Towards machine-checked proofs

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1. Why mechanize definitions and proofs?

2. Coq in a nutshell

3. Representing abstract syntax with binders
   - On paper: the nominal representation
   - In a machine: de Bruijn's representation

Why formalize programming languages?

To obtain precise definitions of programming languages, including:

- dynamic semantics;
- type systems, sometimes known as “static semantics”.

To obtain rigorous proofs of soundness for tools such as

- interpreters,
- compilers,
- type systems (“well-typed programs do not go wrong”),
- type-checkers and type inference engines,
- static analyzers (e.g. abstract interpreters),
- program logics (e.g. Hoare logic, separation logic),
- deductive program provers (e.g. verification condition generators).

Challenge 1: Scale

Hand-written proofs have difficulty scaling up:

- From minimal calculi (λ, π) and toy languages (IMP, MiniML) to large real-world languages such as Java, C, JavaScript, ...
- From textbook compilers to multi-pass optimizing compilers producing code for real processors.
- From textbook abstract interpreters to scalable and precise static analyzers such as Astrée.

Challenge 2: Trust

Hand-written proofs are seldom trustworthy.

- Authors struggle with huge LaTeX documents.
- Reviewers give up on checking huge but boring proofs.

> *Proofs written by computer scientists are boring:*
> *they read as if the author is programming the reader.*
> *(John C. Mitchell)*

- Proof cases are omitted because they are "obvious" or "analogous to the previous case".
- It is difficult to maintain hand-written proofs as the definitions evolve.

Opportunity: machine-assisted proof

Mechanized theorem proving has made great progress.

Landmark examples in mathematics:

- the 4-colour theorem, Gonthier & Werner (2005);
- the Feit-Thompson theorem, Gonthier *et al.* (2013);
- Kepler's conjecture, Hales *et al.* (2015).

Programming language theory is a good match for theorem provers:

- discrete objects (trees); no reals, no analysis, no topology...
- large definitions; proofs with many similar cases;
- syntactic techniques (induction); few deep mathematical concepts.

The POPLmark challenge

In 2005, Aydemir *et al.* challenged the POPL community:

> *How close are we to a world where every paper on programming languages is accompanied by an electronic appendix with machine-checked proofs?*

12 years later, about 20% of the papers at recent POPL conferences come with such an electronic appendix.

Proof assistants

An interactive proof assistant offers:

- A formal specification language,
  in which definitions are written and theorems are stated.
- A set of commands for building proofs,
  either automatically or interactively.
- Often, an independent, automated proof checker,
  so the above commands do not have to be trusted.

Popular proof assistants include Coq, HOL4, Isabelle/HOL.

Computations and functions

Coq offers a pure functional programming language in the style of ML, with recursive functions and pattern-matching.

```
Fixpoint factorial (n: nat) :=
  match n with
  | O   => 1
  | S p => n * factorial p
  end.

Fixpoint concat (A: Type) (xs ys: list A) :=
  match xs with
  | nil => ys
  | x :: xs => x :: concat xs ys
  end.
```

The language is total: all functions terminate. This is enforced by requiring every recursive call to be decreasing w.r.t. the subterm ordering.

Mathematical logic

Propositions can be expressed in this language. They have type `Prop`.

```
Definition divides (a b: N) := exists n: N, b = n * a.

Theorem factorial_divisors:
  forall n i, 1 <= i <= n -> divides i (factorial n).

Definition prime (p: N) :=
  p > 1 /\ (forall d, divides d p -> d = 1 \/ d = p).

Theorem Euclid:
  forall n, exists p, p >= n /\ prime p.
```

The standard logical connectives and quantifiers are available.

Inductive types

An inductive type is a data type.

It is equipped with a finite number of constructors.

Its inhabitants are generated by (finite, well-typed) applications of the constructors.

```
Inductive nat: Type :=
| O: nat
| S: nat -> nat.

Inductive list: Type -> Type :=
| nil:  forall A, list A
| cons: forall A, A -> list A -> list A.
```

E.g., the inhabitants of `nat` are `O`, `S O`, `S (S O)`, etc.

