

# Towards machine-checked proofs

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2023

Mechanization

Coq in a  
nutshell

Syntax with  
binders

Nominal  
de Bruijn

## 1 Why mechanize definitions and proofs?

## 2 Coq in a nutshell

## 3 Representing abstract syntax with binders

The nominal representation

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# Why formalize programming languages?

## Mechanization

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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 ( $\lambda$ ,  $\pi$ ) 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

### Mechanization

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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).

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 Coq, Agda, HOL4, Isabelle/HOL...



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# 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  
  | 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

**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 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

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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 $\alpha$ -equivalence

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

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

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

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

$\alpha$ -equivalence can be defined as follows (Pitts, 2006):

$$\lambda x. t \equiv_{\alpha} \lambda y. \binom{x}{y} t \quad \text{if } y \notin \text{fv}(\lambda x. t) \\ \text{where } \binom{x}{y} \text{ swaps all occurrences of } x \text{ and } y$$



Implicit  $\alpha$ -equivalence

On paper, it is customary to confuse  $\alpha$ -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:

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

If  $\alpha$ -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  $\lambda$ -calculus, this issue does not arise, as there are no quantifiers in types:  $\alpha$ -equivalence and equality of types coincide.

## Explicit $\alpha$ -equivalence

In principle, one should distinguish between:

- **trees** versus **equivalence classes** of trees;
- **equality** = versus  **$\alpha$ -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  $\alpha$ -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  $\alpha$ -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  $\alpha$ -eq. results
- “**let us pick** a name  $x$  outside of ...”

## Free variables

The classic definition of the set of the **free variables** of a  $\lambda$ -term:

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

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:

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

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:

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

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  $\mathbb{T}/\equiv_\alpha$  to  $\mathbb{T}/\equiv_\alpha$ .

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

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

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



## Representations of syntax

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

Several representations come to mind:

- equivalence classes – 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 (2005)** 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!

**POPLmark reloaded (2019)** involves proofs by logical relations.

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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  $\lambda$ ,  
i.e., the **most recently bound** variable;
- 1 denotes the next enclosing  $\lambda$ , 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** –  $\alpha$ -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**?

# $\lambda$ -terms in de Bruijn's notation

The syntax of  $\lambda$ -calculus is simple:

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

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  $\lambda$ -terms of size  $s$  and with at most  $n$  free variables. (Let variables have size 0; let  $\lambda$ -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  $\lambda$ -calculus.  
Abadi, Cardelli, Curien, Lévy, **Explicit substitutions**, 1990.

Let a substitution  $\sigma$  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  $\sigma$  to the term  $t$ ?

It should satisfy the following laws:

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

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

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

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

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

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

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

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

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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 first inductively defining  $t[+1]$  (“**lift**”).

— in fact, one must inductively define  $t[\uparrow^i(+1)]$ .

Then, we define  $\sigma ; +1$ , whence  $\uparrow\sigma$ , whence  $t[\sigma]$  (“**subst**”).



## de Bruijn algebra

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The following equations are **sound**, that is, valid:

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

Furthermore, 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.

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

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

## de Bruijn algebra

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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.

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.

The syntax of  $\lambda$ -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 &gt;&gt; sigma2</code> | substitution composition                |
| $\Uparrow \sigma$     | <code>up sigma</code>               | taking a substitution under a binder    |
| $\Uparrow^n \sigma$   | <code>upn n sigma</code>            | taking a substitution under $n$ binders |
| $t.[u \cdot id]$      | <code>t.[u/]</code>                 | substituting $u$ for 0 in $t$           |

## “lift” as end-of-scope

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  $t[\uparrow^x (+1)]$ .

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

Adopt a nicer **meta-level** notation for it, say “eos  $x$  in  $t$ ”.

The equation discussed **earlier** is now written  $(\text{eos } 0 \text{ in } t)[u \cdot id] = t$ .

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  $\lambda$ -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  $\lambda$ -abstractions and applications.

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

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