Reverse AD at Higher Types: Pure, Principled and Denotationally Correct

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We show how to define source-code transformations for forward- and reverse-mode Automatic Differentiation on a standard higher-order functional language. The transformations generate purely functional code, and they are principled in the sense that their definition arises from a categorical universal property. We give a semantic proof of correctness of the transformations. In their most elegant formulation, the transformations generate code with linear types. However, we demonstrate how the transformations can be implemented in a standard functional language without sacrificing correctness. To do so, we make use of abstract data types to represent the required linear types, e.g. through the use of a basic module system.

CCS Concepts:
- Theory of computation → Denotational semantics; Categorical semantics;
- Mathematics of computing → Differential calculus;
- Software and its engineering → General programming languages;

Additional Key Words and Phrases: automatic differentiation, program correctness, denotational semantics

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1 INTRODUCTION

Automatic Differentiation (AD) is a technique for transforming code that implements a function \( f \) into code that computes \( f \)'s derivative, essentially by using the chain rule for derivatives. Due to its efficiency and numerical stability, AD is the technique of choice whenever derivatives need to be computed for functions that are implemented as programs, particularly in high dimensional settings. Optimization and Monte-Carlo integration algorithms, such as gradient descent and Hamiltonian Monte-Carlo methods, rely crucially on the calculation of derivatives. These algorithms are used in virtually every machine learning and computational statistics application, and the calculation of derivatives is usually the computational bottle-neck. These applications explain the recent surge of interest in AD, which has resulted in the proliferation of popular AD systems such as TensorFlow (Abadi et al. 2016), PyTorch (Paszke et al. 2017), and Stan Math (Carpenter et al. 2015).

AD, roughly speaking, comes in two modes: forward-mode and reverse-mode. When differentiating a function \( \mathbb{R}^n \rightarrow \mathbb{R}^m \), forward-mode tends to be more efficient if \( m \gg n \), while reverse-mode generally is more performant if \( n \gg m \). As most applications reduce to optimization or Monte-Carlo integration of an objective function \( \mathbb{R}^n \rightarrow \mathbb{R} \) with \( n \) very large (today, in the order of \( 10^4 \) – \( 10^7 \)), reverse-mode AD is in many ways the more interesting algorithm.

However, it is also much more complicated to understand and implement than forward AD. Forward AD can be straightforwardly implemented as a structure-preserving program transformation, even on languages with complex features (Shaikhha et al. 2019). As such, it admits an elegant proof of correctness (Huot et al. 2020). By contrast, reverse-AD is only well-understood as a source-code transformation (also called \textit{define-then-run} style AD) on limited programming languages. Typically, its implementations on more expressive languages that have features such as
higher-order functions make use of define-by-run approaches. These approaches first build a computation graph during runtime, effectively evaluating the program until a straight-line first-order program is left, and then they evaluate this new program (Carpenter et al. 2015; Paszke et al. 2017). Such approaches have the severe downside that the differentiated code cannot benefit from existing optimizing compiler architectures. As such, these AD libraries need to be implemented using carefully, manually optimized code, that for example does not contain any common subexpressions. This implementation process is precarious and labour intensive. Further, some whole-program optimizations that a compiler would detect go entirely unused in such systems.

Similarly, correctness proofs of reverse AD have taken a define-by-run approach and have relied on non-standard operational semantics, using forms of symbolic execution (Abadi and Plotkin 2020; Brunel et al. 2020; Mak and Ong 2020). Most work that treats reverse-AD as a source-code transformation does so by making use of complex transformations which introduce mutable state and/or non-local control flow (Pearlmutter and Siskind 2008; Wang et al. 2019). As a result, we are not sure whether and why such techniques are correct. Another approach has been to compile high-level languages to a low-level imperative representation first, and then to perform AD at that level (Innes 2018), using mutation and jumps. This approach has the downside that we might lose important opportunities for compiler optimizations, such as map-fusion and embarrassingly parallel maps, which we can exploit if we perform define-then-run AD on a high-level representation.

A notable exception to these define-by-run and non-functional approaches to AD is (Elliott 2018), which presents an elegant, purely functional, define-then-run version of reverse AD. Unfortunately, their techniques are limited to first-order programs over tuples of real numbers. This paper extends the work of (Elliott 2018) to apply to higher-order programs over (primitive) arrays of reals:

- It defines purely functional define-then-run reverse-mode AD on a higher-order language.
- It shows how the resulting, mysterious looking program transformation arises from a universal property if we phrase the problem in a suitable categorical language. Consequently, the transformations automatically respect equational reasoning principles.
- It explains, from this categorical setting, precisely in what sense reverse AD is the “mirror image” of forward AD.
- It presents an elegant proof of semantic correctness of the AD transformations, based on a semantic logical relations argument, demonstrating that the transformations calculate the derivatives of the program in the usual mathematical sense.
- It shows that the AD definitions and correctness proof are extensible to higher-order primitives such as a map-operation over our primitive arrays.
- It discusses how our techniques are readily implementable in standard functional languages to give purely functional, principled, semantically correct, define-then-run reverse-mode AD.

## 2 KEY IDEAS

Consider a very simple programming language. Types are statically sized arrays $\text{real}^n$ for some $n$, and programs are obtained from a collection of (unary) primitive operations $x : \text{real}^n \rightarrow \text{op}(x) : \text{real}^m$ (intended to implement differentiable functions like linear algebra operations such as addition and products, and sigmoid functions) through sequencing.

Observe that we can straightforwardly implement both forward mode $\mathcal{D}$ and reverse mode AD $\mathcal{D}$ on this language as source-code translations to the larger language of a simply typed $\lambda$-calculus over the ground types $\text{real}^n$ that includes at least the same operations. We translate a type $\tau$ to a pair of types $(\mathcal{D}(\tau)_1, \mathcal{D}(\tau)_2)$ – the former for holding function values (also called primals in the
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AD literature), the latter for holding derivative values (also called tangents or adjoints/cotangents in the AD literature, depending on whether one is considering forward or reverse AD):

\[ \overrightarrow{D}(\text{real}^\tau) \overset{\text{def}}{=} \overrightarrow{D}(\text{real}^n) = (\text{real}^n, \text{real}^n). \]

Terms \( x : \tau + t : \sigma \) can then be translated to pairs of terms

\[ x : \overrightarrow{D}(\tau)_1 \vdash \overrightarrow{D}(t)_1 : \overrightarrow{D}(\sigma)_1 \]
\[ x : \overrightarrow{D}(\tau)_1 \vdash \overrightarrow{D}(t)_2 : \overrightarrow{D}(\tau)_2 \rightarrow \overrightarrow{D}(\sigma)_2 \]

respectively, for forward AD and reverse AD. Indeed, we define, by induction on the syntax:

\[ \overleftarrow{D}(x) \overset{\text{def}}{=} \overrightarrow{D}(x) \overset{\text{def}}{=} (x, \lambda y.y) \]
\[ \overleftarrow{D}(\text{op}(t))_1 \overset{\text{def}}{=} \overrightarrow{D}(\text{op}(t))_1 \overset{\text{def}}{=} \text{op}(t) \]
\[ \overleftarrow{D}(\text{op}(t))_2 \overset{\text{def}}{=} \lambda y.(\text{Dop}(t))\overrightarrow{D}(t)_2 y \]

where we assume that we have chosen suitable terms \( x : \text{real}^\tau \vdash (\text{Dop})(x) : \text{real}^\tau \rightarrow \text{real}^n \) and \( x : \text{real}^n \vdash (\text{Dop})^f(x) : \text{real}^m \rightarrow \text{real}^n \) to represent the derivative and transposed derivative, respectively, of the primitive operation \( \text{op} : \text{real}^n \rightarrow \text{real}^m \).

While this technique works well for performing AD on the limited first-order language we described, it is far from being satisfying. Notably, it has the following two shortcomings:

1. it does not tell us how to perform AD on programs that involve tuples or operations of multiple arguments;
2. it does not tell us how to perform AD on higher-order programs, that is, programs involving \( \lambda \)-abstractions and applications.

The key contributions of this paper are its extension of this transformation (see §7) to apply to a full simply typed \( \lambda \)-calculus (of §3), and its proof that this transformation is correct (see §8).

Shortcoming (1) seems easy to address, at first sight. Indeed, as the (co)tangent vectors to a product of spaces are simply tuples of (co)tangent vectors, one would expect to define

\[ \overrightarrow{D}(\tau * \sigma) \overset{\text{def}}{=} (\overrightarrow{D}(\tau)_1 * \overrightarrow{D}(\sigma)_1), (\overrightarrow{D}(\tau)_2 * \overrightarrow{D}(\sigma)_2) \]
\[ \overleftarrow{D}(\tau * \sigma) \overset{\text{def}}{=} (\overleftarrow{D}(\tau)_1 * \overleftarrow{D}(\sigma)_1), (\overleftarrow{D}(\tau)_2 * \overleftarrow{D}(\sigma)_2). \]

Indeed, this technique straightforwardly applies to forward mode AD:

\[ \overrightarrow{D}((t, s)) \overset{\text{def}}{=} ((\overrightarrow{D}(t)_1, \overrightarrow{D}(s)_1), \lambda y.(\overrightarrow{D}(t)_2(y), \overrightarrow{D}(s)_2(y))) \]
\[ \overleftarrow{D}(\text{fst}) \overset{\text{def}}{=} (\text{fst} \overrightarrow{D}(t)_1, \lambda y.\text{fst} \overrightarrow{D}(t)_2(y)) \]
\[ \overleftarrow{D}(\text{snd}) \overset{\text{def}}{=} (\text{snd} \overrightarrow{D}(t)_1, \lambda y.\text{snd} \overrightarrow{D}(t)_2(y)). \]

For reverse mode AD, however, tuples already present challenges. Indeed, we would like to use the definitions below, but they require terms \( + 0 : \tau \) and \( + t + s : \tau \) for any two \( t, s : \tau \) for each type \( \tau \):

\[ \overrightarrow{D}((t, s)) \overset{\text{def}}{=} ((\overrightarrow{D}(t)_1, \overrightarrow{D}(s)_1), \lambda y.\overrightarrow{D}(t)_2(y) + \overrightarrow{D}(s)_2(y)) \]
\[ \overleftarrow{D}(\text{fst}) \overset{\text{def}}{=} (\text{fst} \overrightarrow{D}(t)_1, \lambda y.\text{fst} \overrightarrow{D}(t)_2(y), 0) \]
\[ \overleftarrow{D}(\text{snd}) \overset{\text{def}}{=} (\text{snd} \overrightarrow{D}(t)_1, \lambda y.0, \overrightarrow{D}(t)_2(y))). \]

These formulae capture the well-known issue of fanout translating to addition in reverse-mode AD, caused by the contravariance of reverse AD in its second component (Pearlmutter and Siskind 2008). Such \( 0 \) and \(+\) could indeed be defined by induction on the structure of types, using \( 0 \) and \(+\) at \( \text{real}^n \). However, more problematically, \( (-, -) \), \( \text{fst} - \) and \( \text{snd} - \) represent explicit uses of structural rules of contraction and weakening at types \( \tau \), which, in a \( \lambda \)-calculus, can also be used implicitly in the typing context \( \Gamma \). Thus, we should also make these implicit uses explicit to account for their presence in the code. Then, we can appropriately translate them into their "mirror image": we map the contraction-weakening comonoids to the monoid structures \((+, 0)\). Here, we see insight (1):
In define-then-run reverse AD, we need to make use of explicit structural rules and "mirror them", which we can do by translating our language into combinators.

Put differently: we define AD on the syntactic category Syn which has types τ as objects and programs (a)βη-equivalence classes of programs x : τ → t : σ as morphisms τ → σ.

Yet the question remains: why should this translation for tuples be correct? What is even less clear is how to address shortcoming (2). What should the space s of tangents D(τ → σ) look like? This is not something we are taught in Calculus 1.01. Instead, we again employ category theory, which leads us to insight (2):

Follow where the categorical structure of the syntax leads you, as doing so produces principled definitions that are easy to prove correct.

With the aim of categorical compositionality in mind, we can not e that our translations compose in the sense that

Both have identities id_A : A → A, id_B : B → B defined by

By the following trick, these equations are functoriality laws. Given a Cartesian closed category (C, ⊗, 1, −×−), define categories E[C] and F[C] as having objects pairs (A_1, A_2) of objects A_1, A_2 of C and morphisms

Both have identities id_{A_1, A_2} ≡ (id_{A_1}, id_{A_2}), where we write Λ for categorical currying and π_2 for the second projection. Composition (A_1, A_2) → (B_1, B_2) → (C_1, C_2) is given by

where we work in the internal language of C. Then, we can see that we have defined two functors:

where we write Syn for the syntactic category of our restrictive first-order language, and we write Syn for that of the full λ-calculus. We would like to extend these to functors

Linear types can help. By using a more fine-grained type system, we can capture the linearity of the derivative. As a result, we can phrase AD on our full language simply as the unique structure-preserving functor that extends the uncontroversial definitions given so far.
To implement this insight, we extend our \( \lambda \)-calculus to a language \( \text{LSyn} \) with limited linear types (in §4): linear function types \( \to \) and a kind of multiplicative conjunction \( !(\_ \otimes \_ \_ ) \), in the sense of the enriched effect calculus (Egger et al. 2009). The algebraic effect giving rise to these linear types, in this instance, is that of the theory of commutative monoids. As we have seen, such monoids are intimately related to reverse AD. Consequently, we demand that every \( f \) with a linear function type \( \tau \to \sigma \) is indeed linear, in the sense that \( f 0 = 0 \) and \( f (t + s) = (f t) + (f s) \). For the categorically inclined reader: that is, we enrich \( \text{LSyn} \) over the category of commutative monoids.