This is well suited to describe the syntax of a programming language.

Inductive predicates

An inductive predicate is equipped with a finite number of constructors, and is generated by (finite, well-typed) applications of the constructors.

```
Inductive even: nat -> Prop :=
| even_zero:
    even 0
| even_plus_2:
    forall n, even n -> even (S (S n)).
```

On paper, this is typically written in the form of inference rules:

$$\frac{}{\texttt{0}\text{ is even}} \qquad \frac{n \text{ is even}}{\texttt{S}\ (\texttt{S}\ n)\text{ is even}}$$

The inhabitants of the type `even n` can be thought of as derivation trees whose conclusion is `even n`.

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Binding and α-equivalence

Most programming languages provide constructs that bind variables, e.g.:

- function abstractions (in terms): $\lambda x.t$
- local definitions (in terms): let $x = t$ in t
- quantifiers (in types): $\forall\alpha.\alpha \rightarrow \alpha$

α-equivalence is a relation that allows renamings of bound variables, e.g.:

$$\lambda x.\, x + 1 \equiv_\alpha \lambda y.\, y + 1 \qquad \forall\alpha.\, \alpha \text{ list} \equiv_\alpha \forall\beta.\, \beta \text{ list}$$

α-equivalence can be defined as follows:

$$\lambda x.t \equiv_\alpha \lambda y.\binom{x}{y}t \qquad \text{if } y \notin fv(\lambda x.t)$$

where $\binom{x}{y}$ swaps all occurrences of x and y

Implicit α-equivalence

On paper, it is customary to confuse α-equivalence $\equiv_\alpha$ with equality $=$.

This plays a role, for instance, in the definition of System *F*.

This is the traditional rule for type-checking a function application:

$$\frac{\Gamma \vdash e_1 : \tau \rightarrow \tau' \qquad \Gamma \vdash e_2 : \tau}{\Gamma \vdash e_1\ e_2 : \tau'}$$

The rule should be written as follows, if α-equivalence was explicit:

$$\frac{\Gamma \vdash e_1 : \tau \rightarrow \tau' \qquad \Gamma \vdash e_2 : \tau_2 \qquad \tau \equiv_\alpha \tau_2}{\Gamma \vdash e_1\ e_2 : \tau'}$$

In simply-typed λ-calculus, this issue does not arise, as there are no quantifiers in types: α-equivalence and equality of types coincide.

Explicit α-equivalence

In principle, one should distinguish between:

- trees versus equivalence classes of trees;
- equality $=$ versus α-equivalence $\equiv_\alpha$.

This sounds easy enough, but leads to subtleties when defining mathematical functions that consume or produce trees... such as:

- program transformations, which produce and consume syntax trees;
- proofs, which produce and consume derivation trees.

Functions on equivalence classes

To define a function f from $\mathbb{T}/{\equiv_\alpha}$ to $\mathbb{T}/{\equiv_\alpha}$,
it suffices to first define a relation F between $\mathbb{T}$ and $\mathbb{T}$,
and to require two conditions:

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and to require two conditions:

- every tree is α-equivalent to some tree in the domain of F:

$$\forall t \in \mathbb{T} \quad \exists t', u' \in \mathbb{T} \quad t \equiv_\alpha t' \wedge t' \; F \; u'$$

  – note: the domain of F need not be $\mathbb{T}$
  – "without loss of generality, let us assume that x does not occur in ..."

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- F is compatible with α-equivalence:

$$\forall t, t', u, u' \in \mathbb{T} \quad t \; F \; u \wedge t' \; F \; u' \wedge t \equiv_\alpha t' \Rightarrow u \equiv_\alpha u'$$

  – note: F need not be deterministic (single-valued)
  – nondeterminism is fine as long as all choices yield α-eq. results
  – "let us pick a name x outside of ..."

