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# Generic pattern unification

We provide a generic second-order unification algorithm for Miller's pattern fragment, implemented in Agda. The syntax with metavariables is parameterised by a notion of signature generalising binding signatures, covering ordered  $\lambda$ -calculus, or (intrinsic) polymorphic syntax such as System F. The correctness of the algorithm is stated and proved on papers using a categorical perspective, based on the observation that the most general unifier is an equaliser in a multi-sorted Lawvere theory, thus generalising the case of first-order unification.

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#### 1 INTRODUCTION

Unification consists in finding a *unifier* of two terms t, u, that is a (metavariable) substitution  $\sigma$ such that  $t[\sigma] = u[\sigma]$ . Unification algorithms try to compute a most general unifier  $\sigma$ , in the sense that given any other unifier  $\delta$ , there exists a unique  $\delta'$  such that  $\delta = \sigma[\delta']$ . First-order unification Robinson [1965] is used in ML-style type inference systems and logic programming languages such as Prolog. More advanced type systems, where variable binding is crucially involved, requires second-order unification Huet [1975], which is undecidable Goldfarb [1981]. However, Miller Miller [1991] identified a decidable fragment: in so-called pattern unification, metavariables are allowed to take distinct variables as arguments. In this situation, we can write an algorithm that either fails in case there is no unifier, or computes the most general unifier.

Recent results in type inference, Dunfield-Krishnaswami Dunfield and Krishnaswami [2019], or Jinxu et. al Zhao et al. [2019], include very large proofs: the former comes with a 190 page appendix, and the latter comes with a Coq proof many thousands of lines long -- and both of these results are for tiny kernel calculi. If we ever hope to extend this kind of result to full programming languages like Haskell or OCaml, we must raise the abstraction level of these proofs, so that they are no longer linear (with a large constant) in the size of the calculus. A close examination of these proofs shows that a large part of the problem is that the type inference algorithms make use of unification, and the correctness proofs for type inference end up essentially re-establishing the entire theory of unification for each algorithm. The reason they do this is because algorithmic typing rules essentially give a first-order functional program with no abstractions over (for example) a signature for the unification algorithm to be defined over, or any axiomatic statement of the invariants the algorithmic typing rules had to maintain.

The present work is a first step towards a general solution to this problem. Our generic unification algorithm implemented in Agda is parameterised by a new notion of signature for syntax with metavariables, whose scope goes beyond the standard binding signatures. One important feature is that the notion of contexts is customisable, making it possible to cover simply-typed secondorder syntax, ordered syntax, or (intrinsic) polymorphic syntax such as System F. We focused on Miller's pattern unification, as this is already a step beyond the above-cited works Dunfield and Krishnaswami [2019]; Zhao et al. [2019] that use plain first-order unification. Moreover, this is necessary for types with binders (e.g., fixed-point operators like  $\mu a.A[a]$ ) as well as for rich type systems like dependent types.

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## Agda implementation

We use Agda as a programming language, not as a theorem prover. We leave for future work the task of mechanising the correctness proof of the algorithm, by investigating the formalisation of various concepts from category theory – a notorious challenge on its own – on which our proof relies on.

Since we focus on providing an effective implementation, the definitions of our data structures typically do not mention the properties. For example, our definition of categories in Agda does not include associativity of composition and neutrality of the identity:

Furthermore, we are not reluctant to using logically inconsistent features to make programming easier: the type hierarchy is collapsed and the termination checker is disabled. We find that dependent types are still helpful in guiding the implementation. In comparison, we previously implemented an ocaml version where the code was much less constrained by the typing discipline, and thus more error-prone.

## Plan of the paper

In section §2, we present our generic pattern unification algorithm, parameterised by our generalised notion of binding signature. 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. Completeness is justified in Section §6. We present some examples of signatures in Section §7. Related work is discussed in Section §8.

#### **General notations**

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

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

#### 2 PRESENTATION OF THE ALGORITHM

In this section, we start by describing a pattern unification algorithm for pure  $\lambda$ -calculus, summarised in Figure 1. Then we present our generic algorithm (Figure 2), and finally show that it indeed describes a terminating algorithm in Section §2.3. Soundness of the algorithm is justified in later sections.

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

Consider the syntax of pure  $\lambda$ -calculus extended with metavariables satisfying the pattern restriction. We list the Agda code in Figure 3, together with more legible inductive rules generating the syntax. We write  $\Gamma$ ;  $n \vdash t$  to mean t is a wellformed  $\lambda$ -term in the context  $\Gamma$ ; n, consisting of two parts:

(1) a metavariable context  $\Gamma = (M_1 : m_1, \dots, M_p : m_p)$ , specifying metavariable symbols  $M_i$  together with their arities, i.e, their number of arguments  $m_i$ , and

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## Judgments

 $\Gamma \vdash \vec{t} = \vec{u} \Rightarrow \sigma \vdash \Delta \iff \sigma : \Gamma \to \Delta \text{ is the most general unifier of } \vec{t} \text{ and } \vec{u}$   $\Gamma \vdash \vec{u} :> \overrightarrow{M(\vec{x})} \Rightarrow \vec{w}; \sigma \vdash \Delta \iff \sigma : \Gamma \to \Delta \text{ extended with } M_i \mapsto w_i \text{ is the most general unifier of } \Gamma \vdash \vec{u} \text{ and } \vec{v}$   $m \vdash \vec{x} = \vec{y} \Rightarrow \vec{z} \vdash p \iff (z_1, \dots, z_p) \text{ are the common positions of } (x_1, \dots, x_m) \text{ and } (y_1, \dots, y_m)$   $n \vdash \vec{x} :> \vec{y} \Rightarrow \vec{l}; \vec{r} \vdash p \iff (l_1, \dots, l_p) \text{ and } (r_1, \dots, r_p) \text{ are the common value positions of } (x_1, \dots, x_m)$ 

#### **Unification Phase**

• Structural rules

$$\frac{\Gamma \vdash () = () \Rightarrow 1_{\Gamma} \dashv \Gamma}{\Gamma \vdash t_{1} = u_{1} \Rightarrow \sigma_{1} \dashv \Delta_{1}} \frac{\Gamma \vdash t_{1} = \vec{u} \Rightarrow ! \dashv \bot}{\Delta_{1} \vdash t_{2}[\sigma_{1}] = u_{2}[\sigma_{1}] \Rightarrow \sigma_{2} \dashv \Delta_{2}} U\Lambda - Split}$$

$$\frac{\Gamma \vdash t_{1} = u_{1} \Rightarrow \sigma_{1} \dashv \Delta_{1}}{\Gamma \vdash t_{1}, t_{2} = u_{1}, u_{2} \Rightarrow \sigma_{1}[\sigma_{2}] \dashv \Delta_{2}} U\Lambda - Split}{\Gamma \vdash t_{1}, t_{2} = u_{1}, u_{2} \Rightarrow \sigma_{1}[\sigma_{2}] \dashv \Delta_{2}}$$

• Rigid-rigid (o, o' are applications,  $\lambda$ -abstractions, or variables)

$$\frac{\Gamma \vdash \vec{t} = \vec{u} \Rightarrow \sigma \dashv \Delta}{\Gamma \vdash o(\vec{t}) = o(\vec{u}) \Rightarrow \sigma \dashv \Delta} \text{U}\Lambda - \text{RigRig} \qquad \frac{o \neq o'}{\Gamma \vdash o(\vec{t}) = o'(\vec{u}) \Rightarrow ! \dashv \bot} \text{U}\Lambda - \text{Clash}$$

• Flex-\*, no cycle

$$\frac{M \notin u \qquad \Gamma \vdash u :> M(\vec{x}) \Rightarrow w; \sigma \vdash \Delta}{\Gamma, M : m \vdash M(\vec{x}) = u \Rightarrow \sigma, M \mapsto w \vdash \Delta} \text{U}\Lambda\text{-NoCycle} \quad + \text{symmetric rule}$$

Flex-Flex, same

$$\frac{m \vdash \vec{x} = \vec{y} \Rightarrow \vec{z} \dashv p}{\Gamma, M : m \vdash M(\vec{x}) = M(\vec{y}) \Rightarrow M \mapsto M'(\vec{z}) \dashv \Gamma, M' : p} \text{U}\Lambda\text{-Flex}$$

• Flex-Rigid, cyclic

$$\frac{M \in u \quad u \neq M(\dots)}{\Gamma, M : m \vdash M(\vec{x}) = u \Rightarrow ! \dashv \bot} \text{U}\Lambda\text{-CYCLIC} \quad + \text{ symmetric rule}$$

## Non-cyclic Phase

Structural rules

Rigid

bound variable

$$\frac{\Gamma \vdash t :> M'(\vec{x}, \vec{n+1}) \Rightarrow w; \sigma \vdash \Delta}{\Gamma \vdash \lambda t :> M(\vec{x}) \Rightarrow \lambda w; \sigma \vdash \Delta} P \Lambda - LAM \qquad \frac{\Gamma \vdash t, u :> M_1(\vec{x}), M_2(\vec{x}) \Rightarrow w_1, w_2; \sigma \vdash \Delta}{\Gamma \vdash t u :> M(\vec{x}) \Rightarrow w_1 w_2; \sigma \vdash \Delta} P \Lambda - APP$$

$$\frac{y=x_i}{\Gamma\vdash y:>M(\vec{x})\Rightarrow i; 1_\Gamma\dashv \Gamma} \text{P}\Lambda\text{-VarOk} \qquad \frac{y\notin \vec{x}}{\Gamma\vdash y:>M(\vec{x})\Rightarrow !; !\dashv \bot} \text{P}\Lambda\text{-VarFail}$$

Flex

$$\frac{n \vdash \vec{x} :> \vec{y} \Rightarrow \vec{l}; \vec{r} \dashv p}{\Gamma, N : n \vdash \mathbb{N}(\vec{x}) \land \mathbb{N}(\vec{y}) \land \mathbb{N}} \land \mathbb{N}(\vec{y}) \lor \mathbb{N} + \mathbb{$$

Fig. 1. Unification for pure  $\lambda$ -calculus (Section §2.1)

## Judgments

$$\Gamma \vdash \vec{t} = \vec{u} \Rightarrow \sigma \vdash \Delta \iff \sigma : \Gamma \rightarrow \Delta \text{ is the most general unifier of } \vec{t} \text{ and } \vec{u}$$

 $\Gamma \vdash \vec{u} :> \overrightarrow{M(x)} \Rightarrow \vec{w}; \sigma \vdash \Delta \iff \sigma : \Gamma \rightarrow \Delta \text{ extended with } M_i \mapsto w_i \text{ is the most general unifier of } \Gamma \vdash \vec{u} := \vec{v}$ 

$$m \vdash x = y \Rightarrow z \dashv p \iff p \xrightarrow{z} m \xrightarrow{x} \dots$$
 is an equaliser in  $\mathcal{A}$ 

$$p \xrightarrow{l} n$$

$$r \downarrow \qquad \qquad |x \text{ is a pullback in } \mathcal{A}$$

$$\dots \xrightarrow{y} \dots$$

## **Unification Phase**

• Structural rules

$$\begin{array}{c|c} \hline \Gamma \vdash () = () \Rightarrow 1_{\Gamma} \dashv \overline{\Gamma} & \hline \bot \vdash \overrightarrow{t} = \overrightarrow{u} \Rightarrow ! \dashv \bot \\ \hline \Gamma \vdash t_{1} = u_{1} \Rightarrow \sigma_{1} \dashv \Delta_{1} & \Delta_{1} \vdash \overrightarrow{t_{2}}[\sigma_{1}] = \overrightarrow{u_{2}}[\sigma_{1}] \Rightarrow \sigma_{2} \dashv \Delta_{2} \\ \hline \Gamma \vdash t_{1}, \overrightarrow{t_{2}} = u_{1}, \overrightarrow{u_{2}} \Rightarrow \sigma_{1}[\sigma_{2}] \dashv \Delta_{2} \\ \hline \end{array}$$
 U-Split

