Unification with binding

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We show correctness of an algorithm computing the most general unifier of a list of term pairs involving binding operations and n-ary metavariables applied to distinct variables. We reason in the framework of Σ-monoids [3], but in the untyped case.

1 Notations

We denote by C^o the opposite category of C. In a category with coproducts, we denote by $in : A_i \hookrightarrow \coprod_i A_i$ the coproduct injection. If F is an endofunctor on a category C, we denote by μF or $\mu Z.F(Z)$ the initial F-algebra.

We denote by $\mathbb{F}$ the full subcategory of sets consisting of finite cardinals: objects are natural numbers and a morphism between n and m is a function $\{0, \dots, n-1\} \to \{0, \dots, m-1\}$.

Given a monad T on a category C, we denote the Kleisli category by Kl_T: objects are objects of C, and morphisms between c and c' are morphisms in C between c and Tc'. Note that there is a bijection between Kleisli morphisms $c \to Tc'$ and T-algebra morphisms $Tc \to Tc'$. We denote by f^* the T-algebra morphism induced by a Kleisli morphism. Composition of g and f is given by $g^* \circ f$. We denote by $I : \mathbb{N} \to Set$ the family of sets mapping n to the nth cardinal set $\{0, \dots, n-1\}$.

We denote metavariables by capital letters $M, N,\dots$

2 Setting

Let Σ be a binding signature. Then, there is a free Σ-monoid monad T on $Set^{\mathbb{N}}$ such that $T(X)$ is the syntax of Σ extended with an n-ary operation for each $x \in X_n$. More precisely, $T(X)_n$ is the set of terms whose free variables are in $\{0, \dots, n-1\}$.

Example 1. Consider the case of λ-calculus. Then, $T(\emptyset)_n$ is the set of λ-terms t taking free variables in $\{0, \dots, n-1\}$.

Consider $X \in Set^{\mathbb{N}}$ such that $X_2 = \{M\}$ and $X_{n \neq 2} = \emptyset$. Then $T(X)_n$ is the set of λ-terms t involving a metavariable M of arity 2 such that $fv(t) \subset \{0, \dots, n-1\}$.

Consider $Y \in Set^{\mathbb{N}}$ such that $Y_2 = \{M, N\}$, $Y_0 = \{C\}$ and $Y_n = \emptyset$ otherwise. Then $T(Y)_n$ is the λ-term t with metavariables M,N of arity 2 and a constant metavariable C such that $fv(t) \subset \{0, \ldots, n-1\}$.

Note that metavariables are allowed to be applied to arbitrary terms here, not only (distinct) variables.

Definition 2. A morphism $X \to T(Y)$ is said *safe* if it factors through $T'(Y) \to T(Y)$, where $T'(Y)_n$ is the subset of $T(Y)_n$ consisting of terms that where metavariables are applied to distinct variables only, rather than arbitrary terms.

Remark 3. $T'(Y)$ is the initial algebra for $Z \mapsto I + Z \boxtimes I + \Sigma(Z)$, where

- we denote by Σ the endofunctor on $Set^{\mathbb{N}}$ corresponding to the binding signature Σ.

- $(Z \boxtimes I)_n = \coprod_p Z_p \times Inj(p, I_n)$. Note that this definition is not functorial in the second argument (unless we restrict to monomorphisms).

Notation 4. We denote by Kl_T the Kleisli category of the monad T: objects are families in $Set^{\mathbb{N}}$ and a morphism $X \to Y$ is a family morphism $X \to T(Y)$.

Remark 5. A (metavariable) substitution is precisely a morphism in the Kleisli category. For example, a Kleisli morphism from X to Y is a morphism $X \to T(Y)$, i.e., for each $n \in \mathbb{N}$, a map $X_n \to T(Y)_n$ which assigns a term taking free variables in $\{0, \ldots, n-1\}$ for each n-ary metavariable.

Remark 6. Consider the "operadic" monoidal product $A \boxtimes B_n = \coprod_p \coprod_{i_1 + \cdots + i_p = n} A_p \times B_{i_1} \times \cdots \times B_{i_p}$ and Σ-monoids for this tensor products, with associated monad T'. In this setting, we think of $T'(X)_n$ as the set of terms withneed to exactly n free variables. Thus, Kleisli morphisms maps metavariables to terms using exactly once each argument.

Definition 7. A family $X \in Set^{\mathbb{N}}$ is said *finite* if $\coprod_n X_n$ is finite.

Our main result consists in the following.

