u} \Rightarrow \sigma \vdash \Delta$ , then  $|\Gamma| \geq |\Delta|$ .*

**Lemma 64.** *If there is a finite derivation tree of  $\Gamma \vdash \vec{t} = \vec{u} \Rightarrow \sigma \vdash \Delta$  such that  $|\Gamma| = |\Delta|$ , then  $\sigma$  is monotone.*

**Corollary 65.** *The unification algorithm as defined in Figure 5 always terminates.*

**Proof** It is straightforward to check that the sizes of the inputs of recursive calls are strictly smaller thanks to the previous lemmas. Let us detail the case of the rule U-SPLIT. We show that the size  $(|\Delta|, ||\delta_1[\sigma]||)$  of the second recursive call is strictly smaller than the size  $(|\Gamma|, ||t_1, \delta_1||)$  of the original input.

If  $|\Delta| < |\Gamma|$  then we are done. Otherwise, by Lemma 63, we have  $|\Delta| = |\Gamma|$ , and by Lemma 64,

$$||\delta_1[\sigma]|| \leq ||\delta_1|| < ||\delta_1|| + ||t_1|| = ||t_1, \delta_1||$$

■

## 6.2 Completeness

In this section, we explain why soundness (Section §4 and Section §5) and termination (Section §6.1) entail completeness. Intuitively, one may worry that the algorithm fails in cases where it should not. In fact, we already checked in the previous sections that failure only occurs when there is no unifier, as expected. Indeed, failure is treated as a free “terminal” unifier, as explained in Section §3.1, by considering the category  $\text{MCon}(S)_\perp$  extending category  $\text{MCon}(S)$  with an error metacontext  $\perp$ . Corollary 19 implies that since the algorithm terminates and computes the coequaliser in  $\text{MCon}(S)_\perp$ , it always finds the most general unifier in  $\text{MCon}(S)$  if it exists, and otherwise returns failure (i.e., the map to the terminal object  $\perp$ ).

## 7 Applications

In this section, we present various examples of pattern-friendly signatures summarised in Tables 1 and 2.



Table 1: Examples of (pattern-friendly) GB-signatures (Definition 23)

Simply-typed  $\lambda$ -calculus (Section §7.2)

Typing rule	$O(\vec{\sigma} \rightarrow \tau) = \dots +$	$\alpha_o = (\dots)$
$\frac{x : \tau \in \Gamma}{\Gamma \vdash x : \tau}$	$\{v_i   i \in  \vec{\sigma} _\tau\}$	$()$
$\frac{\Gamma \vdash t : \tau' \Rightarrow \tau \quad \Gamma \vdash u : \tau'}{\Gamma \vdash t u : \tau}$	$\{a_{\tau'}   \tau' \in T\}$	$\left( \begin{array}{c} \vec{\sigma} \rightarrow (\tau' \Rightarrow \tau) \\ \vec{\sigma} \rightarrow \tau' \end{array} \right)$
$\frac{\Gamma, x : \tau_1 \vdash t : \tau_2}{\Gamma \vdash \lambda x. t : \tau_1 \Rightarrow \tau_2}$	$\{l_{\tau_1, \tau_2}   \tau = (\tau_1 \Rightarrow \tau_2)\}$	$(\vec{\sigma}, \tau_1 \rightarrow \tau_2)$

Simply-typed  $\lambda$ -calculus modulo  $\beta\eta$  (Section §7.3)

Typing rule	$O(\vec{\sigma} \rightarrow \tau) = \dots +$	$\alpha_o = (\dots)$
$\frac{x : (\tau_1, \dots, \tau_n) \Rightarrow \iota \in (\Gamma, \vec{y} : \vec{\tau}_0) \quad \forall i \in \{1, \dots, n\} \Gamma, \vec{y} : \vec{\tau} \vdash t_i : \tau_i}{\Gamma \vdash \lambda \vec{y}. x \vec{t} : \vec{\tau}_0 \Rightarrow \iota}$	$\{a_{j, \tau_1, \dots, \vec{\tau}_0, \iota}   \tau = \vec{\tau}_0 \Rightarrow \iota, j \in  \vec{\sigma} _{\vec{\tau} \Rightarrow \iota}\}$	$\left( \begin{array}{c} \vec{\sigma}, \vec{\tau}_0 \rightarrow \tau_1 \\ \vdots \\ \vec{\sigma}, \vec{\tau}_0 \rightarrow \tau_n \end{array} \right)$