• Rigid-rigid

$$\frac{\Gamma \vdash \vec{t} = \vec{u} \Rightarrow \sigma \vdash \Delta}{\Gamma \vdash o(\vec{t}) = o(\vec{u}) \Rightarrow \sigma \vdash \Delta} \text{U-RigRig} \qquad \frac{o \neq o'}{\Gamma \vdash o(\vec{t}) = o'(\vec{u}) \Rightarrow ! \dashv \bot} \text{U-Clash}$$

• Flex-\*, no cycle

$$\frac{M \notin u \qquad \Gamma \vdash u :> M(x) \Rightarrow w; \sigma \vdash \Delta}{\Gamma, M : m \vdash M(x) = u \Rightarrow \sigma, M \mapsto w \vdash \Delta} \text{U-NoCycle} + \text{symmetric rule}$$

• Flex-Flex, same

$$\frac{m \vdash x = y \Rightarrow z \dashv p}{\Gamma, M : m \vdash M(x) = M(y) \Rightarrow M \mapsto M'(z) \dashv \Gamma, M' : p} \text{U-Flex}$$

• Flex-Rigid, cyclic

$$\frac{M \in u \quad u \neq M(\dots)}{\Gamma. M: m \vdash M(x) = u \Rightarrow ! \dashv \bot} \text{U-CYCLIC} + \text{symmetric rule}$$

## Non-cyclic Phase

• Structural rules

• Rigid

$$\frac{\Gamma \vdash \vec{t} :> M_1(x_1^{o'}), \ldots, M_n(x_n^{o'}) \Rightarrow \vec{u}; \sigma \vdash \Delta \quad o = o'\{x\}}{\Gamma \vdash o(\vec{t}) :> M(x) \Rightarrow o'(\vec{u}); \sigma \vdash \Delta} \text{P-Rig} \quad \frac{o \neq \ldots \{x\}}{\Gamma \vdash o(\vec{t}) :> M(x) \Rightarrow !; ! \vdash \bot} \text{P-Fail}$$

Flex

$$\frac{n \vdash x :> y \Rightarrow l; r \dashv p}{\Gamma, N : n \vdash N(x) :> M(y) \Rightarrow P(l); N \mapsto P(r) \dashv \Gamma, P : p} \text{P-Flex}$$

Fig. 2. Generic pattern unification algorithm (Section §2.2) Proc. ACM Program. Lang., Vol. 1, No. POPL, Article 1. Publication date: January 2024.

Generic pattern unification 1:5

```
\begin{array}{l} \operatorname{data} \ \ \subseteq \ \{A:\operatorname{Set}\}\ (a:A):\operatorname{List}\ A \to \operatorname{Set}\ \text{where} \\ 0:\forall\ \{\ell\} \to a \in (a::\ell) \\ 1+:\forall\ \{x\ \ell\} \to a \in \ell \to a \in (x::\ell) \end{array}
\begin{array}{c} a \in \ell \\ \overline{a \in (a,\ldots)} \quad \overline{a \in \ell} \\ \overline{a \in (x,\ell)} \end{array}
\operatorname{MetaContext}:\operatorname{Set}
```

 $MetaContext = List \mathbb{N}$ 

```
\implies : \mathbb{N} \to \mathbb{N} \to \mathsf{Set}
m \Rightarrow n = \mathsf{Vec} (\mathsf{Fin} \ n) \ m
```

```
data Tm (\Gamma : MetaContext) (n : \mathbb{N}) : Set where

Var : Fin \ n \to Tm \ \Gamma \ n

App : Tm \ \Gamma \ n \to Tm \ \Gamma \ n \to Tm \ \Gamma \ n

Lam : Tm \ \Gamma \ (1 + n) \to Tm \ \Gamma \ n

\_(\_) : \forall \{m\} \to m \in \Gamma \to m \Rightarrow n \to Tm \ \Gamma \ n
```

```
\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 \quad u} \quad \frac{\Gamma; n \vdash 1 \vdash t}{\Gamma; n \vdash \lambda t}
\xrightarrow{x_1, \dots, x_m \in \{1, \dots, n\} \text{ distinct}}
\underline{M : m \in \Gamma} \quad x : m \Rightarrow n
\Gamma; n \vdash M(x_1, \dots, x_m)
```

Fig. 3. Syntax of  $\lambda$ -calculus (Section §2.1)

(2) a variable context, 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 variable context n consist of elements of Fin n, the type of natural numbers between 1 and n. We also use a nameless encoding of metavariable contexts: they are mere lists of metavariable arities, and metavariables are referred to by their index in the list (starting from 0). More concretely, let us focus on the last 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  $\Gamma$ . This constructor also takes an argument of type  $m \Rightarrow n$ , which unfolds as Vec (Fin n) m: this is the type of lists of size m consisting of natural numbers between 1 and n. Note that contrary to our mathematical description, the Agda code does not explicitly enforce that the metavariable arguments are distinct. Anyway, our unification algorithm is only guaranteed to produce correct outputs if this constraint is satisfied in the inputs.

The Agda implementation of metavariable substitution is listed in Figure 5. A *metavariable substitution*  $\sigma: \Gamma \to \Delta$  assigns to each metavariable M of arity m in  $\Gamma$  a term  $\Delta$ ;  $m \vdash \sigma_M$ . In Agda, the type of substitutions between  $\Gamma$  and  $\Delta$  is defined as VecList (Tm  $\Delta$ )  $\Gamma$ , where VecList.t  $X \ell$  is (recursively) defined as the product type X  $a_1 \times \cdots \times X$   $a_n$  for any dependent type  $X: A \to \operatorname{Set}$  and list  $\ell = [a_1, \ldots, a_n]$  of elements of A.

This assignation extends (through a recursive definition) to any term  $\Gamma$ ;  $n \vdash t$ , yielding a term  $\Delta$ ;  $n \vdash t[\sigma]$ . The base case is

$$M(x_1,\ldots,x_m)[\sigma] = \sigma_M\{x\},$$

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

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            id: \forall \{n\} \rightarrow n \Rightarrow n
                                                                                                                                                              : n \Rightarrow n
247
            id \{n\} = Vec.allFin n
249
            o: \forall \{p \ q \ r\} \rightarrow (q \Rightarrow r) \rightarrow (p \Rightarrow q) \rightarrow (p \Rightarrow r)
                                                                                                                                                 x \circ y
            xs \circ [] = []
251
            xs \circ (y :: ys) = Vec.lookup xs y :: (xs \circ ys)
                                                                                                                                         (x_{u_1},\ldots,x_{u_n})
253
            \uparrow: \forall \{p \ q\} \rightarrow p \Rightarrow q \rightarrow (1+p) \Rightarrow (1+q)
255
            \uparrow \{p\}\{q\} \ x = \text{Vec.insert (Vec.map Fin.inject}_1 \ x)
                                                                                                                                                          : p + 1 \Rightarrow q + 1
                                       (Fin.from\mathbb{N} p) (Fin.from\mathbb{N} q)
                                                                                                                                    (x_1,...,x_p,q+1)
                                                                                                                                         \Gamma; n \vdash t
            \{ \} : \forall \{ \Gamma \ n \ p \} \rightarrow \mathsf{Tm} \ \Gamma \ n \rightarrow n \Rightarrow p \rightarrow \mathsf{Tm} \ \Gamma \ p
                                                                                                                                                   \Gamma; p \vdash t\{x\}
            App t u \{ f \} = App (t \{ f \}) (u \{ f \})
261
            Lam \ t \{ f \} = Lam \ (t \{ f \uparrow \})
262
263
            Var i \{ f \} = Var (i \{ f \})
            M(x) \{ f \} = M(f \circ x)
267
                                                                 Fig. 4. Renaming for \lambda-calculus (Section §2.1)
269
             \_ : MetaContext \rightarrow MetaContext \rightarrow Set
270
            \Gamma \longrightarrow \Delta = \text{VecList} (\text{Tm } \Delta) \Gamma
271
272
273
274
            [\_]t : \forall \{\Gamma \ n\} \to \mathsf{Tm} \ \Gamma \ n \to \forall \{\Delta\} \to (\Gamma \longrightarrow \Delta) \to \mathsf{Tm} \ \Delta \ n
275
            App t u [\sigma]t = App (t [\sigma]t) (u [\sigma]t)
276
                                                                                                                                                      \Gamma; n \vdash t
                                                                                                                                                                            \sigma:\Gamma\to\Delta
            Lam t [\sigma]t = Lam (t [\sigma]t)
277
                                                                                                                                                                 \Delta; n \vdash t[\sigma]
            Var i [\sigma]t = Var i
278
            M(x)[\sigma]t = \text{VecList.nth } M \sigma \{x\}
279
280
281
                                                                                                                                               \frac{\sigma: \Gamma_1 \to \Gamma_2 \quad \delta: \Gamma_2 \to \Gamma_3}{\sigma[\delta] \quad : \Gamma_1 \to \Gamma_3}
            []s: \forall \{\Gamma_1 \ \Gamma_2 \ \Gamma_3\} \rightarrow (\Gamma_1 \longrightarrow \Gamma_2) \rightarrow (\Gamma_2 \longrightarrow \Gamma_3) \rightarrow (\Gamma_1 \longrightarrow \Gamma_3)
282
            \delta [\sigma]s = \text{VecList.map}(\lambda \quad t \rightarrow t [\sigma]t) \delta
283
284
285
```

Fig. 5. Metavariable substitution for  $\lambda$ -calculus (Section §2.1)

where  $-\{x\}$  is variable renaming (see Figure 4). For example, the identity substitution  $1_{\Gamma}: \Gamma \to \Gamma$  is defined by the term  $M(1, \ldots, m)$  for each metavariable declaration  $M: m \in \Gamma$ . The composition  $\sigma[\sigma']: \Gamma_1 \to \Gamma_3$  of two substitutions  $\sigma: \Gamma_1 \to \Gamma_2$  and  $\sigma': \Gamma_2 \to \Gamma_3$  is defined as  $M \mapsto \sigma_M[\sigma']$ .

A unifier of two terms  $\Gamma$ ;  $n \vdash t, u$  is a substitution  $\sigma : \Gamma \to \Gamma'$  such that  $t[\sigma] = u[\sigma]$ . A most general unifier of t and u is a unifier  $\sigma : \Gamma \to \Gamma'$  that uniquely factors any other unifier  $\delta : \Gamma \to \Delta$ ,

Fig. 6. Unification of two metavariables for  $\lambda$ -calculus (Section §2.1)

unify-flex-flex : 
$$\forall \{\Gamma \ m \ m' \ n\} \rightarrow m \in \Gamma \rightarrow m \Rightarrow n$$
  
  $\rightarrow m' \in \Gamma \rightarrow m' \Rightarrow n \rightarrow \Gamma \longrightarrow ?$   
unify-flex-flex  $\{\Gamma\} \ M \ x \ M' \ y \ with \ M' \ \ \ \ \ M$ 

... 
$$| \perp =$$
  
let  $p$ ,  $z =$  commonPositions  $x$   $y$  in  
 $\Gamma [M: p] \blacktriangleleft M \mapsto -(z)$ 

$$\frac{M: m \in \Gamma \qquad m \vdash x = y \Rightarrow z \dashv p}{\Gamma \vdash M(x) = M(y) \Rightarrow M \mapsto P(z) \dashv P: p, \Gamma \backslash M}$$
FLEX-EQ

... 
$$| \lfloor M' \rfloor =$$

let  $p, l, r = \text{commonValues } x y \text{ in}$ 
 $\Gamma \setminus M [M': p] \blacktriangleleft M \mapsto (M': p) (l)$ 
 $M' \mapsto (r)$ 

$$M: m, M': m' \in \Gamma \quad M \neq M'$$

$$m \vdash x :> y \Rightarrow l; r \dashv p$$

$$\Gamma \vdash M(x) = M'(y) \Rightarrow$$

$$\begin{pmatrix} M \mapsto P(l) \\ M' \mapsto P(r) \end{pmatrix} \dashv P: p, \Gamma \backslash M \backslash M'$$

in the sense that there exists a unique  $\delta': \Gamma' \to \Delta$  such that  $\delta = \sigma[\delta']$ . We denote this situation by  $\Gamma \vdash t = u \Rightarrow \sigma \dashv \Gamma'$ , leaving the variable context *n* implicit. Intuitively, the symbol  $\Rightarrow$  separates the input and the output of the unification algorithm, which either returns a most general unifier, or fails when there is no unifier at all (for example, when unifying  $t_1$   $t_2$  with  $\lambda u$ ). The type signature of our unification algorithm is thus