Now, we can give more precise types to our derivatives, as we know they are linear functions: for \( x : \tau \to t \), we have \( x : \vec{D}(\tau)_1 \otimes \vec{D}(\tau)_2 : \vec{D}(\tau) \to \vec{D}(\sigma)_2 \) and \( x : \vec{D}(\tau)_1 + \vec{D}(\tau)_2 : \vec{D}(\sigma)_2 \to \vec{D}(\tau)_2 \). Therefore, given any model \( \vec{C} \) of our linear type theory, we generalise our previous construction of the categories \( \vec{C}[\text{C}] \) and \( \vec{C}[\text{C}] \), but now we work with linear functions in the second component. Unlike before, both \( \vec{C}[\text{C}] \) and \( \vec{C}[\text{C}] \) are now Cartesian closed (by §6)!

Thus, we find the following corollary, by the universal property of \( \text{Syn} \). This property states that any well-typed choice of interpretations \( F(\text{op}) \) of the primitive operations in a Cartesian closed category \( \text{C} \) extends to a unique Cartesian closed functor \( F : \text{Syn} \to \text{C} \). It gives a principled definition of AD and explains in what sense reverse AD is the “mirror image” of forward AD.

**Corollary (Definition of AD, §7).** Once we fix the interpretation of the primitives operations \( \text{op} \) to their respective derivatives and transpose derivatives, we obtain unique structure-preserving forward and reverse AD functors \( \vec{D} : \text{Syn} \to \vec{C}[\text{LSyn}] \) and \( \vec{D} : \text{Syn} \to \vec{C}[\text{LSyn}] \).

In particular, the following definitions are forced on us by the theory, producing key insight (4):

For reverse AD, an adjoint at function type \( \tau \to \sigma \), needs to keep track of the incoming adjoints \( v \) of type \( \vec{D}(\sigma)_2 \) for each a primal \( x \) of type \( \vec{D}(\tau)_1 \), on which we call the function. We store these pairs \((x, v)\) in the type \( !\vec{D}(\tau)_1 \otimes \vec{D}(\sigma)_2 \) (which we will see is essentially a quotient of a list of pairs of type \( \vec{D}(\tau)_1 . \vec{D}(\sigma)_2 \)). Less surprisingly, for forward AD, a tangent at function type \( \tau \to \sigma \) consists of a function sending each argument primal of type \( \vec{D}(\tau)_1 \) to the outgoing tangent of type \( \vec{D}(\sigma)_2 \).

\[
\vec{D}(\tau \to \sigma) \overset{\text{def}}{=} (\vec{D}(\tau)_1 \to (\vec{D}(\sigma)_1 = (\vec{D}(\tau)_2 \to \vec{D}(\sigma)_2)), !\vec{D}(\tau)_1 \to \vec{D}(\sigma)_2) \\
\vec{D}(\tau \to \sigma) \overset{\text{def}}{=} (\vec{D}(\tau)_1 \to (\vec{D}(\sigma)_1 \otimes \vec{D}(\tau)_2 \to \vec{D}(\sigma)_2)), !\vec{D}(\tau)_1 \otimes \vec{D}(\sigma)_2)
\]

With these definitions in place, we turn to the correctness of the source-code transformations. To phrase correctness, we first need to construct a suitable denotational semantics with an uncontroversial notion of semantic differentiation. A technical challenge arises, as the usual calculus setting of Euclidean spaces (or manifolds) and smooth functions cannot interpret higher-order functions. To solve this problem, we work with a conservative extension of this standard calculus setting (see §5): the category \( \text{Diff} \) of diffeological spaces. We model our types as diffeological spaces, and programs as smooth functions. By keeping track of a commutative monoid structure on these spaces, we are also able to interpret the required linear types. We write \( \text{Diff}_{\text{CM}} \) for this “linear” category of commutative diffeological monoids and smooth monoid homomorphisms.

By the universal properties of the syntax, we obtain canonical, structure-preserving functors \([\_ ] : \text{LSyn} \to \text{Diff}_{\text{CM}} \) and \([\_ ] : \text{Syn} \to \text{Diff} \) once we fix interpretations \( \mathbb{R}^n \) of \( \text{real}^n \) and well-typed interpretations \( \text{op} \) for each operation \( \text{op} \). These functors define a semantics for our language.

Having constructed the semantics, we can turn to the correctness proof (of §8). The proof consists of a logical relations argument over the semantics, which we phrase categorically, key insight (5):
To show correctness of forward AD, we construct a category 

\[
\text{Diff} \times \mathbb{R}[\text{Diff}_\mathbb{R}]
\]

\[
\overline{\text{Scone}} \rightarrow \text{Diff} \times \mathbb{R}[\text{Diff}_\mathbb{R}]
\]

Once we show that the derivatives of primitive operations \( op \) are correctly implemented, correctness of derivatives of other programs follows from a standard logical relations construction over the semantics that relates a curve to its (co)tangent curve.

To show correctness of forward AD, we construct a category \( \overline{\text{Scone}} \) whose objects are triples \((X, (Y_1, Y_2), P)\) of an object \( X \) of \( \text{Diff} \), an object \((Y_1, Y_2)\) of \( \mathbb{R}[\text{Diff}_\mathbb{R}] \) and a predicate \( P \) on \( \text{Diff}(\mathbb{R}, X) \times \mathbb{R}[\text{Diff}_\mathbb{R}]((\mathbb{R}, \mathbb{R}), (Y_1, Y_2)) \). It has morphisms \( ((X, (Y_1, Y_2)), P) \xrightarrow{(f, (g, h))} ((X', (Y_1', Y_2'), P') \), which are a pair of morphisms \( X \xrightarrow{f} X' \) and \( (Y_1, Y_2) \xrightarrow{(g, h)} (Y_1', Y_2') \) such that for any \((y, (\delta_1, \delta_2)) \in P \), we have that \((y; f, (\delta_1, \delta_2); (g, h)) \in P' \). \( \overline{\text{Scone}} \) is a standard category of logical relations (or subscone), and it is widely known to inherit the Cartesian closure of \( \text{Diff} \times \mathbb{R}[\text{Diff}_\mathbb{R}] \). It also comes equipped with a Cartesian closed functor \( \overline{\text{Scone}} \rightarrow \text{Diff} \times \mathbb{R}[\text{Diff}_\mathbb{R}] \). Therefore, once we fix predicates \( P^f_{\text{real}} \) on \(([[\cdot]], \mathbb{R}[[[\cdot]]])(\text{real}^n) \) and show that all operations \( op \) respect these predicates, it follows that our denotational semantics lifts to a unique structure-preserving functor \( \text{Syn} \xrightarrow{\llbracket \cdot \rrbracket} \overline{\text{Scone}} \), such that the left diagram below commutes (by the universal property of \( \text{Syn} \)).

As a consequence, we can work with \( P^f_{\text{real}} \) \( \overset{\text{def}}{=} \{(f, (g, h)) \mid g = f \text{ and } h = Df \} \), where we write \( Df(x)(v) \) for the usual multivariate calculus derivative of \( f \) at a point \( x \) evaluated at a tangent vector \( v \). By an application of the chain rule for multivariate differentiation, we see that every \( op \) respects this predicate, as long as \([Dop] = D[op] \). The commuting of our diagram then virtually establishes the correctness of forward AD. The only remaining step in the argument is to note that any tangent vector at \([\tau] \equiv \mathbb{R}^N \), for first-order \( \tau \), can be represented by a curve \( \mathbb{R} \rightarrow [\tau] \). For reverse AD, the same construction works, if \([Dop^t] = D[op]^t \), by replacing \( \mathbb{R}[[\cdot]] \) with \( \mathbb{R}[[\cdot]] \) and \( B \) with \( \overline{B} \). We can then choose \( P^r_{\text{real}} \) \( \overset{\text{def}}{=} \{(f, (g, h)) \mid g = f \text{ and } h = x \mapsto (Df(x))^t \} \), as the predicates for constructing \( (\text{real}^n)^t \), where we write \( A^t \) for the matrix transpose of \( A \). We now obtain our main theorem. Crucially, note that this theorem holds even for \( t \) that involve higher-order subprograms.

**THEOREM (CORRECTNESS OF AD, THM. 8.1).** For any typed term \( x : \tau \vdash t : \sigma \) in \( \text{Syn} \) between first-order types \( \tau, \sigma \), we have that \([D^t(t)_2(x)] = D[t](x) \) and \([D^t(t)_2](x) = D[t](x)^t \).

Next, we address the practicality of our method (in §9). The code transformations we employ are not too daunting to implement. We can mechanically translate \( \lambda \)-calculus and functional languages into a (categorical) combinatory form (Curien 1986). However, the implementation of the required linear types presents a challenge. Indeed, types like \(! (\sim) \otimes (\sim) \) and \((\sim) \rightarrow (\sim) \) are absent from functional languages such as Haskell and O’Caml. Luckily, in this instance, we can implement them using abstract data types by making use of a (basic) module system, key insight (6):

Under the hood, \( ! \tau \otimes \sigma \) can consist of a list of values of type \( \tau \star \sigma \). Its API ensures that the list order and the difference between \( xs \equiv [(t, s), (t, s')] \equiv ys \) and \( xs \equiv [(t, s + s') \equiv y s \) cannot be observed: as such, it is a quotient type. Meanwhile, \( \tau \rightarrow \sigma \) can be implemented as a standard function type \( \tau \rightarrow \sigma \) with a limited API that enforces that we can only ever construct linear functions: as such, it is a subtype.
We next phrase the correctness proof of the AD transformations in elementary terms, such that it holds in the applied setting where we use abstract types to implement linear types. Then, we show that our correctness results are meaningful, as they make use of a denotational semantics that is adequate with respect to the standard operational semantics. Finally, to stress the applicability of our method, we sketch its extension to higher-order (primitive) operations, such as \texttt{map}.

### 3 \textsc{\lambda-calculus As a Source Language for Automatic Differentiation}

As a source language for our AD translations, we can begin with a standard, simply typed \textsc{\lambda}-calculus which has ground types \texttt{real^n} of statically sized arrays of \( n \) real numbers, for all \( n \in \mathbb{N} \), and sets \( \text{Op}^n_{n_1, \ldots, n_k} \) of primitive operations \( op \) for all \( k, m, n_1, \ldots, n_k \in \mathbb{N} \). These operations will be interpreted as smooth functions \( (\mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_k}) \rightarrow \mathbb{R}^m \). Examples to keep in mind for \( op \) include:

- constants \( c \in \text{Op}^n \) for each \( c \in \mathbb{R}^n \), for which we slightly abuse notation and write \( c(\langle \rangle) \) as \( c \);
- elementwise addition and product \((+), (*) \in \text{Op}^n_{n, n}\) and matrix-vector product \((* ) \in \text{Op}^n_{n\times m, m} \);
- operations for summing all the elements in an array: \( \text{sum} \in \text{Op}^1 \);
- some non-linear functions like the sigmoid function \( \varsigma \in \text{Op}^1 \).

We intentionally present operations in a schematic way, as primitive operations tend to form a collection that is added to in a by-need fashion, as an AD library develops. The precise operations needed will depend on the applications, but, in statistics and machine learning applications, \( Op \) tends to include a mix of multi-dimensional linear algebra operations and mostly one-dimensional non-linear functions. A typical library for use in machine learning would work with multi-dimensional arrays (sometimes called "tensors"). We focus here on one-dimensional arrays as the issues of how precisely to represent the arrays are orthogonal to the concerns of our development.