Free variables

The classic definition of the set of the free variables of a λ-term:

$$\begin{aligned} fv(x) &= \{x\} \\ fv(\lambda x.t) &= fv(t) \setminus \{x\} \qquad\qquad \text{– no requirement on } x \\ fv(t_1\ t_2) &= fv(t_1) \cup fv(t_2) \end{aligned}$$

A total function from $\mathbb{T}$ to sets of names.

Condition 1 is vacuously satisfied (the relation is defined everywhere).

Condition 2 requires checking the following equality:

$$fv(\lambda x.t) = fv(\lambda y.\binom{x}{y}t) \qquad \text{where } y \notin fv(\lambda x.t)$$

This follows from the fact that fv is equivariant, i.e., commutes with swaps:

$$fv(\pi\, t) = \pi\, fv(t)$$

and from the fact that neither x nor y appear in the set $fv(\lambda x.t)$.

Thus, fv gives rise to a total function from $\mathbb{T}/\equiv_\alpha$ to sets of names.

Capture-avoiding substitution

The classic definition of capture-avoiding substitution:

$$
\begin{aligned}
x[u/x] &= u \\
y[u/x] &= y && \text{if } y \neq x \\
(\lambda z.t)[u/x] &= \lambda z.\, t[u/x] && \text{if } z \notin fv(u) \cup \{x\} \quad \text{– avoid capture!} \\
(t_1\ t_2)[u/x] &= t_1[u/x]\ t_2[u/x]
\end{aligned}
$$

A partial function from $\mathbb{T}$ to $\mathbb{T}$.

Condition 1 holds, as only a finite number of choices for z are forbidden.

Condition 2 requires checking:

$$\lambda z.\, t[u/x] \equiv_\alpha \lambda z'.\, t'[u/x] \qquad \text{where } z, z' \notin fv(u) \cup \{x\} \text{ and } \lambda z.t \equiv_\alpha \lambda z'.t'$$

which follows, again, from the fact that substitution is equivariant.

Thus, this gives rise to a total function from $\mathbb{T}/\equiv_\alpha$ to $\mathbb{T}/\equiv_\alpha$.

Naïve substitution

Naïve substitution does not have the side condition $z \notin fv(u) \cup \{x\}$.

It is a total function from $\mathbb{T}$ to $\mathbb{T}$,
but fails condition 2,
hence does not give rise to a function from $\mathbb{T}/\equiv_\alpha$ to $\mathbb{T}/\equiv_\alpha$.

$$(\lambda y. x + y)[2 \times y/x] \quad = \quad \lambda y. 2 \times y + y \qquad \text{– naïve}$$

$$\begin{aligned} (\lambda y. x + y)[2 \times y/x] &= \\ (\lambda z. x + z)[2 \times y/x] &= \lambda z. 2 \times y + z \qquad \text{– capture-avoiding} \end{aligned}$$

Representations of syntax

How should syntax with binding be represented in a proof assistant?

Several representations come to mind:

- equivalence classes of trees – the nominal approach (Pitts, 2006);
- de Bruijn notation – used in this course (de Bruijn, 1972);
- (parametric) higher-order abstract syntax (Chlipala, 2008);
- the locally nameless representation (Charguéraud, 2009);
- and many more.

One should choose a representation for which the proof assistant has good support.

What about the nominal approach?

The nominal approach is prevalent in informal (paper) proofs.

It is implemented in Nominal Isabelle (Urban, 2008).

- Urban and Narboux (2008) present typical proofs about operational semantics.

It is not well supported in Coq, perhaps for engineering reasons.

- Cohen (2013) shows how to use quotients in Coq (when they exist) and how to construct them (up to certain axioms or hypotheses).

What about other approaches?

The POPLmark challenge proposes a benchmark problem:
a proof of type soundness for $F_{<:}$.

15 solutions have been proposed, using 8 different representations in 7 different proof assistants.

No consensus, yet!

de Bruijn indices

A simple idea: don't use names.

Instead, use pointers from variables back to their binding site.

A second idea: use relative pointers, encoded as natural integers.

- 0 denotes the nearest enclosing λ,
  i.e., the most recently bound variable;
- 1 denotes the next enclosing λ, and so on.