```
data \longrightarrow ? (\Gamma : MetaContext) : Set where
     \blacktriangleleft : \forall \Delta \rightarrow (\Gamma \longrightarrow \Delta) \rightarrow \Gamma \longrightarrow ?
unify: \forall \{\Gamma \ n\} \rightarrow \mathsf{Tm} \ \Gamma \ n \rightarrow \mathsf{Tm} \ \Gamma \ n \rightarrow \mathsf{Maybe} \ (\Gamma \longrightarrow ?)
```

where Maybe X is an inductive type with an error constructor  $\bot$  and a success constructor  $\lfloor - \rfloor$ taking as argument an element of type X.

The unification algorithm recursively inspects the structure of the given terms until reaching a metavariable at the top-level, as seen in Figure 7. In the implementation, we exploit the do notation to propagate failure. For example, in the application case, the program fails if unify t t' does, otherwise it continues with the success return values  $\Delta_1$ ,  $\sigma_1$ .

From a mathematical point of view, it is more convenient to handle failure by considering<sup>2</sup> a formal error metavariable context  $\perp$  in which the only term (in any variable context) is a formal error term!, inducing a unique substitution! :  $\Gamma \to \bot$ , satisfying t[!] = ! for any term t, as demonstrated in the last case when unifying two different rigid term constructors (application,  $\lambda$ -abstraction, or variables). With this extended meaning, the inductive rule for application remains sound, in a sense that will be clarified in Section §3.1. Formally, failure propagation is modelled by the following rule.

<sup>&</sup>lt;sup>2</sup>In Section §3.1, we interpret ⊥ as a terminal object freely added to the category of metavariable contexts and substitutions between them.

 Unification of two metavariables applications  $M(x_1,\ldots,x_m)$  and  $M'(y_1,\ldots,y_{m'})$  is detailed in Figure 6. The algorithm starts by testing whether M' is in  $\Gamma\backslash M$ , which denotes the context  $\Gamma$  without M. Note that this doesn't hold precisely when M=M'. In this case, we need to consider the *vector of common positions* of x and y, that is, the maximal vector of (distinct) positions  $(z_1,\ldots,z_p)$  such that  $x_{\vec{z}}=y_{\vec{z}}$ . We denote<sup>3</sup> such a situation by  $m\vdash x=y\Rightarrow z\dashv p$ . 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, and  $\sigma$  maps M to P(z).

Example 2.1. 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  $M(x, y)[\sigma] = \sigma_M\{1 \mapsto x, 2 \mapsto y\}$  and  $M(z, x)[\sigma] = \sigma_M\{1 \mapsto z, 2 \mapsto x\}$  must be equal,  $\sigma_M$  cannot depend on the variables 1, 2. It follows that the most general unifier is  $M \mapsto M'$ , replacing M with a fresh constant metavariable M'. A similar argument shows that the most general unifier of M(x, y) and M(z, y) is  $M \mapsto M'(z)$ .

The corresponding rule Flex-EQ does not stipulate how to generate the fresh metavariable symbol P. But since M is removed from  $\Gamma$ , the name M becomes fresh and therefore provides a canonical choice. Accordingly, the implementation keeps M but changes its arity to p, resulting in a context denoted by  $\Gamma[M:p]$ .

If  $M \neq M'$ , consider the vectors of common values positions  $(l_1,\ldots,l_p)$  and  $(r_1,\ldots,r_p)$  between  $x_1,\ldots,x_m$  and  $y_1,\ldots,y_{m'}$ , i.e., the pair of maximal lists  $(\vec{l},\vec{r})$  of distinct positions such that  $x_{\vec{l}} = y_{\vec{r}}$ . We denote such a situation by  $m \vdash x :> y \Rightarrow l; r \dashv p$ . 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(l) and M' to P(r).

*Example 2.2.* 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 previously, the corresponding rule Flex-NeQ does not stipulate how to generate the fresh metavariable symbol P. But since both M and M' are removed from the context, either of them can be chosen as a fresh metavariable. The implementation actually picks M'.

Unification of a metavariable application  $M(x_1, \ldots, x_m)$  with a term u is detailed in Figure 8. We have just discussed the case when u is a metavariable. Let us detail the other case. The algorithm starts by checking whether M can be removed from the metavariable context in which u is typed. If not, then  $u \setminus ?_t M$  fails and the do notation propagates the error. This situation described by the failing rule Cycle happens precisely when M occurs in u: since u is not a metavariable, there is no unifier because the size of both hand sides can never match after substitution.

We are left with the case when M does not occur in u. The algorithm then enters a *non-cyclic phase*, which specifically addresses such non-cyclic unification problems: this is what happens in the premise of the rule No-cycle. It uses<sup>4</sup> the notation  $\Gamma \vdash u :> M(\vec{x}) \Rightarrow w; \sigma \dashv \Delta$  for this non-cyclic phase, where u is a term in the metavariable context  $\Gamma$ , while M is a fresh metavariable with respect to  $\Gamma$  and  $\vec{x} = (x_1, \ldots, x_m)$  are distinct variables in the (implicit) variable context of u. The output is the most general unifier of u and  $M(\vec{x})$ , both considered in the extended metavariable context  $M: m, \Gamma$ . This substitution from  $M: m, \Gamma$  to  $\Delta$  is explicitly defined as the extension of a substitution  $\sigma: \Gamma \to \Delta$  with a term  $\Delta; m \vdash w$  for substituting M. The type signature of the non-cyclic phase is thus

```
unify-no-cycle : \forall \{\Gamma \ n\} \rightarrow \mathsf{Tm} \ \Gamma \ n \rightarrow \forall \{m\} \rightarrow m \Rightarrow n \rightarrow \mathsf{Maybe} \ (m :: \Gamma \longrightarrow ?)
```

<sup>&</sup>lt;sup>3</sup>The similarity with the above introduced notation is no coincidence: as we will see (Remark 3.4), both are (co)equalisers. <sup>4</sup>The similarity with the notation for common value positions is no coincidence: both are (co)pullbacks, as we will see in Remark 5.1.

Generic pattern unification 1:9

```
See Figure 8.
                                                                                                                                                                \Gamma \vdash t = t' \Rightarrow \sigma \dashv \Delta
unify (Lam t) (Lam t') = unify t t'
                                                                                                                                                              \frac{\Gamma \vdash \lambda t = \lambda t' \Rightarrow \sigma \dashv \Lambda}{\Gamma \vdash \lambda t = \lambda t' \Rightarrow \sigma \dashv \Lambda}
unify (App tu) (App t'u') = do
                                                                                                                                                              \Gamma \vdash t = t' \Rightarrow \sigma_1 \dashv \Delta_1
    \Delta_1 \blacktriangleleft \sigma_1 \leftarrow \text{unify } t \ t'
                                                                                                                                                   \Gamma \vdash u[\sigma_1] = u'[\sigma_2] \Rightarrow \sigma_2 \dashv \Delta_2
    \Delta_2 \blacktriangleleft \sigma_2 \leftarrow \text{unify } (u [ \sigma_1 ]t) (u' [ \sigma_1 ]t)
                                                                                                                                                   \Gamma \vdash t \ u = t' \ u' \Rightarrow \sigma_1 [\sigma_2] \dashv \Delta_2
    |\Delta_2 \triangleleft \sigma_1 [\sigma_2]s|
unify \{\Gamma\} (Var i) (Var j) with i Fin. \stackrel{f}{=} j
                                                                                                                                     \frac{i \neq j}{\Gamma \vdash \underline{i} = j \Rightarrow ! \dashv \bot} \qquad \overline{\Gamma \vdash \underline{i} = \underline{i} \Rightarrow 1_{\Gamma} \dashv \Gamma}
... | no _ = ⊥
... | yes = | \Gamma \triangleleft id_s |
                                                                                                                                                 o \neq o' (rigid term constructors)
unify _ _ = ⊥
                                                                                                                                                        \Gamma \vdash o(\vec{t}) = o'(\vec{t'}) \Rightarrow ! \dashv \bot
```

Fig. 7. Unification for  $\lambda$ -calculus (Section §2.1): main phase

Fig. 8. Unification with a metavariable application for  $\lambda$ -calculus (Section §2.1)