The types \( \tau, \sigma, \rho \) and terms \( t, s, r \) of our AD source language are as follows:

\[
\begin{align*}
\tau, \sigma, \rho & ::= \quad \text{types} \\
| \quad \text{real}^n & \quad \text{real arrays} \\
| \quad 1 & \quad \text{nullary product} \\
\mid t, s, r & ::= \quad \text{terms} \\
| \quad x & \quad \text{variable} \\
| \quad \text{fst} t & \quad \text{product projections} \\
| \quad \text{snd} t & \quad \text{product projections} \\
| \quad \langle \rangle & \quad \text{product tuples} \\
| \quad \lambda x. t & \quad \text{function abstraction} \\
| \quad t s & \quad \text{function application} \\
| \quad \text{op}(t) & \quad \text{operations/constants} \\
| \quad \text{def} & \quad \text{operation/constant} \\
\end{align*}
\]

The typing rules are in Fig. 1, where we write \( \text{Dom}(op) \overset{\text{def}}{=} \text{real}^{n_1} \ast \ldots \ast \text{real}^{n_k} \), for an operation \( op \in \text{Op}^m_{n_1, \ldots, n_k} \). We will employ the usual syntactic sugar \( \text{let} x = t \text{ in } s \overset{\text{def}}{=} (\lambda x.s)t \). As Fig. 2 displays, we consider the terms of our language up to the standard \( \beta\eta \)-theory. We could consider further equations for our operations, but we do not as we will not need them.

\[
\begin{align*}
\Gamma \vdash x : \tau \quad & \implies \quad \Gamma \vdash t : \text{Dom}(op) \quad \text{and} \quad \text{op} \in \text{Op}^m_{n_1, \ldots, n_k} \\
\Gamma \vdash \langle \rangle : 1 \\
\Gamma \vdash (t_1, s_1) : \tau \ast \sigma \\
\Gamma \vdash \text{fst} t : \tau \\
\Gamma \vdash \text{snd} t : \sigma \\
\Gamma \vdash \lambda x. t : \tau \rightarrow \sigma \\
\Gamma \vdash t : \sigma \rightarrow \tau \\
\Gamma \vdash t : \tau \\
\end{align*}
\]

Fig. 1. Typing rules for the simple language.
We can easily see that 1
As a target language for our AD source code transformations, we consider a language that extends (categorical) combinators. Indeed, there are well-studied mechanical translations from the \(\lambda\)-calculus to the free Cartesian closed category (and back) (Curien 1985; Lambek and Scott 1988). The translation from \(\text{Syn}\) to \(\lambda\)-calculus is self-evident, while the translation in the opposite direction is straightforward after we first convert our \(\lambda\)-terms to de Bruijn indexed form. Concretely,

- **Syn** has types \(\tau, \sigma, \rho\) objects;
- **Syn** has morphisms \(t \in \text{Syn}(\tau, \sigma)\) which are in 1-1 correspondence with terms \(x : \tau \vdash t : \sigma\) up to \(\beta\eta\)-equivalence (which includes \(\alpha\)-equivalence); explicitly, they can be represented by
  - identities: \(\text{id}_\tau \in \text{Syn}(\tau, \tau)\) (corresponding to variables up to \(\alpha\)-equivalence);
  - composition: \(t; s \in \text{Syn}(\tau, \rho)\) for any \(t \in \text{Syn}(\tau, \sigma)\) and \(s \in \text{Syn}(\sigma, \rho)\) (corresponding to the capture avoiding substitution \([t^y\,_g]\) if we represent \(x : \tau \vdash t : \sigma\) and \(y : \sigma \vdash s : \rho\);
  - terminal morphisms: \(\langle \rangle_t \in \text{Syn}(\tau, 1)\);
  - product pairing: \(\langle t, s \rangle \in \text{Syn}(\tau \sigma \rho)\) for any \(t \in \text{Syn}(\tau, \sigma)\) and \(s \in \text{Syn}(\tau, \rho)\);
  - product projections: \(\text{fst}_\tau \sigma \rho \in \text{Syn}(\tau \sigma \rho, \tau)\) and \(\text{snd}_\tau \sigma \rho \in \text{Syn}(\tau \sigma \rho, \sigma)\);
  - function evaluation: \(\text{ev}_{\tau, \sigma, \rho} \in \text{Syn}((\tau \rightarrow \sigma) \sigma \rho, \sigma)\);
  - currying: \(\Lambda_{\tau, \sigma, \rho} (t) \in \text{Syn}(\tau, \sigma \rightarrow \rho)\) for any \(t \in \text{Syn}(\tau \sigma \rho)\);
  - constants and operations: \(\text{op} \in \text{Syn}(\text{real}^m, \ldots, \text{real}^m)\) for any \(\text{op} \in \text{Op}_{n_1, \ldots, n_k}\).
- all subject to the usual equations of a Cartesian closed category (Lambek and Scott 1988).

We can easily see that 1 and \(\bullet\) give finite products in \(\text{Syn}\), while \(\rightarrow\) gives categorical exponentials. Syn has the following universal property: for any Cartesian closed category \(C\), \(1, \times, \Rightarrow\), we obtain a unique Cartesian closed functor \(F : \text{Syn} \rightarrow C\), once we choose objects \(F\text{real}^n\) of \(C\) as well as make well-typed choices of \(C\)-morphisms, for each \(\text{op} \in \text{Op}_{n_1, \ldots, n_k}\):

\[
Fop : (\text{Freal}^{n_1} \times \ldots \times \text{Freal}^{n_k}) \rightarrow \text{Freal}^m.
\]

### 4 A \(\lambda\)-Calculus with Linear Types as an Idealised AD Target Language

As a target language for our AD source code transformations, we consider a language that extends the language of §3 with limited linear types. We could opt to work with a full linear logic as in (Benton 1994) or (Barber and Plotkin 1996). Instead, however, we will only include the bare minimum of linear type formers that we actually need to phrase the AD transformations. The resulting language is closely related to, but more minimal than, the Enriched Effect Calculus of (Egger et al. 2009). We limit our language in this way because we want to stress that the resulting code transformations can easily be implemented in existing functional languages such as Haskell or O’Caml. As we discuss in §9, the idea will be to make use of a module system to implement the required linear types as abstract data types.

In our idealised target language, we consider **linear types** (also called computation types) \(\underline{\tau}, \underline{\sigma}, \underline{\rho}\), in addition to the **Cartesian types** (also called value types) \(\tau, \sigma, \rho\) that we have considered so far. We think of Cartesian types as denoting spaces and linear types as denoting spaces equipped with an algebraic structure. As we are interested in studying differentiation, the relevant space structure in this instance is a geometric structure that suffices to define differentiability. Meanwhile, the

\[
t = \langle \rangle \quad \text{fst} (\langle t, s \rangle) = t \quad \text{snd} (\langle t, s \rangle) = s \quad t = (\text{fst} t, \text{snd} t) \quad (\lambda x.t) s = t[x/s] \quad t \equiv \lambda x.t x
\]

Fig. 2. Standard \(\beta\eta\)-laws for products and functions. We write \(\equiv_{x_1, \ldots, x_n}\) to indicate that the variables \(x_1, \ldots, x_n\) need to be fresh in the left hand side. Equations hold on pairs of terms of the same type. As usual, we only distinguish terms up to \(\alpha\)-renaming of bound variables.
relevant algebraic structure on linear types turns out to be that of a commutative monoid, as this algebraic structure is needed to phrase Automatic Differentiation algorithms. Indeed, we will use the linear types to denote spaces of (co)tangent vectors to the spaces of primal denoted by Cartesian types. These spaces of (co)tangents form a commutative monoid under addition.

Concretely, we extend the types and terms of our language as follows:

\[
\begin{align*}
\tau, \sigma, \rho \colon & \quad \text{linear types} \quad | \quad \tau \ast \sigma \quad \text{binary product} \\
& \quad | \quad \mathbb{R}^n \quad \text{real array} \quad | \quad \tau \rightarrow \sigma \quad \text{function} \\
& \quad | \quad 1 \quad \text{unit type} \quad | \quad !\tau \otimes \sigma \quad \text{tensor product} \\
\end{align*}
\]

\[
\begin{align*}
\tau, \sigma, \rho \colon & \quad \text{Cartesian types} \quad | \quad \tau \otimes \sigma \quad \text{linear function} \\
& \quad | \quad \ldots \quad \text{as in §3} \\
t, s, r \colon & \quad \text{terms} \quad | \quad !t \otimes s \quad \text{tensor product} \\
& \quad | \quad \ldots \quad \text{as in §3} \quad | \quad \lambda x.t \mid t\{s\} \quad \text{linear fun. abstraction/application} \\
& \quad | \quad \text{lop}(t; s) \quad \text{linear operation} \quad | \quad 0 \mid t + s \quad \text{monoid structure.}
\end{align*}
\]

We work with linear operations \( \text{lop} \in \text{LOp}_{m_1, \ldots, n_k; n'_1, \ldots, n'_l} \), which are intended to represent functions which are linear (in the sense of respecting 0 and +) in the last \( l \) arguments but not in the first \( k \). We write \( \text{Dom}(\text{lop}) \overset{\text{def}}{=} \mathbb{R}^{n_1} \ast \ldots \ast \mathbb{R}^{n_k} \) and \( \text{LDom}(\text{lop}) \overset{\text{def}}{=} \mathbb{R}^{n'_1} \ast \ldots \ast \mathbb{R}^{n'_l} \) for \( \text{lop} \in \text{LOp}_{m_1, \ldots, n_k; n'_1, \ldots, n'_l} \). These operations can include e.g. dense and sparse matrix-vector multiplications. Their purpose is to serve as primitives that we can use to implement derivatives \( \text{Dop}(x; y) \) and \( \text{(Dop)}^f(x; y) \) of the operations \( \text{lop} \) from the source language as terms that are linear in \( y \).

In addition to the judgement \( \Gamma \vdash t : \tau \), which we encountered in §3, we now consider an additional judgement \( \Gamma; x : \tau \vdash t : \sigma \). While we think of the former as denoting a (structure-preserving) function between spaces, we think of the latter as a (structure-preserving) function from the space which \( \Gamma \) denotes to the space of (structure-preserving) monoid homomorphisms from the denotation of \( \tau \) to that of \( \sigma \). In this instance, “structure-preserving” will mean differentiable.

Fig. 3 displays the typing rules of our language. We consider the terms of this language up to the \( \beta\eta+ \)-equational theory of Fig. 4. It includes \( \beta\eta \)-rules as well as monoid and homomorphism laws.

## 5 DE NOTATIONAL SEMANTICS OF THE SOURCE AND TARGET LANG UAGES

### 5.1 Preliminaries

**Category theory.** We assume familiarity with categories \( C, \mathcal{D} \), functors \( F, G : C \rightarrow \mathcal{D} \), natural transformations \( \alpha, \beta : F \rightarrow G \), and their theory of (co)limits and adjunctions. We write:

- unary, binary, and \( l \)-ary products as \( \times, X_1 \times X_2, \) and \( \prod_{i \in I} X_i \), writing \( \pi_i \) for the projections and \( ()_i, (x_1, x_2), \) and \( (x_i)_{i \in I} \) for the tupling maps;
- unary, binary, and \( l \)-ary coproducts as \( 0, X_1 + X_2, \) and \( \sum_{i \in I} X_i \), writing \( t_i \) for the injections and \( []_i, [x_1, x_2], \) and \( [x_i]_{i \in I} \) for the cotupling maps;
- exponentials as \( Y \Rightarrow X \), writing \( \Lambda \) and ev for the currying and evaluation maps.

**Monoids.** A monoid \( (|X|, 0_X, +_X) \) consists of a set \( |X| \) with an element \( 0_X \in |X| \) and a function \( (+_X) : |X| \times |X| \rightarrow |X| \) such that \( 0_X +_X x = x = x +_X 0_X \) for any \( x \in |X| \) and \( x +_X (x' +_X x'') = (x +_X x') +_X x'' \) for any \( x, x', x'' \in |X| \). A monoid \( (|X|, 0_X, +_X) \) is called commutative if \( x +_X x' = x' +_X x \) for all \( x, x' \in |X| \). Given monoids \( X \) and \( Y \), a function \( f : |X| \rightarrow |Y| \) is called a homomorphism of monoids if \( f(0_X) = 0_Y \) and \( f(x +_X x') = f(x) +_Y f(x') \). We write \( \text{CMon} \) for the
Fig. 3. Typing rules for the idealised AD target language with linear types.

| Case | Typing rule                                                                 |
|------|-----------------------------------------------------------------------------|
| 1    | $\Gamma \vdash t : \text{Dom(lo)} \quad \Gamma ; x : \tau \vdash s : \text{LDom(lo)} \quad (\text{lo} \in \text{LOp}^{\text{lin}}_{n_1, \ldots, n_k, m'_1, \ldots, m'_l})$ |
| 2    | $\Gamma ; x : \tau \vdash x : \tau$                                       |
| 3    | $\Gamma ; x : \tau \vdash t : \sigma \quad \Gamma ; x : \tau \vdash s : \rho$ |
| 4    | $\Gamma ; x : \tau \vdash t : \sigma \otimes \rho$                        |
| 5    | $\Gamma ; x : \tau \vdash t : \sigma \text{?} \rho$                       |
| 6    | $\Gamma ; x : \tau \vdash \text{fst} t : \sigma$                         |
| 7    | $\Gamma ; x : \tau \vdash \text{snd} t : \rho$                          |
| 8    | $\Gamma ; y : \sigma ; x : \tau \vdash t : \rho \quad \Gamma ; x : \tau \vdash t : \sigma \rightarrow \rho$ |
| 9    | $\Gamma ; x : \tau \vdash t : \sigma \rightarrow \rho$                   |
| 10   | $\Gamma ; x : \tau \vdash t : \sigma \rightarrow s : \rho$              |
| 11   | $\Gamma ; x : \tau \vdash t : \sigma \rightarrow s : \rho$              |
| 12   | $\Gamma ; x : \tau \vdash t : \sigma \rightarrow !y \otimes z : \rho'$  |
| 13   | $\Gamma ; x : \tau \vdash t : \sigma \rightarrow !y \otimes z : \rho'$  |
| 14   | $\Gamma ; x : \tau \vdash t : \sigma \rightarrow s : \sigma$            |
| 15   | $\Gamma ; x : \tau \vdash t : \sigma \rightarrow s : \sigma$            |

Fig. 4. Equational rules for the idealised, linear AD language, which we use on top of the rules of Fig. 2. In addition to standard \(\beta\eta\)-rules for \(!(-) \otimes (-)\) and \(\rightarrow\)-types, we add rules making \((0, +)\) into a commutative monoid on the terms of each linear type as well as rules which say that terms of linear types are homomorphisms in their linear variable. Equations hold on pairs of terms of the same type.

category of commutative monoids and their homomorphisms. We will sometimes write \(\sum_{i=1}^n x_i\) for \((x_1 + x_2 + \ldots) + x_n\).

