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# Abstract

The  $\lambda\sigma$ -calculus is a refinement of the  $\lambda$ -calculus where substitutions are manipulated explicitly. The  $\lambda\sigma$ -calculus provides a setting for studying the theory of substitutions, with pleasant mathematical properties. It is also a useful bridge between the classical  $\lambda$ -calculus and concrete implementations.

### 1 Introduction

Substitution is the éminence grise of the  $\lambda$ -calculus. The classical  $\beta$  rule,

$$(\lambda x.a)b \rightarrow_{\beta} a\{b/x\}$$

uses substitution crucially though informally. Here a and b denote two terms, and  $a\{b/x\}$  represents a where all free occurrences of x are replaced with b. This substitution does not belong in the calculus proper, but rather in an informal meta-level. Similar situations arise in dealing with all binding constructs, from universal quantifiers to type abstractions.

A naive reading of the  $\beta$  rule suggests that the substitution of b for x should happen at once, when the rule is applied. In implementations, substitutions invariably happen in a more controlled way. This is due to practical considerations, relevant in the implementation of both logics and programming languages. The term  $a\{b/x\}$  may contain many copies of b (for instance, if a = xxxx); without sophisticated structure-sharing mechanisms [13], performing substitutions immediately causes a size explosion.

Therefore, in practice, substitutions are delayed and explicitly recorded; the application of substitutions is independent, and not coupled with the  $\beta$  rule. The correspondence between the theory and its implementations becomes highly nontrivial, and the correctness of the implementations can be compromised.

In this paper we study the  $\lambda\sigma$ -calculus, a refinement of the  $\lambda$ -calculus [1] where substitutions are manipulated explicitly. Substitutions have syntactic representations, and if a is a term and s is a substitution then the term a[s] represents a with the substitution s. We can now express a  $\beta$  rule with delayed substitution, called *Beta*:

$$(\lambda x.a)b \longrightarrow_{Beta} a[(b/x) \cdot id]$$

where  $(b/x) \cdot id$  is syntax for the substitution that replaces x with b and affects no other variable ("." represents extension and *id* the identity substitution). Of course, additional rules are needed to distribute the substitution later on.

The  $\lambda\sigma$ -calculus is a suitable setting for studying the theory of substitutions, where we can express and prove desirable mathematical properties. For example, the calculus is Church-Rosser and it is a conservative extension of the  $\lambda$ -calculus. Moreover, the  $\lambda\sigma$ -calculus is strongly connected with the categorical understanding of the  $\lambda$ -calculus, where a substitution is interpreted as a composition [5].

We propose the  $\lambda\sigma$ -calculus as a step in closing the gap between the classical  $\lambda$ -calculus and concrete implementations. The calculus is a vehicle in designing, understanding, verifying, and comparing implementations of the  $\lambda$ -calculus, from interpreters to machines. Other applications are in the analysis of typechecking algorithms for higher-order languages and in the mechanization of logical systems.

When one considers weak reduction strategies, the treatment of substitutions can remain quite simple and then our approach may seem overly general. Weak reduction strategies do not compute in the scope of  $\lambda$ 's. Then, there arise no nested substitutions or substitutions in the scope of  $\lambda$ 's. All substitutions are at the top level, as simple environments. An ancestor of the  $\lambda\sigma$ -calculus, the  $\lambda\rho$ -calculus, suffices in this setting [5].

However, strong reduction strategies are useful in general, both in logics and in typechecking higher-

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order programming languages. In fact, strong reduction strategies are useful in all situations where symbolic matching has to be conducted in the scope of binders. Thus, a general treatment of substitutions is required, where substitutions may occur at the top level and deep inside terms.

In some respects, the  $\lambda\sigma$ -calculus resembles the calculi of combinators, particularly those of categorical combinators [4]. The  $\lambda\sigma$ -calculus and the combinator calculi all give full formal accounts of the process of computation, without suffering from unpleasant complications in the (informal) handling of variables. They all make it easy to derive machines for the  $\lambda$ -calculus and to show the correctness of these machines. ¿From our perspective, the advantage of the  $\lambda\sigma$ -calculus over combinator calculi is that it remains closer to the original  $\lambda$ -calculus.

There are actually several versions of the calculus of substitutions. We start out by discussing an untyped calculus. The main value of the untyped calculus is for studying evaluation methods. We give reduction rules that extend those of the classical  $\lambda$ -calculus and investigate their confluence. We concentrate on a presentation that relies on De Bruijn's numbering for variables [2], and briefly discuss presentations with more traditional variable names.

Then we proceed to consider typed calculi of substitutions, in De Bruijn notation. We discuss typing rules for a first-order system and for a higherorder system; we prove some of their central properties. The typing rules are meant to serve in designing typechecking algorithms. In particular, their study has been of help for both soundness and efficiency in the design of the Quest typechecking algorithm [3].

We postpone discussion of the untyped calculi to section 3 and of the typed calculi to sections 4 and 5. We now proceed with a gentle technical overview.

### 2 Informal overview

We start with a review of De Bruijn notation, and then preview untyped, first-order, and second-order calculi of substitutions.

#### 2.1 De Bruijn notation

In De Bruijn notation, variable occurrences are replaced with positive integers (called De Bruijn indices); binding occurrences of variables become unnecessary. The positive integer **n** refers to the variable bound by the **n**-th surrounding  $\lambda$  binder, for example:

$$\lambda x \cdot \lambda y \cdot xy$$
 becomes  $\lambda \lambda 21$ 

In first-order typed systems, the binder types must be preserved, for example:

$$\lambda x: A.\lambda y: B.xy$$
 becomes  $\lambda A.\lambda B.$  21

In second-order systems, type variables too are replaced with De Bruijn indices:

$$\Lambda A.\lambda x: A.x$$
 becomes  $\Lambda \lambda 1.1$ 

De Bruijn notation is unreadable, but it leads to simple formal systems. Hence we use indices in inference rules, but variable names in examples.

Classical  $\beta$  reduction and substitution must be adapted for De Bruijn notation. In order to reduce  $(\lambda a)b$ , it does not suffice to substitute b into a in the appropriate places. If there are occurrences of 2, 3, 4, ... in a, these become "one off," since one of the  $\lambda$ binders surrounding a has been removed. Hence, all the remaining free indices in a must be decremented; the desired effect is obtained with an infinite substitution: the  $\beta$  rule becomes

$$(\lambda a)b \rightarrow_{\beta} a\{b/1, 1/2, 2/3, \ldots\}$$

When pushing this substitution inside a, we may come across a  $\lambda$  term  $(\lambda c)\{b/1, 1/2, 2/3, \ldots\}$ . In this case, we must be careful to avoid replacing the occurrences of 1 in c with b, since these occurrences correspond to a bound variable and the substitution should not affect them. Hence we must "shift" the substitution. In addition, we must "lift" all the indices of b in order to prevent captures. We obtain  $\lambda c\{1/1, b\{2/1, 3/2, \ldots\}/2, 2/3, \ldots\}$ .

This informal introduction to De Bruijn notation should suffice to give the flavor of things to come.

### 2.2 An untyped calculus

We shall study a simple set of algebraic operators that perform all these index manipulations—without ...'s, even though we treat infinite substitutions that replace all indexes. If s represents the infinite substitution  $\{a_1/1, a_2/2, a_3/3, \ldots\}$ , we write a[s] for a with the substitution s. A term of the form a[s] is called a *closure*. The change from  $\{\}$ 's to []'s emphasizes that the substitution is no longer a meta-level operation.

The syntax of the untyped  $\lambda\sigma$ -calculus is:

Terms	$a ::= 1 \mid ab \mid \lambda a \mid a[s]$
Substitutions	$s ::= id  \uparrow  a \cdot s   s \circ t$

This syntax of substitutions corresponds to the index manipulations described in the previous section:

• *id* is the identity substitution  $\{i/i\}$  (for all *i*).

- ↑ (shift) is the substitution {(i+1)/i}; for example, 1[↑] = 2. Thus, we need only the index 1; n+1 is coded as 1[↑<sup>n</sup>], where ↑<sup>n</sup> is the composition of n shifts, ↑ ... ↑. We also write ↑<sup>0</sup> for id.
- i[s] is the value of the De Bruijn index i in the substitution s, also written s(i) when s is viewed as a function.
- $a \cdot s$  (the cons of a onto s) is the substitution  $\{a/1, s(i)/(i+1)\}$ ; for example,

•  $s \circ t$  (the composition of s and t) is the substitution such that  $a[s \circ t] = a[s][t]$ , hence  $s \circ t = \{s(i)/i\} \circ t = \{s(i)[t]/i\}$  and, for example,

$$id \circ t = \{id(i)[t]/i\} = \{t(i)/i\} = t \\ \uparrow \circ (a \cdot s) = \{\uparrow(i)[a \cdot s]/i\} = \{s(i)/i\} = s$$

At this point, we have shown most of the algebraic properties of the substitution operations. In addition, composition is associative and distributes over cons (that is,  $(a \cdot s) \circ t = a[s] \cdot (s \circ t)$ ). Moreover, the last example above indicates that  $\uparrow \circ s$  is the "rest" of s, without the first component of s; thus,  $\mathbf{1}[s] \cdot (\uparrow \circ s) = s$ .