```
unify-flex-* : \forall \{\Gamma \ m \ a\} \rightarrow m \in \Gamma \rightarrow m \Rightarrow a \rightarrow \operatorname{Tm} \Gamma \ a \rightarrow \operatorname{Maybe} (\Gamma \longrightarrow ?)
unify-flex-* M \ x \ (N \ (y \ )) = \lfloor \operatorname{unify-flex-flex} M \ x \ N \ y \rfloor

unify-flex-* M \ x \ u = \operatorname{do}
u \leftarrow u \setminus ?_t \ M
\Delta \blacktriangleleft t \ , \sigma \leftarrow \operatorname{unify-no-cycle} u \ x
\lfloor \Delta \blacktriangleleft M \mapsto t \ , \sigma \rfloor
unify-flex-* M \ x \ u = \operatorname{do}
u \leftarrow u \setminus ?_t \ M
\Delta \blacktriangleleft t \ , \sigma \leftarrow \operatorname{unify-no-cycle} u \ x
| \Delta \blacktriangleleft M \mapsto t \ , \sigma |
| \Delta \blacktriangleleft M \mapsto t \ , \sigma |
```

Note that contrary to the above notation, because of the nameless encoding, the fresh metavariable symbol M is not explicit.

Remark 2.3. The symbol :> evokes the pruning involved in this phase. Indeed, one intuition behind the non-cyclic unification of  $M(\vec{x})$  and u consists in taking  $u[x_i \mapsto i]$  as a definition for M. This only makes sense if the free variables of u are among  $\vec{x}$ : if u is a variable that does not occur in  $\vec{x}$ , then obviously there is no unifier. However, it is possible to remove the outbound variables in u if they only occur in metavariable arguments, by restricting the arities of those metavariables. We accordingly call  $\sigma: \Gamma \to \Delta$  the pruning substitution. As an example, if u is a metavariable application  $N(\vec{x}, \vec{y})$ , then although the free variables are not all included in  $\vec{x}$ , there is still a most general unifier, and the corresponding pruning substitution essentially replaces N with M, discarding the outbound variables  $\vec{y}$ .

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unify-no-cycle (M(x)) y =
    | unify-flex-flex (1+ M) \times 0 y |
                                                                                                                      M': m', \Gamma \vdash M(x) = M'(y) \Rightarrow t, \sigma \dashv \Delta
                                                                                                                             \Gamma \vdash M(x) :> M'(y) \Rightarrow t : \sigma \dashv \Delta
unify-no-cycle (M(x)) y =
    | unify-flex-flex (1+ M) x 0 y |
unify-no-cycle (Lam t) x = do
                                                                                                                                \Gamma \vdash t :> M'(x \uparrow) \Rightarrow t'; \sigma \dashv \Delta
    \Delta \blacktriangleleft t', \sigma \leftarrow \text{unify-no-cycle } t(x \uparrow)
                                                                                                                                \Gamma \vdash \lambda t :> M(x) \Rightarrow \lambda t'; \sigma \dashv \Delta
    | \Delta \triangleleft \text{Lam } t', \sigma |
                                                                                                                                  \frac{i=x_j}{\Gamma \vdash \underline{i} :> M(x) \Rightarrow \underline{j}; 1_{\Gamma} \dashv \Gamma}
unify-no-cycle \{\Gamma\} (Var i) x with i \{x\}^{-1}
... | __ = __
                                                                                                                                    \frac{i \notin \vec{x}}{\Gamma \vdash i :> M(x) \Rightarrow !; ! \dashv \bot}
... | | j | = | \Gamma \triangleleft Var j, id_s |
unify-no-cycle (App t u) x = do
    \Delta_1 \blacktriangleleft t', \sigma_1 \leftarrow \text{unify-no-cycle } t x
                                                                                                                               \Gamma \vdash t :> M_1(x) \Rightarrow t'; \sigma_1 \dashv \Delta_1
    \Delta_2 \blacktriangleleft u', \sigma_2 \leftarrow \text{unify-no-cycle} (u [\sigma_1]t) x
                                                                                                                        \Delta_1 \vdash u[\sigma_1] :> M_2(x) \Rightarrow u'; \sigma_2 \dashv \Delta_2
    [\Delta_2 \blacktriangleleft App(t'[\sigma_2]t)u', \sigma_1[\sigma_2]s]
                                                                                                                  \frac{\Gamma \vdash t \ u :> M(x) \Rightarrow t'[\sigma_2] \ u' : \sigma_1[\sigma_2] + \Delta_2}{\Gamma \vdash t \ u :> M(x) \Rightarrow t'[\sigma_2] \ u' : \sigma_1[\sigma_2] + \Delta_2}
```

Fig. 9. Non-cyclic unification for  $\lambda$ -calculus (Section §2.1)

The non-cyclic phase proceeds recursively as in Figure 9. The metavariable case is straightforward. In the variable case,  $i\{x\}^{-1}$  returns the index j such that  $i=x_j$ , or fails if no such j exist. For  $\lambda$ -abstraction, a fresh variable M' is introduced for the body of the  $\lambda$ -abstraction which is additionally applied to the bound variable n+1, as it should not be pruned. Keeping in mind the intuition that  $M=\lambda M'$ , if M' is to be substituted with t', then M should be substituted with  $\lambda t'$ , thus justifying the conclusion of the rule.

This ends our description of the unification algorithm, in the specific case of pure  $\lambda$ -calculus. The purpose of this work is to present a generalisation, by parameterising the algorithm by a signature specifying a syntax.

#### 2.2 Generalisation

## To adapt

Our algorithm is parameterised by a notion of signature generalising binding signatures Aczel [2016] to account for syntax with metavariables.

To recall, a binding signature  $(O, \alpha)$  specifies for each natural number n a set of n-ary operation symbols  $O_n$  and for each  $o \in O_n$ , an arity  $\alpha_o = (\overline{o}_1, \dots, \overline{o}_n)$  as a list of natural numbers specifying how many variables are bound in each argument. For example, pure  $\lambda$ -calculus is specified by  $O_1 = \{lam\}, O_2 = \{app\}, \alpha_{app} = (0, 0), \alpha_{lam} = (1), \text{ and } O_n = \emptyset \text{ for any natural number } n \notin \{1, 2\}.$ 

Our algorithm is parameterised by a *generalised binding signature*, or GB-signature, a notion we will formally introduce in Definition 3.11, and is implemented in Agda code as shown in Figure 10. A GB-signature consists in a tuple  $(\mathcal{A}, O, \alpha)$  consisting of

• a small category  $\mathcal{A}$  whose objects are called *arities* or *variable contexts*, and whose morphisms are called *renamings*;

Generic pattern unification 1:11

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538 539 Tms  $\Gamma$  as = VecList.t (Tm  $\Gamma$ ) (Vec.toList as)

```
In the following, Vec X n is the type of vectors of elements of X of size n. Given two vectors
\ell = [a_1, \dots, a_n] and \ell' = [a'_1, \dots, a'_n] of objects of the same category, the type \ell \lor \Rightarrow \ell' is
recursively defined as the type (a_1 \Rightarrow a'_1) \times \cdots \times (a_n \Rightarrow a'_n).
record Signature: Set where
   field
      A: Category
   module A = Category \mathcal{A}
   module V = VecMor \mathcal{A}
   field
      O: \mathbb{N} \to A.Obj \to Set
      \alpha: \forall \{n \ a\} \rightarrow (o: \bigcirc n \ a) \rightarrow \text{Vec A.Obj } n
      - The last two fields account for functoriality
      \{a\}: \forall \{n\}\{a\} \rightarrow \bigcirc n \ a \rightarrow \forall \{b\} \ (f: a \land A \Rightarrow b) \rightarrow \bigcirc n \ b
      ^{\land}: \forall \{a\}\{b\}(f: a \land A.\Rightarrow b)\{n\}(o: \bigcirc n \ a) \rightarrow (\alpha \ o) \lor A.\Rightarrow (\alpha \ (o \ f \ b))
MetaContext : Set
MetaContext = List A.Obj
Tms : MetaContext \rightarrow \forall \{n\}(v : \text{Vec A.Obj } n) \rightarrow \text{Set}
data Tm (\Gamma: MetaContext) (a: A.Obj) : Set where
   Rigid: \forall \{n\} (o: \bigcirc n \ a) \rightarrow \mathsf{Tms} \ \Gamma (\alpha \ o) \rightarrow \mathsf{Tm} \ \Gamma \ a
   Flexible : \forall \{m\} (M : m \in \Gamma)(f : m \land A \Rightarrow a) \rightarrow \mathsf{Tm} \Gamma a
```

Fig. 10. Definition of signatures and associated syntax in Agda

- for each variable context a and natural number n, a set of n-ary operation symbols  $O_n(a)$ ;
- for each operation symbol  $o \in O_n(a)$ , a list of variable contexts  $\alpha_o = (\overline{o}_1, \dots, \overline{o}_n)$

such that O and  $\alpha$  are functorial in a suitable sense (see Remark 2.7 below). Intuitively,  $O_n(a)$  is the set of n-ary operation symbols available in the variable context a.

*Definition 2.4.* The syntax specified by a GB-signature  $(\mathcal{A}, O, \alpha)$  is inductively generated by the two following rules.

$$\frac{o \in O_n(a) \quad \Gamma; \overline{o}_1 \vdash t_1 \quad \dots \quad \Gamma; \overline{o}_n \vdash t_n}{\Gamma; a \vdash o(t_1, \dots, t_n)} RIG$$

$$\frac{M : m \in \Gamma \quad x \in \hom_{\mathcal{A}}(m, a)}{\Gamma; a \vdash M(x)} FLEX$$

where a context  $\Gamma$ ; a consists of a variable context a and a metavariable context  $\Gamma$ , as a metavariable arity function from a finite set of metavariable symbols to the set of objects of  $\mathcal{A}$ . We call a term rigid if it is of the shape  $o(\ldots)$ , flexible if it is  $M(\ldots)$ .

*Remark 2.5.* The syntax in the empty metavariable context does not depend on the morphisms in  $\mathcal{A}$ . In fact, by restricting the morphisms in the category of arities to identity morphisms, any

 GB-signature induces an indexed container Altenkirch and Morris [2009] generating the same syntax without metavariables.

*Example 2.6.* Binding signatures can be compiled into GB-signatures. More specifically, a syntax specified by a binding signature  $(O, \alpha)$  is also generated by the GB-signature  $(\mathbb{F}_m, O', \alpha')$ , where

- $\mathbb{F}_m$  is the category of finite cardinals and injections between them;
- $O'_n(p) = \{v_1, \ldots, v_p\} \sqcup \{o_p | o \in O_n\};$
- $\alpha'_{v_i} = ()$  and  $\alpha'_{o_p} = (p + \overline{o}_1, \dots, p + \overline{o}_n)$  for any  $i, p, n \in \mathbb{N}, o \in O_n$ .

Note that variables  $v_i$  are explicitly specified as nullary operations and thus do not require a dedicated generating rule, contrary to what happens with binding signatures. Moreover, the choice of renamings (i.e., morphisms in the category of arities) is motivated by the Flex rule. Indeed, if M has arity  $m \in \mathbb{N}$ , then a choice of arguments in the variable context  $a \in \mathbb{N}$  consists of a list of distinct variables in the variable context a, or equivalently, an injection between the cardinal sets m and a, that is, a morphism in  $\mathbb{F}_m$  between m and a.

GB-signatures capture multi-sorted binding signatures such as simply-typed  $\lambda$ -calculus, or polymorphic syntax such as System F (see Section §7).

Remark 2.7. In the notion of GB-signature, functoriality ensures that the generated syntax supports renaming: given a morphism  $f: a \to b$  in  $\mathcal{A}$  and a term  $\Gamma; a \vdash t$ , we can recursively define a term  $\Gamma; b \vdash t\{f\}$ . The case of metavariables is simple:  $M(x)\{f\} = M(f \circ x)$ . For an operation  $o(t_1, \ldots, t_n)$ , functoriality provides the following components:

- an operation symbol  $o\{f\} \in O_n(b)$ ;
- a morphism  $f_i^o : \overline{o}_i \to \overline{o\{f\}}_i$  for each  $i \in \{1, ..., n\}$ .

Then,  $o(t_1, ..., t_n)\{f\}$  is defined as  $o\{f\}\{t_1\{f_1^o\}, ..., t_n\{f_n^o\}\}$ .

Unification can be formulated by following the same route as in Section §2.1. A metavariable substitution  $\sigma$  from  $\Gamma = (M_1 : m_1, ..., M_p : m_p)$  to  $\Delta$  is a list of terms  $(\sigma_1, ..., \sigma_p)$  such that  $\Delta$ ;  $m_i \vdash \sigma_i$ . Given a term  $\Gamma$ ;  $a \vdash t$ , we can recursively define the substituted term  $\Delta$ ;  $a \vdash t[\sigma]$  by  $o(\vec{t})[\sigma] = o(\vec{t}[\sigma])$  and  $M_i(x)[\sigma] = \sigma_i\{x\}$ .