Ordered  $\lambda$ -calculus (Section §7.4)

Typing rule	$O(\vec{\sigma}   \vec{\omega} \rightarrow \tau) = \dots +$	$\alpha_o = (\dots)$
$\frac{x : \tau \in \Gamma}{\Gamma   \cdot \vdash x : \tau}$	$\{v_i   i \in  \vec{\sigma} _\tau \text{ and } \vec{\omega} = ()\}$	$()$
$\frac{}{\Gamma   x : \tau \vdash x : \tau}$	$\{v^>   \vec{\omega} = ()\}$	$()$
$\frac{\Gamma   \Omega \vdash t : \tau' \Rightarrow \tau \quad \Gamma   \cdot \vdash u : \tau'}{\Gamma   \Omega \vdash t u : \tau}$	$\{a_{\tau'}   \tau' \in T\}$	$\left( \begin{array}{c} \vec{\sigma}   \vec{\omega} \rightarrow (\tau' \Rightarrow \tau) \\ \vec{\sigma}   () \rightarrow \tau' \end{array} \right)$
$\frac{\Gamma   \Omega_1 \vdash t : \tau' \Rightarrow \tau \quad \Gamma   \Omega_2 \vdash u : \tau'}{\Gamma   \Omega_1, \Omega_2 \vdash t^> u : \tau}$	$\{a_{\tau'}^{\vec{\omega}_1, \vec{\omega}_2}   \tau' \in T \text{ and } \vec{\omega} = \vec{\omega}_1, \vec{\omega}_2\}$	$\left( \begin{array}{c} \vec{\sigma}   \vec{\omega}_1 \rightarrow (\tau' \Rightarrow \tau) \\ \vec{\sigma}   \vec{\omega}_2 \rightarrow \tau' \end{array} \right)$
$\frac{\Gamma, x : \tau_1   \Omega \vdash t : \tau_2}{\Gamma   \Omega \vdash \lambda x. t : \tau_1 \Rightarrow \tau_2}$	$\{l_{\tau_1, \tau_2}   \tau = (\tau_1 \Rightarrow \tau_2)\}$	$(\vec{\sigma}, \tau_1   \vec{\omega} \rightarrow \tau_2)$
$\frac{\Gamma   \Omega, x : \tau_1 \vdash t : \tau_2}{\Gamma   \Omega \vdash \lambda^> x. t : \tau_1 \Rightarrow \tau_2}$	$\{l_{\tau_1, \tau_2}^>   \tau = (\tau_1 \Rightarrow \tau_2)\}$	$(\vec{\sigma}, \tau_1   \vec{\omega} \rightarrow \tau_2)$

We start in Section §7.1 with a variant of pure  $\lambda$ -calculus where metavariable arguments are sets rather than lists. In Section §7.2, we present simply-typed  $\lambda$ -calculus, as an example of syntax specified by a multi-sorted binding signature. We then explain in Section §7.3 how we can handle  $\beta$  and  $\eta$  equations by working on the normalised syntax. Next, we introduce an example of unification for ordered syntax in Section §7.4, and finally we present an example of polymorphic such as System F, in Section §7.5.1.

