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Towards Specifying Symbolic Computation

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Differentiation

- An important task of calculus is to find the derivative of a function.
- A function $f : \mathbb{R} \rightarrow \mathbb{R}$ is differentiable at a if

$$\lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

exists. If this limit exists, it is denoted by $f'(a)$ and is called the derivative of f at a. The function f' is called the derivative of f.
- Computing the derivative of function from the definition of a derivative is generally very difficult.

Symbolic Differentiation

- It is much easier to compute derivatives using an algorithm that repeatedly applies symbolic differentiation rules such as:

$$\frac{d}{dx}(c) = 0 \text{ where } c \text{ is a constant.}$$

$$\frac{d}{dx}(u+v) = \frac{d}{dx}(u) + \frac{d}{dx}(v).$$

$$\frac{d}{dx}(x^n) = \begin{cases} 0 & \text{if } n = 0 \\ n \cdot x^{n-1} & \text{if } n > 0. \end{cases}$$

$$\frac{d}{dx}(\ln(x)) = \frac{1}{x}.$$

$$\frac{d}{dx}(u(v)) = \frac{d}{dv}(u(v)) \cdot \frac{d}{dx}(v).$$

- Notice that these rules operate on expressions with variables, not on functions.

The Symbolic Differentiation Problem

- Consider the function

$$\begin{aligned} f &= \lambda\, x : \mathbb{R}\, .\, \ln(x^2 - 1) \\ &= \lambda\, x : \mathbb{R}\, .\, \mathrm{if}(|x| > 1, \ln(x^2 - 1), \bot). \end{aligned}$$

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- The derivative calculators on the web return

$$g = \lambda\, x : \mathbb{R} \,.\, \frac{2x}{x^2 - 1}$$

as the derivative of f, which might mean

$$\lambda\, x : \mathbb{R} \,.\, \mathrm{if}(|x| \neq 1, \frac{2x}{x^2 - 1}, \bot).$$

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$$\lambda\, x : \mathbb{R} \,.\, \mathrm{if}(|x| \neq 1, \frac{2x}{x^2 - 1}, \perp).$$

- But this is wrong! The derivative of f is

$$f' = \lambda\, x : \mathbb{R} \,.\, \mathrm{if}(|x| > 1, \frac{2x}{x^2 - 1}, \perp).$$

Syntax-Based Mathematical Algorithms

- A syntax-based mathematical algorithm (SBMA) manipulates the syntax of expressions in a mathematically meaningful way.
  - SBMAs are commonplace in mathematics.
  - Symbolic differentiation algorithms are examples of SBMAs.

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  1. The computational behavior is the relationship between its input and output expressions.
  2. The mathematical meaning is the relationship between what its input and output expressions mean mathematically.

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- A SBMA has two fundamental properties:
  1. The computational behavior is the relationship between its input and output expressions.
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- Explains symbolic differentiation in derivative calculators.

Specification of SBMAs

- A correct implementation requires a correct specification.
- Interplay of syntax and semantics makes specification difficult.
- This is because:
    1. Manipulating syntax is complex.
    2. Difficult to disentangle the interplay of syntax and semantics.
    3. Benign syntactic manipulations generate undefined expressions.

Specification of Symbolic Differentiation

- Let $\mathcal{L}$ be the set of expressions built by the usual operators on $\mathbb{R}$.
- Let $\mathrm{diff} : \mathcal{L} \to \mathcal{L}$ be the SBMA that repeatedly applies symbolic differentiation rules.
- The specification of diff is: For all $e \in \mathcal{L}$,
  if $f = (\lambda\, x : \mathbb{R} \,.\, e)$ is differentiable at a, then $f'(a)$ is

  $$(\lambda\, x : \mathbb{R} \,.\, \mathrm{diff}(e))(a).$$

- Note: If f is not differentiable at a, then f' is not defined at a.