Example 5.1. The real numbers \(\mathbb{R}\) form a commutative monoid with 0 and + equal to the number 0 and addition of numbers.

Example 5.2. Given commutative monoids \((X_i)_{i \in I}\), we can form the product monoid \(\prod_{i \in I} X_i\) with underlying set \(\prod_{i \in I} |X_i|, 0 = (0x_i)_{i \in I}\) and \((x_i)_{i \in I} + (y_i)_{i \in I} \text{ def } = (x_i + y_i)_{i \in I}\).

Ex. 5.2 gives the categorical product in \(\text{Cmon}\). We can, for example, construct a commutative monoid structure on any Euclidean space \(\mathbb{R}^k\) by combining the one on \(\mathbb{R}\) with the product monoid structure.

Example 5.3. Given a set \(S\), we can form the free commutative monoid \(!S\) on \(S\). \(|S|\) is defined as the set of functions \(f : S \rightarrow \mathbb{N}\) to the natural numbers \(\mathbb{N}\) that have finite support in the sense that \(f(s) \neq 0\) for only finitely many \(s\). (That is, \(|S|\) is the set of finite multisets of elements of \(S\).) We define \(0_{!S}\) to be the function that is constantly 0 and \((f +_{!S} g)(s) \text{ def } = f(s) + g(s)\). Observe that any element of \(!S\) arises as a finite sum \(\sum_{i=1}^n \delta(s_i)\) for \(s_i \in S\), if we write \(\delta : S \rightarrow \mathbb{Z}|S|\) for the function \(\delta(s)(s) = 1\) and \(\delta(s)(s') = 0\) for \(s \neq s'\).
Example 5.4. Given two monoids \(X\) and \(Y\), we can form their tensor product \(X \otimes Y\). Define \(|X \otimes Y|\) as \(|(X \times Y)|/\sim\) where we identify \(0 \otimes y \sim 0, x \otimes 0 \sim 0, x \otimes y + x' \otimes y \sim (x + x') \otimes y\) and \(x \otimes y + x \otimes y' \sim x \otimes (y + y')\). Here, we write \(\otimes\) for the function \(|X| \times |Y| \to |X \otimes Y|\) defined by \(x \otimes y \def \delta(x,y)\). \(X \otimes Y\) is a commutative monoid by the monoid operations that are induced from \(|X \times Y|\).

Commutative monoid homomorphisms \(X \otimes Y \to Z\) are in 1-1-correspondence with bilinear functions \(f : |X| \times |Y| \to |Z|\) (i.e. \(f(0,y) = 0, f(x,0) = 0, f(x + x', y + y') = f(x, y) + f(x', y) + f(x, y') + f(x', y')). This follows as we can uniquely extend such an \(f\) bilinearly to a map \(X \otimes Y \to Z\).

Finally, a category \(C\) is called \(\text{CMon}\)-enriched if we have a commutative monoid structure on each homset \(C(C', C'') \to C(C, C'')\). Finite products in a category \(C\) are well-known to be biproducts (i.e. simultaneously products and coproducts) if and only if \(C\) is \(\text{CMon}\)-enriched (see e.g. (Fiore 2007)): define \([[]] = 0\) and \([f, g] = [\pi_1; f + \pi_2; g]\) and, conversely, \(0 = [[]]\) and \([f + g] = (\text{id}, \text{id}; [f, g])\).

5.2 Abstract Semantics

The language of §3 has a canonical interpretation in any Cartesian closed category \((C, \times, \Rightarrow, \bot)\), once we fix \(C\)-objects \([\text{real}^n]\) to interpret \(\text{real}^n\) and \(C\)-morphisms \([\text{op}] \in C(\lbrack\text{Dom}(\text{op})\rbrack, [\text{real}^m])\) to interpret \(\text{op} \in \text{Op}^m_{n_1, \ldots, n_k}\). We interpret (Cartesian) types \(\tau\) and contexts \(\Gamma\) as \(C\)-objects \([\tau]\) and \([\Gamma]\):

\[
[1] \def 1 \quad [\tau \times \sigma] \def [\tau] \times [\sigma] \quad [\tau \to \sigma] \def [\tau] \Rightarrow [\sigma] \quad [x_1 : \tau_1, \ldots, x_n : \tau_n] \def [\tau_1] \times \ldots \times [\tau_n].
\]

We interpret terms \(\Gamma \vdash t : \tau\) as morphisms \([t] \in C(\lbrack\Gamma\rbrack, [\tau]\rbrack)\): \([x_1 : \tau_1, \ldots, x_n : \tau_n \vdash k : \tau_k] \def [\pi_k(t)] \quad ([t,s]) \def ([t], [s]) \quad [\text{fst}] \def [\pi_1] \quad [\text{snd}] \def [\pi_2] \quad [\lambda x.t] \def \Lambda([t]) \quad [t,s] \def ([t], [s]);\) ev.

This is an instance of the universal property of \(\text{Syn}\) mentioned in §3.

We discuss how to extend \([-\,]\) to apply to the full target language of §4. Suppose that \(\mathcal{D} : C^{op} \to \text{Cat}\) is a locally indexed category, i.e. a (strict) contravariant functor from \(C\) to the category \(\text{Cat}\) of categories, such that \(\text{ob} \mathcal{D}(C) = \text{ob} \mathcal{D}(C')\) and \(\mathcal{D}(f)(D) = D\) for any object \(D\) of \(\text{ob} \mathcal{D}(C)\) and any \(f : C' \to C\) in \(C\). We say that \(\mathcal{D}\) is \(\text{biadditive}\) if each category \(\mathcal{D}(C)\) has (chosen) finite biproducts \((1, x)\) and \(\mathcal{D}(f)\) preserves them, for any \(f : C' \to C\) in \(C\), in the sense that \(\mathcal{D}(f)(1) = 1\) and \(\mathcal{D}(f)(D \times D') = \mathcal{D}(f)(D) \times \mathcal{D}(f)(D')\). We say that it supports \(-\otimes(\text{\&})\)-types and \(\Rightarrow\)-types, if \(\mathcal{D}(\pi_1)\) has a left adjoint \(!C' \otimes_C -\) and a right adjoint functor \(C' \Rightarrow C\Rightarrow -\), for each product projection \(\pi_1 : C \times C' \to C\) in \(C\), satisfying a Beck-Chevalley condition: \(!C' \otimes_C D = !C' \otimes_C D\) and \(C' \Rightarrow D = C' \Rightarrow D\) for any \(C, C''\) in \(C\). We simply write \(!C'\otimes D\) and \(C' \Rightarrow D\).

Let us write \(\Phi\) and \(\Psi\) for the natural isomorphisms \(\mathcal{D}(C)(C' \otimes D, D') \cong \mathcal{D}(C \times C')(D, D')\) and \(\mathcal{D}(C \times C')(D, D') \cong \mathcal{D}(C)(D', C\Rightarrow D')\). We say that \(\mathcal{D}\) supports Cartesian \(\Rightarrow\)-types if the functor \(C^{op} \to \text{Set}\); \(C \vdash \mathcal{D}(C)(D, D')\) is representable for any objects \(D, D'\) of \(\mathcal{D}\). That is, we have objects \(D \Rightarrow D'\) of \(\mathcal{C}\) with isomorphisms \(\Lambda : \mathcal{D}(C)(D', D') \cong \mathcal{D}(C, D \Rightarrow D')\), which are natural in \(C\).

We call a \(\mathcal{D}\) satisfying all these conditions a \(\text{categorical model}\) of the language of §4. If we choose \(\mathcal{D}\)-objects \([\text{real}^n]\) to interpret \(\text{real}^n\) and compatible \(\mathcal{D}\)-morphisms \([\text{op}]\) in \(\mathcal{D}(\lbrack\text{Dom}(\text{op})\rbrack)(\lbrack\lbrack\text{Dom}(\text{op})\rbrack\rbrack, [\text{real}^k])\) for each \(\text{Lop}^m_{n_1, \ldots, n_k, n'_1, \ldots, n'_l}\), then we can interpret linear types \(\tau\) as objects \([\tau]\) of \(\mathcal{D}\):

\[
[1] \def 1 \quad [\tau \times \sigma] \def [\tau] \times [\sigma] \quad [\tau \to \sigma] \def [\tau] \Rightarrow [\sigma] \quad [\tau \otimes \sigma] \def [\tau] \otimes [\sigma].
\]
We can interpret \( \tau \to \sigma \) as the \( C \)-object \( \llbracket \tau \to \sigma \rrbracket \equiv \llbracket \tau \rrbracket \to \llbracket \sigma \rrbracket \). Finally, we can interpret terms \( \Gamma \vdash t : \tau \) as morphisms \( \llbracket t \rrbracket \) in \( C(\llbracket \Gamma \rrbracket, \llbracket \tau \rrbracket) \) and terms \( \Gamma; x : \tau \vdash t : \sigma \) as \( \llbracket t \rrbracket \) in \( D(\llbracket \Gamma \rrbracket)(\llbracket \tau \rrbracket, \llbracket \sigma \rrbracket) \):

\[
\llbracket \Gamma; x : \tau \vdash x : \tau \rrbracket \equiv \text{id}_{\llbracket \tau \rrbracket}, \quad \llbracket \langle \rangle \rrbracket \equiv () \quad \llbracket \langle t, s \rangle \rrbracket \equiv ([t], [s]), \quad \llbracket \text{fst} \rrbracket \equiv \pi_1, \quad \llbracket \text{snd} \rrbracket \equiv \pi_2.
\]

\[
\llbracket \lambda x.t \rrbracket \equiv \Psi([t]), \quad \llbracket [t] s \rrbracket \equiv D((\llbracket \text{id}, [t] \rrbracket))(\Psi^{-1}([t])) \quad \llbracket t \otimes s \rrbracket \equiv D((\llbracket \text{id}, [t] \rrbracket))(\Phi(\text{id})); ([\llbracket \sigma \rrbracket] \otimes [s])
\]

\[
\llbracket \text{case } t \text{ of } !y \otimes x \to s \rrbracket \equiv \llbracket t \rrbracket; \Phi^{-1}([s]) \quad \llbracket \Delta x.t \rrbracket \equiv \Delta([t]) \quad \llbracket [t] s \rrbracket \equiv \Delta^{-1}([t]); [s]
\]

\[
\llbracket \emptyset \rrbracket \equiv [] \quad \llbracket t + s \rrbracket \equiv (\text{id}, \text{id}); ([t], [s]).
\]

Observe that we interpret \( \& \) and \( + \) using the biproduct structure of \( D \).

**Proposition 5.5.** The interpretation \([\cdot]\) of the language of §4 in categorical models is both sound and complete with respect to the \( \beta\eta^+ \)-equational theory: \( t \equiv^+ s \) iff \( \llbracket t \rrbracket = [s] \) in each such model.

Soundness follows by case analysis on the \( \beta\eta^+ \)-rules. Completeness follows by the construction of the syntactic model \( \text{LSyn} : \text{Syn}^{pp} \to \text{Cat} \) which we describe next.