Table 2: The (pattern-friendly) GB-signature of (syntactic) system F (Section §7.5.1)

Typing rule	$O(p \vec{\sigma} \rightarrow \tau) = \dots +$	$\alpha_o = (\dots)$
$\frac{x : \tau \in \Gamma}{n \Gamma \vdash x : \tau}$	$\{v_i   i \in  \vec{\sigma} _\tau\}$	$()$
$\frac{n \Gamma \vdash t : \tau' \Rightarrow \tau \quad n \Gamma \vdash u : \tau'}{n \Gamma \vdash t u : \tau}$	$\{a_{\tau'}   \tau' \in S_n\}$	$\left( \begin{array}{c} n \vec{\sigma} \rightarrow \tau' \Rightarrow \tau \\ n \vec{\sigma} \rightarrow \tau' \end{array} \right)$
$\frac{n \Gamma, x : \tau_1 \vdash t : \tau_2}{n \Gamma \vdash \lambda x. t : \tau_1 \Rightarrow \tau_2}$	$\{l_{\tau_1, \tau_2}   \tau = (\tau_1 \Rightarrow \tau_2)\}$	$(n \vec{\sigma}, \tau_1 \rightarrow \tau_2)$
$\frac{n \Gamma \vdash t : \forall \tau_1 \quad \tau_2 \in S_n}{n \Gamma \vdash t \cdot \tau_2 : \tau_1 [\tau_2]}$	$\{A_{\tau_1, \tau_2}   \tau = \tau_1 [\tau_2]\}$	$(n \vec{\sigma} \rightarrow \forall \tau_1)$
$\frac{n+1 wk(\Gamma) \vdash t : \tau}{n \Gamma \vdash \Lambda t : \forall \tau}$	$\{\Lambda_{\tau'}   \tau = \forall \tau'\}$	$(n+1 wk(\vec{\sigma}) \rightarrow \tau')$

### 7.1 Metavariable arguments as sets

If we think of the arguments of a metavariable as specifying the available variables, then it makes sense to assemble them in a set rather than in a list. This motivates considering the category  $\mathcal{A} = \mathbb{I}$  whose objects are natural numbers and a morphism  $n \rightarrow p$  is a subset of  $\{1, \dots, p\}$  of cardinal  $n$ . Equivalently,  $\mathbb{I}$  can be taken as subcategory of  $\mathbb{F}_m$  consisting of strictly increasing injections, or as the subcategory of the augmented simplex category consisting of injective functions. Then, a metavariable takes as argument a set of variables, rather than a list of distinct variables. In this approach, unifying two metavariables (see the rules U-FLEX and P-FLEX) amount to computing a set intersection.

### 7.2 Simply-typed $\lambda$ -calculus

In this section, we present the example of simply-typed  $\lambda$ -calculus. Our treatment generalises to any multi-sorted binding signature (Fiore and Hur, 2010).

Let  $T$  denote the set of simple types generated by a set of base types and a binary arrow type construction  $- \Rightarrow -$ . Let us now describe the category  $\mathcal{A}$  of arities, or scopes, and renamings between them. An arity  $\vec{\sigma} \rightarrow \tau$  consists of a list of input types  $\vec{\sigma}$  and an output type  $\tau$ . A term  $t$  in  $\vec{\sigma} \rightarrow \tau$  considered as a scope is intuitively a well-typed term  $t$  of type  $\tau$  potentially using variables whose types are specified by  $\vec{\sigma}$ . A valid choice of arguments for a metavariable  $M : (\vec{\sigma} \rightarrow \tau)$  in scope  $\vec{\sigma}' \rightarrow \tau'$  first requires  $\tau = \tau'$ , and consists of an injective renaming  $\vec{r}$  between  $\vec{\sigma} = (\sigma_1, \dots, \sigma_m)$  and  $\vec{\sigma}' = (\sigma'_1, \dots, \sigma'_n)$ , that is, a choice of distinct positions  $(r_1, \dots, r_m)$  in  $\{1, \dots, n\}$  such that  $\vec{\sigma} = \sigma'_{\vec{r}}$ .

This discussion determines the category of arities as  $\mathcal{A} = \mathbb{F}_m[T] \times T$ , where  $\mathbb{F}_m[T]$  is the category of finite lists of elements of  $T$  and injective renamings between them. Table 1 summarises the definition of the endofunctor  $F$  on  $[\mathcal{A}, \text{Set}]$  specifying the syntax, where  $|\vec{\sigma}|_\tau$  denotes the number (as a cardinal set) of occurrences of  $\tau$  in  $\vec{\sigma}$ .