Using this notation, we can write the Beta rule as

$$(\lambda a)b \rightarrow_{Beta} a[b \cdot id]$$

To complement this rule, we can write rules to evaluate 1, for instance

$$\mathbf{1}[c \cdot s] \rightarrow c$$

and rules to push substitution inwards, for instance

$$(cd)[s] \rightarrow (c[s])(d[s])$$

In particular, we can derive an intriguing law for the distribution of substitution over  $\lambda$ :

$$(\lambda c)[s] \to \lambda(c[\mathbf{1} \cdot (s \circ \uparrow)])$$

This law uses all the operators (except id), and suggests that this choice of operators is natural, perhaps inevitable. In fact, there are many possible variations, but we shall not discuss them here.

Explicit substitutions complicate the structure of bindings somewhat. For example, consider the term  $(\lambda(\mathbf{1}[2 \cdot id]))[a \cdot id]$ . We may be tempted to think that **1** is bound by  $\lambda$ , as it would be in a standard De Bruijn reading. However, the substitution  $[2 \cdot id]$  intercepts the index, giving the value **2** to **1**. Then, after crossing over  $\lambda$ , the index **2** is renamed to **1** and receives the value *a*. One should keep these complications in mind in examining  $\lambda\sigma$  formulas—for example, in deciding whether a formula is closed, in the usual sense.

#### 2.3 A first-order calculus

When we move to a typed calculus, we introduce types both in terms and in substitutions. We assume a set of constant types K. The syntax becomes:

$\mathbf{Types}$	$A ::= K \mid A \to B$
Environments	$E ::= nil \mid A, E$
Terms	$a ::= 1 \mid ab \mid \lambda A.a \mid a[s]$
Substitutions	$s ::= id \mid \uparrow \mid a{:}A \cdot s \mid s \circ t$

The environments are used in the type inference rules, as is commonly done, to record the types of the free variables of terms. Naturally, in this setting, environments are indexed by De Bruijn indices. The environment  $A_1, A_2, \ldots, A_n, nil$  associates type  $A_i$  with index **i**. For example, the axiom for **1** and the rule for  $\lambda$  abstraction are:

$$A, E \vdash \mathbf{1} : A$$
$$\underline{A, E \vdash b : B}$$
$$\overline{E \vdash \lambda A.b : A \to B}$$

In the first-order  $\lambda \sigma$ -calculus, environments also serve as the "types" of substitutions. We write  $s \therefore E$ to say that the substitution s "has" the environment E. For example, the typing rule for cons is:

$$\frac{E \vdash a : A \qquad E \vdash s \therefore E'}{E \vdash a : A \cdot s \therefore A, E'}$$

The main use of this new notion is in typing closures. Since s provides the context in which a should be understood, the approach is to compute the environment E' of s, and then type a in that environment:

$$\frac{E \vdash s \therefore E' \quad E' \vdash a : A}{E \vdash a[s] : A}$$

#### 2.4 A second-order calculus

When we move to a second-order system, new subtleties appear, because substitutions may contain types, and environments may contain place-holders for types; for example,  $Bool::Ty \cdot id$ . Ty, nil.

The typing rules become more complex because types may contain type variables, which must be looked up in the appropriate environments (this problem arises in full generality with dependent types [12]). In particular, the typing axiom for **1** shown above becomes the rule:

$$\frac{E \vdash A :: \mathrm{Ty}}{A, E \vdash \mathbf{1} : A[\uparrow]}$$

The extra shift is required because A is understood in the environment E in the hypothesis, while it is understood in A, E in the conclusion. An alternative (but heavy) solution would be to have separate index sets for ordinary term variables and for type variables, and to manipulate separate term and type environments as well.

Another instance of this phenomenon is in the rule for  $\lambda$  abstraction, given above. Notice that A must have been proved to be a type in the environment E, while B is understood in A, E in the assumption. Then  $A \to B$  is understood in E in the conclusion. This means that the indices of B are "one off" in  $A \to B$ . The rule for application takes this into account; a substitution is applied to B to "unshift" its indices:

$$\frac{E \vdash b : A \rightarrow B \quad E \vdash a : A}{E \vdash b(a) : B[a:A \cdot id]}$$

The  $B[a:A \cdot id]$  part is reminiscent of the rule found in calculi for dependent types, and this is the correct technique for the version of such calculi with explicit substitutions. However, since here we do not deal with dependent types, a will never be substituted in B (B will never contain the index 1). The substitution is still needed to shift the other indices in B.

The main difficulty in our second-order calculus arises in typing closures. The approach described for the first order, while still viable, is not sufficient. For example, if *not* is the usual negation on *Bool*, we certainly want to be able to type

$$(\lambda \mathbf{1}.not(\mathbf{1}))[Bool \cdot id]$$

or, in a more familiar notation,

Let 
$$X = Bool$$
 in  $\lambda x: X.not(x)$ 

(We interpret Let via a substitution, not via a  $\lambda$ .) Our strategy for the first-order calculus was to type the substitution, obtaining an environment  $(X::Ty) \cdot id$ , and then type  $\lambda x: X.not(x)$  in  $(X::Ty) \cdot id$ . Unfortunately, to type this term, it does not suffice to know that X is a type; we must know that X is Bool. To solve this difficulty, we have rules to push a substitution inside a term and then type the result. As in calculi with dependent types, the tasks of deriving types and applying substitutions are inseparable.

Finally, as discussed below, surprises arise in writing down the precise rules; for example the rule for typing conses has to be modified. Even the form of the judgement  $E \vdash s \therefore E'$  must be reconsidered.

Higher-order calculi (possibly with dependent type constructions) are also of theoretical and practical importance. We do not discuss them formally below, however, for we believe that the main complications arise already at the second order.

### 3 The untyped $\lambda \sigma$ -calculus

In this section we present the untyped  $\lambda\sigma$ -calculus. We propose a basic set of equational axioms for the  $\lambda\sigma$ -calculus in De Bruijn notation. The equations induce a rewriting system; this rewriting system suffices for the purposes of computation. We show that the rewriting system is confluent, and thus provides a convenient theoretical basis for more deterministic implementations of the  $\lambda\sigma$ -calculus. We also consider some variants of the axiom system and treatments using variable names.

As in the classical  $\lambda$ -calculus, actual implementations would resort to particular rewriting strategies. We discuss a normal-order strategy for  $\lambda\sigma$  evaluation. Then we focus on a more specialized reduction system, still based on normal order, which provides a suitable basis for abstract  $\lambda\sigma$  machines. We describe one machine, which extends Krivine's weak reduction machine [11] with strong reduction.

#### 3.1 The basic rewriting system

The syntax of the untyped  $\lambda\sigma$ -calculus is the one given in the informal overview,

$\mathbf{Terms}$	$a ::= 1   ab   \lambda a   a[s]$
${f Substitutions}$	$s ::= id  \uparrow  a \cdot s   s \circ t$

Notice that we have not included metavariables over the sorts of terms and substitutions—we consider only closed terms, and this suffices for our purposes. (In De Bruijn notation, the variables  $1, 2, \ldots$  are constants rather than metavariables.)

In this notation, we now define an equational theory for the  $\lambda\sigma$ -calculus, by proposing a set of equations as axioms. When they are all oriented from left to right, the equations become rewrite rules and give rise to a rewriting system. The equations fall into two subsets: a singleton *Beta*, the equivalent of the classical  $\beta$  rule, and ten rules for manipulating substitutions, which we call  $\sigma$  collectively.

Beta 
$$(\lambda a)b = a[b \cdot id]$$

$$VarId \qquad \mathbf{1}[id] = \mathbf{1}$$

$$VarCons \qquad \mathbf{1}[a \cdot s] = a$$

$$App \qquad (ab)[s] = (a[s])(b[s])$$

$$Abs \qquad (\lambda a)[s] = \lambda(a[\mathbf{1} \cdot (s \circ \uparrow)])$$

$$Clos \qquad a[s][t] = a[s \circ t]$$

 $IdL \qquad id \circ s = s$ 

 $\begin{array}{ll} ShiftId & \uparrow \circ id = \uparrow \\ ShiftCons & \uparrow \circ (a \cdot s) = s \\ Map & (a \cdot s) \circ t = a[t] \cdot (s \circ t) \\ Ass & (s_1 \circ s_2) \circ s_3 = s_1 \circ (s_2 \circ s_3) \end{array}$ 

The equational theory follows from these axioms and rules for replacing equals for equals.

Our choice of presentation is guided by the structure of terms and substitutions. The *Beta* rule eliminates  $\lambda$ 's and creates substitutions; the function of the other rules is to eliminate substitutions. Two rules deal with the evaluation of **1**. The next three deal with pushing substitutions inwards. The remaining five express substitution computations. We prove below that the substitution rules always produce unique normal forms; we denote by  $\sigma(a)$  the  $\sigma$ normal form of a.

The classical  $\beta$  rule is not directly included, but it can be simulated. The crucial fact is that, if  $a_1, \ldots, a_n, \ldots$  is a sequence of consecutive integers after some point, then the meta-level substitution  $\{a_1/1, \ldots, a_n/n, \ldots\}$  corresponds closely to an explicit substitution:

**Proposition 3.1** If there exist  $m \ge 0$  and  $p \ge 0$  such that  $a_{m+q} = \mathbf{p} + \mathbf{q}$  for all  $q \ge 1$ , then  $a\{a_1/1, \ldots, a_n/n, \ldots\} = \sigma(a[a_1 \cdot a_2 \cdot \ldots \cdot a_m \cdot \uparrow^p]).$ 

Therefore, the simulation of the  $\beta$  rule consists in first applying *Beta* and then  $\sigma$  until a  $\sigma$  normal form is reached.