Figure 2 summarises our generic algorithm, parameterised by a GB-signature, and a few more parameters: a solver for the equation

$$o = o'\{x\},\tag{1}$$

where o' is the unknown (see the rules P-Rig and P-Fail, detailed below), and a construction of equalisers and pullbacks in  $\mathcal{A}$ , highlighted in blue. These are used to compute the most general unifier of two metavariable applications in the rules U-Flex and P-Flex. Specialised to pure  $\lambda$ -calculus, they correspond to the rules U $\Lambda$ -Flex and P $\Lambda$ -Flex: indeed, the vector of common positions of  $\vec{x}$  and  $\vec{y}$  can be characterised as their equaliser in  $\mathbb{F}_m$ , when thinking of lists as functions from a finite cardinal, while the vectors of common value positions can be characterised as a pullback.

The main differences with the example of pure  $\lambda$ -calculus presented above in Figure 1 is that the vector notation is dropped for arguments of metavariables, since they are abstracted as morphisms in a category<sup>5</sup>. Moreover, the case for operations and variables are merged in the non-cyclic phase with the rules P-Rig and P-Fail that both handle non-cyclic unification of M(x) with  $o(\vec{t})$ . If  $o = o'\{x\}$  for some o', then the rule P-Rig applies; otherwise, the rule P-Fail outputs an error. Let us explain how they specialise for a syntax specified by a binding signature as in Example 2.6. In this case, x is a list of distinct variables  $(x_1, \ldots, x_m)$ . If o is a variable  $v_i$ , then the side condition  $o = o'\{x\}$  means that i is  $x_j$  for some variable  $o' = v_j$ . Thus, those rules account for the rules PA-Varok and PA-Varfail. On the other hand, if o is actually  $o_n$ , i.e., an operation symbol o

<sup>&</sup>lt;sup>5</sup>See Section §7.1 for an example where metavariables arguments are sets rather than lists.

Generic pattern unification

 considered in the variable context n, then, by definition of the functorial action,  $o_n = o_m\{x\}$ . Thus, the rule P-Rig always applies with  $o' = o_m$ . Moreover,  $x_i^o$  is in fact the morphism from  $m + \overline{o}_i$  to  $n + \overline{o}_i$  defined as  $x + \overline{o}_i$ , corresponding to the list  $(\vec{x}, n + 1, \dots, n + \overline{o}_i)$ . Thus, the rule P-Rig unfolds as

$$\frac{\Gamma \vdash \vec{t} :> ..., M_i(\vec{x}, n+1, ..., n+1+\overline{o}_i), ... \Rightarrow \vec{u}; \sigma \dashv \Delta}{\Gamma \vdash o(\vec{t}) :> M(\vec{x}) \Rightarrow o(\vec{u}); \sigma \dashv \Delta}.$$

Correctness of our generic algorithm relies on additional assumptions on the GB-signature that we introduce in Definition 3.12. In particular all morphisms in  $\mathcal{A}$  must be monomorphic: this ensures that Equation (1) has at most one solution (see Property 3.14.(i) below).

#### 2.3 Progress and termination

Each inductive rule in Figure 2 provides an elementary step for the construction of the most general unifier. To ensure that this set of rules describes a terminating algorithm, we essentially need two properties: *progress*, i.e., there is always one rule that applies given some input data, and *termination*, i.e., there is no infinite sequence of rule applications. The former is ensured by Agda's type-checker. In this section we sketch the proof of the latter termination property, following a standard argument. Roughly, it consists in realising that for each rule, the premises are strictly smaller than the conclusion, for an adequate notion of input size. First, we define the size  $|\Gamma|$  of a metavariable context  $\Gamma$  as the number of its declared metavariables. We extend this definition to the case where  $\Gamma = \bot$ , by taking  $|\bot| = 0$ . We also recursively define the size |It| of a term t by ||M(x)|| = 1 and  $||o(\overline{t})|| = 1 + ||\overline{t}||$ , with  $||\overline{t}|| = \sum_i ||t_i||$ . Note that no term is of empty size.

Let us first quickly justify termination of the non-cyclic phase. We define the size of a judgment  $\Gamma \vdash \vec{t} :> \overrightarrow{M(x)} \Rightarrow \vec{w}; \sigma \vdash \Delta$  as  $||\vec{t}||$ . It is straightforward to check that the sizes of the premises are strictly smaller than the size of the conclusion, for the two recursive rules P-Split and P-Rig of the non-cyclic phase, thanks to the following lemmas.

LEMMA 2.8. For any term  $\Gamma$ ;  $a \vdash t$  and substitution  $\sigma : \Gamma \to \Delta$ , if  $\sigma$  is a metavariable renaming, i.e.,  $\sigma_M$  is a metavariable application for any  $M : m \in \Gamma$ , then  $||t[\sigma]|| = ||t||$ .

Lemma 2.9. If there is a finite derivation tree of  $\Gamma \vdash \vec{t} :> \overrightarrow{M(x)} \Rightarrow \vec{w}; \sigma \dashv \Delta$  and  $\Delta \neq \bot$ , then  $|\Gamma| = |\Delta|$  and  $\sigma$  is a metavariable renaming.

The size invariance in the above lemma is actually used in the termination proof of the main unification phase, where the size of a judgment  $\Gamma \vdash t = u \Rightarrow \sigma \dashv \Delta$  is defined as the pair  $(|\Gamma|, ||t||)$ . More precisely, it is used in the following lemma that ensures size decreasing (with respect to the lexicographic order) in the two recursive rules U-Split and U-RigRig.

LEMMA 2.10. If there is a finite derivation tree of  $\Gamma \vdash \vec{t} = \vec{u} \Rightarrow \sigma \dashv \Delta$ , then  $|\Gamma| \geq |\Delta|$ , and moreover if  $|\Gamma| = |\Delta|$  and  $\Delta \neq \bot$ , then  $\sigma$  is a metavariable renaming.

#### 3 CATEGORICAL SEMANTICS

It remains to prove that each rule is sound, e.g., for the rule U-Split, if the output of the premises are most general unifiers, then so is the conclusion. To do so, the next sections 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  $S = (\mathcal{A}, O, \alpha)$  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 Barr and Wells [1990]; Rydeheard and Burstall [1988]. We furthermore provide a formal justification for the error metavariable context  $\bot$ .

Lemma 3.1. Metavariable contexts and substitutions (with their composition) between them define a category MCon(S).

This relies on functoriality of GB-signatures that we will spell out formally in the next section. There, we will see in Lemma 3.19 that this category fully faithfully embeds in a Kleisli category for a monad generated by S on  $[\mathcal{A}, \operatorname{Set}]$ .

Remark 3.2. MCon(S) is the opposite category of a multi-sorted Lawvere theory: the sorts are the objects of  $\mathcal{A}$ . This theory is not freely generated by operations unless  $\mathcal{A}$  is discrete, in which case we recover (multi-sorted) first-order unification. Even the GB-signature induced (as in Example 2.6) by an empty binding signature is not "free".

Since a substitution is precisely a list of terms sharing the same metavariable context  $\Gamma$ , a unification problem for two list of terms is equivalently given by a pair of parallel substitutions

$$\Gamma \xrightarrow{\sigma_1} \Delta$$
.

LEMMA 3.3. The most general unifier of two lists of terms  $\Delta$ ;  $n_i \vdash t_i, u_i$ , if it exists, is characterised as the coequaliser of  $\vec{t}$  as  $\vec{u}$  as substitutions from  $(N_1 : n_1, ...)$  to  $\Delta$ .

*Remark 3.4.* This justifies a common interpretation as (co)equalisers of the two variants of the notation  $-\vdash -=-\Rightarrow -\dashv -$  involved in Figure 2.

Pattern unification is often stated as the existence of a coequaliser on the condition that there is a unifier. It turns out that we can get rid of this condition by considering the category MCon(S) freely extended with a terminal object  $\bot$ , as we now explain.

Definition 3.5. Given a category  $\mathcal{B}$ , let  $\mathcal{B}_{\perp}$  denote the category  $\mathcal{B}$  extended freely with a terminal object  $\perp$ .

*Notation 3.6.* We denote by ! any terminal morphism to  $\perp$  in  $\mathcal{B}_{\perp}$ .

Adding a terminal object results in adding a terminal cocone to all diagrams. As a consequence, we have the following lemma.

Lemma 3.7. 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) I has a colimit in  $\mathcal{B}_{\perp}$ .

The following result is also useful.

Lemma 3.8. Given a category  $\mathscr{B}$ , the canonical embedding functor  $\mathscr{B} \to \mathscr{B}_{\perp}$  creates colimits.

This ensures in particular that coproducts in MCon(S), which are computed as union of metavariable contexts, are also coproducts in  $MCon_{\perp}(S)$ .

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

COROLLARY 3.9. Any coequaliser in  $\mathrm{MCon}(S)$  is also a coequaliser in  $\mathrm{MCon}_{\perp}(S)$ . Moreover, whenever there is no unifier of two lists of terms, then the coequaliser of the corresponding parallel arrows in  $\mathrm{MCon}_{\perp}(S)$  exists: it is the terminal cocone on  $\perp$ .

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734 735 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 3.12).

Theorem 3.10. Given any pattern-friendly signature S, the category  $MCon_{\perp}(S)$  has coequalisers.

## 3.2 Initial Algebra Semantics for GB-signatures

Definition 3.11. A generalised binding signature, or GB-signature, is a tuple  $(\mathcal{A}, \mathcal{O}, \alpha)$  consisting of

- a small category  $\mathcal{A}$  of arities and renamings between them;
- a functor  $O_{-}(-): \mathbb{N} \times \mathcal{A} \to \text{Set of operation symbols};$
- a functor  $\alpha: \int J \to \mathcal{A}$

where  $\int J$  denotes the category of elements of  $J: \mathbb{N} \times \mathcal{A} \to \text{Set mapping } (n, a) \text{ to } O_n(a) \times \{1, \dots, n\},$  defined as follows:

- objects are tuples (n, a, o, i) such that  $o \in O_n(a)$  and  $i \in \{1, ..., n\}$ ;
- a morphism between (n, a, o, i) and (n', a', o', i') is a morphism  $f : a \to a'$  such that n = n', i = i' and  $o\{f\} = o'$  where  $o\{f\}$  denotes the image of o by the function  $O_n(f) : O_n(a) \to O_n(a')$ . introduce the reverse partial notation for the P-RIG rule?

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

*Definition 3.12.* A GB-signature  $S = (\mathcal{A}, O, \alpha)$  is said *pattern-friendly* if

- (1)  $\mathcal{A}$  has finite connected limits;
- (2) all morphisms in  $\mathcal{A}$  are monomorphic;
- (3) each  $O_n(-): \mathcal{A} \to \text{Set}$  preserves finite connected limits;
- (4)  $\alpha$  preserves finite connected limits.

*Remark 3.13.* The first condition is equivalent to the existence of equalisers and pullbacks in  $\mathcal{A}$ , since any finite connected limit can be constructed from those.

These conditions ensure the following two properties.

*Property 3.14.* The following properties hold.