Theorem 8. *Let $V \rightrightarrows T(W)$ be a pair of safe morphisms between finite families V and W. If there is a coequalising Kleisli morphism, then there is coequaliser in $Kl(T)$.*

We use an explicit construction, detailed in the next section. This theorem allows to compute the most general unifier of two terms.

Corollary 9. *Let $t, u \in T(V)_n$ for some finite family $V \in Set^{\mathbb{N}}$ (thought as a specification of metavariables). If there exists a substitution unifying t and u, then there exists a most general unifier, i.e., a substitution $V \to T(W)$ such that any other unifying substitution uniquely factors through it.*

Proof. Giving two terms $t, u \in T(V)_n$ amounts to giving two parallel morphisms $yn \rightrightarrows T(V)$, where yn denotes the family defined by $yn_p = \emptyset$ if $p \neq n$ and yn_n is a singleton set. The most general unifier, if it exists, is the coequaliser of t and u. $\square$

More generally, we can compute any finite colimit under the same condition.

Corollary 10. *Let $J : D \to Kl_T$ be a finite diagram selecting safe Kleisli morphisms and finite families. If there is a cocone, then J has a colimit.*

Proof. This follows from the computation of colimits as coequalisers and coproducts [4, Theorem V.2.2]. □

Let us finish this section by introducing some useful definitions, notations, and lemmas.

Lemma 11. *Free T-algebras extend to functors $\mathbb{F} \to Set$ preserving pullbacks, where $\mathbb{F}$ is the full subcategory of sets consisting in finite cardinals. Action on morphisms is given by renaming. Moreover, Kleisli morphisms are compatible with renaming.*

Proof. See Appendix A. □

Notation 12. If $n \in \mathbb{N}$, we denote the nth cardinal set $\{0, \ldots, n-1\}$ by n.

If $n \in \mathbb{N}$, we denote by yn the yoneda embedding into $Set^{\mathbb{N}}$, i.e., $yn(p)$ is empty if $n \neq p$ and a singleton set otherwise. We call *representable* any family which is isomorphic to some yn.

$I \in Set^{\mathbb{N}}$ denotes the family $I_n = n$.

Lemma 13. *Any family $X \in Set^{\mathbb{N}}$ is isomorphic to a coproduct of representable families. A family X is finite if and only if such a coproduct is finite.*

Proof. Clearly, any family X is isomorphic to $\coprod_n X_n yn \simeq \coprod_n \coprod_{x \in X_n} yn$. □

Notation 14. We represent a finite family $X \in Set^{\mathbb{N}}$ as a finite (metavariable) context $x_1 : n_1, \ldots, x_p : n_p$ where $x_i \in X_{n_i}$.

3 Algorithm

The algorithm takes as input

- a (finite) metavariable context $\Gamma \in Set^{\mathbb{N}}$, that we denote by a list $M_1 : m_1, \ldots M_n : m_n$ of metavariable symbols M_i with their associated arities m_i;

- a list of term pairs $t_i =_{n_i} u_i$, where n_i that t_i and u_i takes free variables in $\{0, \ldots, n_i - 1\}$

It outputs:

- a metavariable context Δ

- a Kleisli map $\sigma : \Gamma \to T(\Delta)$, that is a substitution assigning to each metavariable $M : m$ declared in Γ a term with m free variables involving metavariables Δ.

In this section we inductively specify the algorithm through the judgement

$$\Gamma \vdash t_1 =_{n_1} u_1, \dots t_p =_{n_p} u_p \Rightarrow \sigma \dashv \Delta$$

that we sometimes abbreviate as

$$\Gamma \vdash \vec{t} =_{\vec{n}} \vec{u} \Rightarrow \sigma \dashv \Delta$$

The completeness statement (proven by induction) is the following.

Proposition 15. *Given a list of safe term pairs $\vec{t} = \vec{u}$ taking metavariables in Γ, if there exists a (finite) derivation tree of $\Gamma \vdash \vec{t} =_{\vec{n}} \vec{u} \Rightarrow \sigma \dashv \Delta$, then σ is the most general unifier. Moreover such a derivation tree exists as long as there exists at least one unifier.*

We will justify this proposition by showing that each introduced rule is sound, in the sense that that it supports the induction step. We omit the proof that if the conclusion involves safe terms, the also do the premises.

At most one rule is applyable given an input $\vec{t} = \vec{u}$.