As usual, we want a confluence theorem. This theorem will guarantee that all rewrite sequences yield identical results, and thus that the strategies used by different implementations are equivalent:

**Theorem 3.2** Beta +  $\sigma$  is confluent.

The proof does *not* rely on standard rewriting techniques, as  $Beta + \sigma$  does not pass the Knuth-Bendix test (but  $\sigma$  does). We come back to this point below.

Instead, the proof relies on the termination and confluence of  $\sigma$ , the confluence of the classical  $\lambda$ -calculus, and Hardin's interpretation technique [7].

First we show that  $\sigma$  is noetherian (that is,  $\sigma$  reductions always terminate) and confluent.

#### **Proposition 3.3** $\sigma$ is noetherian and confluent.

Since  $\sigma$  is noetherian, let us examine the form of  $\sigma$  normal forms. A substitution in normal form is necessarily in the form  $a_1 \cdot (a_2 \cdot (\dots (a_m \cdot U) \dots))$  where U is either *id* or a composition  $\uparrow \circ (\dots (\uparrow \circ \uparrow) \dots)$ . A term in normal form is entirely free of substitutions,

except in subterms such as  $1[\uparrow^n]$ , which codes the De Bruijn index n+1. Thus, a term in normal form is a classical  $\lambda$ -calculus term (modulo the equivalence of  $1[\uparrow^n]$  and n+1).

In summary, the syntax of  $\sigma$  normal forms is:

**Terms**  $a ::= \mathbf{1} | \mathbf{1} [\uparrow^n] | ab | \lambda a$ **Substitutions**  $s ::= id | \uparrow^n | a \cdot s$ 

After these remarks on  $\sigma$ , we can apply Hardin's interpretation technique to show that the full  $\lambda \sigma$  system is confluent. First, we review Hardin's method. Let X be a set equipped with two relations R and S. Suppose that R is noetherian and confluent, and denote by R(x) the R normal form of x; that  $S_R$  is a relation included in  $(R \cup S)^*$  on the set of R normal forms; and that, for any x and y in X, if S(x, y) then  $S_R^*(R(x), R(y))$ . An easy diagram chase yields that if  $S_R$  is confluent then so is  $(R \cup S)^*$ .

In our case, we take R to be the relation induced by  $\sigma$ , that is, R(x, y) holds if x reduces to y with the  $\sigma$  rules. We take  $S_R$  to be classical  $\beta$  conversion, that is,  $S_R(x, y)$  holds if y is obtained from x by replacing a subterm of the form  $(\lambda a)b$  with  $\sigma(a[b \cdot id])$ .

Thus two lemmas suffice for proving confluence:

**Lemma 3.4**  $\beta$  is confluent on  $\sigma$  normal forms.

**Lemma 3.5** If  $a \to_{Beta} b$  then  $\sigma(a) \to_{\beta}^{*} \sigma(b)$ . If  $s \to_{Beta} t$  then  $\sigma(s) \to_{\beta}^{*} \sigma(t)$ .

### 3.2 Variants

Some subsystems of  $\sigma$  are reasonable first steps to deterministic evaluation algorithms. We can restrict  $\sigma$  in three different ways. The rule *Clos* can be removed. The inference rule

$$\frac{s=s'\quad t=t'}{s\circ t=s'\circ t'}$$

can be removed, and the inference rule for the closure operator can be restricted to

$$\frac{s=s'}{\mathbf{1}[s]=\mathbf{1}[s']}$$

These restrictions (even cumulated) do not prevent us from obtaining  $\sigma$  normal forms and confluence, through the interpretation technique.

Confluence properties suggest a second kind of variant. Although  $Beta + \sigma$  is confluent, when we view it as a standard rewriting system on first-order terms it is not even locally confluent. The subtle point is that we have proved confluence on closed  $\lambda\sigma$  terms, that is, on terms exclusively constructed from the operators of the  $\lambda\sigma$ -calculus. In contrast, checking critical pairs involves considering open terms over this signature, with metavariables (that is, variables  $\mathbf{x}$  and  $\mathbf{u}$ ranging over terms and substitutions, different from De Bruijn indexes  $1, 2, \ldots$ ).

Consider, for example, the critical pair:

$$\begin{array}{ll} ((\lambda a)b)[u] & \rightarrow^{\star} & a[b[u] \cdot u] \\ ((\lambda a)b)[u] & \rightarrow^{\star} & a[b[u] \cdot (u \circ id)] \end{array}$$

For local confluence, we would want the equation  $(s \circ id) = s$ , but this equation is not a theorem of  $\sigma$ . Similar critical pair considerations suggest the addition of four new rules:

$$Id a[id] = a$$

$$IdR s \circ id = s$$

$$VarShift 1 \cdot \uparrow = id$$

$$SCons 1[s] \cdot (\uparrow \circ s) = s$$

These additional rules are well justified from a theoretical point of view. However, confluence on closed terms can be established without them, and they are not computationally significant. Moreover some of them are admissible (that is, every closed instance is provable). More precisely *Id* and *IdR* are admissible in  $\sigma$ , and *SCons* is admissible in  $\sigma + VarShift$ .

We should particularly draw attention to the last rule, *SCons.* It expresses that a substitution is equal to its first element appended in front of the rest. This rule is reminiscent of the surjective-pairing rule, which deserved much attention in the classical  $\lambda$ calculus. Klop has showed that surjective pairing destroys confluence for the  $\lambda$ -calculus [10].

Similarly, we conjecture that our system is not confluent when we have metavariables for both terms and substitutions. (Local confluence still holds.) The following term, inspired by Klop's counterexample [10], seems to work as a counterexample to confluence:

 $Y(Y(\lambda\lambda\mathbf{x}[\mathbf{1}[\mathbf{u}\circ(\mathbf{1}\cdot id)]\cdot(\uparrow\circ(\mathbf{u}\circ((\mathbf{21})\cdot id)))]))$ 

where Y is a fixpoint combinator,  $\mathbf{x}$  is a term metavariable, and  $\mathbf{u}$  is a substitution metavariable.

The reader may wonder what thwarts the techniques used in the last subsection. The point is that in Lemma 3.5, our reduction to the classical substitution lemma depended on the syntax of substitutions in normal form, which is not so simple any more (the syntax allows in particular expressions of the form  $\mathbf{u} \circ (\mathbf{1} \cdot id)$ , as in the claimed counterexample).

We can go half way in adding metavariables. If we add only term metavariables, the syntax of substitution  $\sigma$  normal forms is unchanged. This protects us from the claimed counterexample. There are two additional cases for term  $\sigma$  normal forms:

**Terms** 
$$a ::= \mathbf{1} | \mathbf{1} [\uparrow^n] | ab | \lambda a | \mathbf{x} | \mathbf{x} [s]$$

We believe that confluence can be proved in this case by the interpretation technique. Confluence on normal forms would be obtained through an encoding of the normal forms in the  $\lambda$ -calculus extended with constants, which is known to be confluent (**x** becomes a constant; **x**[s] becomes a constant applied to the elements of s).

### **3.3** The $\lambda\sigma$ -calculus with names

Let us discuss a more traditional formulation of the calculus, with variable names  $x, y, z, \ldots$ , as a small digression. Two ways seem viable.

In one approach, we consider the syntax:

 $\begin{array}{ll} \mathbf{Terms} & a ::= x \mid ab \mid \lambda x.a \mid a[s] \\ \mathbf{Substitutions} & s ::= id \mid (a/x) \cdot s \mid s \circ t \end{array}$ 

The corresponding theory includes axioms such as:

Beta 
$$(\lambda x.a)b = a[(b/x) \cdot id]$$

$$Var1 x[(a/x) \cdot s] = a$$

$$Var2 \qquad x[(a/y) \cdot s] = x[s] \qquad (x \neq y)$$

$$Var3 \qquad x[id] = x$$

Abs 
$$(\lambda x.a)[s] = \lambda y.(a[(y/x) \cdot s])$$
  
(y occurs in neither a nor s)

The rules correspond closely to the basic ones presented in De Bruijn notation. The *Abs* rule does not require a shift operator, but involves a condition on variable occurrences. (The side condition could be weakened.) The consideration of the critical pairs generated by the previous rules immediately suggests new rules, for example:

$$(a/x) \cdot ((b/y) \cdot s) = (b/y) \cdot ((a/x) \cdot s) \qquad (x \neq y)$$

These are unpleasant rules. The given rule destroys the existence of substitution normal forms. Intuitively, we may take this as a hint that this calculus with names does not really enjoy nice confluence features. In this respect, the calculus in De Bruijn notation seems preferable.