Rational Expressions and Rational Functions

- A rational expression (in x over $\mathbb{Q}$) is an expression that denotes a member of $\mathbb{Q}(x)$, the field of fractions of polynomials in x.
- A rational function (in x over $\mathbb{Q}$) is an expression $(\lambda\, x : \mathbb{Q} \,.\, r)$ where r is a rational expression.
  - Denotes a function of type $\mathbb{Q} \to \mathbb{Q}$.
- Notice that x plays different roles here.
- It is useful to normalize rational expressions.
  - For example, $x - 2 + \frac{x+1}{x-1}$ normalizes to $\frac{x-3}{x-1}$
  - But x/x normalizes to 1 and
    $1/x - 1/x$ normalizes to 0.
- It is also useful to normalize rational functions ... but how?

The Rational Function Normalization Problem

- Consider the rational function $f = \lambda\, x : \mathbb{Q} \, . \, \frac{x^4-1}{x^2-1}$.
- In computer algebra systems, $\frac{x^4-1}{x^2-1}$ is interpreted both as a rational expression and as a rational function.
- This leads to the following problem:
  - The value of $\frac{x^4-1}{x^2-1}$ for $x = 1$ is undefined.
  - $\frac{x^4-1}{x^2-1}$ normalizes to $x^2 + 1$.
  - The value of $x^2 + 1$ for $x = 1$ is 2.
  - So f is effectively normalized to $g = \lambda\, x : \mathbb{Q} \, . \, x^2 + 1$, but $f \neq g$.
- Hence CASs do not correctly normalize rational functions!

Specification of Rational Function Normalization

- Let $\mathcal{L}$ be the set of rational functions.
- A quasinormal form is a rational expression p/q in which there are no common irreducible polynomials of degree ≥ 2.
- Let $\mathsf{norm} : \mathcal{L} \to \mathcal{L}$ be the SBMA that normalizes a rational function $\lambda\, x : \mathbb{Q} \,.\, r$ by quasinormalizing r.
- The specification of norm is: For all $(\lambda\, x : \mathbb{Q} \,.\, r) \in \mathcal{L}$,
  1. $\mathsf{norm}(\lambda\, x : \mathbb{Q} \,.\, r) = (\lambda\, x : \mathbb{Q} \,.\, r')$ where r' is quasinormal and
  2. $(\lambda\, x : \mathbb{Q} \,.\, r)$ and $\mathsf{norm}(\lambda\, x : \mathbb{Q} \,.\, r)$ denote the same function.

Formal Specification of SBMAs

- Consider the specification of diff: For all $e \in \mathcal{L}$, if $f = (\lambda\, x : \mathbb{R}\,.\ e\ )$ is differentiable at a, then $f'(a)$ is

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- This should be written: For all $e \in \mathcal{L}$, if $f = (\lambda\, x : \mathbb{R}\, .\ [\![e]\!]\ )$ is differentiable at a, then $f'(a)$ is

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Formal Specification of SBMAs

- Consider the specification of diff: For all $e \in \mathcal{L}$, if $f = (\lambda\, x : \mathbb{R}\,.\; e\,)$ is differentiable at a, then $f'(a)$ is

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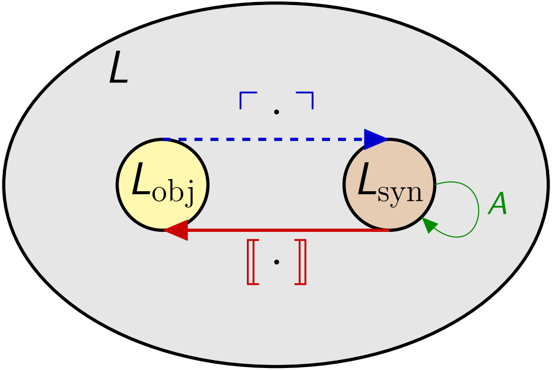
  $$(\lambda\, x : \mathbb{R}\,.\; [\![\mathrm{diff}(e)]\!]\,)(a)$$

  where $[\![e]\!]$ is the value of the expression denoted by e.
- To formally specify and apply SBMAs we need a reflection infrastructure with quotation $\ulcorner \cdot \urcorner$ and evaluation $[\![\cdot]\!]$ operators.