- (i) The action of  $O_n : \mathcal{A} \to \text{Set}$  on any renaming is an injection: given any  $o \in O_n(b)$  and renaming  $f : a \to b$ , there is at most one  $o' \in O_n(a)$  such that  $o = o'\{f\}$ .
- (ii) Let  $\mathcal{L}$  be the functor  $\mathcal{A}^{op} \to \mathrm{MCon}(S)$  mapping a morphism  $x \in \mathrm{hom}_{\mathcal{A}}(b,a)$  to the substitution  $(X:a) \to (X:b)$  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  $\mathrm{MCon}(S)$ .

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



(ii) The proof is deferred to the end of this section.

The first property is used for soundness of the rules P-Rig and P-Fail. The second one is used to justify unification of two metavariables applications as pullbacks and equalisers in  $\mathcal{A}$ , in the rules U-Flex and P-Flex.

*Remark 3.15.* A metavariable application  $\Gamma$ ;  $a \vdash M(x)$  corresponds to the composition  $\mathcal{L}x[in_M]$ , where  $in_M$  is the coproduct injection  $(X : m) \cong (M : m) \hookrightarrow \Gamma$ .

The rest of this section can be safely skipped at first reading: we provide Initial Algebra Semantics for the generated syntax that we exploit to prove Property 3.14.(ii).

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

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

Lemma 3.16. F is finitary and generates a free monad T. Moreover, TX is the initial algebra of  $Z \mapsto X + FZ$ .

PROOF. 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].

LEMMA 3.17. The syntax generated by a GB-signature (see Definition 2.4) is recovered as free algebras for F. More precisely, given a metavariable context  $\Gamma = (M_1 : m_1, ..., M_p : m_p)$ ,

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

where  $\underline{\Gamma}: \mathcal{A} \to \operatorname{Set}$  is defined as the coproduct of representable functors  $\coprod_i ym_i$ , mapping a to  $\coprod_i \operatorname{hom}_{\mathcal{A}}(m_i, a)$ .

*Notation 3.18.* Given a metavariable context  $\Gamma$ . We sometimes denote  $\Gamma$  just by  $\Gamma$ .

If  $\Gamma = (M_1: m_1, ..., M_p: m_p)$  and  $\Delta$  are metavariable contexts, a Kleisli morphism  $\sigma: \Gamma \to T\Delta$  is equivalently given (by 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 metavariable contexts  $\mathrm{MCon}(S)$  and the Kleisli category of T

LEMMA 3.19. The category MCon(S) is equivalent to the full subcategory of  $Kl_T$  spanned by coproducts of representable functors.

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

Lemma 3.20. 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  $\mathscr{C}$  of  $[\mathcal{A}, \operatorname{Set}]$  consisting of functors preserving finite connected limits if and only if the last two conditions of Definition 3.12 holds.

Proof. See Appendix §A.

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

LEMMA 3.21. & is closed under limits, coproducts, and filtered colimits. Moreover, it is cocomplete.

PROOF. Cocompleteness follows from Adámek and Rosicky [1994, Remark 1.56], since  $\mathscr E$  is the category of models of a limit sketch, and is thus locally presentable, by Adámek and Rosicky [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)].

Generic pattern unification 1:17

COROLLARY 3.22. T restricts as a monad on  $\mathscr C$  freely generated by the restriction of F as an endofunctor on  $\mathscr C$  (Lemma 3.20).

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

We now turn to the proof of Property 3.14.(ii).

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

Lemma 3.23. Let  $\mathscr{D}$  denote the opposite category of  $\mathscr{A}$  and  $K: \mathscr{D} \to \mathscr{C}$  the factorisation of  $\mathscr{C} \to [\mathscr{A}, \operatorname{Set}]$  by the Yoneda embedding. Then,  $K: \mathscr{D} \to \mathscr{C}$  preserves finite connected colimits.

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

$$y = J \circ K. \tag{2}$$

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

$$\mathscr{C}(K \lim F, X) \cong [\mathcal{A}, \operatorname{Set}](JK \lim F, JX) \qquad (J \text{ is fully faithful})$$

$$\cong [\mathcal{A}, \operatorname{Set}](y \lim F, JX) \qquad (By \text{ Equation (2)})$$

$$\cong JX(\lim F) \qquad (By \text{ the Yoneda Lemma.})$$

$$\cong \lim(JX \circ F) \qquad (X \text{ preserves finite connected limits})$$

$$\cong \lim([\mathcal{A}, \operatorname{Set}](yF-, JX)] \qquad (By \text{ the Yoneda Lemma})$$

$$\cong \lim([\mathcal{A}, \operatorname{Set}](JKF-, JX)] \qquad (By \text{ Equation (2)})$$

$$\cong \lim \mathscr{C}(KF-, X) \qquad (J \text{ is full and faithful})$$

$$\cong \mathscr{C}(\operatorname{colim} KF, X) \qquad (By \text{ left continuity of the hom-set bifunctor})$$

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

PROOF OF PROPERTY 3.14.(II). Let  $T_{|\mathscr{C}|}$  be the monad T restricted to  $\mathscr{C}$ , following Corollary 3.22. Since  $K: \mathscr{D} \to \mathscr{C}$  preserves finite connected colimits (Lemma 3.23), composing it with the left adjoint  $\mathscr{C} \to Kl_{T_{|\mathscr{C}|}}$  yields a functor  $\mathscr{D} \to Kl_{T_{|\mathscr{C}|}}$  also preserving those colimits. Since it factors as  $\mathscr{D} \xrightarrow{\mathcal{L}} \mathrm{MCon}(S) \hookrightarrow Kl_{T_{|\mathscr{C}|}}$ , where the right functor is full and faithful,  $\mathcal{L}$  also preserves finite connected colimits.

#### 4 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 main unification phase in Figure 2, which computes a coequaliser in  $\mathrm{MCon}_{\perp}(S)$ . More specifically, we discuss the rule sequential rule U-Split (Section §4.1), the rule U-Flex unifying metavariable with itself (Section §4.2), and the failing rule U-Cyclic for cyclic unification of a metavariable with a term which includes it deeply (Section §4.3).

## 4.1 Sequential unification (rule U-SPLIT)

The rule U-Split follows from 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.

$$A_1 \xrightarrow[u_1]{t_1} \Gamma \xrightarrow{\sigma_1} \Delta_1 \qquad A_2 \qquad \Delta_1 \xrightarrow{\sigma_2} \Delta_2$$

$$u_2 \xrightarrow[\Gamma]{\sigma_1} \times A_1 \xrightarrow{\sigma_2} \Delta_2$$

$$A_1 + A_2 \xrightarrow[u_1, u_2]{t_1, t_2} \Gamma \xrightarrow{\sigma_2 \circ \sigma_1} \Delta_2$$

## 4.2 Flex-Flex, same metavariable (rule U-FLEX)

Here we detail unification of M(x) and M(y), for  $x, y \in \text{hom}_{\mathcal{A}}(m, a)$ . By Remark 3.15,  $M(x) = \mathcal{L}x[in_M]$  and  $M(y) = \mathcal{L}y[in_M]$ . We exploit the following lemma with  $u = \mathcal{L}x$  and  $v = \mathcal{L}y$ .

Lemma 4.1. In any category, denoting morphism composition  $g \circ f$  by f[g], the following rule applies:

$$\frac{B + u = v \Rightarrow h + C}{B + D + u[in_B] = v[in_B] \Rightarrow h + 1_D + C + D}$$

In other words, if the below left diagram is a coequaliser, then so is the below right diagram.

$$A \xrightarrow{u} B - \xrightarrow{h} C \qquad A \xrightarrow{u} B \xrightarrow{in_B} B + D \xrightarrow{h+1_D} C + D$$

It follows that it is enough to compute the coequaliser of  $\mathcal{L}x$  and  $\mathcal{L}y$ . Furthermore, by Property 3.14.(ii), it is the image by  $\mathcal{L}$  of the equaliser of x and y, thus justifying the rule U-Flex.

## 4.3 Flex-rigid, cyclic (rule U-CYCLIC)

The rule U-Cyclic handles unification of M(x) and a term u such that u is rigid and M occurs in u. In this section, we show that indeed there is no unifier. More precisely, we prove Corollary 4.6 below, stating that if there is a unifier of a term u and a metavariable application M(x), then either M occurs at top-level in u, or it does not occur at all. The argument follows the basic intuition that  $\sigma_M = u[M \mapsto \sigma_M]$  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 4.2. The size<sup>6</sup>  $|t| \in \mathbb{N}$  of a 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 4.3. 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 4.4. For any term  $\Gamma, M : m; a \vdash t$ , if  $|t|_M = 0$ , then  $\Gamma; a \vdash t$ . Moreover, for any  $\Gamma = (M_1 : m_1, \ldots, M_n : m_n)$ , well-formed term t in context  $\Gamma; a$ , and substitution  $\sigma : \Gamma \to \Delta$ , we have  $|t[\sigma]| = |t| + \sum_i |t|_{M_i} \times |\sigma_i|$ .

<sup>&</sup>lt;sup>6</sup>The difference with the notion of size introduced in Section §2.3 is that metavariables are of size 0.

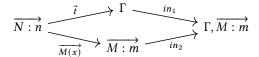
 COROLLARY 4.5. For any term t in context  $\Gamma, M : m; a$ , substitution  $\sigma : \Gamma \to \Delta$ , morphism  $x \in \hom_{\mathcal{A}}(m, a)$  and u in context  $\Delta; u$ , we have  $|t[\sigma, M \mapsto u]| \ge |t| + |u| \times |t|_M$  and |M(x)[u]| = |u|.

COROLLARY 4.6. Let t be a term in context  $\Gamma, M : m$ ; a and  $x \in \hom_{\mathcal{A}}(m, a)$  such that  $(\sigma, M \mapsto u) : (\Gamma, M : m) \to \Delta$  unifies t and M(x). Then, either t = M(y) for some  $y \in \hom_{\mathcal{A}}(m, a)$ , or  $\Gamma; a \vdash t$ .

PROOF. Since  $t[\sigma, u] = M(x)[u]$ , we have  $|t[\sigma, u]| = |M(x)[u]|$ . Corollary 4.5 implies  $|u| \ge |t| + |u| \times |t|_M$ . Therefore, either  $|t|_M = 0$  and we conclude by Lemma 4.4, or  $|t|_M > 0$  and |t| = 0, so that t is M(y) for some y.

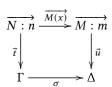
#### 5 SOUNDNESS OF THE NON-CYCLIC PHASE

In this section, we assume a pattern-friendly GB-signature S and prove soundness of the main rule of the non-cyclic phase. This phase handles unification of a list of terms  $\Gamma$ ;  $n_i \vdash t_i$  with a list of fresh metavariable applications  $M_1(x_1), \ldots, M_p(x_p)$ , in the extended metavariable context  $\Gamma, M_1 : m_1, \ldots, M_p : x_p$ . Categorically speaking, we are looking at the following coequalising diagram in MCon(S).



The P-Split rule is a straightforward adaption of the U-Split rule specialised to those specific coequaliser diagrams.

Remark 5.1. A unifier  $\Gamma, \overline{M}: m \to \Delta$  splits into two components: a substitution  $\sigma: \Gamma \to \Delta$  and a substitution  $\overrightarrow{u}$  from N: n to M: m such that  $t_i[\sigma] = u_i\{x_i\}$  for each  $i \in \{1, \dots, p\}$ . Moreover, the coequaliser  $\sigma, \overrightarrow{u}: (\Gamma, \overline{M:m}) \to \Delta$  is equivalently characterised as a pushout



This justifies a common interpretation as pushouts of the two variants of the notation  $- \vdash - :> - \Rightarrow -$ ; – involved in Figure 2, in  $\mathcal{A}^{op}$  and MCon(S).