Proposition 16. *There is at most one derivation tree of $\Gamma \vdash \vec{t} =_{\vec{n}} \vec{u} \Rightarrow \sigma \dashv \Delta$.*

Let us list indeed the rules according to the input $\vec{t} = \vec{u}$ in the conclusion:

- Empty list $\vec{t} = \vec{u} = ()$, in Section 3.1;

- Non empty, non singleton lists, $t_0 = u_0, \vec{t} = \vec{u}$, in Section 3.2;

- $M(\vec{x}) = N(\vec{y})$, in Section 3.3;

- $o(\vec{t}) = o(\vec{u})$ and $x = y$ in Section 3.4;

- $M(\vec{x}) = o(\vec{t})$, in Section 3.5;

- $M(\vec{x}) = x_i$, in Section 3.6.

Let us mention the missing cases, which can never be unified anyway.

- $o(\vec{t}) = o'(\vec{u})$ when $o \neq o'$;

- $M(\vec{x}) = y$ when $y \notin \vec{x}$

- $o(\vec{t}) = x$

3.1 Empty list

$$\overline{\Gamma \vdash () \Rightarrow id \dashv \Gamma}$$

Soundness is straightforward.

3.2 Stepwise construction

We can restrict to the case of a single coequaliser.

$$\frac{\Gamma \vdash t_0 =_{n_0} u_0 \Rightarrow \sigma_0 \dashv \Delta_1 \qquad \Delta_1 \vdash \vec{t}[\sigma_0] =_{\vec{n}} \vec{u}[\sigma_0] \Rightarrow \sigma \dashv \Delta_2 \qquad \vec{t} \text{ is not empty}}{\Gamma \vdash t_0 =_{n_0} u_0, \vec{t} =_{\vec{n}} \vec{u} \Rightarrow \sigma \circ \sigma_0 \dashv \Delta_2}$$

Soundness of this rule follows from the following general categorical lemma.

Lemma 17. *Let $f_1, g_1 : A_1 \to B$ and $f_2, g_2 : A_2 \to B$ be morphisms in some category. Then the coequaliser of the induced parallel morphism $A_1 \coprod A_2 \rightrightarrows B$ is the morphism $B \to C \to D$ defined as follows (assuming the involved coequalisers exist):*

1. $B \to C$ is the coequaliser of $A_1 \rightrightarrows B$;

2. $C \to D$ is the coequaliser of $A_2 \rightrightarrows B \to C$.

Corollary 18. *The above rule is sound.*

Proof. Assume there is a common unifier for $t_0 = u_0, \vec{t} = \vec{u}$. By induction hypothesis, the premises are derivable and thus the rule can be applied. Moreover, again by induction hypothesis, the premises produce most general unifiers. The output substitution of the conclusion is also the most general unifier, thanks to the previous lemma by specialising it to the Kleisli category Kl_T, taking $A_1 = yn_0$ and $A_2 = \coprod_i yn_i$. □

3.3 Case $M(x_1, \ldots, x_m) =_q N(y_1, \ldots, y_n)$

We need to make the distinction whether $M = N$ or not.

$$\frac{(i_1, \ldots, i_p) \text{ is the family of common positions: } x_{\vec{i}} = y_{\vec{i}}}{\Gamma \vdash M(\vec{x}) =_q M(\vec{y}) \Rightarrow M(1, \ldots, m) \mapsto N(i_1, \ldots i_p) \dashv \Gamma \backslash \{M\}, N : p}$$

The premise states that $i : p \to m$ is the equaliser of $\vec{x}, \vec{y} : m \to q$ in $\mathbb{F}$.

$$\frac{M \neq N \qquad (i_1, \ldots, i_p) \text{ and } (j_1, \ldots, j_p) \text{ are maximal such that } x_{\vec{i}} = y_{\vec{j}}}{\Gamma \vdash M(\vec{x}) =_q N(\vec{y}) \Rightarrow M(1, \ldots, m) \mapsto O(i_1, \ldots i_p), N(1, \ldots, n) \mapsto O(j_1, \ldots, j_p) \dashv \Gamma \backslash \{M, N\}, O : p}$$

The premise states that $m \xleftarrow{i} p \xrightarrow{j} n$ is a pullback of $m \xrightarrow{\vec{x}} q \xleftarrow{\vec{y}} n$ in $\mathbb{F}$.

Proposition 19. *The above rules are sound.*

Proof. We prove that the output substitution is the most general unifier.