There is an alternative solution, with the shift operator. The syntax is now:

Terms
$$a ::= x \mid ab \mid \lambda x.a \mid a[s]$$
Substitutions $s ::= id \mid \uparrow \mid (a/x) \cdot s \mid s \circ t$ 

In this notation, intuitively,  $x[\uparrow]$  refers to x after the first binder. The equations are the ones of the  $\lambda\sigma$ -calculus in De Bruijn notation except for:

 $Beta \qquad (\lambda x.a)b = a[(b/x) \cdot id]$   $Var1 \qquad x[(a/x) \cdot s] = a$   $Var2 \qquad x[(a/y) \cdot s] = x[s] \qquad (x \neq y)$   $Var3 \qquad x[id] = x$   $Abs \qquad (\lambda x.a)[s] = \lambda x.(a[(x/x) \cdot (s \circ \uparrow)])$ 

This framework may be useful for showing the differences between dynamic and lexical scopes in programming languages. The rules here correspond to lexical binding, but dynamic binding is obtained by erasing the shift operator in rule Abs.

#### **3.4** A normal-order strategy

As usual, we want a complete rewriting strategy—a deterministic method for finding a normal form whenever one exists. Here we study normal-order strategies (the leftmost-outermost redex is chosen at each step). Completeness follows from the completeness of the normal-order strategy for the  $\lambda$ -calculus.

The normal-order algorithm naturally decomposes into two parts: a weak normal-order algorithm, for obtaining weak head normal forms, and recursive calls on this algorithm. In our setting, weak head normal forms are defined as follows:

**Definition 3.6** A weak head normal form (what for short) is a  $\lambda \sigma$  term of the form  $\lambda a$  or  $\mathbf{n} a_1 \cdots a_m$ .

We write  $\stackrel{n}{\longrightarrow}_{\beta}$  for the usual (one step) weak normalorder  $\beta$  reduction in the  $\lambda$ -calculus, and write  $\stackrel{n}{\rightarrow}$  for the (one step) weak normal-order  $Beta + \sigma$  reduction in the  $\lambda\sigma$ -calculus. Clearly,  $\stackrel{n}{\longrightarrow}_{\beta}$  and  $\stackrel{n}{\rightarrow}$  are related:

**Proposition 3.7** If  $a \xrightarrow{n} b$  then either  $\sigma(a) \xrightarrow{n}_{\beta} \sigma(b)$ or  $\sigma(a)$  and  $\sigma(b)$  are identical. The  $\xrightarrow{n}$  reduction of a terminates (with a weak head normal form) iff the  $\xrightarrow{n}_{\beta}$  reduction of  $\sigma(a)$  terminates.

**Corollary 3.8**  $\xrightarrow{n}$  is a complete strategy.

We can also define a system  $\stackrel{wn}{\rightarrow}$ , which incorporates some slight optimizations (present also in our abstract machine, below). In  $\stackrel{wn}{\rightarrow}$ , the rule

$$((\lambda a)[s])b \xrightarrow{wn} a[b \cdot s]$$

replaces the rules

$$\begin{aligned} & (\lambda a)b \xrightarrow{n} a[b \cdot id] \\ & (\lambda a)[s] \xrightarrow{n} \lambda(a[\mathbf{1} \cdot (s \circ \uparrow)]) \end{aligned}$$

The new rule is an optimization justified by the  $\sigma$  reduction steps

$$((\lambda a)[s])b \xrightarrow{n^{\star}} a[(\mathbf{1} \cdot (s \circ \uparrow)) \circ (b \cdot id)] \to^{\star} a[b \cdot s]$$

which is not allowed in  $\xrightarrow{n}$ .

Both  $\xrightarrow{n}$  and  $\xrightarrow{wn}$  are weak in the sense that they do not reduce under  $\lambda$ 's. In addition,  $\xrightarrow{wn}$  is also weak in the sense that substitutions are not pushed under  $\lambda$ 's. In this respect,  $\xrightarrow{wn}$  models environment machines while  $\xrightarrow{n}$  is closer to combinator reduction machines.

We do not exactly get weak head normal forms for instance,  $\stackrel{wn}{\rightarrow}$  does not reduce even  $(\lambda 11)(\lambda 11)$  or  $(1[(\lambda 11) \cdot id])(\lambda 11)$ . This motivates a syntactic restriction which entails no loss of generality: we start with closures, and all conses have the form  $a[s] \cdot t$ . Under this restriction, we cannot start with  $(\lambda 11)(\lambda 11)$ , but instead have to write  $((\lambda 11)(\lambda 11))[id]$ , which has the expected, nonterminating behavior. We obtain:

**Proposition 3.9** If  $a \xrightarrow{wn} b$  then either  $\sigma(a)$  and  $\sigma(b)$  are identical or  $\sigma(a) \xrightarrow{n}_{\beta} \sigma(b)$ . The  $\xrightarrow{wn}$  reduction terminates (with a term of the form  $(\lambda a)[s]$  or  $na_1 \dots a_m$ ) iff the  $\xrightarrow{n}_{\beta}$  reduction of  $\sigma(a)$  terminates.

#### 3.5 Towards an implementation

As a further refinement, we adapt  $\stackrel{wn}{\rightarrow}$ , to manipulate only expressions of the forms a[t] and  $s \circ t$ . The substitution t corresponds to the "global environment," whereas substitutions deeper in a or s correspond to "local declarations." In defining our machine, we take the view that the linear representation of a can be read as a sequence of machine instructions acting on the graph representation of t.

In this approach, some of the original rules are no longer acceptable, since they do not yield expressions of the desired forms. For example, the reduct of the App rule, (a[s])(b[s]), is not a closure. In order to reduce (ab)[s], we have to reduce a[s] to a weak head normal form first. In the machine discussed below, we use a stack for storing b[s].

The following reducer whnf() embodies these modifications to  $\stackrel{wn}{\rightarrow}$ . The reducer takes a pair of arguments, the term a and the substitution s of a closure, and returns another pair, of one of the forms  $(na_1 \cdots a_m, id)$  and  $(\lambda a', s')$ . To compute whnf(), the following axioms and rules should be applied, in the order of their listing. We proceed by cases on the structure of a, and when a is n by cases on the structure of s, and when s is a composition  $t \circ t'$  by cases on the structure of t.

$$whnf(\lambda a, s) = (\lambda a, s)$$

$$\begin{split} \frac{whnf(a,s) = (\lambda a',s')}{whnf(ab,s) = whnf(a',b[s]\cdot s')} \\ \hline whnf(ab,s) = whnf(a',b[s]\cdot s') \\ \hline whnf(ab,s) = (a'(b[s]),id) \\ whnf(ab,s) = (a'(b[s]),id) \\ whnf(n,id) = (n,id) \\ whnf(n,\uparrow) = (n+1,id) \\ whnf(1,a[s]\cdot t) = whnf(a,s) \\ whnf(n+1,a\cdot s) = whnf(n,s) \\ whnf(n,s\circ s') = whnf(n[s],s') \\ whnf(n[id],s) = whnf(n[s],s') \\ whnf(n[id],s) = whnf(n+1,s) \\ whnf(n[1[a\cdot s],s') = whnf(n+1,s) \\ whnf(n[1[a\cdot s],s') = whnf(n[s],s') \\ whnf(n[s\circ s'],s'') = whnf(n[s],s') \\ whnf(n[s],s' = whnf(n[s],s') \\ whnf(a[s],s') = whnf(n[s],s' \circ s'') \\ whnf(n[s],s') = whnf(a,s\circ s') \end{split}$$

A simple extension of the rules yields normal forms:

$$\frac{whnf(a,s) = (\lambda a',t)}{nf(a,s) = \lambda(nf(a', \mathbf{1} \cdot (t \circ \uparrow)))}$$
$$\frac{whnf(a,s) = (\mathbf{n}(a_1[s_1]) \dots (a_m[s_m]), id)}{nf(a,s) = \mathbf{n}(nf(a_1,s_1)) \dots (nf(a_m,s_m))}$$

The precise soundness property of whnf() is:

**Proposition 3.10** Given a and s, whnf(a,s) = (a', s') is provable if and only if  $\sigma(a'[s'])$  is the weak head normal form of  $\sigma(a[s])$ .

The last step we consider is the derivation of a transition machine from the rules for whnf(). One basic idea is to implement the recursive call on a[s] during the evaluation of (ab)[s] by using a stack to store the argument b[s]. Thus, the stack contains closures.

The following table represents an extension of Krivine's abstract machine [11, 5]. The first column represents the "current state," the second one represents the "next state." Each line has to be read as a transition from a triplet (Subst, Term, Stack) to a triplet of the same nature. To evaluate a program a in the global environment s, the machine is started in state  $(s, a, \langle \rangle)$ , where  $\langle \rangle$  is the empty stack. The machine repeatedly uses the first applicable rule. The machine stops when no transition is applicable any more. These termination states have one of the forms  $(id, n, a_1 \cdots a_m)$  and  $(s, \lambda a, \langle \rangle)$ , which represent  $na_1 \cdots a_m$  and  $(\lambda a)[s]$ , respectively.

The machine can be restarted when it stops, and then we have a full normal form  $\lambda$  reducer.