- **Objects of \( \text{LSyn}(\tau) \)** are linear types \( \sigma \) of our target language.
- **Morphisms in \( \text{LSyn}(\tau')(\sigma, \rho) \)** are terms \( x : \tau; y : \sigma \vdash t : \rho \) modulo (\( \alpha \)\( \beta\eta^+ \))-equivalence.
- **Identities in \( \text{LSyn}(\tau) \)** are represented by the terms \( x : \tau; y : \sigma \vdash t : \rho \).
- **Composition of \( x : \tau; y_1 : \sigma_1 \vdash t : \sigma_2 \)** and \( x : \tau; y_2 : \sigma_2 \vdash t : \sigma_3 \) in \( \text{LSyn}(\tau) \) is defined by the capture avoiding substitution \( x : \tau; y_1 : \sigma_1 \vdash s[\llbracket t \rrbracket] : \sigma_3 \).
- **Change of base \( \text{LSyn}(t) : \text{LSyn}(\tau) \to \text{LSyn}(\tau') \)** along \( (x' : \tau') \vdash t : \tau \in \text{Syn}(\tau', \tau) \) is defined by \( \text{LSyn}(t)(x : \tau; y : \sigma \vdash s : \rho) \equiv x' : \tau'; y : \sigma \vdash s[\llbracket t \rrbracket] : \rho \).
- **All type formers are interpreted as would be expected based on their notation, using their introduction and elimination rules for the required structural isomorphisms.**

### 5.3 Diffeological Spaces

Diffeological Spaces. Throughout this paper, we will have an instance of the abstract semantics of our languages in mind, as we intend to interpret \( \text{real}^n \) as the usual Euclidean space \( \mathbb{R}^n \) and to interpret each program \( x_1 : \text{real}^{n_1}, \ldots, x_k : \text{real}^{n_k} \vdash t : \text{real}^m \) as a smooth \((C^\infty-)\) function \( \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_k} \to \mathbb{R}^m \). One challenge is that the usual settings for multivariate calculus and differential geometry do not form Cartesian closed categories, making the interpretation of higher types impossible (see Huot et al. 2020, Appx. A)). One solution, recently employed by (Huot et al. 2020), is to work with **diffeological spaces** (Iglesias-Zemmour 2013; Souriau 1980), which generalise the usual notions of differentiability from Euclidean spaces and smooth manifolds to apply to higher types (as well as a range of other types such a sum and inductive types). We will also follow this route and use such spaces to construct our concrete semantics. Other valid options for a concrete semantics exist: convenient vector spaces (Blute et al. 2012; Frölicher 1988), Frölicher spaces (Frölicher 1982), or synthetic differential geometry (Kock 2006), to name a few. We choose to work with diffeological spaces mostly because they seem to us to provide simplest way to define and analyse the semantics of a rich class of language features.

Diffeological spaces formalise the important intuition that a higher-order function is smooth if it sends smooth functions to smooth functions, meaning that we can never use it to build non-smooth first-order functions. This intuition is reminiscent of a logical relation, and it is realised by **directly axiomatising smooth maps into the space**, rather than treating smoothness as a derived property.
Definition 5.6. A diffeological space \(X = (|X|, \mathcal{P}_X)\) consists of a set \(|X|\) together with, for each \(n \in \mathbb{N}\) and each open subset \(U\) of \(\mathbb{R}^n\), a set \(\mathcal{P}^U_X\) of functions \(U \rightarrow |X|\) called plots, such that

- (constant) all constant functions are plots;
- (rearrangement) if \(f : V \rightarrow U\) is a smooth function and \(p \in \mathcal{P}^U_X\), then \(f; p \in \mathcal{P}^V_X\);
- (gluing) if \( \{ p_i \in \mathcal{P}^U_X \}_{i \in I} \) is a compatible family of plots \( (x \in U_i \cap U_j \Rightarrow p_i(x) = p_j(x)\) and \( (U_i)_{i \in I}\) covers \(U\), then the gluing \( p : U \rightarrow |X| : x \in U_i \mapsto p_i(x)\) is a plot.

We think of plots as the maps that are axiomatically deemed “smooth”. We call a function \(\mathcal{Y}\) between diffeological spaces smooth if, for all plots \(p \in \mathcal{P}^U_X\), we have that \(p \circ f \in \mathcal{P}^V_Y\). We write \(\text{Diff}(X, Y)\) for the set of smooth maps from \(X\) to \(Y\). Smooth functions compose, and so we have a category \(\text{Diff}\) of diffeological spaces and smooth functions. We give some examples of such spaces.

Example 5.7 (Manifold diffeology). Given any open subset \(X\) of a Euclidean space \(\mathbb{R}^n\) (or, more generally, a smooth manifold \(X\)), we can take the set of smooth \((C^\infty)\) functions \(U \rightarrow X\) in the traditional sense as \(\mathcal{P}^U_X\). Given another such space \(X'\), then \(\text{Diff}(X, X')\) coincides precisely with the set of smooth functions \(X \rightarrow X'\) in the traditional sense of calculus and differential geometry.

Put differently, the categories \(\text{CartSp}\) of Euclidean spaces and \(\text{Man}\) of smooth manifolds with smooth functions form full subcategories of \(\text{Diff}\).

Example 5.8 (Product diffeology). Given diffeological spaces \((X_i)_{i \in I}\), we can equip \(\prod_{i \in I} |X_i|\) with the product diffeology: \(\mathcal{P}^U_{\prod_{i \in I} X_i} \overset{\text{def}}{=} \left\{ (\alpha_i)_{i \in I} \mid \alpha_i \in \mathcal{P}^U_{X_i} \right\}\).

Example 5.9 (Functional diffeology). Given diffeological spaces \(X, Y\), we can equip \(\text{Diff}(X, Y)\) with the functional diffeology \(\mathcal{P}^U_{X \times Y} \overset{\text{def}}{=} \{ \Lambda(\alpha) \mid \alpha \in \text{Diff}(U \times X, Y)\}\).

Examples 5.8 and 5.9 give us the categorical product and exponential objects, respectively, in \(\text{Diff}\). The embeddings of \(\text{CartSp}\) and \(\text{Man}\) into \(\text{Diff}\) preserve products (and coproducts).

We work with the concrete semantics, where we fix \(\mathcal{C} = \text{Diff}\) as the target for interpreting Cartesian types and their terms. That is, by choosing the interpretation \([\text{real}^n]\) \(\overset{\text{def}}{=} \mathbb{R}^n\), and by interpreting each \(\text{op} \in \text{Op}^m_{n_1, \ldots, n_k}\) as the smooth function \([\text{op}] : \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_k} \rightarrow \mathbb{R}^m\) that it is intended to represent, we obtain a unique interpretation \([\_] : \text{Syn} \rightarrow \text{Diff}\).

Commutative Diffeological Monoids. To interpret linear types and their terms, we need a semantic setting \(\mathcal{D}\) that is both compatible with \(\text{Diff}\) and enriched over the category of commutative monoids. We choose to work with commutative diffeological monoids. That is, commutative monoids internal to the category \(\text{Diff}\).

Definition 5.10. A diffeological monoid \(X = (|X|, \mathcal{P}_X, 0_X, +_X)\) consists of a diffeological space \((|X|, \mathcal{P}_X)\) with a monoid structure \((0_X \in |X|, (+_X) : |X| \times |X| \rightarrow |X|)\), such that \(+_X\) is smooth. We call a diffeological monoid commutative if the underlying monoid structure on \(|X|\) is commutative.

We write \(\text{Diff}_{\text{CM}}\) for the category whose objects are commutative diffeological monoids and whose morphisms \((|X|, \mathcal{P}_X, 0_X, +_X) \rightarrow (|Y|, \mathcal{P}_Y, 0_Y, +_Y)\) are functions \(f : |X| \rightarrow |Y|\) that are both smooth \((|X|, \mathcal{P}_X) \rightarrow (|Y|, \mathcal{P}_Y)\) and monoid homomorphisms \((|X|, 0_X, +_X) \rightarrow (|Y|, 0_Y, +_Y)\). Given that \(\text{Diff}_{\text{CM}}\) is \(\text{CMon}\)-enriched, finite products are biproducts.

Example 5.11. The real numbers \(\mathbb{R}\) form a commutative diffeological monoid \(\mathbb{R}\) by combining its standard diffeology with its usual commutative monoid structure \((0, +)\). Similarly, \(\mathbb{N} \in \text{Diff}_{\text{CM}}\) by equipping \(\mathbb{N}\) with \((0, +)\) and the discrete diffeology, in which plots are locally constant functions.
Example 5.12. We form the (categorical) product in \( \text{Diff}_{CM} \) of \((X_i)_{i \in I}\) by equipping \( \prod_{i \in I} |X_i| \) with the product diffeology and product monoid structure.

Example 5.13. Given a commutative diffeological monoid \( X \), we can equip the monoid \(!(|X|, 0_X, +_X)\) with the free monoid diffeology: \( \mathcal{P}_X^U \overset{\text{def}}{=} \{ \sum_{i=1}^n \alpha_i \delta \mid n \in \mathbb{N} \text{ and } \alpha_i \in \mathcal{P}_X^U \} \).

Example 5.14. Given commutative diffeological monoids \( X \) and \( Y \), we can equip the tensor product monoid \((|X|, 0_X, +_X) \otimes (|Y|, 0_Y, +_Y)\) with the tensor product diffeology:
\[
\mathcal{P}_X^U \otimes \mathcal{P}_Y^U \overset{\text{def}}{=} \{ \sum_{i=1}^n \alpha_i \otimes \beta_i \mid n \in \mathbb{N} \text{ and } \alpha_i \in \mathcal{P}_X^U, \beta_i \in \mathcal{P}_Y^U \}.
\]

In this paper, we will only make use of the combined operation \( X \otimes Y \) (read: \(!|X| \otimes Y\)).

Example 5.15. Given commutative diffeological monoids \( X \) and \( Y \), we can define a commutative diffeological monoid \( X \rightarrow Y \) with underlying set \( \text{Diff}_{CM}(X, Y), \) \( X \rightarrow Y(x) \overset{\text{def}}{=} 0_Y, \) \( (f +_{X \rightarrow Y} g)(x) \overset{\text{def}}{=} f(x) +_Y g(x) \) and \( \mathcal{P}_X^U \rightarrow Y \overset{\text{def}}{=} \{ \alpha : U \rightarrow |X \rightarrow Y| \mid \alpha \in \mathcal{P}_U (|X|, \mathcal{P}_X) \rightarrow (|Y|, \mathcal{P}_Y) \} \).

In this paper, we will primarily be interested in \( X \rightarrow Y \) as a diffeological space, and we will mostly disregard its monoid structure, until §§9.3.

Example 5.16. Given a diffeological space \( X \) and a commutative diffeological monoid \( Y \), we can define a commutative diffeological monoid structure \( X \Rightarrow Y \) on \( X \Rightarrow (|Y|, \mathcal{P}_Y) \) by using the pointwise monoid structure: \( 0 \Rightarrow Y(x) = 0_Y \) and \( (f +_{X \Rightarrow Y} g)(x) = f(x) +_Y g(x) \).

Given \( f \in \text{Diff}(X, Y) \), we can define \(!f \in \text{Diff}_{CM}(|X|, Y)\) by \(!f(\sum_{i=1}^n x_i) = \sum_{i=1}^n f(x_i)\). ! is a left adjoint to the obvious forgetful functor \( \text{Diff}_{CM} \rightarrow \text{Diff} \), while \( !(X \times Y) \cong !X \otimes !Y \) and \( !1 \cong !\mathbb{N} \).

Seeing that \( (\mathbb{N}, \otimes, \rightarrow) \) defines a symmetric monoidal closed structure on \( \text{Diff}_{CM} \), cognoscenti will recognise that \( (\text{Diff}, 1, \times, \Rightarrow) \cong (\text{Diff}_{CM}, 1, \otimes, \Rightarrow) \) is a model of intuitionistic linear logic (Mellies 2009). In fact, seeing that \( \text{Diff}_{CM} \) is \( \text{CMon} \)-enriched, the model is biadditive (Fiore 2007).

However, we do not need such a rich type system. For us, the following suffices. Define \( \text{Diff}_{CM}(X) \), for \( X \in \text{ob Diff} \), to have the objects of \( \text{Diff}_{CM} \) and homsets \( \text{Diff}_{CM}(X)(Y, Z) \overset{\text{def}}{=} \text{Diff}(X, Y \Rightarrow Z) \).

Identities are defined as \( x \mapsto (y \mapsto y) \) and composition \( f \circ \text{Diff}_{CM}(X, g) \) is defined by \( x \mapsto (f(x), \text{Diff}_{CM}(X, g)(x)) \).

Given \( f \in \text{Diff}(X, X'), \) we define change-of-base \( \text{Diff}_{CM}(X') \rightarrow \text{Diff}_{CM}(X) \) as \( \text{Diff}_{CM}(f)(g) \overset{\text{def}}{=} f \circ \text{Diff}_{CM}(X, g) \).

\( \text{Diff}_{CM}(-) \) defines a locally indexed category. By taking \( C = \text{Diff} \) and \( D(-) = \text{Diff}_{CM}(-) \), we obtain a concrete instance of our abstract semantics. Indeed, we have natural isomorphisms

\[
\text{Diff}(X, (!X' \otimes Y) \Rightarrow Z) \cong \text{Diff}_{CM}(X)(!X' \otimes Y, Z) \cong \text{Diff}_{CM}(X \times X')(Y, Z) \cong \text{Diff}_{CM}(X)(Y, X' \Rightarrow Z) \cong \text{Diff}(X, X \times X', Y \Rightarrow Z) \cong \text{Diff}(X, X \times Y \Rightarrow Z)
\]

\[
\text{Diff}(X, \times X', Y \Rightarrow Z) \cong \text{Diff}_{CM}(X \times X')(Y, Z) \circ \text{Diff}_{CM}(X)(Y, X' \Rightarrow Z) \cong \text{Diff}_{CM}(X)(Y, X \Rightarrow Z)
\]

\[
\Phi(f)(x, x')(y) \overset{\text{def}}{=} f(x)(\delta(x') \otimes y) \quad \Psi(f)(x)(y) \overset{\text{def}}{=} f(x)(y)(x').
\]

\( \Phi^{-1}(f)(x) = \sum_{i=1}^n (\delta(x'_i) \otimes y_i) = \sum_{i=1}^n f(x, x'_i)(y_i) \quad \Psi^{-1}(f)(x, y)(x') = f(x)(y)(x') \).