Let us consider the first rule. We decompose Γ as $M : m, \Gamma'$ the coproduct of ym and Γ'. The term $M(\vec{x})$ corresponds to the composition of $yq \xrightarrow{M(\vec{x})}$

$T(ym) \hookrightarrow T(\Gamma)$. More abstractly, we want to compute the coequaliser, in Kl_T, of

for $A = yq$, $B = ym$, $C = \Gamma'$. It is enough to compute the coequaliser of $f : B \to D$ of $A \rightrightarrows B$, for the desired coequaliser is then $B+C \xrightarrow{f+C} D+C$. So we need to compute the coequaliser of $yq \rightrightarrows T(ym)$. As we explain in Section A, the functor $\mathbb{N} \xrightarrow{y} Set^{\mathbb{N}} \to Kl_T$ extends to a functor $\mathbf{y} : \mathbb{F} \to Kl_T^{op}$ such that the coequaliser is precisely that of $\mathbf{y}\vec{x}$ and $\mathbf{y}\vec{y}$. Since $\mathbf{y}$ preserves equalisers (Lemma 36), the coequaliser is $ym \xrightarrow{\mathbf{y}i} T(yp)$, where $i : p \to m$ is the equaliser of $\vec{x}$ and $\vec{y}$.

The second rule can be justified similarly. $\qquad\square$

3.4 Case $o(\vec{t}) = o(\vec{u})$ and $x = y$

$$\frac{o \text{ has binding arity } \vec{n} \qquad \Gamma \vdash \vec{t} =_{q+\vec{n}} \vec{u} \Rightarrow \sigma \dashv \Delta}{\Gamma \vdash o(\vec{t}) =_q o(\vec{u}) \Rightarrow \sigma \dashv \Delta}$$

Lemma 20. *This rule is sound.*

Proof. The result follows from the fact that a substitution unifies $o(\vec{t}) = o(\vec{u})$ if and only if it unifies $\vec{t}$ with $\vec{u}$. $\qquad\square$

$$\overline{\Gamma \vdash x =_q x \Rightarrow id \dashv \Gamma}$$

3.5 Case $M(\vec{x}) = o(\vec{u})$

$$\frac{o \text{ has binding arity } (n_1, \ldots, n_p) \qquad M \text{ does not occur in } \vec{u}}{\Gamma \backslash \{M\}, \vec{N} : m + \vec{n} \vdash N_1(0, \ldots, n_1 - 1, x_1 + n_1, \ldots, x_m + n_1) =_{q+n_1} u_1, \cdots \Rightarrow \sigma \dashv \Delta}{\Gamma \vdash M(\vec{x}) =_q o(\vec{u}) \Rightarrow \sigma \circ M(1, \ldots m) \mapsto o(\vec{N}) \dashv \Delta}$$

Lemma 21. *The above rule are sound.*

Proof. If there is a unifier, then M can't appear in $\vec{u}$ for size reason. Let us write Γ as $M : m, \Gamma'$, the coproduct of ym and Γ'. The term $M(\vec{x})$ corresponds to the composition of $yq \to T(ym)$ selecting $M(\vec{x})$ with the coproduct injection $T(ym) \hookrightarrow T(\Gamma)$. As M does not appear in $o(\vec{u})$, the corresponding morphism

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$yq \to T(\Gamma)$ factors through the coproduct injection $T(\Gamma') \hookrightarrow T(\Gamma)$. In other words, we want to compute the coequaliser (in Kl_T) of

with $A = yq$, $B = ym$ and $C = \Gamma'$. This is equivalent to the pushout of $B \leftarrow A \to C$. The morphism $A \to C$ corresponding to $o(\vec{u})$ factors as $yq \xrightarrow{u} T(\Gamma')^{(\vec{n})} \xrightarrow{o} T(\Gamma')$.

Now, let us study the category of unifiers. A unifier $ym \to T(\Delta) \leftarrow \Gamma'$ must maps M to some $o(\dots)$, so that $ym \to T(\Delta)$ factors as $ym \to T(\Delta)^{(\vec{n})} \xrightarrow{o} T(\Delta)$. In other words, a unifier is a family Δ with morphisms $f : \Gamma' \to T(\Delta)$ and $g : ym \to T(\Delta)^{(\vec{n})}$ such that the following diagram commutes:

Now, since f^* is a T-algebra morphism, commutation of the previous diagram is equivalent to commutation of the following one:

Since o is injective, this is equivalent to commutation of the following dia-

gram.

$$yq \xrightarrow{M(\vec{x})} T(ym)$$
$$u \downarrow \qquad \qquad \downarrow g^*$$
$$T(\Gamma')^{(\vec{n})} \xrightarrow[f^{*(\vec{n})}]{} T(\Delta)^{(\vec{n})}$$