The induced signature is pattern-friendly and so the generic pattern unification algorithm applies. Equalisers and pullbacks are computed following the same pattern as in pure  $\lambda$ -calculus. For example, to unify  $M(\vec{x})$  and  $M(\vec{y})$ , we first compute the vector  $\vec{z}$  of common positions between  $\vec{x}$  and  $\vec{y}$ , thus satisfying  $x_{\vec{z}} = y_{\vec{z}}$ . Then, the most general unifier maps  $M : (\vec{\sigma} \rightarrow \tau)$  to the term  $P(\vec{z})$ , where the arity  $\vec{\sigma}' \rightarrow \tau'$  of the fresh metavariable  $P$  is the only possible choice such that  $P(\vec{z})$  is a valid term in the scope  $\vec{\sigma} \rightarrow \tau$ , that is,  $\tau' = \tau$  and  $\vec{\sigma}' = \sigma_{\vec{z}}$ .

### 7.3 Simply-typed $\lambda$ -calculus modulo $\beta\eta$

Let us explain how we account for Miller's original setting: simply-typed  $\lambda$ -calculus modulo  $\beta$  and  $\eta$ -equations. Let us denote a type  $\sigma_1 \Rightarrow \dots \Rightarrow \sigma_n \Rightarrow \iota$  by  $\vec{\sigma} \Rightarrow \iota$ , where  $\iota$  is a base type. Note that any type can be written in this way, uniquely. We consider the same set of scopes as in the previous section, but with different morphisms as we explain now. As a preliminary remark, note that any scope  $\vec{\sigma} \rightarrow (\vec{\tau} \Rightarrow \iota)$ , induces a type  $\vec{\sigma}, \vec{\tau} \Rightarrow \iota$ . A morphism between two scopes respectively inducing the types  $\vec{\tau} \Rightarrow \iota$  and  $\vec{\tau}' \Rightarrow \iota'$  is a morphism between the scopes  $\vec{\tau} \rightarrow \iota$  and  $\vec{\tau}' \rightarrow \iota'$  in the sense of the previous section. As a consequence, our category of scopes is equivalent to  $\mathbb{F}_m[T] \times B$  where  $B$  is the set of base types.

We follow Cheney's presentation (Cheney, 2005, Section 2.2) of the equation-free syntax of  $\beta$ -short  $\eta$ -long normal forms with metavariables. Table 1 shows the base syntax which is generated by a single rule combining application and abstraction.

Let us now describe the enriched syntax. We write  $M :: \vec{\tau} \Rightarrow \iota \in \Gamma$  to mean that the type induced by the scope of  $M$  declared in  $\Gamma$  is  $\vec{\tau} \Rightarrow \iota$ . The introduction rule for metavariables is the following.

$$\frac{M :: (\tau_1, \dots, \tau_n) \Rightarrow \iota \in \Gamma \quad (x_1, \dots, x_n) \text{ are distinct variables in } \vec{\sigma}, \vec{\tau}' \text{ of type } \vec{\tau}}{\Gamma; \vec{\sigma} \vdash \lambda_{\vec{\tau}} M(\vec{x}) : \vec{\tau}' \Rightarrow \iota}$$

Thanks to our modified notion of scope morphism, this rule indeed complies with our introduction rule for metavariables, in the sense that it requires the same data.

Let us note that the metavariable arities  $\vec{\sigma} \rightarrow \tau \Rightarrow \tau'$  and  $\vec{\sigma}, \tau \rightarrow \tau'$  are equivalent in the sense that they share the same metavariable introduction rule.