The prime motivating examples of morphisms in this category are derivatives. Recall that the derivative at \( x \), \( Df(x) \), and transposed derivative at \( x \), \( (Df)^T(x) \), of a smooth function \( f : \mathbb{R}^n \rightarrow \mathbb{R}^m \) are defined as the unique functions \( Df(x) : \mathbb{R}^n \rightarrow \mathbb{R}^m \) and \( (Df)^T(x) : \mathbb{R}^m \rightarrow \mathbb{R}^n \) satisfying

\[
Df(x)(v) = \lim_{\delta \rightarrow 0} \frac{f(x + \delta \cdot v) - f(x)}{\delta} \quad (Df)^T(x)(w) \cdot v = w \cdot Df(x)(v),
\]

where we write \( v \cdot u' \) for the inner product \( \sum_{i=1}^n (\pi_1 v)(\pi_1 u') \) of vectors \( v, u' \in \mathbb{R}^n \). Now, for a morphism \( f \in \text{Diff}(\mathbb{R}^n, \mathbb{R}^m) \), \( Df \) and \( (Df)^T \) give morphisms in \( \text{Diff}_{CM}(\mathbb{R}^n)(\mathbb{R}^m, \mathbb{R}^m) \) and \( \text{Diff}_{CM}(\mathbb{R}^n)(\mathbb{R}^m, \mathbb{R}^n) \), respectively.
rectively. Indeed, derivatives $Df(x)$ of $f$ at $x$ are linear functions, as are transposed derivatives $(Df)\mathbf{T}(x)$. Both depend smoothly on $x$ in case $f$ is $C^\omega$-smooth. Note that the derivatives are not merely linear in the sense of preserving 0 and +. They are also multiplicative in the sense that $(Df)(x)(c \cdot v) = c \cdot (Df)(x)(v)$. We could have captured this property by working with vector spaces internal to $\textbf{Diff}$. However, we will not need this property to phrase or establish correctness of AD. Therefore, we restrict our attention to the more straightforward structure of monoids.

By interpreting $[\text{real}^n] \overset{\text{def}}{=} \mathbb{R}^n$ and by interpreting each operation $\text{lop} \in \text{LOp}$ as the smooth function $[\text{lop}] : (\mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_k}) \rightarrow (\mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_k}) \rightarrow \mathbb{R}^m$ that is intended to represent, we obtain a canonical interpretation of our target language in $\text{Diff}_\text{CM}$.

6 PAIRING PRIMALS WITH THEIR TANGENTS/ADJOINTS, CATEGORICALLY

In this section, we show that any categorical model $\mathcal{D} : C^{op} \rightarrow \text{Cat}$ of our target language gives rise to two Cartesian closed categories $\Sigma_C \mathcal{D}$ and $\Sigma_C \mathcal{D}^{op}$ (which we wrote $\mathcal{L}[D]$ and $\mathcal{L}[D]$ in §2). We believe these observations of Cartesian closure are novel. Surprisingly, they are highly relevant for obtaining a principled understanding of AD on a higher-order language: the former for forward AD, and the latter for reverse AD. Applying these constructions to the syntactic category $\text{LSyn} : \text{Syn}^{op} \rightarrow \text{Cat}$ of our language, we produce a canonical definition of the AD macros, as the canonical interpretation of the $\lambda$-calculus in the Cartesian closed categories $\Sigma_\text{SynLSyn}$ and $\Sigma_\text{SynLSyn}^{op}$. In addition, when we apply this construction to the denotational semantics $\text{Diff}_\text{CM} : \text{Diff}^{op} \rightarrow \text{Cat}$ and invoke a categorical logical relations technique, known as subsconing, we find an elegant correctness proof of the source code transformations. The abstract construction delineated in this section is in many ways the theoretical crux of this paper.

6.1 Grothendieck Constructions on Strictly Indexed Categories

Recall that for any strictly indexed category, i.e. a (strict) functor $\mathcal{D} : C^{op} \rightarrow \text{Cat}$, we can consider its total category (or Grothendieck construction) $\Sigma_C \mathcal{D}$, which is a fibred category over $C$ (see (Johnstone 2002, sections A1.1.7, B1.3.1)). We can view it as a $\Sigma$-type of categories, which generalizes the Cartesian product. Concretely, its objects are pairs $(A_1, A_2)$ of objects $A_1$ of $C$ and $A_2$ of $\mathcal{D}(A_1)$. Its morphisms $(A_1, A_2) \rightarrow (B_1, B_2)$ are pairs $(f_1, f_2)$ of a morphism $f_1 : A_1 \rightarrow B_1$ in $C$ and a morphism $f_2 : A_2 \rightarrow \mathcal{D}(f_1)(B_2)$ in $\mathcal{D}(A_1)$. Identities are $\text{id}_{(A_1, A_2)} \overset{\text{def}}{=} (\text{id}_{A_1}, \text{id}_{A_2})$ and composition is $(f_1, f_2) \cdot (g_1, g_2) \overset{\text{def}}{=} (f_1 \cdot g_1, f_2 \cdot \mathcal{D}(f_1)(g_2))$. Further, given a strictly indexed category $\mathcal{D} : C^{op} \rightarrow \text{Cat}$, we can consider its fibrewise dual category $\mathcal{D}^{op} : C^{op} \rightarrow \text{Cat}$, which is defined as the composition $C^{op} \overset{F}{\rightarrow} \text{Cat} \overset{\text{op}}{\rightarrow} \text{Cat}$. Thus, we can apply the same construction to $\mathcal{D}$ to obtain a category $\Sigma_C \mathcal{D}^{op}$.

6.2 Categorical Structure of $\Sigma_C \mathcal{D}$ and $\Sigma_C \mathcal{D}^{op}$ for Locally Indexed Categories

§6.1 applies, in particular, to the locally indexed categories of §5. In this case, we will analyze the categorical structure of $\Sigma_C \mathcal{D}$ and $\Sigma_C \mathcal{D}^{op}$. For reference, we first give a concrete description.

$\Sigma_C \mathcal{D}$ is the following category:

- objects are pairs $(A_1, A_2)$ of objects $A$ of $C$ and $A_2$ of $\mathcal{D}$;
- morphisms $(A_1, A_2) \rightarrow (B_1, B_2)$ are pairs $f : A_1 \rightarrow B_1 \in C$ and $f_2 : A_2 \rightarrow B_2 \in \mathcal{D}(A_1)$;
- identities $\text{id}_{(A_1, A_2)}$ are $(\text{id}_{A_1}, \text{id}_{A_2})$;
- composition $(A_1, A_2) \overset{(f, f_2)}\rightarrow (B_1, B_2) \overset{(g, g_2)}\rightarrow (C_1, C_2)$ is given by $(f \cdot g, f_2 \cdot \mathcal{D}(f)(g_2))$.

$\Sigma_C \mathcal{D}^{op}$ is the following category:

- objects are pairs $(A_1, A_2)$ of objects $A$ of $C$ and $A_2$ of $\mathcal{D}$;
• morphisms \((A_1, A_2) \to (B_1, B_2)\) are pairs \(f : A_1 \to B_1 \in C\) and \(f_2 : B_2 \to A_2 \in \mathcal{D}(A_1)\);
• identities \(\text{id}_B(A_1, A_2)\) are \((\text{id}_{A_1}, \text{id}_{A_2})\);
• composition \((A_1, A_2) \xrightarrow{(f, f_2)} (B_1, B_2) \xrightarrow{(g, g_2)} (C_1, C_2)\) is given by \((f; g, \mathcal{D}(f))(g_2); f_2\).

We examine the categorical structure present in \(\Sigma_C \mathcal{D}\) and \(\Sigma_C \mathcal{D}^{op}\). As this structure are of such importance in our development, we discuss in detail.

**Proposition 6.1.** \(\Sigma_C \mathcal{D}\) has terminal object \(\mathbb{1} = (\mathbb{1}, \mathbb{1})\), binary product \((A_1, A_2) \times (B_1, B_2) = (A_1 \times B_1, A_2 \times B_2)\), and exponential \((A_1, A_2) \Rightarrow (B_1, B_2) = (A_1 \Rightarrow (B_1 \times (A_2 \rightarrow B_2)), A_1 \Rightarrow B_2)\).

**Proof (sketch).** We have natural bijections
\[
\Sigma_C \mathcal{D}((A_1, A_2), (\mathbb{1}, \mathbb{1})) = C(A_1, \mathbb{1}) \times \mathcal{D}(A_1)(A_2, \mathbb{1}) \cong \mathbb{1} \times \mathbb{1} \cong \mathbb{1} \quad \{ \mathbb{1} \text{ are terminal in } C \text{ and } \mathcal{D}(A_1) \}
\]
\[
\Sigma_C \mathcal{D}((A_1, A_2), (B_1 \times C_1, B_2 \times C_2)) = C(A_1, B_1 \times C_1) \times \mathcal{D}(A_1)(A_2, B_2 \times C_2) \cong C(A_1, B_1) \times C(A_1, C_1) \times \mathcal{D}(A_1)(A_2, B_2) \times \mathcal{D}(A_1)(A_2, C_2) \cong \Sigma_C \mathcal{D}((A_1, A_2), (B_1, B_2)) \times \Sigma_C \mathcal{D}((A_1, A_2), (C_1, C_2))
\]
\[
\Sigma_C \mathcal{D}((A_1, A_2) \times (B_1, B_2), (C_1, C_2)) = \Sigma_C \mathcal{D}((A_1 \times B_1, A_2 \times B_2), (C_1, C_2)) = C(A_1 \times B_1, C_1) \times \mathcal{D}(A_1)\mathcal{D}(A_1)(A_2 \times B_2, C_2) \cong C(A_1 \times B_1, B_2) \times \mathcal{D}(A_1)(A_2, C_1) \times \mathcal{D}(A_1)(A_2, B_2) \times \mathcal{D}(A_1)(A_2, C_2)
\]
\[
\Sigma_C \mathcal{D}((A_1, A_2), (B_1 \Rightarrow C_1, B_2 \Rightarrow C_2)) = \Sigma_C \mathcal{D}((A_1, A_2), (B_1 \Rightarrow (C_1 \times (B_2 \rightarrow C_2)), B_1 \Rightarrow C_2)) = \Sigma_C \mathcal{D}((A_1, A_2), (B_1, B_2) \Rightarrow (C_1, C_2)).
\]

\[\Box\]

We observe that we need \(\mathcal{D}\) to have biproducts (equivalently: to be \(\mathbf{CMon} \) enriched) in order to show Cartesian closure. Further, we need linear \(\Rightarrow\)-types and Cartesian \(\rightarrow\)-types.

**Proposition 6.2.** \(\Sigma_C \mathcal{D}^{op}\) has terminal object \(\mathbb{1} = (\mathbb{1}, \mathbb{1})\), binary product \((A_1, A_2) \times (B_1, B_2) = (A_1 \times B_1, A_2 \times B_2)\), and exponential \((A_1, A_2) \Rightarrow (B_1, B_2) = (A_1 \Rightarrow (B_1 \times (B_2 \rightarrow A_2)), A_1 \otimes B_2)\).