Subst	Term	Stack	Subst	Term	Stack
1	n	S	id	n+1	S
$a[s] \cdot t$	1	S	s	a	S
$a \cdot s$	n+1	S	s	n	S
$s \circ s'$	n	S	s'	n[s]	S
s	ab	S	s	a	$b[s] \cdot S$
s	$\lambda a$	$b \cdot S$	$b \cdot s$	a	S
s	$n[\mathit{id}]$	S	s	n	S
s	$n[\uparrow]$	S	s	n+1	S
s'	$\mathtt{1}[a \cdot s]$	S	s'	a	S
s'	$n+1[a \cdot s]$	S	s'	n[s]	S
$s^{\prime\prime}$	$\mathtt{n}[s \circ s']$	S	$s' \circ s''$	n[s]	S
s'	a[s]	S	$s \circ s'$	a	S

Specifically, when the machine terminates with the triplet  $(s, \lambda a, \langle \rangle)$ , we restart it in the initial state  $(1 \cdot (s \circ \uparrow), a, \langle \rangle)$ , and when the machine terminates with the triplet  $(id, n, a_1[s_1] \cdot \ldots \cdot a_n[s_n] \cdot \langle \rangle)$ , we restart *n* copies of the machine in the states  $(s_1, a_1, \langle \rangle), \ldots, (s_n, a_n, \langle \rangle)$ .

The machine is correct:

**Proposition 3.11** Starting in the state  $(s, a, \langle \rangle)$ , the machine terminates in  $(id, n, a_1 \cdot \ldots \cdot a_m)$  iff  $whnf(a, s) = (na_1 \ldots a_m, id)$ , and it terminates in  $(s, \lambda a, \langle \rangle)$  iff  $whnf(a, s) = (\lambda a, s)$ .

By now, we are far away from the wildly nondeterministic basic rewriting system of Section 3.1. However, through the derivations, we have managed to keep some understanding of the successive refinements and to guarantee their correctness. In great part, this has been possible because the  $\lambda\sigma$ -calculus is more concrete than the  $\lambda$ -calculus, and hence an easier starting point.

### 4 First-order theories

In the previous section, we have seen how to derive a machine that can be used as a sensible implementation of the untyped  $\lambda\sigma$ -calculus, and in turn of the untyped  $\lambda$ -calculus. Different implementation issues arise in typed systems. For typed calculi, we need not just an execution machine, but also a typechecker. As will become apparent when we discuss second-order systems, explicit substitutions can also help in deriving typecheckers. Thus, we want a typechecker for the  $\lambda\sigma$ -calculus.

At the first order, the typechecker does not present much difficulty. In addition to the usual rules for a classical system L1, we must handle the typechecking of substitutions. Inspection of the rules of L1 shows that this can be done easily, since the rules are deterministic.

In this section we describe the first-order typed  $\lambda\sigma$ calculus. We prove that it preserves types under reductions, and that it is sound with respect to the  $\lambda$ -calculus. We move on to the second-order calculus in the next section. We start by recalling the syntax and the type rules of the first-order  $\lambda$ -calculus with De Bruijn's notation.

$\mathbf{Types}$	$A ::= K \mid A \to B$
Environments	$E ::= nil \mid A, E$
$\mathbf{Terms}$	$a ::= \mathbf{n} \mid \lambda A.a \mid ab$

 $A, E \vdash \mathbf{1} : A$ 

#### Definition 4.1 (Theory L1)

 $E \vdash \mathbf{n} \cdot B$ 

(L1-var)

(

L1-varn) 
$$\frac{E + \mathbf{n} : B}{A, E \vdash \mathbf{n+1} : B}$$

(L1-lambda) 
$$\frac{A, E \vdash b : B}{E \vdash \lambda A.b : A \rightarrow B}$$

(L1-app) 
$$\frac{E \vdash b: A \to B \quad E \vdash a: A}{E \vdash ba: B}$$

We do not include the  $\beta$  rule, because we now focus on typechecking—rather than on evaluation.

The first-order  $\lambda\sigma$ -calculus has the syntax:

$\mathbf{Types}$	$A ::= K \mid A \to B$
Environments	$E ::= nil \mid A, E$
$\mathbf{Terms}$	$a ::= 1 \mid ab \mid \lambda A.a \mid a[s]$
${f Substitutions}$	$s ::= id  \uparrow  a : A \cdot s   s \circ t$

The type rules come in two groups, one for giving types to terms, and one for giving environments to substitutions. The two groups interact through the rule for closures.

#### Definition 4.2 (Theory S1)

(S1-var)  $A, E \vdash \mathbf{1} : A$ 

(S1-lambda) 
$$\frac{A, E \vdash b : B}{E \vdash \lambda A.b : A \rightarrow}$$

(S1-app) 
$$\begin{array}{c} E \vdash b: A \to B \quad E \vdash a: A \\ \hline E \vdash ba: B \end{array}$$

В

(S1-clos) 
$$\underbrace{ \begin{array}{c} E \vdash s \therefore E' \quad E' \vdash a : A \\ E \vdash a[s] : A \end{array} }$$

$$(S1-id) E \vdash id \therefore E$$

(S1-shift) 
$$A, E \vdash \uparrow \therefore E$$

(S1-cons) 
$$\frac{E \vdash a : A \qquad E \vdash s \therefore E'}{E \vdash a : A \cdot s \therefore A, E'}$$

(S1-comp) 
$$\frac{E \vdash s'' \therefore E'' \quad E'' \vdash s' \therefore E'}{E \vdash s' \circ s'' \therefore E'}$$

In S1, we include neither the *Beta* nor the  $\sigma$  axioms.

Clearly, typechecking is decidable in S1. We proceed to show that S1 is sound. As a preliminary, we prove two lemmas. The first lemma relies on the notion of  $\sigma$  normal form, which was defined in the previous section. We use a modified version of the  $\sigma$  rules for typed terms; four of the rules change.

$$\begin{array}{ll} VarCons & 1[a:A \cdot s] = a \\ Abs & (\lambda A.a)[s] = \lambda A.(a[1:A \cdot (s \circ \uparrow)]) \\ ShiftCons & \uparrow \circ (a:A \cdot s) = s \end{array}$$

$$Map \qquad (a:A\cdot s)\circ t = a[t]:A\cdot (s\circ t)$$

The typed version of  $\sigma$  enjoys the properties of the untyped version.

A term in  $\sigma$  normal form is typeable in S1 iff it is typeable in L1, and  $\sigma$  reduction  $\rightarrow_{\sigma}$  preserve typings:

**Lemma 4.3** For all a in  $\sigma$  normal form,  $E \vdash_{S1} a:A$  iff  $E \vdash_{L1} a:A$ .

**Lemma 4.4 (Subject reduction)** If  $a \to_{\sigma} a'$  and  $E \vdash_{S1} a:A$ , then  $E \vdash_{S1} a':A$ . Similarly, if  $s \to_{\sigma} s'$  and  $E' \vdash_{S1} s \therefore E''$ , then  $E' \vdash_{S1} s' \therefore E''$ .

Together, the two lemmas give us soundness:

**Proposition 4.5 (Soundness)** If  $E \vdash_{S_1} a:A$  then  $E \vdash_{L_1} \sigma(a):A$ .

One may wonder whether a completeness result holds, as a converse to our soundness result. Unfortunately, the answer is no. For instance, if L1 gives a type to *a* but not to *b*, then S1 cannot give a type to  $\mathbf{1}[a \cdot b \cdot id]$ , while L1 gives a type to  $\sigma(\mathbf{1}[a \cdot b \cdot id])$ , that is, to *a*. However, if L1 gives types to *a* and *b*, then S1 gives a type to  $\mathbf{1}[a \cdot b \cdot id]$ . Conversely, if S1 gives a type to  $\mathbf{1}[a \cdot b \cdot id]$ , then L1 gives types to *a* and *b*.

These observations suggest a reformulation of the soundness and completeness claim. Informally, one would like to show that S1 can give a type to a term iff L1 can give a type to the normal forms of the term and of some subterms that  $\sigma$  normalization discards.

#### 5 Second-order theories

Type rules and typecheckers are also needed for second-order calculi. Unfortunately, the situation is more complex than at the first order, because types include binding constructs (quantifiers). These interact with substitutions in the same subtle ways in which  $\lambda$  interacts with substitutions. (We have no equivalent of  $\beta$  reduction here, but this too reappears in higher-order typed systems.)

In implementing a typechecker (or proofchecker) for the second or higher orders, we face the same concerns of efficient handling of substitution and correctness of implementation that pushed us from the untyped  $\lambda$ -calculus to the untyped  $\lambda\sigma$ -calculus. It is nice to discover that we can apply the same concept of explicit substitutions to tackle typechecking problems as well.

In order to carry out this plan, we must first obtain a second-order system with explicit substitutions, which already incurs several difficulties. Then we must refine the system, and obtain an actual typechecking algorithm. During this enterprise, we should keep in mind the goal of deriving an algorithm that is correct and close to a sensible implementation by virtue of handling substitutions explicitly.

Second-order theories are considerably more complex than untyped or first-order theories, both in number of rules and in subtlety. The complication is already apparent in the De Bruijn formulation of the ordinary second-order  $\lambda$ -calculus (L2, below). The complication intensifies in the second-order  $\lambda\sigma$ calculus (S2) because of unexpected difficulties. (We mentioned some of them in the overview.)

We begin with a description of L2, then we define S2 and prove that it is sound with respect to L2. Unlike L1, L2, and even S1, the new system S2 is not deterministic. Therefore, we also define a secondorder typechecking algorithm S2alg, and prove that it is sound with respect to S2.