### 7.4 Ordered $\lambda$ -calculus

Our setting handles linear ordered  $\lambda$ -calculus, consisting of  $\lambda$ -terms using all the variables in context. In this context, a metavariable  $M$  of arity  $m \in \mathbb{N}$  can only be used in the scope  $m$ , and there is no freedom in choosing the arguments of a metavariable application, since all the variables must be used, in order. Thus, there is no need to even mention those arguments in the syntax. It is thus not surprising that ordered  $\lambda$ -calculus is already handled by first-order unification, where metavariables do not take any argument, by considering ordered  $\lambda$ -calculus as a multi-sorted Lawvere theory where the sorts are the scopes, and the syntax is generated by operations  $L_n \times L_m \rightarrow L_{n+m}$  and abstractions  $L_{n+1} \rightarrow L_n$ .

Our generalisation can handle calculi combining ordered and unrestricted variables, such as the calculus underlying ordered linear logic described in Polakow and Pfenning (2000). In this section we detail this specific example. Note that this does not fit into Schack-Nielsen

and Schürman’s pattern unification algorithm (Schack-Nielsen and Schürmann, 2010) for linear types where exchange is allowed (the order of their variables does not matter).

The set  $T$  of types is generated by a set of atomic types and two binary arrow type constructions  $\Rightarrow$  and  $\multimap$ . The syntax extends pure  $\lambda$ -calculus with a distinct application  $t^> u$  and abstraction  $\lambda^> u$ . Variables contexts are of the shape  $\vec{\sigma}|\vec{\omega} \rightarrow \tau$ , where  $\vec{\sigma}$ ,  $\vec{\omega}$ , and  $\tau$  are taken in  $T$ . The idea is that a term in such a context has type  $\tau$  and must use all the variables of  $\vec{\omega}$  in order, but is free to use any of the variables in  $\vec{\sigma}$ . Assuming a metavariable  $M$  of arity  $\vec{\sigma}|\vec{\omega} \rightarrow \tau$ , the above discussion about ordered  $\lambda$ -calculus justifies that there is no need to specify the arguments for  $\vec{\omega}$  when applying  $M$ . Thus, a metavariable application  $M(\vec{x})$  in the scope  $\vec{\sigma}'|\vec{\omega}' \rightarrow \tau'$  is well-formed if  $\tau = \tau'$  and  $\vec{x}$  is an injective renaming from  $\vec{\sigma}$  to  $\vec{\sigma}'$ . Therefore, we take  $\mathcal{A} = \mathbb{F}_m[T] \times T^* \times T$  for the category of arities, where  $T^*$  denotes the discrete category whose objects are lists of elements of  $T$ . The remaining components of the GB-signature are specified in Table 1: we alternate typing rules for the unrestricted and the ordered fragments (variables, application, abstraction).

Pullbacks and equalisers are computed essentially as in Section §7.2. For example, the most general unifier of  $M(\vec{x})$  and  $M(\vec{y})$  maps  $M$  to  $P(\vec{z})$  where  $\vec{z}$  is the vector of common positions of  $\vec{x}$  and  $\vec{y}$ , and  $P$  is a fresh metavariable of arity  $\sigma_{\vec{z}}|\vec{\omega} \rightarrow \tau$ .

## 7.5 Intrinsic polymorphic syntax

### 7.5.1 Syntactic system $F$

We present intrinsic System  $F$ , in the spirit of Hamana (2011). The Agda implementation of the friendly GB-signature can be found in the supplemental material.

The syntax of types in type scope  $n$  is inductively generated as follows, following the De Bruijn level convention.

$$\frac{1 \leq i \leq n}{n \vdash i} \quad \frac{n \vdash t \quad n \vdash u}{n \vdash t \Rightarrow u} \quad \frac{n + 1 \vdash t}{n \vdash \forall t}$$

Let  $S : \mathbb{F}_m \rightarrow \text{Set}$  be the functor mapping  $n$  to the set  $S_n$  of types for system  $F$  taking free type variables in  $\{1, \dots, n\}$ . In other words,  $S_n = \{\tau | n \vdash \tau\}$ . Intuitively, a metavariable arity  $n|\vec{\sigma} \rightarrow \tau$  specifies the number  $n$  of free type variables, the list of input types  $\vec{\sigma}$ , and the output type  $\tau$ , all living in  $S_n$ . This provides the underlying set of objects of the category  $\mathcal{A}$  of arities. A term  $t$  in  $n|\vec{\sigma} \rightarrow \tau$  considered as a scope is intuitively a well-typed term of type  $\tau$  potentially involving ground variables of type  $\vec{\sigma}$  and type variables in  $\{1, \dots, n\}$ .