**Proof (sketch).** We have natural bijections
\[
\Sigma_C \mathcal{D}^{op}((A_1, A_2), (\mathbb{1}, \mathbb{1})) = C(A_1, \mathbb{1}) \times \mathcal{D}(A_1)(\mathbb{1}, A_2) \cong \mathbb{1} \times \mathbb{1} \cong \mathbb{1} \quad \{ \mathbb{1} \text{ terminal in } C, \text{ initial in } \mathcal{D}(A_1) \}
\]
\[
\Sigma_C \mathcal{D}^{op}((A_1, A_2), (B_1 \times C_1, B_2 \times C_2)) = C(A_1, B_1 \times C_1) \times \mathcal{D}(A_1)(B_2, C_2) \cong C(A_1, B_1) \times C(A_1, C_1) \times \mathcal{D}(A_1)(B_2, C_2) \cong C(A_1, B_1) \times \mathcal{D}(A_1)(B_2, B_1) \times \mathcal{D}(A_1)(B_2, C_2)
\]
\[
\Sigma_C \mathcal{D}^{op}((A_1, A_2) \times (B_1, B_2), (C_1, C_2)) = \Sigma_C \mathcal{D}^{op}((A_1 \times B_1, A_2 \times B_2), (C_1, C_2)) = C(A_1 \times B_1, C_1) \times \mathcal{D}(A_1)(B_1 \times C_2, A_2) \times \mathcal{D}(A_1)(B_2, C_2) \times \mathcal{D}(A_1)(B_1, B_2) \times \mathcal{D}(A_1)(B_2, C_2)
\]
\[
\Sigma_C \mathcal{D}^{op}((A_1, A_2), (B_1 \Rightarrow (C_1 \times (B_2 \rightarrow C_2))), B_1 \Rightarrow C_2)) = \Sigma_C \mathcal{D}^{op}((A_1, A_2), (B_1 \Rightarrow (C_1 \times (B_2 \rightarrow C_2)), B_1 \Rightarrow C_2)) = \Sigma_C \mathcal{D}^{op}((A_1, A_2), (B_1, B_2) \Rightarrow (C_1, C_2)).
\]

\[\Box\]
Correct Reverse AD at Higher Types

\[ C(A \times B_1, C_1 \times (C_2 \to B_2)) \times D(A_1 \times B_1)(C_2, A_2) \quad \text{is product in } C \]

\[ \triangleq C(A_1, A_1 \Rightarrow (C_1 \times (C_2 \to B_2))) \times D(A_1 \times B_1)(C_2, A_2) \quad \text{is exponential in } C \]

\[ \triangleq C(A_1, B_1 \Rightarrow (C_1 \times (C_2 \to B_2))) \times D(A_1)(!B_1 \otimes C_2, A_2) \quad \text{is } (-) \otimes (-) \text{-types} \]

\[ = \Sigma_C D^{op}((A_1, A_2), (B_1 \Rightarrow (C_1 \times (C_2 \to B_2)), !B_1 \otimes C_2)) \]

\[ = \Sigma_C D^{op}((A_1, A_2), (B_1, B_2) \Rightarrow (C_1, C_2)). \]

\[ \square \]

Observe that we need the biproduct structure of \( D \) to construct finite products in \( \Sigma C D^{op} \). Further, we need Cartesian \( -\circ - \)-types and \( !(-) \otimes (-) \)-types to construct exponentials, but not biproducts.

7 DEFINING THE CORE ALGORITHMS: AD SOURCE-CODE TRANSFORMATIONS

As \( \Sigma_{\text{Syn}} \text{LSyn} \) and \( \Sigma_{\text{Syn}} \text{LSyn}^{op} \) are both Cartesian closed categories by §6, the universal property of \( \text{Syn} \) yields unique structure-preserving morphisms, \( \overrightarrow{\text{Syn}}(-) : \text{Syn} \to \Sigma_{\text{Syn}} \text{LSyn} \) (forward AD) and \( \overleftarrow{\text{Syn}}(-) : \text{Syn} \to \Sigma_{\text{Syn}} \text{LSyn}^{op} \) (reverse AD), once we fix a compatible definition for the macros on \( \text{real}^n \) and basic operations \( \text{op} \). By definition of equality in \( \text{Syn} \), \( \Sigma_{\text{Syn}} \text{LSyn} \) and \( \Sigma_{\text{Syn}} \text{LSyn}^{op} \), these macros automatically respect equational reasoning principles, in the sense that \( t \overset{\beta}{=} s \) implies that \( \overrightarrow{\text{Syn}}(t) \overset{\beta}{=} \overrightarrow{\text{Syn}}(s) \) and \( \overleftarrow{\text{Syn}}(t) \overset{\beta}{=} \overleftarrow{\text{Syn}}(s) \).

We need to choose suitable terms \( \text{Dop}(x; y) \) and \( \text{Dop}^f(x; y) \) to represent the forward- and reverse-mode derivatives of the basic operations \( \text{op} \in \text{Op}^m_{n_1, \ldots, n_k} \). For example, for elementwise multiplication \((\ast) \in \text{Op}^m_n\), we can define \( D(\ast)(x; y) = (\text{fst } x) \ast (\text{snd } y) + (\text{snd } x) \ast (\text{fst } y) \) and \( D(\ast)^f(x; y) = \langle(\text{snd } x) \ast y, (\text{fst } x) \ast y\rangle \), where we use (linear) elementwise multiplication \((\ast) \in \text{LOp}^m_{n, n} \). We represent derivatives as linear functions. This representation allows for efficient Jacobian-vector/adjoint product implementations, which avoid first calculating a full Jacobian and next taking a product. Such implementations are known to be important to achieve performant AD systems.

\( \overrightarrow{\text{Syn}}(\text{real}^n)_1 \overset{\text{def}}{=} \text{real}^n \quad \overrightarrow{\text{Syn}}(\text{real}^n)_2 \overset{\text{def}}{=} \text{real}^n \quad \overrightarrow{\text{Syn}}(\text{real}^m) \overset{\text{def}}{=} \text{real}^n \quad \overrightarrow{\text{Syn}}(\text{real}^m) \overset{\text{def}}{=} \text{real}^n \)

\( \overleftarrow{\text{Syn}}(\text{op})_1 \overset{\text{def}}{=} \text{op} \quad \overleftarrow{\text{Syn}}(\text{op})_2 \overset{\text{def}}{=} x : \text{real}^m \ast \ldots \ast \text{real}^n_k \rightarrow \text{Dop}(x; y) : \text{real}^m \quad \overleftarrow{\text{Syn}}(\text{op})_2 \overset{\text{def}}{=} x : \text{real}^m \ast \ldots \ast \text{real}^n_k \rightarrow \text{Dop}^f(x; y) : \text{real}^m \ast \ldots \ast \text{real}^n_k \)

For the AD transformations to be correct, it is important that these derivatives of language primitives are implemented correctly in the sense that

\[ [x; y \dagger \text{Dop}(x; y)] = D[\text{op}] \quad [x; y \dagger \text{Dop}^f(x; y)] = D[\text{op}]^f. \]

In practice, AD library developers tend to assume the subtle task of correctly implementing such derivatives \( \text{Dop}(x; y) \) and \( \text{Dop}^f(x; y) \) whenever a new primitive operation \( \text{op} \) is added to the library.

The extension of the AD macros \( \overrightarrow{\text{Syn}} \) and \( \overleftarrow{\text{Syn}} \) to the full source language are now canonically determined, as the unique Cartesian closed functors that extend the previous definitions, following the categorical structure described in §6. Because of the counter-intuitive nature of the Cartesian closed structures on \( \Sigma_{\text{Syn}} \text{LSyn} \) and \( \Sigma_{\text{Syn}} \text{LSyn}^{op} \), we list the full macros explicitly in Appx. A.

8 PROVING REVERSE AND FORWARD AD DENOATIONALLY CORRECT

In this section, we will show that the source code transformations described in §7 correctly implement mathematical derivatives. We make correctness precise as the statement that for programs \( x : \tau \dagger t : \sigma \) between first-order types \( \tau \) and \( \sigma \), i.e. types not containing any function type constructors, we have that \( [\overrightarrow{\text{Syn}}(t)_2] = D[t] \) and \( [\overleftarrow{\text{Syn}}(t)_2] = (D[t])^f \), where \( [-] \) is the semantics of §5. The proof mainly consists of logical relations arguments over the semantics in \( \Sigma_{\text{Diff}} \text{Diff}_{\text{CM}} \) and

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This logical relations proof can be phrased in elementary terms, but the resulting argument is very technical and would be hard to discover. Instead, we prefer to phrase it in terms of a categorical subsconing construction, a more abstract and elegant perspective on logical relations. We discovered the proof by taking this categorical perspective, and, while we have verified the elementary argument (see Appx. B), we would not otherwise have come up with it.

8.1 Preliminaries

**Subsconing.** Logical relations arguments provide a powerful proof technique for demonstrating properties of typed programs. The arguments proceed by induction on the structure of types. Here, we briefly review the basics of categorical logical relations arguments, or *subsconing constructions*. We restrict to the level of generality that we need here, but we would like to point out that the theory applies much more generally.

Consider a Cartesian closed category \((C, \mathbb{1}, \times, \Rightarrow)\). Suppose that we are given a functor \(F : C \to \text{Set}\) to the category \(\text{Set}\) of sets and functions which preserves finite products in the sense that \(F(\mathbb{1}) \cong \mathbb{1}\) and \(F(C \times C') \cong F(C) \times F(C')\). Then, we can form the subscone of \(F\), or category of logical relations over \(F\), which is Cartesian closed (Johnstone et al. 2007):

- objects are pairs \((C, P)\) of an object \(C\) of \(C\) and a predicate \(P \subseteq FC\);
- morphisms \((C, P) \to (C', P')\) are \(C\) morphisms \(f : C \to C'\) which respect the predicates in the sense that \(F(f)(P) \subseteq P'\);
- identities and composition are as in \(C\);
- \((\mathbb{1}, F\mathbb{1})\) is the terminal object, and products and exponentials are given by \((C, P) \times (C', P') = (C \times C', \{\alpha \in F(C \times C') \mid F(\pi_1)(\alpha) \in P \text{ and } F(\pi_2)(\alpha) \in P'\})\) and \((C, P) \Rightarrow (C', P') = (C \Rightarrow C', \{F(\pi_2)(y) \mid y \in F((C \Rightarrow C') \times C) \text{ s.t. } F(\pi_2)(y) \in P \implies F(ev)(y) \in P'\})\).

Forgetting about the predicates gives a faithful Cartesian closed functor \(\pi_1\) from the subscone to \(C\).

In typical applications, \(C\) can be the syntactic category of a language (like \(\text{Syn}\)), the codomain of a denotational semantics \([\cdot]\) (like \(\text{Diff}\)), or a product of the above, if we want to consider \(n\)-ary logical relations instead of logical predicates. Typically, \(F\) tends to be a hom-functor (which always preserves products), like \(C(\mathbb{1}, -)\) or \(C(C_0, -)\), for some important object \(C_0\). When applied to the syntactic category \(\text{Syn}\) and \(F = \text{Syn}(\mathbb{1}, -)\), the formulae for products and exponentials in the subscone clearly reproduce the usual recipes in traditional, syntactic logical relations arguments. As such, subsconing generalises standard logical relations methods.

8.2 Subsconing for Correctness of AD

We will apply the subsconing construction above to

\[
\begin{align*}
C &= \text{Diff} \times \Sigma_{\text{Diff} \text{Diff}_{\text{CM}}} \\
F &= \text{Diff} \times \Sigma_{\text{Diff} \text{Diff}_{\text{CM}}}((\mathbb{R}, (\mathbb{R}, \mathbb{R})), -) \\
F &= \text{Diff} \times \Sigma_{\text{Diff} \text{Diff}_{\text{CM}}}((\mathbb{R}, (\mathbb{R}, \mathbb{R})), -)
\end{align*}
\]

for forward AD

\[
\begin{align*}
C &= \text{Diff} \times \Sigma_{\text{Diff} \text{Diff}_{\text{CM}}}^{op} \\
F &= \text{Diff} \times \Sigma_{\text{Diff} \text{Diff}_{\text{CM}}}^{op}((\mathbb{R}, (\mathbb{R}, \mathbb{R})), -) \\
F &= \text{Diff} \times \Sigma_{\text{Diff} \text{Diff}_{\text{CM}}}^{op}((\mathbb{R}, (\mathbb{R}, \mathbb{R})), -)
\end{align*}
\]

for reverse AD,

where we note that \(\text{Diff}, \Sigma_{\text{Diff} \text{Diff}_{\text{CM}}}, \text{and } \Sigma_{\text{Diff} \text{Diff}_{\text{CM}}}^{op}\) are Cartesian closed (given the arguments of §5 and §6) and that the product of Cartesian closed categories is again Cartesian closed. Let us write \(\text{SScone}\) and \(\text{SScone}\), respectively, for the resulting categories of logical relations.

Seeing that \(\text{SScone}\) and \(\text{SScone}\) are Cartesian closed, we obtain unique Cartesian closed functors \(\langle - \rangle^f : \text{Syn} \to \text{SScone}\) and \(\langle - \rangle^r : \text{Syn} \to \text{SScone}\) once we fix an interpretation of \(\text{real}^n\) and all operations \(\text{op}\). We write \(P^f_r\) and \(P^r_r\), respectively, for the relations \(\pi_2(\tau)^f\) and \(\pi_2(\tau)^r\). Let us interpret

\[
\langle \text{real}^n \rangle^f \defeq ((\mathbb{R}^n, (\mathbb{R}^n, \mathbb{R}^n)), P^f_{\text{real}^n} \defeq \{(f, (g, h)) \mid f = g \text{ and } h = Df\})
\]

\[
\langle \text{real}^n \rangle^r \defeq ((\mathbb{R}^n, (\mathbb{R}^n, \mathbb{R}^n)), P^r_{\text{real}^n} \defeq \{(f, (g, h)) \mid f = g \text{ and } h = (Df)^f\})
\]
where we write $Df$ for the semantic derivative of $f$ (see §5). We need to verify, respectively, that $\langle [\text{op}], ([Df](t_1)), [Df](t_2)) \rangle$ and $\langle [\text{op}], ([Df](t_1)), [Df](t_2)) \rangle$ respect the logical relations $P^f$ and $P^r$. This respecting of relations follows immediately from the chain rule for multivariate differentiation.