In the following sections, we detail soundness of the rules for the rigid case (Section §5.1) and then for the flex case (Section §5.2).

## 5.1 Rigid (rules P-Rig and P-Fail)

The rules P-Rig and P-Fail handle non-cyclic unification of M(x) with  $\Gamma$ ;  $a \vdash o(\overline{t})$  in the metavariable context  $\Gamma$ , M:m for some  $o \in O_n(a)$ . By Remark 5.1, a unifier is given by a substitution  $\sigma:\Gamma\to\Delta$  and a term u such that

$$o(\vec{t}[\sigma]) = u\{x\}. \tag{3}$$

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 (3). Therefore,  $u = o'(\vec{v})$  for some  $o' \in O_n(m)$  and  $\vec{v} = (v_1, \ldots, v_n)$  is a list of terms such that  $\Delta; \overline{o'}_i \vdash v_i$ . Then,  $u\{x\} = (o'\{x\})(v_1\{x_1^{o'}\}, \ldots)$ . It follows from Equation (3) that  $o = o'\{x\}$ , and  $t_i[\sigma] = v_i\{x_i^{o'}\}$ .

Note that there is at most one o' such that  $o = o'\{x\}$ , by Property 3.14.(i). In this case, a unifier is equivalently given by a substitution  $\sigma : \Gamma \to \Delta$  and a list of terms  $\vec{v} = (v_1, \dots, v_n)$  such that

  $\Delta; \overline{o'}_i \vdash v_i$  and  $t_i[\sigma] = v_i\{x_i^{o'}\}$ . But, by Remark 5.1, this is precisely the data for a unifier of  $\vec{t}$  and  $M_1(x_i^{o'}), \ldots, M_n(x_n^{o'})$ . This actually induces an isomorphism between the two categories of unifiers, thus justifying the rules P-Rig and P-Fail.

## 5.2 Flex (rule P-FLEX)

The rule P-FLEX handles unification of  $\Gamma$ , N:n;  $a \vdash N(x)$  and M(y) where M is fresh in  $\Gamma$ , N:n. Note that M(y), as a substitution  $(A:a) \to (M:m)$ , is isomorphic to  $\mathcal{L}y$ , while  $N(x) = \mathcal{L}x[in_N]$ , by Remark 3.15. Thanks to the following lemma, it is actually enough to compute the pushout of  $\mathcal{L}x$  and  $\mathcal{L}y$ .

LEMMA 5.2. In any category, denoting morphism composition by  $f \circ g = g[f]$ , the following rule applies

$$\frac{X \vdash g :> f \Rightarrow u; \sigma \dashv Z}{X + Y \vdash g[in_1] :> f \Rightarrow u[in_1]; \sigma + Y \dashv Z + Y}$$

In other words, if the diagram below left is a pushout, then so is the right one.

$$\begin{array}{ccccc}
A & \xrightarrow{f} & B \\
\downarrow g & \downarrow u \\
X & & Z \\
X & --\sigma & Z & in_1 \downarrow & in_1 \\
& & & X & Y & --\sigma & Y & Z + Y
\end{array}$$

By Property 3.14.(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.

#### **6 COMPLETENESS**

In this section, we explain why soundness (Section §5 and Section §4) and termination (Section §2.3) entail completeness. Intuitively, one may worry that the algorithm fails in cases where it should not. In fact, soundness already ensures that this cannot happen because failure is really handled as a coequaliser, on par with most general unifiers. As explained in Section §3.1, this is done by considering the category  $\mathrm{MCon}_{\perp}(S)$  extending category  $\mathrm{MCon}(S)$  with a (dignified) error object  $\perp$ . Corollary 3.9 implies that since the algorithm terminates and computes the coequaliser in  $\mathrm{MCon}_{\perp}(S)$ , it always finds the most general unifier in  $\mathrm{MCon}(S)$  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. We start in Section §7.1 with a variant of pure  $\lambda$ -calculus where metavariable arguments are sets rather than lists. Then, in Section §7.2, we present simply-typed  $\lambda$ -calculus, as an example of syntax specified by a multi-sorted binding signature. Next, we introduce an example of unification for ordered syntax in Section §7.3, and finally we present an example of polymorphic such as System F, in Section §7.4.

#### 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  $n \to p$  is a subset of  $\{1, \ldots, p\}$  of cardinal n. For instance,  $\mathbb{I}$  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 atomic types and a binary arrow type construction  $-\Rightarrow$  –. Let us now describe the category  $\mathcal A$  of arities, or variable contexts, and renamings between them. An arity  $\vec{\sigma} \to \tau$  consists of a list of input types  $\vec{\sigma}$  and an output type  $\tau$ . A term t in  $\vec{\sigma} \to \tau$  considered as a variable context 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  $M: (\vec{\sigma} \to \tau)$  in variable context  $\vec{\sigma}' \to \tau'$  first requires  $\tau = \tau'$ , and consists of an injective renaming  $\vec{r}$  between  $\vec{\sigma} = (\sigma_1, \ldots, \sigma_m)$  and  $\vec{\sigma}' = (\sigma'_1, \ldots, \sigma'_n)$ , that is, a choice of distinct positions  $(r_1, \ldots, r_m)$  in  $\{1, \ldots, n\}$  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  $[\mathcal{A}, \operatorname{Set}]$  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  $M: (\vec{\sigma} \to \tau)$  to the term  $P(\vec{z})$ , where the arity  $\vec{\sigma}' \to \tau'$  of the fresh metavariable P is the only possible choice such that  $P(\vec{z})$  is a valid term in the variable context  $\vec{\sigma} \to \tau$ , that is,  $\tau' = \tau$  and  $\vec{\sigma}' = \sigma_{\vec{z}}$ .

## 7.3 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 variable context 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 variable contexts, and the syntax is generated by operations  $L_n \times L_m \to L_{n+m}$  and abstractions  $L_{n+1} \to L_n$ .

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.

The set T of types is generated by a set of atomic types and two binary arrow type constructions  $\Rightarrow$  and  $\Rightarrow$ . The syntax extends pure  $\lambda$ -calculus with a distinct application  $t^>u$  and abstraction  $\lambda^>u$ . Variables contexts are of the shape  $\vec{\sigma}|\vec{\omega}\to\tau$ , 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  $\vec{\sigma}|\vec{\omega}\to\tau$ , 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 variable context  $\vec{\sigma}'|\vec{\omega}'\to\tau'$  is well-formed if

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

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

	Typing rule	$O_n(\vec{\sigma} \vec{\omega} \to \tau) = \dots +$	$\alpha_o = (\ldots)$
Ordered λ-calculus (Section §7.3)	$\frac{x:\tau\in\Gamma}{\Gamma \cdot\vdash x:\tau}$	$\{v_i i\in  \vec{\sigma} _{\tau} \text{ and } \vec{\omega}=()\}$	()
	$\overline{\Gamma x:\tau\vdash x:\tau}$	$\{v^{>} \vec{\omega}=()\}$	()
	$\frac{\Gamma \Omega \vdash t : \tau' \Rightarrow \tau  \Gamma  \cdot \vdash u : \tau'}{\Gamma \Omega \vdash t \ u : \tau}$	$\{a_{\tau'} \tau'\in T\}$	$\begin{pmatrix} \vec{\sigma}   \vec{\omega} \to (\tau' \Rightarrow \vec{\sigma}   () \to \tau' \end{pmatrix}$
	$\frac{\Gamma \Omega_1 \vdash t : \tau' \twoheadrightarrow \tau  \Gamma \Omega_2 \vdash u : \tau'}{\Gamma \Omega_1, \Omega_2 \vdash t^> u : \tau}$	$\{a_{\tau'}^{\vec{\omega}_1,\vec{\omega}_2} \tau'\in T \text{ and } \vec{\omega}=\vec{\omega}_1,\vec{\omega}_2\}$	$ \begin{pmatrix} \vec{\sigma}   \vec{\omega}_1 \to (\tau' \Rightarrow \vec{\sigma}   \vec{\omega}_2 \to \tau' \end{pmatrix} $
	$\frac{\Gamma, x : \tau_1   \Omega \vdash t : \tau_2}{\Gamma   \Omega \vdash \lambda x . t : \tau_1 \Rightarrow \tau_2}$	$\{l_{\tau_1,\tau_2} \tau=(\tau_1\Rightarrow\tau_2)\}$	$(\vec{\sigma}, \tau_1   \vec{\omega} \rightarrow \tau_2$
	$\frac{\Gamma \Omega, x : \tau_1 \vdash t : \tau_2}{\Gamma \Omega \vdash \lambda^{>} x.t : \tau_1 \twoheadrightarrow \tau_2}$	$\{l_{\tau_1,\tau_2}^{>} \tau=(\tau_1\twoheadrightarrow\tau_2)\}$	$(\vec{\sigma}, \tau_1   \vec{\omega} \rightarrow \tau_2$

System F (Section §7.4)

Typing rule	$O_n(p \vec{\sigma} \vdash \tau) = \dots +$	$\alpha_o = (\ldots)$
$\frac{x:\tau\in\Gamma}{n \Gamma\vdash x:\tau}$	$\{v_i i\in  \vec{\sigma} _\tau\}$	0
$\frac{n \Gamma \vdash t : \tau' \Rightarrow \tau  n \Gamma \vdash u : \tau'}{n \Gamma \vdash t \; u : \tau}$	$\{a_{\tau'} \tau'\in S_n\}$	$ \left( \begin{array}{c} n \vec{\sigma} \to \tau' \Rightarrow \tau \\ n \vec{\sigma} \to \tau' \end{array} \right) $
$\frac{n \Gamma, x : \tau_1 \vdash t : \tau_2}{n \Gamma \vdash \lambda x.t : \tau_1 \Rightarrow \tau_2}$	$\{l_{\tau_1,\tau_2} \tau=(\tau_1\Rightarrow\tau_2)\}$	$(n \vec{\sigma},\tau_1\to\tau_2)$
$\frac{n \Gamma \vdash t : \forall \tau_1  \tau_2 \in S_n}{n \Gamma \vdash t \cdot \tau_2 : \tau_1[\tau_2]}$	$\{A_{\tau_1,\tau_2} \tau=\tau_1[\tau_2]\}$	$(n \vec{\sigma} \to \forall \tau_1)$
$\frac{n+1 wk(\Gamma) \vdash t : \tau}{n \Gamma \vdash \Lambda t : \forall \tau}$	$\{\Lambda_{\tau'} \tau=\forall\tau'\}$	$(n+1 wk(\vec{\sigma}) \to \tau')$

  $\tau = \tau'$  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  $T^*$  denote 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  $\sigma_{\vec{z}}|\vec{\omega} \to \tau$ .

## 7.4 Intrinsic polymorphic syntax

We present intrinsic System F, in the spirit of Hamana [2011]. The syntax of types in type variable context n is inductively generated as follows, following the De Bruijn level convention.

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

Let  $S: \mathbb{F}_m \to \operatorname{Set}$  be the functor mapping n to the set  $S_n$  of types for system F taking free type variables in  $\{1,\ldots,n\}$ . In other words,  $S_n=\{\tau|n\vdash\tau\}$ . Intuitively, a metavariable arity  $n|\vec{\sigma}\to\tau$  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  $n|\vec{\sigma}\to\tau$  considered as a variable context is intuitively a well-typed term of type  $\tau$  potentially involving ground variables of type  $\vec{\sigma}$  and type variables in  $\{1,\ldots,n\}$ .