A metavariable  $M : (n|\sigma_1, \dots, \sigma_p \rightarrow \tau)$  in the scope  $n'|\vec{\sigma}' \rightarrow \tau'$  must be supplied with a choice  $(\eta_1, \dots, \eta_n)$  of  $n$  distinct type variables among the set  $\{1, \dots, n'\}$  such that  $\tau[\vec{\eta}] = \tau'$ , as well as an injective renaming  $\vec{\sigma}[\vec{\eta}] \rightarrow \vec{\sigma}'$ , i.e., a list of distinct positions  $r_1, \dots, r_p$  such that  $\vec{\sigma}[\vec{\eta}] = \sigma'_{\vec{r}}$ .

This defines the data for a morphism in  $\mathcal{A}$  between  $(n|\vec{\sigma} \rightarrow \tau)$  and  $(n'|\vec{\sigma}' \rightarrow \tau')$ . The intrinsic syntax of system  $F$  can then be specified as in Table 2. The induced GB-signature is pattern-friendly. For example, morphisms in  $\mathcal{A}$  are easily seen to be monomorphic; we detail in Section §7.5.3 the proof that  $\mathcal{A}$  has finite connected limits.

Pullbacks and equalisers in  $\mathcal{A}$  are essentially computed as in Section §7.2, by computing the vector of common (value) positions. For example, given a metavariable  $M$  of arity  $m|\vec{\sigma} \rightarrow \tau$ , to unify  $M(\vec{w}|\vec{x})$  with  $M(\vec{y}|\vec{z})$ , we compute the vector of common positions

$\vec{p}$  between  $\vec{w}$  and  $\vec{y}$ , and the vector of common positions  $\vec{q}$  between  $\vec{x}$  and  $\vec{z}$ . Then, the most general unifier maps  $M$  to the term  $P(\vec{p}|\vec{q})$ , where  $P$  is a fresh metavariable. Its arity  $m'|\vec{\sigma}' \rightarrow \tau'$  is the only possible one for  $P(\vec{p}|\vec{q})$  to be well-formed in the scope  $m|\vec{\sigma} \rightarrow \tau$ , that is,  $m'$  is the size of  $\vec{p}$ , while  $\tau' = \tau[p_i \mapsto i]$  and  $\vec{\sigma}' = \sigma_{\vec{q}}[p_i \mapsto i]$ .

### 7.5.2 System F modulo $\beta\eta$

In this section, we sketch how we can handle system F modulo  $\beta\eta$  in the spirit of Section §7.3, by devising a signature for normal forms. To make the syntax more legible, we depart from the previous presentation and instead consider system F as a pure type system. We also ignore the De Bruijn encoding. A scope is now of the shape  $\vec{y} : \vec{u} \rightarrow \tau$ , where

- $\vec{y} : \vec{u}$  is a list of variable declarations  $y_1 : u_1, \dots, y_n : u_n$  where  $u_i$  is either  $*$ , meaning that  $y_i$  is a type variable, or a type which is well-formed in context involving all the type variables occurring before  $y_i$  in the scope;
- $\tau$  is a type well-formed in  $\vec{y} : \vec{u}$ .

We use the notation  $\prod(\alpha : u).\tau$ , where  $\tau$  may depend on  $\alpha$ , to mean either  $\forall\alpha.\tau_2$  in case  $u = *$ , or  $u \Rightarrow \tau$  otherwise (in the latter case,  $\tau$  does not depend on  $\alpha$ ).