The syntax and the type rules for the second-order  $\lambda$ -calculus are:

Types	$A ::= \mathbf{n} \mid A \to B \mid \forall A$
Environments	$E ::= nil \mid A, E \mid Ty, E$
$\mathbf{Terms}$	$a ::= \mathbf{n} \mid \lambda A.a \mid \Lambda a \mid ab \mid aB$

#### Definition 5.1 (Theory L2)

(L2-nil)	$\vdash nil$ env
(L2-ext)	$\vdash E  \text{env}  E \vdash A$
(LL OAU)	

A, E

env

:: Ty

(L2-ext2)	$\begin{array}{c c} \vdash E & \mathrm{env} \\ \hline \vdash & \mathrm{Ty}, E & \mathrm{env} \end{array}$
(L2-tvar)	$\frac{\vdash E  \text{env}}{\text{Ty}, E \vdash 1 :: \text{Ty}}$
(L2-tvarn)	$\frac{E \vdash \mathbf{n} :: \mathrm{Ty}  E \vdash A :: \mathrm{Ty}}{A, E \vdash \mathbf{n+1} :: \mathrm{Ty}}$
(L2-tvarn2)	$\frac{E \vdash \mathbf{n} :: \mathrm{Ty}}{\mathrm{Ty}, E \vdash \mathbf{n+1} :: \mathrm{Ty}}$
(L2-tfun)	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
(L2-tgen)	$\frac{\mathbf{Ty}, E \vdash B :: \mathbf{Ty}}{E \vdash \forall B :: \mathbf{Ty}}$
(L2-var)	$\frac{E \vdash A :: \mathrm{Ty}}{A, E \vdash 1 : A\{\uparrow\}}$
(L2-varn)	$\frac{E \vdash \mathbf{n} : B \qquad E \vdash A :: \mathrm{Ty}}{A, E \vdash \mathbf{n+1} : B\{\uparrow\}}$
(L2-varn $2)$	$\frac{E \vdash \mathbf{n} : B}{\text{Ty}, E \vdash \mathbf{n+1} : B\{\uparrow\}}$
(L2-lambda)	$\begin{array}{ccc} A, E \ \vdash \ b : B \\ \hline E \ \vdash \ \lambda A.b : A \rightarrow B \end{array}$
(L2-Lambda)	$\begin{array}{c c} \text{Ty}, E \vdash b : B \\ \hline E \vdash \Lambda b : \forall B \end{array}$
(L2-app)	$\begin{array}{cccc} E \ \vdash \ b : A \rightarrow B & E \ \vdash \ a : A \\ \hline E \ \vdash \ b(a) : B\{a : A \cdot id\} \end{array}$
(L2-App)	$\frac{E \vdash b : \forall B  E \vdash A :: \mathrm{Ty}}{E \vdash b(A) : B\{A :: \mathrm{Ty} \cdot id\}}$

We now move on to the S2 system, with the following syntax:

Types	$A ::= 1 \mid A \to B \mid \forall A \mid A[s]$
Environments	$E ::= nil \mid A, E \mid Ty, E$
Terms	$a ::= 1 \mid \lambda A.a \mid \Lambda a \mid ab \mid aB \mid a[s]$
$\mathbf{Substitutions}$	$s ::= id \mid \uparrow \mid a {:} A \cdot s \mid A {::} \mathrm{Ty} \cdot s \mid s \circ t$

In the previous section, we have seen how to formulate a first-order  $\lambda\sigma$ -calculus (S1) by adding one closure rule and a group of substitution rules to the first-order  $\lambda$ -calculus (L1). In S1, the task of deriving types can be separated from the task of applying substitutions. As indicated in the informal overview, this approach does not extend to S2. The rules of S2 described below are structured in such a way that substitutions are automatically pushed inside terms during typechecking. The unfortunate side effect is a small explosion in the number of rules. We do not include an analogue for S1-clos (in fact, we conjecture that it is admissible).

S2 is formulated with equivalence judgments, for example judgments of the form  $E \vdash a \sim b : A$ . This judgment means that a and b are equivalent terms of type A in the environment E. We can recover the standard judgments, with definitions such as

$$E \vdash a : A =_{def} E \vdash a \sim a : A$$

In S2, equivalence judgments are needed because it is not always possible to prove directly  $E \vdash a : A$ , but only  $E \vdash b : A$  for a term b that is  $\sigma$ -equivalent to a (as in the example above). Formally, in order to prove  $E \vdash a \sim a : A$ , we first prove  $E \vdash a \sim b : A$ , and then use symmetry and transitivity. Similarly, it is not always possible to prove directly  $E \vdash a : A$ , but instead  $E \vdash a : B$  for a type B that is  $\sigma$ -equivalent to A—then we "retype" a from B to A.

We have seen in section 2 how the typing axiom for 1 has to be modified. Similar considerations show that the rule for conses, S1-cons, needs to be modified as well, and suggest the following, tentative rule:

Note that, in the hypothesis, we require that a have type A[s] rather than A: the reason is that A is wellformed in E' rather than in E. Furthermore, we require that s and t be equivalent substitutions of type E', but in truth their type is irrelevant. This suggests a new approach: we deal with judgments of the form

$$E \vdash s \sim t \quad subst_p$$

where p records the length |E'| of E'.

In fact, we could hardly do more than keep track of the lengths of substitutions. As the following example illustrates, the type of a substitution cannot be determined satisfactorily. In the tentative rule above, let E = nil, s = t = Bool::Ty  $\cdot id$ , a = b = true, and A = 1 and B = Bool. We obtain

$$nil \vdash true: \mathbf{1} \cdot s \sim true: Bool \cdot t \therefore \mathbf{1}:: Ty, nil$$

where we would more naturally expect Bool::Ty, nil. The information that 1 is Bool is not found in the environment: s has to be used to check that 1 is indeed Bool. It seems thus that the type of a substitution cannot be intrinsically defined.

With these explanations in mind, the reader should be able to approach the rules of the theory S2.

#### Definition 5.2 (Theory S2) See appendix 7.

S2 is sound, in the following sense:

#### Proposition 5.3 (Soundness)

- 1. If  $E \vdash_{S2} a \sim b : A$ then  $\sigma(E) \vdash_{L2} \sigma(a) : \sigma(A) \text{ and } \sigma(a) = \sigma(b).$
- 2. If  $E \vdash_{S2} A \sim B :: Ty$ then  $\sigma(E) \vdash_{L2} \sigma(A) :: Ty$  and  $\sigma(A) = \sigma(B)$ .
- 3. If  $\vdash_{S2} E \sim E'$  env then  $\vdash_{L2} \sigma(E)$  env and  $\sigma(E) = \sigma(E')$ .
- 4. If  $E \vdash_{S2} s \sim s'$  subst<sub>p</sub> then for some m and n
  - $\sigma(s) = G_1 \cdot \ldots \cdot G_m \cdot \uparrow^n$  and  $\sigma(s') = G'_1 \cdot \ldots \cdot G'_m \cdot \uparrow^n$ ,
  - for all  $q \leq m$ , either  $G_q = G'_q = A ::$  Ty and  $\sigma(E) \vdash_{L_2} A ::$  Ty for some A, or  $G_q = a:A$ ,  $G'_q = a:A'$ ,  $\sigma(A[\uparrow^q \circ s]) = \sigma(A'[\uparrow^q \circ s'])$ , and  $\sigma(E) \vdash_{L_2} a: \sigma(A[\uparrow^q \circ s])$ for some a, A, and A',

• 
$$p = m + |E| - n$$
.

As for S1, we speculate that the soundness claim for S2 can be strengthened, and that a converse completeness result then holds.

We now provide a typechecking algorithm S2alg for the second-order calculus. The algorithm is formulated as a set of rules, for easy comparison with S2.

For terms that are not closures, S2alg and L2 operate identically. However, these are the least interesting cases: an actual implementation would manipulate only closures (as in subsection 3.5). In order to typecheck a term a[s], the strategy is to analyze simpler and simpler components of a while accumulating more and more complex substitutions in s. When we reach an index, we extract the relevant information from the substitution or from the environment.

Informally, the algorithmic flow of control for each rule is: start with the given parts of the conclusion, recursively do what the assumptions on top require, accumulate the results, and from them produce the unknown parts of the conclusion. For example, if we want to type a in the environment E, we select an

inference rule of S2alg by inspecting the shape of its conclusion. Then we move on to the assumptions of this rule, recursively; we solve the typing problems presented by each of them, and collect the results to produce a type for the original term a.

Some of the rules involve tests for type equivalence; two auxiliary "reduction" judgments are used:

$$E \vdash s \rightsquigarrow s' \quad subst_p \quad \text{and} \quad E \vdash A \rightsquigarrow A'::Ty$$

In these judgments, s' and A' are in a sort of weak head normal form, namely: s' is never a composition and if A' is a closure then it has the form  $1[\uparrow^n]$ .

#### Definition 5.4 (S2alg) See appendix 8.

To show that S2alg really defines an algorithm, we first notice that only one rule can be applied bottomup in each situation. For the judgments  $E \vdash A$ ::Ty and  $E \vdash A \rightsquigarrow A'$ ::Ty, we test applicability by cases on A; when A = B[s], by cases on B; and when B = 1by cases on the reduction of s. For  $E \vdash a : A$ , we proceed by cases on a; when a = b[s], by cases on b; and when b = 1 by cases on the reduction of s. For  $E \vdash s \quad subst_p$ , we proceed by cases on s, and when  $s = t \circ u$  by cases on t. For  $E \vdash s \rightsquigarrow s' \quad subst_p$ , we proceed by cases on s; when  $s = t \circ u$ , by cases on t; and when  $t = \uparrow$  by cases on the reduction of u. Finally,  $E \vdash A \leftrightarrow B$ :: Ty is handled by cases on the reductions of A and B.