Now, a morphism $u : yk \to Y^{(\vec{n})}$ is equivalently given by a morphism $u' :$
$y(k+\vec{n}) \to Y$, where $y(k+\vec{n})$ denotes the coproduct $\coprod_i y(k+n_i)$. Then u can be
retrieved from u' as the composition $yk \xrightarrow{d} y(k+\vec{n})^{(\vec{n})} \xrightarrow{u'^{(\vec{n})}} Y^{(\vec{n})}$. Thus, a unifier
is given by a family Δ together with Kleisli morphisms $g' : y(m + \vec{n}) \to T(\Delta)$
and $h : \Gamma' \to T(\Delta)$ such that the following diagram commutes.

$$y(q + \vec{n}) \xrightarrow{M(\vec{x})'} T(y(m + \vec{n})) \qquad\qquad (1)$$
$$u' \downarrow \qquad\qquad\qquad \downarrow g'^*$$
$$T(\Gamma') \xrightarrow{f^*} T(\Delta)$$

Thus, a unifier is a cocone over the pushout diagram

$$y(q + \vec{n}) \xrightarrow{M(\vec{x})'} T(y(m + \vec{n}))$$
$$u' \downarrow$$
$$T(\Gamma')$$

The premise is precisely computing this colimit, producing $\sigma : \Gamma' + y(m + \vec{n}) \to$
$T(\Delta)$:

$$\Gamma\backslash\{M\}, \vec{N} : m+\vec{n} \vdash N_1(0,\dots,n_1{-}1, x_1{+}n_1, \dots, x_m{+}n_1) =_{q+n_1} u_1, \dots \Rightarrow \sigma \dashv \Delta$$

The desired unifier is then the composition of σ with the coproduct morphism
(in Kl_T) $\Gamma' + ym \xrightarrow{id_{\Gamma'}+v} T(\Gamma' + y(m + \vec{n}))$, where v is the composite $ym \to$
$T(y(m + \vec{n}))^{(\vec{n})} \xrightarrow{o} T(y(m + \vec{n}))$. $\qquad\qquad \square$

3.6 Case $M(\vec{x}) = x_i$

$$\overline{\Gamma \vdash M(\vec{x}) =_q x_i : M(1,\dots,m) \mapsto i \dashv \Gamma\backslash\{M\}}$$

A symmetric rule must be introduced as well.

3.7 Termination

This section is devoted to the proof of the following proposition.

Proposition 22. *There is no infinite derivation tree of $\Gamma \vdash \vec{t} =_{\vec{n}} \vec{u} \Rightarrow \sigma \dashv \Delta$.*

The main difficulty to show termination is that the case $M(\vec{x}) = o(\vec{u})$ involves a recursive call with an extended context, while all the other rules are reducing or keeping the same context size. One way to solve this issue consists in avoiding creating new metavariables. Instead, we could first (potentially) reduce the arities of metavariables appearing in $o(\vec{u})$ so that they don't refer to free variables outside $\vec{x}$ and then directly instantiate M with the resulting term. This seems to be a bit tedious to describe precisely (not to mention to prove correctness).

It turns out that after encountering the case $M(\vec{x}) = o(\vec{u})$, the algorithm virtually enters a phase where the left handsides will always be distinct metavariables that don't appear in the right handsides. We say that the unification problem is *directed* if it is of this shape.

Lemma 23. *If there is a finite derivation of $\Gamma \vdash \vec{t} =_{\vec{n}} \vec{u} \Rightarrow \sigma \dashv \Delta$ where $\vec{t} = \vec{u}$ is directed, then all the involved nodes are directed..*

The difficult case is the stepwise rule. It relies on the following lemma.

Lemma 24. *Let $\Gamma \vdash t_0, \vec{t} = u_0, \vec{u}$ be a directed unification problem, and assume given a finite derivation tree $\Gamma \vdash t_0 = u_0 \Rightarrow \sigma \dashv \Delta$. Then, $\vec{t}[\sigma] = \vec{u}[\sigma]$ is directed.*
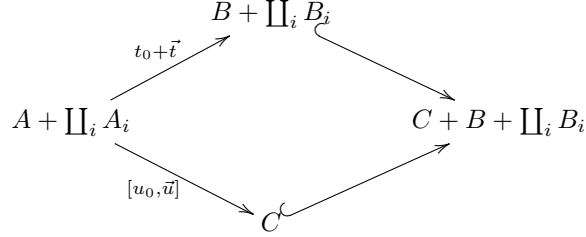
This in turn requires the following lemma proved by induction.