$\lambda x.x$ is $\lambda 0$.

$\lambda f.\lambda x.f\ x$ is $\lambda\lambda(1\ 0)$.

Why is this a good idea?

de Bruijn syntax has several strengths:

- it is easily defined;
- it is inductive – terms are trees, no quotient is required;
- it is canonical – α-equivalence is just equality.

Its drawbacks are well-known, too:

- terms are more difficult to read – a printer may be needed;
- definitions and theorems can seem difficult to write and read – mostly a matter of habit?

λ-terms in de Bruijn's notation

The syntax of λ-calculus is simple:

$$t ::= x \mid \lambda t \mid t\ t \qquad \text{where } x \in \mathbb{N}$$

In Coq:

```
Inductive term :=
| Var: nat -> term
| Lam: term -> term
| App: term -> term -> term.
```

Suggested exercises

Exercise: In OCaml, implement conversions between the nominal representation and de Bruijn's representation, both ways.

Exercise: In OCaml, implement an exhaustive enumeration of the λ-terms of size *s* and with at most *n* free variables. (Let variables have size 0; let λ-abstractions and applications contribute 1.)

Exercise: Use this exhaustive enumeration to test that the above conversions are inverses of each other.

Substitution

— *Substitution is the éminence grise of the λ-calculus.*

Abadi, Cardelli, Curien, Lévy, Explicit substitutions, 1990.

Substitutions

Let a substitution σ be a total function of variables $\mathbb{N}$ to terms $\mathbb{T}$.

It can also be thought of as an infinite sequence $\sigma(0) \cdot \sigma(1) \cdot \ldots$

Let *id* be the identity substitution: $id(x) = x$.

- $0 \cdot 1 \cdot 2 \cdot \ldots$

Let $+i$ be the lift substitution: $(+i)(x) = x + i$.

- $i \cdot (i + 1) \cdot (i + 2) \cdot \ldots$

Let $t \cdot \sigma$ be the cons substitution that maps 0 to t and $x + 1$ to $\sigma(x)$.

- $t \cdot \sigma(0) \cdot \sigma(1) \cdot \ldots$

id can in fact be viewed as sugar for $0 \cdot (+1)$.

Substitution application and composition

Can we define $t[\sigma]$, the application of the substitution σ to the term t?

It should satisfy the following laws:

$$
\begin{aligned}
x[\sigma] &= \sigma(x) \\
(\lambda t)[\sigma] &= ? \\
(t_1\ t_2)[\sigma] &= t_1[\sigma]\ t_2[\sigma]
\end{aligned}
$$

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(\lambda t)[\sigma] &= \lambda(t[0 \cdot ?]) \\
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\end{aligned}
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x[\sigma] &= \sigma(x) \\
(\lambda t)[\sigma] &= \lambda(t[0 \cdot (\sigma \,;\, +1)]) \\
(t_1\ t_2)[\sigma] &= t_1[\sigma]\ t_2[\sigma]
\end{aligned}
$$

and the composition of two substitutions $\sigma_1 \,;\, \sigma_2$ should satisfy:

$$(\sigma_1 \,;\, \sigma_2)(x) = (\sigma_1(x))[\sigma_2]$$

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$$\begin{aligned} x[\sigma] &= \sigma(x) \\ (\lambda t)[\sigma] &= \lambda(t[\Uparrow \sigma]) \\ (t_1\ t_2)[\sigma] &= t_1[\sigma]\ t_2[\sigma] \end{aligned}$$

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$$(\sigma_1\,;\,\sigma_2)(x) = (\sigma_1(x))[\sigma_2]$$

These equations are mutually recursive, so do not form a valid definition.