The following invariants can be used to show that the algorithm considers all the cases that may arise when the input terms are well typed:

- If  $E \vdash s \rightsquigarrow s'$  subst<sub>p</sub> then s' has one of the forms  $id, \uparrow^n, a: A \cdot t$ , and  $A:: Ty \cdot t$ .
- If  $E \vdash A \rightsquigarrow A' ::$  Ty then A' has one of the forms  $\mathbf{1}, \mathbf{1}[\uparrow^n], B \to C$ , and  $\forall B$ .

Finally, the algorithm always terminates, with success or failure, because every rule either reduces the size of terms or moves terms towards a normal form.

The algorithm S2alg is sound with respect to S2. For example, if  $E \vdash_{S2alg} A ::$  Ty then we can prove  $E \vdash_{S2} A \sim A ::$  Ty. We conjecture that the algorithm is also complete, in the sense that for example if  $E \vdash_{S2} A \sim A' ::$  Ty then  $E \vdash_{S2alg} A ::$  Ty.

## 6 Conclusion

The usual presentations of the  $\lambda$ -calculus discreetly play down the handling of substitutions. This helps in developing the metatheory of the  $\lambda$ -calculus, at a suitable level of abstraction. We hope to have demonstrated the benefits of a more explicit treatment of substitutions, both for untyped systems and typed systems. The theory and the manipulation of explicit substitutions can be delicate, but useful for correct and efficient implementations.

Acknowledgements We have benefited from discussions on untyped systems with P. Crégut, T. Hardin, E. Muller, and A. Suárez, and from C. Hibbard's editorial help.

### 7 Appendix: Theory S2

### 7.1 Type equivalence

$$\frac{E \vdash A \sim B :: Ty}{E \vdash B \sim A :: Ty}$$

$$\frac{E \vdash A \sim B :: Ty \qquad E \vdash B \sim C :: Ty}{E \vdash A \sim C :: Ty}$$

$$\frac{\vdash E \ env}{Ty, E \vdash 1 \sim 1 :: Ty}$$

$$\frac{E \vdash A \sim A' :: Ty \qquad A, E \vdash B \sim B' :: Ty}{E \vdash A \rightarrow B \sim A' \rightarrow B' :: Ty}$$

$$\frac{E \vdash A \rightarrow B \sim A' \rightarrow B' :: Ty}{E \vdash A \oplus B \sim \forall B' :: Ty}$$

$$\frac{E \vdash 1 :: Ty \qquad E \vdash A :: Ty}{E \vdash 4 [t] \sim 1 [t] :: Ty}$$

$$\frac{E \vdash 1 :: Ty \qquad E \vdash A :: Ty}{A, E \vdash 1[t] \sim 1[t] :: Ty}$$

$$\frac{E \vdash 1 :: Ty \qquad E \vdash A :: Ty}{Ty, E \vdash 1[t] \sim 1[t] :: Ty}$$

$$\frac{E \vdash 1 [t^n] :: Ty \qquad E \vdash A :: Ty}{A, E \vdash 1[t]^{n+1}] \sim 1[t^{n+1}] :: Ty}$$

$$\frac{E \vdash 1[t^n] :: Ty \qquad E \vdash A :: Ty}{Ty, E \vdash 1[t]^{n+1}] \sim 1[t^{n+1}] :: Ty}$$

$$\frac{E \vdash 1[t^{n+1}] \sim 1[t^{n+1}] \sim 1[t^{n+1}] :: Ty}{Ty, E \vdash 1[t^{n+1}] \sim 1[t^{n+1}] :: Ty}$$

$$\frac{E \vdash A :: Ty \cdot s \ subst_p \qquad E \vdash 1[s'] :: Ty}{E \vdash 1[s] \sim 1[s'] :: Ty}$$

$$\frac{E \vdash A[s] \rightarrow B[1:A.(s \circ t)] :: Ty}{E \vdash (\forall B][s] \sim \forall (B[1::Ty \cdot (s \circ t)]) :: Ty}$$

$$\frac{E \vdash A[s][t] \sim A[s \circ t] :: Ty}{E \vdash A[s][t] \sim A[s \circ t] :: Ty}$$

$$\frac{E \vdash A[s][t] \sim A[s \circ t] :: Ty}{E \vdash A[s][t] \sim A[s \circ t] :: Ty}$$

# 7.2 Term equivalence

# 7.3 Substitution equivalence

$$\frac{E \vdash s \sim t \quad subst_p}{E \vdash t \sim s \quad subst_p}$$

$$\frac{E \vdash s \sim t \ subst_p}{E \vdash s \sim u \ subst_p} = \frac{E \vdash t \sim u \ subst_p}{E \vdash id \sim id \ subst_{|E|}}$$

$$\frac{E \vdash id \sim id \ subst_{|E|}}{E \vdash id \sim id \ subst_{|E|}}$$

$$\frac{E \vdash A :: Ty}{A, E \vdash \uparrow \sim \uparrow \ subst_{|E|}}$$

$$\frac{E \vdash env}{Ty, E \vdash \uparrow \sim \uparrow \ subst_{|E|}}$$

$$\frac{E \vdash s \sim t \ subst_p \ E \vdash A[s] \sim B[t] :: Ty}{E \vdash a \sim b:A[s]}$$

$$\frac{E \vdash A \sim B :: Ty \ E \vdash s \sim t \ subst_{p+1}}{E \vdash A:: Ty \cdot s \sim B:: Ty \cdot t \ subst_{p+1}}$$

$$\frac{E \vdash s \sim s' \ subst_p}{E \vdash id \circ s \sim s' \ subst_p}$$

$$\frac{E \vdash s \sim s' \ subst_p}{E \vdash \uparrow \circ id \sim \uparrow \ subst_p}$$

$$\frac{E \vdash s \sim s' \ subst_p}{E \vdash \uparrow \circ (A:: Ty \cdot s) \sim s' \ subst_p}$$

$$\frac{E \vdash s \sim s' \ subst_p}{E \vdash \uparrow \circ (A:: Ty \cdot s) \sim s' \ subst_p}$$

$$\frac{E \vdash s \sim s' \ subst_p}{E \vdash \uparrow \circ (A:: Ty \cdot s) \sim s' \ subst_p}$$

$$\frac{E \vdash s \sim s' \ subst_p}{E \vdash (a:A \cdot s) \circ t \sim a[t]:A \cdot (s \circ t) \ subst_p}$$

$$\frac{E \vdash A = [t]:A \cdot (s \circ t) \ subst_p}{E \vdash (s \circ t) \circ u \sim s \circ (t \circ u) \ subst_p}$$

$$\frac{E \vdash s \sim t \ subst_p}{E \vdash (s \sim t \ subst_p} \vdash E \sim C' \ env}{E' \vdash s \sim t \ subst_p}$$

# 7.4 Environment equivalence

# 8 Appendix: Algorithm S2alg

# 8.1 Inference for types

$\frac{\vdash E  env}{\mathrm{Ty}, E \vdash 1 :: \mathrm{Ty}}$
$\frac{E \vdash A :: Ty}{E \vdash A \rightarrow B :: Ty}$
$\frac{\text{Ty}, E \vdash B :: \text{Ty}}{E \vdash \forall B :: \text{Ty}}$
$\frac{\text{Ty}, E \vdash s \rightsquigarrow id  subst_p}{\text{Ty}, E \vdash 1[s] :: \text{Ty}}$
$\frac{E \vdash 1 :: \mathrm{Ty}  E \vdash A :: \mathrm{Ty}}{A, E \vdash 1[\uparrow] :: \mathrm{Ty}}$
$\frac{E \vdash 1 :: \mathrm{Ty}}{\mathrm{Ty}, E \vdash 1[\uparrow] :: \mathrm{Ty}}$
$\frac{E \vdash 1[\uparrow^n] :: \mathrm{Ty}  E \vdash A :: \mathrm{Ty}}{A, E \vdash 1[\uparrow^{n+1}] :: \mathrm{Ty}}$
$\frac{E \vdash 1[\uparrow^n] :: \mathrm{Ty}}{\mathrm{Ty}, E \vdash 1[\uparrow^{n+1}] :: \mathrm{Ty}}$
$\frac{E \vdash s \rightsquigarrow A :: \mathrm{Ty} \cdot t  subst_p}{E \vdash 1[s] :: \mathrm{Ty}}$
$\frac{E \vdash s \rightsquigarrow \uparrow^n  subst_p  E \vdash 1[\uparrow^n] :: \mathrm{Ty}}{E \vdash 1[s] :: \mathrm{Ty}}$
$\frac{E \vdash A[s] :: \mathrm{Ty}}{A[s], E \vdash B[1 : A \cdot (s \circ \uparrow)] :: \mathrm{Ty}}$ $\frac{E \vdash (A \to B)[s] :: \mathrm{Ty}}{E \vdash (A \to B)[s] :: \mathrm{Ty}}$
$\frac{\text{Ty}, E \vdash B[1::\text{Ty} \cdot (s \circ \uparrow)] :: \text{Ty}}{E \vdash (\forall B)[s] :: \text{Ty}}$
$\frac{E \vdash A[s \circ t] :: \mathrm{Ty}}{E \vdash A[s][t] :: \mathrm{Ty}}$