Note that any type can be written as  $\prod(y_1 : u_1) \prod \dots \prod(y_n : u_n).\iota$ , abbreviated as  $\prod(\vec{y} : \vec{u}).\iota$ , where  $\iota$  is a type variable. Any scope  $(\vec{y} : \vec{u}) \rightarrow \prod(\vec{z} : \vec{v}).\iota$ , induces a type  $\prod(\vec{y} : \vec{u})(\vec{z} : \vec{v}).\iota$ . A morphism between two scopes inducing the types  $\prod(\vec{y} : \vec{u}).\iota$  and  $\prod(\vec{z} : \vec{v}).\iota'$  is an injective renaming  $\rho$  between  $\vec{y} : \vec{u}$  and  $\vec{z} : \vec{v}$  such that  $\iota[\rho] = \iota'$ .

Let us now describe the base syntax. We write  $\Gamma \vdash t : *$  to mean that  $t$  is a type well-formed in  $\Gamma$  and we do not make any syntactic distinction between type and term abstractions.

The base syntax is generated by the following rule, where  $\iota$  denotes a type variable, and  $u_i$  or  $v_i$  are either types or  $*$ .

$$\frac{\Gamma, \vec{y} : \vec{u} \vdash x : \iota \quad \begin{array}{c} \Gamma, \vec{y} : \vec{u} \vdash t_1 : v_1 \quad \tau_1[\alpha_1 \mapsto t_1] = \prod(\alpha_2 : v_2).\tau_2 \\ \Gamma, \vec{y} : \vec{u} \vdash t_2 : v_2 \quad \tau_2[\alpha_2 \mapsto t_2] = \prod(\alpha_3 : v_3).\tau_3 \\ \dots \quad \tau_n[\alpha_n \mapsto t_n] = \iota \end{array}}{\Gamma \vdash \lambda \vec{y}.x : \prod(\vec{y} : \vec{u}).\iota \quad \Gamma \vdash \lambda \vec{y}.x \vec{t} : \prod(\vec{y} : \vec{u}).\iota}$$

Let us now describe the enriched syntax. We write  $M :: \prod(\vec{y} : \vec{u}).\iota$  to mean that the type induced by the arity of  $M$  is  $\prod(\vec{y} : \vec{u}).\iota$ . The introduction rule for metavariables is the following.

$$\frac{M :: \prod(\vec{x} : \vec{t}).\iota \in \Gamma \quad (\alpha_1, \dots, \alpha_n) \text{ are distinct variables in } \vec{y}, \vec{z} \text{ of sort } \vec{t}}{\Gamma; \vec{y} : \vec{u} \vdash \lambda \vec{z}.M(\vec{\alpha}) : \prod(\vec{z} : \vec{v}).\iota'}$$

As in Section §7.3, thanks to our modified notion of scope morphism, this rule indeed complies with our introduction rule for metavariables, in the sense that it requires the same data.

### 7.5.3 Proof that $\mathcal{A}$ has finite connected limits (Section 7.5.1 on system F)

In this section, we show that the category  $\mathcal{A}$  of arities for System F (Section §7.5.1) has finite connected limits. First, note that  $\mathcal{A}$  is the op-lax colimit of the functor from  $\mathbb{F}_m$  to the category of small categories mapping  $n$  to  $\mathbb{F}_m[S_n] \times S_n$ . Let us introduce the category  $\mathcal{A}'$  whose definition follows that of  $\mathcal{A}$ , but without the output types: objects are pairs of a natural number  $n$  and an element of  $S_n$ . Formally, this is the op-lax colimit of  $n \mapsto \mathbb{F}_m[S_n]$ .

**Lemma 66.**  *$\mathcal{A}'$  has finite connected limits, and the projection functor  $\mathcal{A}' \rightarrow \mathbb{F}_m$  preserves them.*

**Proof** The crucial point is that  $\mathcal{A}'$  is not only op-fibred over  $\mathbb{F}_m$  by construction, it is also fibred over  $\mathbb{F}_m$ . Intuitively, if  $\vec{\sigma} \in \mathbb{F}_m[S_n]$  and  $f : n' \rightarrow n$  is a morphism in  $\mathbb{F}_m$ , then  $f_! \vec{\sigma} \in \mathbb{F}_m[S_{n'}]$  is essentially  $\vec{\sigma}$  restricted to elements of  $S_n$  that are in the image of  $S_f$ . We can now apply (Gray, 1966, Corollary 4.3), since each  $\mathbb{F}_m[S_n]$  has finite connected limits.