Lemma 25. *Assume there is a finite derivation of $\Gamma, \Gamma' \vdash \vec{t} = \vec{u} \Rightarrow \sigma \dashv \Delta$, such that metavariables in $\vec{t}, \vec{u}$ are in Γ. Then, there exists Δ' such that $\Delta \simeq \Delta', \Gamma'$ and σ through this isomorphism, is of the shape $\sigma' + id_{\Gamma'}$. In other words, the output substitution preserves any unused metavariable and never use them for instantiation otherwise.*
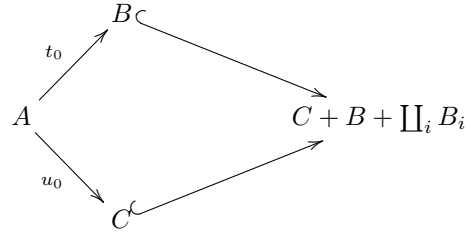
Proof of Lemma 24. Note that a directed unification problem $\vec{t} = \vec{u}$ corresponds to a diagram in Kl_T of the shape

$$
\begin{array}{ccc}
 & \coprod_i B_i & \\
\overset{\vec{t}}{\nearrow} & & \searrow \\
\coprod_i A_i & & C + \coprod_i B_i \\
\underset{\vec{u}}{\searrow} & & \nearrow \\
 & C &
\end{array}
$$

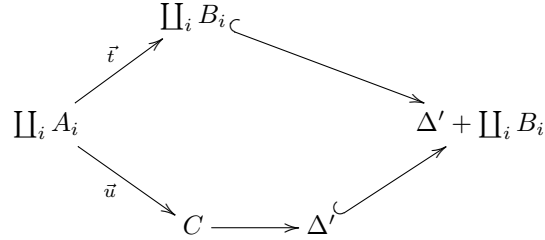In particular, a directed unification problem $t_0, \vec{t} = u_0, \vec{u}$ has this shape:

$$B + \coprod_i B_i$$

$$A + \coprod_i A_i \xrightarrow{\;t_0 + \vec{t}\;} \qquad \qquad C + B + \coprod_i B_i$$

$$\xrightarrow{[u_0, \vec{u}]} C$$

The most general unifier of t_o and u_0 corresponds to the coequaliser of

$$B$$
$$A \xrightarrow{t_0} \quad u_0 \qquad C + B + \coprod_i B_i$$
$$C$$

By Lemma 25, the coequaliser computed by the derivation of $\Gamma \vdash t_0 = u_0 \Rightarrow \sigma \dashv \Delta$ has the shape

$$B$$
$$A \xrightarrow{t_0} \; \xrightarrow{u_0} \quad C + B + \coprod_i B_i \xrightarrow{\;\sigma' + \coprod_i B_i\;} \Delta' + \coprod_i B_i$$
$$C$$
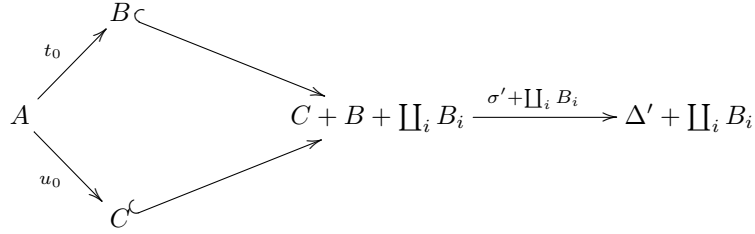
Now, $\vec{t}[\sigma] = \vec{u}[\sigma]$ corresponds to the diagram

$$\coprod_i B_i$$
$$\coprod_i A_i \xrightarrow{\vec{t}} \; \xrightarrow{\vec{u}} \quad \Delta' + \coprod_i B_i$$
$$C \longrightarrow \Delta'$$

which is indeed directed. $\qquad \qquad \square$

Now we can prove easily

Lemma 26. *If there is a finite derivation tree of* $\Gamma \vdash \vec{t} =_{\vec{n}} \vec{u} \Rightarrow \sigma \dashv \Delta$, *then*

- $|\Gamma| \geq |\Delta|$

- if $|\Gamma| = |\Delta|$, then σ is a renaming, in the sense that it instantiates metavariables with metavariables.

- if $\vec{t} = \vec{u}$ is directed, then $|\Gamma| = |\Delta| + |\vec{t}|$, where $|\vec{t}|$ is the length of $\vec{t}$, as a list.

Finally, to prove termination, we consider the lexicographic order induced by the context size and the size of the involved terms to each judgement $\Gamma \vdash \vec{t} =_{\vec{n}} \vec{u} \Rightarrow \sigma \dashv \Delta$. More precisely,

- the context size is defined as the length of Γ if it is not directed, or as the total number of metavariables involved in the right handsides otherwise.

