

Towards machine-checked proofs

MPRI FUN

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1 Why mechanize definitions and proofs?

2 Rocq in a nutshell

3 Representing abstract syntax with binders

de Bruijn's representation

The nominal representation

Why formalize programming languages?

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To obtain **precise definitions** of programming languages.

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.
- Proof cases are **omitted** because they are “obvious”.
- It is difficult to **maintain** hand-written proofs as definitions evolve.

Opportunity: machine-assisted proof

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Mechanized theorem proving has made great progress.

Landmark examples in mathematics:

- the 4-color th.: Haken & Appel (1976), Gonthier & Werner (2005);
- the Feit-Thompson theorem: Gonthier *et al.* (2013);
- Kepler's conjecture: Hales *et al.* (2015);
- The Liquid Tensor Experiment: Commelin *et al.* (2022).

Programming language theory is a **good match** for proof assistants:

- 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?

Today, over 20% of the papers at POPL come with such an 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.

Barendregt and Wiedijk,
The Challenge of Computer Mathematics, 2005.

Popular proof assistants include Rocq, Agda, HOL4, Isabelle/HOL...

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Computations and functions

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

```
Fixpoint factorial (n: nat) :=  
  match n with  
    | 0    => 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

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

Definition divides $(a\ b: N) := \text{exists } n: N, b = n * a.$

Theorem factorial_divisors:

forall $n\ i, 1 \leq i \leq n \rightarrow \text{divides } i\ (\text{factorial } n).$

Definition prime $(p: N) :=$

$p > 1 \wedge (\text{forall } d, \text{divides } d\ p \rightarrow d = 1 \vee d = p).$

Theorem Euclid:

forall $n, \text{exists } p, p \geq n \wedge \text{prime } p.$

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 repeated application of the constructors.

```
Inductive nat: Type :=
```

```
| 0: 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 `0`, `S 0`, `S (S 0)`, etc.

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

Inductive predicates

An **inductive predicate** is equipped with a finite number of constructors, and is generated by repeated application 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:

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

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:

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

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

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

On paper, usually,

- the concepts of names and binding are **not** clearly defined;
- one **confuses** α -equivalence \equiv_{α} with equality $=$.

Representations of syntax

How should syntax with binding be mathematically defined,
on paper or in a proof assistant?

Several representations come to mind:

- **de Bruijn** notation – used in this course (**de Bruijn, 1972**);
- equivalence classes – the **nominal** approach (**Pitts, 2006**);
- (parametric) **higher-order abstract syntax** (**Chlipala, 2008**);
- the **locally nameless** representation (**Charguéraud, 2009**);
- the solutions of the **POPLmark challenge (2005)** involve 8 different representations, and there are more.

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

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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?

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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;
- definitions and theorems can seem difficult to read and write
 - mostly a matter of **habit**?

λ -terms in de Bruijn's notation

The syntax of λ -calculus is simple:

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

In Rocq:

```
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

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- Substitution is the *éminence grise* of the λ -calculus.
Abadi, Cardelli, Curien, Lévy, **Explicit substitutions**, 1990.

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 $\sigma(0) \cdot \sigma(1) \cdot \dots$

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

- $0 \cdot 1 \cdot 2 \cdot \dots$

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

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

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

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

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:

$$x[\sigma] = \sigma(x)$$

$$(\lambda t)[\sigma] = ?$$

$$(t_1 \ t_2)[\sigma] = t_1[\sigma] \ t_2[\sigma]$$

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:

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

Substitution application and composition

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

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

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:

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

$\uparrow \sigma$ can be understood as “the substitution σ , moved under one binder”.

The (left-to-right) **composition** of two substitutions $\sigma_1 ; \sigma_2$ should satisfy:

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

Substitution application and composition

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$$\begin{aligned} x[\sigma] &= \sigma(x) \\ (\lambda t)[\sigma] &= \lambda(t[\uparrow\sigma]) \\ (t_1 \ t_2)[\sigma] &= t_1[\sigma] \ t_2[\sigma] \end{aligned} \quad \text{where } \uparrow\sigma \text{ stands for } 0 \cdot (\sigma ; +1)$$

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The (left-to-right) **composition** of two substitutions $\sigma_1 ; \sigma_2$ should satisfy:

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

Unfortunately, these equations are mutually recursive,
so **they are not accepted as a valid definition**
by a proof assistant such as Rocq.

Work-around (1): define lifting first

To work around this problem, one first defines $t[\sigma]$ in the special case where σ is $\uparrow^i(+1)$.

This yields a function of two arguments, **lifting**, written $\uparrow^i t$:

$$\begin{aligned}\uparrow^i(x) &= x + i \\ \uparrow^i(\lambda t) &= \lambda(\uparrow^{i+1} t) \\ \uparrow^i(t_1 t_2) &= \uparrow^i t_1 \uparrow^i t_2\end{aligned}$$

This definition is accepted by a proof assistant. (Why?)

$\uparrow^i t$ can be understood as “the term t , moved under i binders”.

Work-around (2): define substitution next

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Then, one can define $\uparrow\sigma$ as the substitution that maps 0 to 0 and that maps $x + 1$ to $\uparrow^1(\sigma(x))$.

Exercise: Check that $\uparrow\sigma$ is equal to $0 \cdot (\sigma; +1)$ as desired.

Finally, one defines substitution:

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

This definition is accepted by a proof assistant. (Why?)

de Bruijn algebra

The following equations are **valid**, that is, universally true:

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

Furthermore, these equations form a **complete** theory: that is, if an equation (which involves just the above concepts) is valid then it **is a logical consequence** of the above equations (Schäfer *et al.*, 2015).

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

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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.**

Does $t[+1][u \cdot id] = t$ hold? **Yes.**

- In nominal style, this would be written: $t[u/x] = t$ if $x \notin fv(t)$.
- de Bruijn style is less familiar, but has **no side condition**.

And so on, and so forth.

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

We do not really care about these proofs – a machine can find them.

Rocq tactics for de Bruijn algebra

The Rocq library **AutoSubst** offers two tactics:

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

I use AutoSubst version 1 because it suffices for my needs.

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.

See [DemoSyntaxReduction](#).

AutoSubst key notations

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

Reading “lift” as an end-of-scope mark

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Suppose we are building a term in a context where n variables exist and we wish to refer to a subterm t that was built in a context where one of our variables, say x , where $0 \leq x < n$, did not exist.

We cannot just refer to t . Instead, we must use $t[\uparrow^x(+1)]$, that is, $\uparrow^x t$.

Is this ugly low-level index arithmetic?

Yes and no: one can read it as an **end-of-scope** mark for the variable x .

One can adopt a nicer **meta-level** notation for it, say “*unbind x in t* ”.

The equation discussed **earlier** is then written $(\text{unbind } 0 \text{ in } t)[u \cdot \text{id}] = t$. That is, replacing 0 with u in a term where 0 is not in scope has no effect.

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

Calculi of explicit substitutions

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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.

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Binding and α -equivalence

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- 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, a relation on trees, can be defined as follows (Pitts, 2006):

$$\frac{y \notin \text{fv}(\lambda x. t) \quad u = \binom{x}{y} t}{\lambda x. t \equiv_{\alpha} \lambda y. u}$$

where $\binom{x}{y}$ swaps **all** occurrences of the names x and y in the term t .

Implicit α -equivalence

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

This plays a role, for instance, in the definition of System F , where types contain universal quantifiers.

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

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

If α -equivalence was explicit, the rule would be written as follows:

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

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_{α} .

A **term** is an equivalence class of trees.

This sounds easy enough, but leads to subtleties when defining mathematical **functions** that consume or produce terms... 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_α to \mathbb{T}/\equiv_α ,
it suffices to first define a **relation** F between \mathbb{T} and \mathbb{T} ,
and to require two conditions:

Functions on equivalence classes

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it suffices to first define a **relation** F between \mathbb{T} and \mathbb{T} ,
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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- note: the domain of F need not be \mathbb{T}
- “without loss of generality, **let us assume** that x does not occur in ...”

- 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

This is the classic definition of the set of the **free variables** of a tree:

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

It is 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:

$$fv(\lambda x.t) = fv(\lambda y.({}_y^x)t) \quad \text{where } y \notin fv(\lambda x.t)$$

This follows from the fact that fv is **equivariant**,
that is, fv commutes with every permutation π :

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

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_α to sets of names.

Capture-avoiding substitution

This is the classic definition of capture-avoiding substitution:

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

It is 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:

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

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 $z \notin \text{fv}(u) \cup \{x\}$.

It is a total function from \mathbb{T} to \mathbb{T} ,
but **does not satisfy** condition 2,
hence does **not** give rise to a function from \mathbb{T}/\equiv_α to \mathbb{T}/\equiv_α .

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

$$(\lambda y. x + y)[2 \times y/x] =$$

$$(\lambda z. x + z)[2 \times y/x] = \lambda z. 2 \times y + z \quad - \text{capture-avoiding}$$

The nominal approach in proof assistants

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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 Rocq, perhaps for engineering reasons.

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