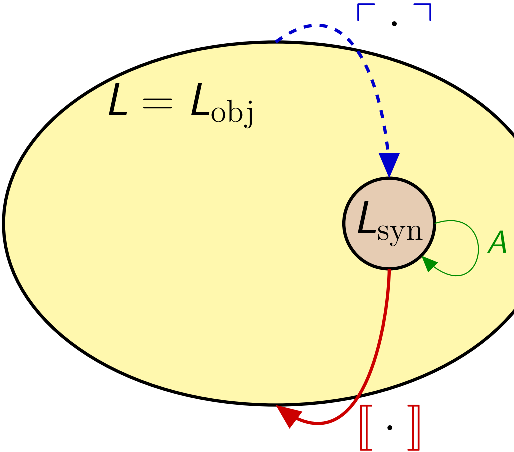
Reflection Infrastructure



$\mathrm{CTT}_{\mathrm{qe}}$ and $\mathrm{CTT}_{\mathrm{uqe}}$

- $\mathrm{CTT}_{\mathrm{qe}}$ is a version of Church's type theory that has a built-in global reflection infrastructure.

Global Reflection Infrastructure



$\mathrm{CTT}_{\mathrm{qe}}$ and $\mathrm{CTT}_{\mathrm{uqe}}$

- $\mathrm{CTT}_{\mathrm{qe}}$ is a version of Church's type theory that has a built-in global reflection infrastructure.
- By modifying the HOL Light proof assistant, we have produced a rudimentary implementation of $\mathrm{CTT}_{\mathrm{qe}}$ called HOL Light QE.
- Unlike $\mathrm{CTT}_{\mathrm{qe}}$, $\mathrm{CTT}_{\mathrm{uqe}}$ is a variant of $\mathrm{CTT}_{\mathrm{qe}}$ that admits undefined expressions and partial functions.
- $\mathrm{CTT}_{\mathrm{uqe}}$ is well suited for specifying SBMAs that manipulate expressions that may be undefined such as diff.

Specification of diff in $\mathrm{CTT}_{\mathrm{uqe}}$

$$
\begin{array}{l}
\forall\, u_\epsilon \;.\\
\quad \mathsf{if}\ (\mathsf{DiffExpr}_{\epsilon\to o}\, u_\epsilon)\\
\qquad (\mathsf{DiffExpr}_{\epsilon\to\epsilon}(\mathsf{diff}_{\epsilon\to\epsilon}\, u_\epsilon) \wedge\\
\qquad\ \forall\, a_r \;.\\
\qquad\quad (\mathsf{deriv}_{(r\to r)\to r\to r}\,(\lambda\, x_r \;.\; [\![u_e]\!]_r)\, a_r){\downarrow} \supset\\
\qquad\qquad \mathsf{deriv}_{(r\to r)\to r\to r}\,(\lambda\, x_r \;.\; [\![u_e]\!]_r)\, a_r = (\lambda\, x_r \;.\; [\![\mathsf{diff}_{\epsilon\to\epsilon}\, u_e]\!]_r)\, a_r\\
\qquad (\mathsf{diff}_{\epsilon\to\epsilon}\, u_\epsilon){\uparrow}
\end{array}
$$

Future Work

- Show that global reflection, as realized in $\mathrm{CTT}_{\mathrm{qe}}$ and $\mathrm{CTT}_{\mathrm{uqe}}$, is a viable approach for reasoning about SBMAs.
- Continue the development of HOL Light QE.
- Define several examples of SBMAs in HOL Light QE.
- Prove in HOL Light QE the mathematical meanings of these SBMAs from their definitions.

Conclusion

- An SBMA is an algorithm that manipulates the syntactic structure of expressions to achieve a mathematical task.
- The interplay of syntax and semantics inherent in SBMAs can make them tricky to implement and specify.
- The formal specification of SBMAs requires a reflection infrastructure with quotation and evaluation operators.
- $\mathrm{CTT}_{\mathrm{qe}}$ and $\mathrm{CTT}_{\mathrm{uqe}}$ have built-in global reflection infrastructures well suited for specifying, defining, and reasoning about SBMAs.