A metavariable  $M:(n|\sigma_1,\ldots,\sigma_p\to\tau)$  in the variable context  $n'|\vec{\sigma}'\to\tau'$  must be supplied with

- a choice  $(\eta_1, \dots, \eta_n)$  of *n* distinct type variables among  $\{1, \dots, n'\}$ , such that  $\tau[\vec{\eta}] = \tau'$ , and
- an injective renaming  $\vec{\sigma}[\vec{\eta}] \to \vec{\sigma}'$ , i.e., a list of distinct positions  $r_1, \ldots, r_p$  such that  $\vec{\sigma}[\vec{\eta}] = \sigma'_{\vec{\tau}}$ .

This defines the data for a morphism in  $\mathcal{A}$  between  $(n|\vec{\sigma} \to \tau)$  and  $(n'|\vec{\sigma}' \to \tau')$ . The intrinsic syntax of system F can then be specified as in Table 1. The induced GB-signature is pattern-friendly. For example, morphisms in  $\mathcal{A}$  are easily seen to be monomorphic; we detail in Appendix §B the proof of the following statement.

#### Lemma 7.1. $\mathcal{A}$ 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  $m|\vec{\sigma} \to \tau$ , 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  $m'|\vec{\sigma}' \to \tau'$  is the only possible one for  $P(\vec{p}|\vec{q})$  to be well-formed in the variable context  $m|\vec{\sigma} \to \tau$ , that is, m' is the size of  $\vec{p}$ , while  $\tau' = \tau[p_i \mapsto i]$  and  $\vec{\sigma}' = \sigma_{\vec{q}}[p_i \mapsto i]$ .

## 8 RELATED WORK

First-order unification has been explained from a lattice-theoretic point of view by Plotkin Plotkin [1970], and later categorically analysed in Barr and Wells [1990]; Goguen [1989]; Rydeheard and Burstall [1988, 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.

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

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everything is explicitly scoped: terms come with their support, metavariables always appear with their scope of allowed variables.

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.

Cheney Cheney [2005] shows that nominal unification and pattern unification problems are inter-translatable. As he 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.

#### 9 CONCLUSION

We presented a generic unification algorithm for Miller's pattern fragment with its associated categorical semantics, parameterised by a new notion of signature for syntax with metavariables. In the future, we plan to a implement a reusable library based on this work. We also plan to see how this work applies to dependently-typed languages, going beyond polymorphic syntax. Finally, we are interesting in further extending the setting to cover unification modulo equations, or linear syntax without restriction on the order the variables are used.

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Generic pattern unification 1:25

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#### **PROOF OF LEMMA 3.20**

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*Notation A.1.* Given a functor  $F: I \to \mathcal{B}$ , we denote the limit (resp. colimit) of F by  $\int_{i \in I} F(i)$  or  $\lim F$  (resp.  $\int_{-i}^{i:I} F(i)$  or colim F) and the canonical projection  $\lim F \to Fi$  by  $p_i$  for any object i of I.

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

LEMMA A.2. 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  $\mathscr C$  of  $[\mathcal A,\operatorname{Set}]$  consisting of functors preserving finite connected limits if and only if each  $O_n \in \mathscr{C}$ , and  $\alpha : \int J \to \mathcal{A}$  preserves finite limits.

We first introduce a bunch of intermediate lemmas.

- Lemma A.3. If  $\mathscr{B}$  is a small category with finite connected limits, then a functor  $G:\mathscr{B}\to\operatorname{Set}$ preserves those limits if and only if  $\int \mathcal{B}$  is a coproduct of filtered categories.
  - PROOF. This is a direct application of Adámek et al. [2002, Theorem 2.4 and Example 2.3.(iii)].
- COROLLARY A.4. Assume  $\mathcal{A}$  has finite connected limits. Then  $J: \mathbb{N} \times \mathcal{A} \to \operatorname{Set}$  preserves finite connected limits if and only if each  $O_n : \mathcal{A} \to \operatorname{Set}$  does.
- PROOF. This follows from  $\int J \cong \coprod_{n \in \mathbb{N}} \coprod_{j \in \{1,...,n\}} \int O_n$ .
- Lemma A.5. Let  $F: \mathscr{B} \to \operatorname{Set}$  be a functor. For any functor  $G: I \to \int F$ , denoting by H the composite functor  $I \xrightarrow{G} \int F \to \mathcal{B}$ , there exists a unique  $x \in \lim(F \circ H)$  such that  $Gi = (Hi, p_i(x))$ .
- 1218 PROOF.  $\int F$  is isomorphic to the opposite of the comma category y/F, where  $y: \mathcal{B}^{op} \to \mathbb{R}$ 1219 [B, Set] is the Yoneda embedding. The statement follows from the universal property of a comma 1220 category.
- LEMMA A.6. Let  $F: \mathcal{B} \to \operatorname{Set}$  and  $G: I \to \int F$  such that F preserves the limit of  $H: I \xrightarrow{G} \int F \to I$ 1222  $\mathcal{B}$ . Then, there exists a unique  $x \in F \lim H$  such that  $Gi = (Hi, Fp_i(x))$  and moreover,  $(\lim H, x)$  is 1223 the limit of G. 1224

 PROOF. The unique existence of  $x \in F \lim H$  such that  $Gi = (Hi, Fp_i(x))$  follows from Lemma A.5 and the fact that F preserves  $\lim H$ . Let  $\mathscr C$  denote the full subcategory of  $[\mathscr B, \operatorname{Set}]$  of functors preserving  $\lim G$ . Note that  $\int F$  is isomorphic to the opposite of the comma category K/F, where  $K: \mathscr B^{op} \to \mathscr C$  is the Yoneda embedding, which preserves colim G, by an argument similar to the proof of Lemma 3.23. 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 A.7. Let I be a small category,  $\mathscr{B}$  and  $\mathscr{B}'$  be categories with I-limits (i.e., limits of any diagram over I). Let  $F: \mathscr{B} \to \operatorname{Set}$  be a functor preserving those colimits. Then,  $\int F$  has I-limits, preserved by the projection  $\int F \to \mathscr{B}$ . Moreover, a functor  $G: \int F \to \mathscr{B}'$  preserves them if and only if for any  $d: I \to \mathscr{B}$  and  $x \in F \lim d$ , the canonical morphism  $G(\lim d, x) \to \int_{i:I} G(d_i, Fp_i(x))$  is an isomorphism.

PROOF. By Lemma A.6, a diagram  $d': I \to \int F$  is equivalently given by  $d: I \to \mathcal{B}$  and  $x \in F \lim d$ , recovering d' as  $d'_i = (d_i, Fp_i(x))$ , and moreover  $\lim d' = (\lim d, x)$ .

COROLLARY A.8. Assuming that  $\mathcal{A}$  has finite connected limits and each  $O_n$  preserves finite connected limits, the finite limit preservation on  $\alpha:\int J\to\mathcal{A}$  of Lemma A.2 can be reformulated as follows: given a finite connected diagram  $d:D\to\mathcal{A}$  and element  $o\in O_n(\lim d)$ , the following canonical morphism is an isomorphism

$$\overline{o}_j \to \int_{i \cdot D} \overline{o\{p_i\}_j}$$

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

PROOF. This is a direct application of Corollary A.7 and Corollary A.4.

Lemma A.9 (Limits commute with dependent pairs). Given functors  $K:I\to \operatorname{Set}$  and  $G:\int K\to \operatorname{Set}$ , the following canonical morphism is an isomorphism

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

Proof. It is straightforward to check that both sets share the same universal property.  $\Box$ 

Proof of Lemma A.2. Let  $d: I \to \mathcal{A}$  be a finite connected diagram and X be a functor preserving finite connected limits. Then,

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

Generic pattern unification 1:27

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

$$\int_{i} F(X)_{d_{i}} = \coprod_{n} \coprod_{o \in \int_{i} O_{n}(d_{i})} X_{\int_{i:I} \overline{p_{i}(o)_{1}}} \times \cdots \times X_{\int_{i:I} \overline{p_{i}(o)_{n}}}$$
(4)

Now, let us prove the only if statement first. Assuming that  $\alpha : \int J \to \mathcal{A}$  and each  $O_n$  preserves finite connected limits. Then,

$$\int_{i} F(X)_{d_{i}} \cong \coprod_{n} \coprod_{o \in \int_{i} O_{n}(d_{i})} X_{\int_{i:I} \overline{p_{i}(o)_{1}}} \times \cdots \times X_{\int_{i:I} \overline{p_{i}(o)_{n}}}$$
(By Equation (4))
$$\cong \coprod_{n} \coprod_{o \in O_{n}(\lim d)} X_{\int_{i:I} \overline{o\{p_{i}\}_{1}}} \times \cdots \times X_{\int_{i:I} \overline{o\{p_{i}\}_{n}}}$$
(By assumption on  $O_{n}$ )
$$\cong \coprod_{n} \coprod_{o \in O_{n}(\lim d)} X_{\overline{o}_{1}} \times \cdots \times X_{\overline{o}_{n}}$$
(By Corollary A.8)
$$= F(X)_{\lim d}$$

Conversely, let us assume that F restricts to an endofunctor on  $\mathscr{C}$ . Then,  $F(1) = \coprod_n O_n$  preserves finite connected limits. By Lemma A.3, each  $O_n$  preserves finite connected limits. By Corollary A.8, it is enough to prove that given a finite connected diagram  $d:D\to \mathcal{A}$  and element  $o\in O_n(\lim d)$ , the following canonical morphism is an isomorphism

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

Now, we have

$$\int_{i:I} F(X)_{d_i} \cong F(X)_{\lim d}$$
 (By assumption)
$$= \coprod_{n} \coprod_{o \in O_i(\lim d)} X_{\overline{o}_1} \times \dots \times X_{\overline{o}_n}$$

On the other hand,

$$\int_{i:I} F(X)_{d_{i}} \cong \coprod_{n} \coprod_{o \in \int_{i} O_{n}(d_{i})} X_{\int_{i:I} \overline{p_{i}(o)_{1}}} \times \cdots \times X_{\int_{i:I} \overline{p_{i}(o)_{n}}}$$
(By Equation (4))
$$= \coprod_{n} \coprod_{o \in O_{n}(\lim d)} X_{\int_{i:I} \overline{o\{p_{i}\}_{1}}} \times \cdots \times X_{\int_{i:I} \overline{o\{p_{i}\}_{n}}}$$
(O<sub>n</sub> preserves finite connected limits)

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

#### **B** PROOF OF LEMMA 7.1

In this section, we show that the category  $\mathcal A$  of arities for System F (Section §7.4) 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 B.1.  $\mathcal{A}'$  has finite connected limits, and the projection functor  $\mathcal{A}' \to \mathbb{F}_m$  preserves them.

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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  $f: n' \to n$  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.

PROOF OF LEMMA 7.1. Since  $S: \mathbb{F}_m \to \text{Set}$  preserves finite connected limits,  $\int S$  has finite connected limits and the projection functor to  $\mathbb{F}_m$  preserves them by Corollary A.7.

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  $\mathcal{A}' \to \mathbb{F}_m \leftarrow \int S$ . But since  $\int S \to \mathbb{F}_m$  is a fibration, and thus an isofibration, by Joyal and Street [1993] this weak pullback can be computed as a pullback, which is  $\mathcal{A}$ .