- the size of a non empty term list $||\vec{t}||$ is defined as $|\vec{t}| - 1 + \Sigma_i ||t_i||$

- the size of a term $||o(\vec{t})||$ is defined as $1 + ||\vec{t}||$, and $||M|| = ||x|| = 0$.

It is easy to show that each recursive call is decreasing with respect to this order. The crucial point, in the stepwise rule, is the following lemma.

Lemma 27. *If σ is a renaming, then $||t[\sigma]|| = ||t||$.*

References

[1] Thorsten Altenkirch, James Chapman, and Tarmo Uustalu. Monads need not be endofunctors. *Logical Methods in Computer Science*, 11(1), 2015.

[2] Peio Borthelle, Tom Hirschowitz, and Ambroise Lafont. A cellular Howe theorem. In Holger Hermanns, Lijun Zhang, Naoki Kobayashi, and Dale Miller, editors, *Proc. 35th ACM/IEEE Symposium on Logic in Computer Science* ACM, 2020.

[3] Marcelo Fiore and Dmitrij Szamozvancev. Formal metatheory of second-order abstract syntax. *Proceedings of the ACM on Programming Languages*, 6(POPL), 2022.

[4] Saunders Mac Lane. *Categories for the Working Mathematician*. Number 5 in Graduate Texts in Mathematics. Springer, 2nd edition, 1998.

A Free T-algebras preserve pullbacks

In this section we show that renaming turn free T-algebras into functors $\mathbb{F} \to Set$ preserving pullbacks. In fact, we are going to show it for the initial T-algebra, since a free T-algebra on $X \in Set^{\mathbb{N}}$ is equivalently the initial Σ'-monoid, for Σ' the binding signature extending Σ with first order operations as specified by X.

Let us first explain where renaming comes from. Every binding signature Σ induces an endofunctor on $Set^{\mathbb{N}}$ that we still denote by Σ. For example, in the case of λ-calculus, $\Sigma(X)_n = X_n \times X_n + X_{n+1}$.

Lemma 28. *Denoting Σ^* the free monad $\Sigma^* X = \mu Z.X + \Sigma(Z)$ induced by a binding signature Σ, the initial Σ-monoid is $\Sigma^* I$.*

Proof. See [2, Theorem 2.15]. $\qquad\square$

Lemma 29. *Given a binding signature Σ, the free monad Σ^* lifts to the category $Set^{\mathbb{F}}$. Denoting $\underline{I}$ the canonical embedding $\mathbb{F} \to Set$, renaming on $\Sigma^* I$ is given by the renaming structure on $\Sigma^* \underline{I}$.*

Proof. Renaming on $\Sigma^* I$ is induced by substitution. Substitution on $\Sigma^* I$ induced by a monoid structure on them (for a monoidal structure on $Set^{\mathbb{F}}$ or $Set^{\mathbb{N}}$, as in [1]) induced by a strength $\Sigma(A) \otimes B \to \Sigma(A \otimes B)$.
  TODO $\qquad\square$

Lemma 30. *The previous lemma induces a functor $\mathcal{U} : Kl_T \to Set^{\mathbb{F}}$.*

What remains to show is that this renaming preserves pullbacks. Let us reason on the category $Set^{\mathbb{F}}$ on which Σ^* lifts, as we just argued. Now, $\Sigma^* I$ is computed as the initial algebra of $H : Set^{\mathbb{F}} \to Set^{\mathbb{F}}$ mapping X to $I + \Sigma(X)$. This means that $\Sigma^* I$ is the colimit over the initial ω-chain

$$\emptyset \to H(\emptyset) \to \cdots \to H..H(..(\emptyset..)) \to \ldots$$

Since pullback preserving functors are preserved by filtered colimits (as filtered colimits commute with finite limits), it is enough to show that each functor $H^{\circ n}(\emptyset)$ preseves pullbacks, which again amounts to showing that H preserves functors preservings pullbacks.