This can be worked around by defining $t[+i]$ first ("lift"),
then $\sigma\,;\,+i$, whence $\Uparrow\sigma$, whence $t[\sigma]$ ("subst").

de Bruijn algebra

The following equations are sound, that is, valid:

$$
\begin{aligned}
(\lambda t)[\sigma] &= \lambda(t[0 \cdot (\sigma \,;\, +1)]) \\
(t_1\ t_2)[\sigma] &= t_1[\sigma]\ t_2[\sigma] \\
0[t \cdot \sigma] &= t \\
(+1) \,;\, (t \cdot \sigma) &= \sigma
\end{aligned}
\qquad
\begin{aligned}
id \,;\, \sigma &= \sigma \\
\sigma \,;\, id &= \sigma \\
(\sigma_1 \,;\, \sigma_2) \,;\, \sigma_3 &= \sigma_1 \,;\, (\sigma_2 \,;\, \sigma_3) \\
(t \cdot \sigma_1) \,;\, \sigma_2 &= t[\sigma_2] \cdot (\sigma_1 \,;\, \sigma_2)
\end{aligned}
$$

Furthermore, they are complete (Schäfer *et al.*, 2015).

That is, if an equation based on the following grammar is valid, then it logically follows from the above equations.

$$
\begin{aligned}
t &::= 0 \mid \lambda t \mid t\ t \mid t[\sigma] \mid T \\
\sigma &::= +1 \mid t \cdot \sigma \mid \sigma \,;\, \sigma \mid \Sigma
\end{aligned}
$$

Schäfer *et al.* also prove that validity is decidable.

de Bruijn algebra

Decidability means that the machine can answer questions for us.

Does $t[id] = t$ hold? Yes.

Does $t[\sigma_1][\sigma_2] = t[\sigma_1 ; \sigma_2]$ hold? Yes.

And so on, and so forth.

For proofs of the above two equations, see Schäfer *et al.*, Fact 6.

Yet, we do not really care about these proofs – a machine can find them.

Coq tactics for de Bruijn algebra

The Coq library Autosubst offers two tactics:

- `autosubst` proves an equation between terms or substitutions;
- `asimpl` simplifies a goal in which a term or substitution appears.

λ-terms with AutoSubst

The syntax of λ-calculus can be declared as follows:

```
Inductive term :=
| Var:           var -> term
| Lam:   {bind term} -> term
| App: term -> term -> term.
```

AutoSubst defines `var` as a synonym for `nat`
and `{bind term}` as a synonym for `term`.

AutoSubst defines substitution application, composition, etc., for us.

AutoSubst key notations

$t \cdot \sigma$	`t .: sigma`	substitution "cons"
$+i$	`ren (+i)`	the substitution $+i$
id	`ids`	the identity substitution
$t[\sigma]$	`t.[sigma]`	substitution application
$\sigma_1 ; \sigma_2$	`sigma1 >> sigma2`	substitution composition
$\Uparrow \sigma$	`up sigma`	taking a substitution under a binder
$\Uparrow^n \sigma$	`upn n sigma`	taking a substitution under *n* binders
$t.[u \cdot id]$	`t.[u/]`	substituting *u* for 0 in *t*

“lift” as end-of-scope

Suppose we are writing a program in de Bruijn’s notation.

Suppose we are in a context where n variables exist
and we wish to refer to a subterm t that has $n - 1$ free variables.
That is, t does not know about one of our variables, say i, where $0 \leq i < n$.

We cannot just refer to t, as some indices would be off by one.

Instead, we must use $t[\Uparrow^i (+1)]$.

Ugly, low-level index arithmetic? No: read it as an end-of-scope mark.

Adopt a nicer notation for it, say “eos i in t”.

There is no syntax for it in the λ-calculus; it is a meta-level notation.

A related, object-level end-of-scope construct, “abdmal”,
has been studied by Hendriks and van Oostrom (2003).

Calculi of explicit substitutions

Similarly, we have viewed substitution application as a meta-level operation. There is no syntax for it in the λ-calculus.

In the $\lambda\sigma$-calculus, however, there is syntax for substitutions and substitution application, and a set of small-step reduction rules that explain how substitutions interact with λ-abstractions and applications.

Abadi, Cardelli, Curien, Lévy, Explicit substitutions, 1990.

Curien, Hardin, Lévy, Confluence properties of weak and strong calculi of explicit substitutions, 1992.