■

We are now ready to prove that  $\mathcal{A}$  has finite connected limits.

**Lemma 67.**  *$\mathcal{A}$  has finite connected limits.*

**Proof** Since  $S : \mathbb{F}_m \rightarrow \text{Set}$  preserves finite connected limits,  $\int S$  has finite connected limits and the projection functor to  $\mathbb{F}_m$  preserves them by Corollary 43.

Now, the 2-category of small categories with finite connected limits and functors preserving those between them is the category of algebras for a 2-monad on the category of small categories (Blackwell et al., 1989). Thus, it includes the weak pullback of  $\mathcal{A}' \rightarrow \mathbb{F}_m \leftarrow \int S$ . But since  $\int S \rightarrow \mathbb{F}_m$  is a fibration, and thus an isofibration, by (Joyal and Street, 1993) this weak pullback can be computed as a pullback, which is  $\mathcal{A}$ .

■

## 8 Related work

First-order unification has been explained from a lattice-theoretic point of view by Plotkin (1970), and later categorically analysed by Rydeheard and Burstall (1988); Goguen (1989); Barr and Wells (1990, Section 9.7) as coequalisers. However, there is little work on understanding pattern unification algebraically, with the notable exception of Vezzosi and Abel (2014), working with normalised terms of simply-typed  $\lambda$ -calculus. The present paper can be thought of as a generalisation of their work as sketched in their conclusion, although our treatment of their case study differs (Section §7.3).

Although our notion of signature has a broader scope since we are not specifically focusing on syntax where variables can be substituted, our work is closer in spirit to the presheaf approach (Fiore et al., 1999) to binding signatures than to the nominal approach (Gabbay and Pitts, 1999) in that everything is explicitly scoped: terms come with their scope, metavariables always appear with their patterns.

Nominal unification (Urban et al., 2003) is an alternative to pattern unification where metavariables are not supplied with the list of allowed variables. Instead, substitution can capture variables. Nominal unification explicitly deals with  $\alpha$ -equivalence as an external

relation on the syntax, and as a consequence deals with freshness problems in addition to unification problems.

Nominal unification and pattern unification problems are inter-translatable (Cheney, 2005; Levy and Villaret, 2012). As Cheney notes, this result indirectly provides semantic foundations for pattern unification based on the nominal approach. In this respect, the present work provides a more direct semantic analysis of pattern unification, leading us to the generic algorithm we present, parameterised by a general notion of signature for the syntax.

Pattern unification has also been studied from the viewpoint of logical frameworks (Pientka, 2003; Nanevski et al., 2003, 2008; Abel and Pientka, 2011) using contextual types to characterise metavariables. LF-style signatures handle type dependency, but there are also GB-signatures which cannot be encoded with an LF signature. For example, GB-signatures allow us to express pattern unification for ordered lambda terms (Section §7.4).

In the dependently-typed setting, Pfenning (1991) provides unification and antiunification algorithms in the pattern fragment for the calculus of constructions. Gundry (2013, Chapter 4) presents a pattern unification algorithm for a dependent type theory, as a component of his type inference algorithm. It actually implements "dynamic pattern unification", which addresses unification problems that do not necessarily fit into the pattern fragment at first.

Our semantics for metavariables has been engineered so that it can *only* interpret metavariable instantiations in the pattern fragment, and cannot interpret full metavariable instantiations, contrary to prior semantics of metavariables, e.g., Hu et al. (2022) or Hamana (2004). This restriction gives our model much stronger properties, enabling us to characterise each part of the pattern unification algorithm in terms of universal properties. This lets us extend Rydeheard and Burstall's proof to the pattern case.

**Conflicts of interest.** Ambroise Lafont is part of the INRIA team PARTOUT.

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