Lemma 31. *The endofunctor $H : Set^{\mathbb{F}} \to Set^{\mathbb{F}}$ maps functors preserving pullbacks to functors preserving pullbacks.*

Proof. Let F be a functor $\mathbb{F} \to Set$ preserving pullbacks. Let

$$\begin{array}{ccc} A & \longrightarrow & B \\ \downarrow & & \downarrow \\ C & \longrightarrow & D \end{array}$$

be a pullback in $\mathbb{F}$. Let us show that the following square is a pullback.

$$\begin{array}{ccc} H(F)_A & \longrightarrow & H(F)_B \\ \downarrow & & \downarrow \\ H(F)_C & \longrightarrow & H(F)_D \end{array}$$

Since pullbacks commute with coproducts in Set, this is enough to show that the following square is a pullback

$$\begin{array}{ccc}
\Sigma(F)_A & \longrightarrow & \Sigma(F)_B \\
\downarrow & & \downarrow \\
\Sigma(F)_C & \longrightarrow & \Sigma(F)_D
\end{array}$$

This follows from the fact that $\Sigma(F)$ is isomorphic to some $\coprod_i F^{(\vec{n_i})}$, and coproducts commute with connected limits. $\square$

Notation 32. Let $Set_p^{\mathbb{F}}$ be the full subcategory of functors preserving pullbacks.

Lemma 33. *The functor $\mathbb{N} \xrightarrow{y} Set^{\mathbb{N}} \to Kl_T$ extends to a functor $\mathbf{y} : \mathbb{F}^o \to Kl_T$ such that $Kl_T(\mathbf{y}m, X) \simeq Set_p^{\mathbb{F}}(Jm, TX)$ is natural in m.*

Proof. The isomorphism $Kl_T(ym, X) \simeq TX_m \simeq Set^{\mathbb{F}}(Jm, TX)$ means that the following diagram commutes up to isomorphism

$$\begin{array}{ccccc}
\mathbb{N} & \xrightarrow{y} & (Set^{\mathbb{N}})^o & \longrightarrow & Kl_T^o \\
\downarrow & & & & \downarrow{\scriptstyle y} \\
\mathbb{F} & \xrightarrow{y} & (Set^{\mathbb{F}})^o & \xrightarrow[Set^{\mathcal{U}}]{y} Set^{Set^{\mathbb{F}}} & Set^{Kl_T}
\end{array}$$

where y denotes the yoneda embedding. Since the left vertical morphism is bijective on objects and the right vertical morphism is full and faithful, there is a filling of this square $\mathbf{y} : \mathbb{F}^o \to Kl_T$ making triangles both commute up to isomorphism (TODO: find references) $\square$

Remark 34. Another way to define $\mathbf{y}$ goes as follows. There is a Σ-monoid monad T' on $Set^{\mathbb{F}}$ and T is actually isomorphic to $RT'L$, where L is the left Kan extension and R its right adjoint (precomposition by $\mathbb{N} \to \mathbb{F}$). As a consequence, there is a fully faithful Kleisli extension

$$\begin{array}{ccc}
Set^{\mathbb{N}} & \xrightarrow{L} & Set^{\mathbb{F}} \\
\downarrow & & \downarrow \\
Kl_T & \longrightarrow & Kl_{T'}
\end{array}$$

Then, we can define $\mathbf{y}$ as filling the square

$$\begin{array}{ccc}
\mathbb{N} & \longrightarrow & Kl_T^o \\
\downarrow & & \downarrow \\
\mathbb{F} & \longrightarrow & Kl_{T'}^o
\end{array}$$

Remark 35. Given a morphism $f : m \to n$ in $\mathbb{F}$, the induced morphism $\mathbf{y}f : yn \to T(ym)$ selects the term $t \in T(ym)_n$ defined as renaming the canonical term $M(0, \ldots, m-1) \in T(ym)_m$, corresponding to the unit $ym \to T(ym)$, along f. In other words, $\mathbf{y}f$ selects the term $M(f_0, \ldots f_{m-1})$.

Lemma 36. $\mathbf{y}^o : \mathbb{F} \to Kl_T^o$ *preserves pullbacks, hence finite connected limits.*

Proof. We have a natural isomorphism $Kl_T(\mathbf{y}m, X) \simeq Set_p^{\mathbb{F}}(Jm, TX)$, where J is the yoneda embedding in $\mathbb{F}^o \to Set^{\mathbb{F}}$: $Jn_m = m^n$. It follows that $\mathbf{y}$ preserves any colimit that J preserves. Now, since J is the yoneda embedding, J preserves pullbacks, as we restrict to the category of presheaves preserving pullbacks. $\square$

Corollary 37. *Let* $f : p \to q$ *be an injective map. Then, the induced map* $\mathbf{y}f : yq \to T(yp)$ *is epimorphic.*

Proof. The proof follows from Lemma 36 by noting that $f : A \to B$ is monomorphic if and only if the following square is a pullback.

$$
\begin{array}{ccc}
A & \xrightarrow{\;id\;} & A \\
{\scriptstyle id}\downarrow & & \downarrow{\scriptstyle f} \\
A & \xrightarrow[\;f\;]{} & B
\end{array}
$$

$\square$