# 8.2 Inference for terms

$$\frac{E \vdash A :: \mathrm{Ty}}{A, E \vdash \mathbf{1} : A[\uparrow]}$$

$$\frac{E \vdash A :: Ty \qquad A, E \vdash b : B}{E \vdash \lambda A, b : A \rightarrow B}$$

$$\frac{Ty, E \vdash b : B}{E \vdash \Lambda b : \forall B}$$

$$\frac{E \vdash b : A \rightarrow B \qquad E \vdash a : A}{E \vdash b(a) : B[a:A \cdot id]}$$

$$\frac{E \vdash b : \forall B \qquad E \vdash A :: Ty}{E \vdash b(A) : B[A::Ty \cdot id]}$$

$$\frac{A, E \vdash s \rightsquigarrow id \ subst_p}{A, E \vdash 1[s] : A[t]]}$$

$$\frac{E \vdash 1 : A \qquad E \vdash B :: Ty}{B, E \vdash 1[t] : A[t]]}$$

$$\frac{E \vdash 1 : A}{Ty, E \vdash 1[t] : A[t]}$$

$$\frac{E \vdash 1[t^n] : A \qquad E \vdash B :: Ty}{B, E \vdash 1[t^{n+1}] : A[t]}$$

$$\frac{E \vdash s \rightsquigarrow a: A \leftarrow subst_p}{E \vdash 1[s] : A[t]}$$

$$\frac{E \vdash s \rightsquigarrow a: A \leftarrow subst_p}{E \vdash 1[s] : A[t]}$$

$$\frac{E \vdash s \rightsquigarrow a: A \leftarrow subst_p}{E \vdash 1[s] : A[t]}$$

$$\frac{E \vdash s \rightsquigarrow t = b[1 : A \cdot (s \circ t)] : B}{E \vdash (\lambda A, b)[s] : A[s] \rightarrow B}$$

$$\frac{Ty, E \vdash b[1::Ty \cdot (s \circ t)] : B}{E \vdash (\lambda b)[s] : A[s] \rightarrow B}$$

$$\frac{E \vdash b[s] : A \rightarrow B \qquad E \vdash a[s] : A'}{E \vdash (b(a))[s] : B[a[s] : A \cdot id]}$$

$$\frac{E \vdash b[s] : A \rightarrow B \qquad E \vdash a[s] : A'}{E \vdash (b(a))[s] : B[A[s] ::Ty \cdot id]}$$

$$\frac{E \vdash b[s] : \forall B \qquad E \vdash A[s] ::Ty \cdot id]}{E \vdash (b(A))[s] : B[A[s] ::Ty \cdot id]}$$

# 8.3 Inference for substitutions

$$\frac{\vdash E \quad env}{E \vdash id \quad subst_{|E|}}$$

$$\frac{E \vdash A :: Ty}{A, E \vdash \uparrow \quad subst_{|E|}}$$

$$\frac{\vdash E \quad env}{Ty, E \vdash \uparrow \quad subst_{|E|}}$$

$$\frac{E \vdash a : B \quad E \vdash s \quad subst_{|E|}}{E \vdash a : A \cdot s \quad subst_{p+1}}$$

$$\frac{E \vdash A :: Ty \quad E \vdash s \quad subst_{p+1}}{E \vdash A :: Ty \cdot s \quad subst_{p+1}}$$

$$\frac{E \vdash s \quad subst_{p}}{E \vdash id \circ s \quad subst_{p}}$$

$$\frac{E \vdash s \quad subst_{p+1}}{E \vdash \uparrow \circ s \quad subst_{p}}$$

$$\frac{E \vdash a[t] : A \cdot (s \circ t) \quad subst_{p}}{E \vdash (a : A \cdot s) \circ t \quad subst_{p}}$$

$$\frac{E \vdash A[t] :: Ty \cdot (s \circ t) \quad subst_{p}}{E \vdash (A :: Ty \cdot s) \circ t \quad subst_{p}}$$

$$\frac{E \vdash s \circ (t \circ u) \quad subst_{p}}{E \vdash (s \circ t) \circ u \quad subst_{p}}$$

# 8.4 Substitution reduction

$$\begin{array}{c|c} \vdash E & env \\ \hline E \vdash id \rightsquigarrow id \quad subst_{|E|} \\ \hline E \vdash id \rightsquigarrow id \quad subst_{|E|} \\ \hline E \vdash A ::: Ty \\ \hline A, E \vdash \uparrow \rightsquigarrow \uparrow \quad subst_{|E|} \\ \hline \hline H = env \\ \hline Ty, E \vdash \uparrow \rightsquigarrow \uparrow \quad subst_{|E|} \\ \hline E \vdash A[s] ::: Ty \quad E \vdash a : B \\ \hline E \vdash B \leftrightarrow A[s] ::: Ty \quad E \vdash s \quad subst_{p+1} \\ \hline E \vdash a : A \cdot s \rightsquigarrow a : A \cdot s \quad subst_{p+1} \\ \hline E \vdash A :: Ty \quad E \vdash s \quad subst_{p+1} \\ \hline \hline E \vdash A :: Ty \cdot s \rightsquigarrow A :: Ty \cdot s \quad subst_{p+1} \\ \hline \hline E \vdash A :: Ty \cdot s \rightsquigarrow s \quad subst_{p} \\ \hline \hline E \vdash id \circ s \rightsquigarrow s' \quad subst_{p} \end{array}$$

$$\frac{E \vdash s \rightsquigarrow id \quad subst_{p+1}}{E \vdash \uparrow \circ s \rightsquigarrow \uparrow \quad subst_{p}}$$

$$\frac{E \vdash s \rightsquigarrow \uparrow^{n} \quad subst_{p+1}}{E \vdash \uparrow \circ s \rightsquigarrow \uparrow^{n+1} \quad subst_{p}}$$

$$\frac{E \vdash s \rightsquigarrow a : A \cdot s' \quad subst_{p+1}}{E \vdash s' \rightsquigarrow s'' \quad subst_{p}}$$

$$\frac{E \vdash s \rightsquigarrow A :: Ty \cdot s' \quad subst_{p}}{E \vdash \uparrow \circ s \rightsquigarrow s'' \quad subst_{p}}$$

$$\frac{E \vdash s \rightsquigarrow A :: Ty \cdot s' \quad subst_{p}}{E \vdash \uparrow \circ s \rightsquigarrow s'' \quad subst_{p}}$$

$$\frac{E \vdash s \land A :: Ty \cdot s' \quad subst_{p}}{E \vdash \uparrow \circ s \rightsquigarrow s'' \quad subst_{p}}$$

$$\frac{E \vdash a[t] : A \cdot (s \circ t) \quad subst_{p}}{E \vdash (a : A \cdot s) \circ t \rightsquigarrow a[t] : A \cdot (s \circ t) \quad subst_{p}}$$

$$E \vdash (A :: Ty \cdot s) \circ t \rightsquigarrow A[t] :: Ty \cdot (s \circ t) \quad subst_{p}$$

$$\frac{E \vdash s \circ (t \circ u) \rightsquigarrow v \quad subst_{p}}{E \vdash (s \circ t) \circ u \leadsto v \quad subst_{p}}$$

# 8.5 Type reductions

$$\frac{\vdash E \quad env}{\text{Ty}, E \vdash \mathbf{1} \sim \mathbf{1} :: \text{Ty}}$$

$$\frac{E \vdash A[s \circ t] \rightsquigarrow B :: \mathrm{Ty}}{E \vdash A[s][t] \rightsquigarrow B :: \mathrm{Ty}}$$

$$\frac{E \vdash A \rightsquigarrow \mathbf{1} :: \mathrm{Ty} \quad E \vdash A' \rightsquigarrow \mathbf{1} :: \mathrm{Ty}}{E \vdash A \leftrightarrow A' :: \mathrm{Ty}}$$

$$\begin{array}{cccc} E \ \vdash \ A \rightsquigarrow B \rightarrow C :: \mathrm{Ty} \\ E \ \vdash \ A' \rightsquigarrow B' \rightarrow C' :: \mathrm{Ty} \\ \hline E \ \vdash \ B' :: \mathrm{Ty} & B, E \ \vdash \ C \leftrightarrow C' :: \mathrm{Ty} \\ \hline \hline E \ \vdash \ A \leftrightarrow A' :: \mathrm{Ty} \end{array}$$

$$\begin{array}{cccc} E \ \vdash \ A \rightsquigarrow \forall B ::: \mathrm{Ty} & E \ \vdash \ A' \rightsquigarrow \forall B' :: \mathrm{Ty} \\ & \mathrm{Ty}, E \ \vdash \ B \leftrightarrow B' :: \mathrm{Ty} \\ \hline & E \ \vdash \ A \leftrightarrow A' :: \mathrm{Ty} \end{array}$$

$$\frac{E \vdash A \rightsquigarrow \mathbf{1}[\uparrow^n] :: \mathrm{Ty} \quad E \vdash A' \rightsquigarrow \mathbf{1}[\uparrow^n] :: \mathrm{Ty}}{E \vdash A \leftrightarrow A' :: \mathrm{Ty}}$$

### 8.7 Inference for environments

$$\vdash nil env$$

$$\vdash E env E \vdash A :: Ty$$

$$\vdash A, E env$$

$$\vdash E env$$

$$\vdash Ty, E env$$

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