Consequently, we obtain our Cartesian closed functors $([-])^f$ and $([-])^r$.

Further, observe that we have a Cartesian closed functor $\Sigma_L\text{Syn} \to \Sigma_{\text{DiffCM}}$, defined by $\Sigma_L\text{Syn} \to \Sigma_{\text{DiffCM}}$, $\Sigma_L\text{Syn} \to \Sigma_{\text{DiffCM}}$. As a consequence, the two squares below commute. Indeed, going

$$
\text{Syn} \xrightarrow{(\text{id}, \tilde{D})} \text{Syn} \times \Sigma_{\text{DiffCM}} \times \Sigma_{\text{Syn}L\text{Syn}} \quad \text{Syn} \xrightarrow{(\text{id}, \tilde{D})} \text{Syn} \times \Sigma_{\text{DiffCM}} \times \Sigma_{\text{Syn}L\text{Syn}}
$$

around the squares in both directions define Cartesian closed functors that agree on their action on $\text{real}$ and all operations $\text{op}$. Therefore, by the universal property of $\text{Syn}$, they must coincide. In particular, $\langle [t], ([Df](t_1)), [Df](t_2)) \rangle$ is a morphism in $\text{Syn}L\text{Syn}$ and therefore respects the relations $P^f$ for any well-typed term $t$ of the source language of §3. Similarly, $\langle [t], ([Df](t_1)), [Df](t_2)) \rangle$ is a morphism in $\text{Syn}L\text{Syn}$ and therefore respects the relations $P^r$.

Most of the work is now in place to show correctness of AD. We finish the proof below. To ease notation, we work with terms in a context with a single type. Doing so is not a restriction as our language has products, and the theorem holds for arbitrary terms between first-order types.
Theorem 8.1 (Correctness of AD). For programs \( x : \tau \vdash t : \sigma \) between first-order types \( \tau \) and \( \sigma \),
\[
\text{Diff}(t_1) = [t] \quad \text{Diff}(t_2) = D[t] \quad \text{Diff}(t_1) = [t] \quad \text{Diff}(t_2) = D[t]
\]
where we write \( D \) for the usual calculus derivative and \((-)^t\) for the matrix transpose.

Proof (sketch). First, we focus on \( \text{Diff} \). Let \( x \in \text{Diff}(\tau_1) = [t] \equiv \mathbb{R}^N \) and \( v \in \text{Diff}(\tau_2) \equiv \mathbb{R}^N \) (for some \( N \)). Then, there is a smooth curve \( y : \mathbb{R} \to [t] \), such that \( y(0) = x \) and \( D_y(0)(1) = v \). Clearly, \( (y, (y, Dy)) \in \mathbb{R}^t \). As \((\llbracket t \rrbracket, (\llbracket \text{Diff}(t_1) \rrbracket, \llbracket \text{Diff}(t_2) \rrbracket))\) respects the logical relation \( P^t \), we have
\[
(y', [t], [t], \llbracket \text{Diff}(t_1) \rrbracket, x \mapsto r \mapsto \llbracket \text{Diff}(t_2) \rrbracket((y(x))(Dy(x)(r)))) = (y, (y, Dy)); ([t], (\llbracket \text{Diff}(t_1) \rrbracket, \llbracket \text{Diff}(t_2) \rrbracket)) \in P^t,
\]
where we use the definition of composition in \( \text{Diff} \times \Sigma_{\text{Diff}} \text{Diff}_{\text{CM}} \). Therefore, \( y'; [t] = y; [t] \) and, by the chain rule, \( x \mapsto r \mapsto D[t](y(x))(Dy(x)(r)) = D[y'; [t] = x \mapsto r \mapsto \llbracket \text{Diff}(t_2) \rrbracket((y(x))(Dy(x)(r))). \)
Evaluating the former at 0 gives \( [t](x) = \llbracket \text{Diff}(t_1) \rrbracket(x) \). Similarly, evaluating the latter at 0 and 1 gives \( D[t](x)(v) = \llbracket \text{Diff}(t_2) \rrbracket(x)(v) \).

Next, we turn to \( \text{Diff} \). Let \( x \in \text{Diff}(\tau_1) = [t] \equiv \mathbb{R}^N \) and \( v \in \text{Diff}(\tau_2) \equiv \mathbb{R}^N \) (for some \( N \)). Let \( y_1 : \mathbb{R} \to [t] \) be a smooth curve such that \( y_1(0) = x \) and \( D_y(0)(1) = e_i \), where we write \( e_i \) for the \( i \)-th standard basis vector of \( \mathbb{R}^N \). Clearly, \( (y_1, (y_1, Dy_1')) \in P^t \). As \((\llbracket t \rrbracket, (\llbracket \text{Diff}(t_1) \rrbracket, \llbracket \text{Diff}(t_2) \rrbracket))\) respects the logical relation \( P^t \), we have \( (y_1, [t], [t], \llbracket \text{Diff}(t_1) \rrbracket, x \mapsto w \mapsto D_y_1(x')(\llbracket \text{Diff}(t_2) \rrbracket((y_1(x))(w)))) = (y_1, (y_1, Dy_1')); ([t], (\llbracket \text{Diff}(t_1) \rrbracket, \llbracket \text{Diff}(t_2) \rrbracket)) \in P^t, \)
by using the definition of composition in \( \text{Diff} \times \Sigma_{\text{Diff}} \text{Diff}_{\text{CM}} \). Consequently, \( y_1; [t] = y_1; [t] \) and, by the chain rule,
\[
x \mapsto w \mapsto D_y_1(x')(D[t](y_1(x))'(w)) = D[y_1; [t] = x \mapsto w \mapsto D_y_1(x')(\llbracket \text{Diff}(t_2) \rrbracket((y_1(x))(w))).
\]
Evaluating the former at 0 gives \( [t](x) = \llbracket \text{Diff}(t_1) \rrbracket(x) \). Similarly, evaluating the latter at 0 and \( v \) gives us \( e_i \cdot D[t](x')(v) = e_i \cdot \llbracket \text{Diff}(t_2) \rrbracket(x)(v) \). As this equation holds for all basis vectors \( e_i \) of \( \llbracket \text{Diff}(\tau) \rrbracket \), we find that \( D[t](x) = \sum_{i=1}^{N} e_i \cdot \llbracket \text{Diff}(t_2) \rrbracket(x)(v) \).

9. PRACTICAL RELEVANCE AND IMPLEMENTATION IN FUNCTIONAL LANGUAGES

Most popular functional languages, such as Haskell and O’Caml, do not natively support linear types. As such, the transformations described in this paper may seem hard to implement. However, as we will argue in this section, we can easily implement the limited linear types necessary for phrasing the transformations as abstract data types by using merely a basic module system.

Specifically, we explain how to implement \( (-) \otimes (-) \) and Cartesian \( (-) \rightarrow (-) \)-types. We first convey some intuitions, and then we discuss the required API, the AD transformations, their semantics and correctness, and, finally, we explain how the API can be implemented.

Based on the denotational semantics, \( \tau \rightarrow \sigma \)-types should hold (representations of) functions \( f \) from \( \tau \) to \( \sigma \) that are homomorphisms of the monoid structures on \( \tau \) and \( \sigma \). We will see that these types can be implemented using an abstract data type that holds certain basic linear functions (extensible as the library evolves) and is closed under the identity, composition, argument swapping, and currying (to be discussed later). Again, based on the semantics, \( \! \tau \otimes \sigma \) should contain (representations of) finite multisets \( \sum_{i=1}^{n} \delta_{(t_i, s_i)} \) of pairs \((t_i, s_i)\), where \( t_i \) is of type \( \tau \) and \( s_i \) is of type \( \sigma \), and where we identify \( x + \delta_{(t, s)} \) and \( x + \delta_{(t', s')} \).

9.1 An Alternative, Applied Target Language for AD Based on Abstract Data Types

Next, we discuss an extension of the source language of §3 with two abstract data type formers \( \text{LFun} \) and \( \text{Tens} \), as it can serve as an alternative, applied target language for our transformation. This language is essentially equivalent to that of §4, but it no longer distinguishes between linear
and Cartesian types. To be precise, we extend the source language with the types and terms

\[
\begin{align*}
\tau, \sigma, \rho & ::= \text{types} & \text{Tens}(\tau, \sigma) & \text{tensor types} \\
\ldots & \text{as in §3} & \text{LFun}(\tau, \sigma) & \text{linear function}
\end{align*}
\]

\[
\begin{align*}
t, s, r & ::= \text{terms} & \text{lswap} t & \text{swapping args} \\
\ldots & \text{as in §3} & \text{leval}, & \text{linear evaluation} \\
\text{lop}(t) & \text{linear operations lop} & \{ (t, -) \} & \text{singletons} \\
0_r & \text{zero} & \text{lcur}^{-1} t & \text{Tens-elim} \\
\tau \cdot s & \text{plus} & \text{lfst} & \text{linear projection} \\
\tau & \text{linear composition} & \text{lsnd} & \text{linear projection} \\
\text{lapp}(t, s) & \text{linear application} & \text{lpair}(t, s) & \text{linear pairing},
\end{align*}
\]

which are typed according to the rules of Fig. 5.

We can use this extension of the source language as an alternative target language for our AD transformations. In fact, we could define a translation \((-)\)\text{\,} such as the extension with higher-order primitive operations that we consider in §§9.6.

![Fig. 5. Typing rules for the alternative target language.](image)
9.2 AD Macros Targeting the Applied Language with Abstract Types

Assume that we have chosen suitable terms \( x : \text{Dom}(\text{op}) \vdash \text{Dop}(x) : \text{LFun}(\text{Dom}(\text{op}), \text{real}^n) \) and \( x : \text{Dom}(\text{op}) \vdash \text{Dop}'(x) : \text{LFun}(\text{real}^m, \text{Dom}(\text{op})) \) for representing the forward and reverse derivatives of operations \( \text{op} \in \text{Op}^n_{\text{dom}} \).

For forward AD, we translate each type \( \tau \) into a pair of types \((\overline{\delta}(\tau)_1, \overline{\delta}(\tau)_2)\). We also translate each term \( x : \tau \vdash t : \sigma \) into a pair of terms \( x : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_1 : \overline{\delta}(\tau)_1 \) and \( x : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_2 : \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\sigma)_2) \). We then define \( \overline{\delta}(-) \) on types as

\[
\overline{\delta}(\text{real}^n)_{1,2} \equiv \text{real}^n \quad \overline{\delta}(1)_{1,2} \equiv 1 \quad \overline{\delta}(\tau \ast \sigma)_{1,2} \equiv \overline{\delta}(\tau)_1 \ast \overline{\delta}(\sigma)_1 \quad \overline{\delta}(\tau \ast \sigma)_{2,2} \equiv \overline{\delta}(\tau)_2 \ast \overline{\delta}(\sigma)_2
\]

On programs, we define it as

\[
\overline{\delta}(\text{op})_{1,2} \equiv \text{op} \quad \overline{\delta}(\text{idr})_{1,2} \equiv x \vdash \text{Dop}(x) \quad \overline{\delta}(\text{lfst})_{1,2} \equiv x \vdash \overline{\delta}(\tau)_1 \vdash x : \overline{\delta}(\tau)_1 \quad \overline{\delta}(\text{idr})_{2,2} \equiv \text{lid}
\]

where \( x : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_1 : \overline{\delta}(\sigma)_1 \) and \( y : \overline{\delta}(\sigma)_1 \vdash \overline{\delta}(s)_1 : \overline{\delta}(\rho)_1 \)

\[
x_1 : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_2 : \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\sigma)_2) \text{ and } y_1 : \overline{\delta}(\sigma)_1 \vdash \overline{\delta}(s)_2 : \text{LFun}(\overline{\delta}(\sigma)_2, \overline{\delta}(\rho)_2)
\]

For reverse AD, we translate each type \( \tau \) into a pair of types \((\overline{\delta}(\tau)_1, \overline{\delta}(\tau)_2)\). We also translate each term \( x : \tau \vdash t : \sigma \) into a pair of terms \( x : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_1 : \overline{\delta}(\tau)_1 \) and \( x : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_2 : \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\sigma)_2) \). We define \( \overline{\delta}(-) \) on types as

\[
\overline{\delta}(\text{real}^n)_{1,2} \equiv \text{real}^n \quad \overline{\delta}(1)_{1,2} \equiv 1 \quad \overline{\delta}(\tau \ast \sigma)_{1,2} \equiv \overline{\delta}(\tau)_1 \ast \overline{\delta}(\sigma)_1 \quad \overline{\delta}(\tau \ast \sigma)_{2,2} \equiv \overline{\delta}(\tau)_2 \ast \overline{\delta}(\sigma)_2
\]

\[
\overline{\delta}(\tau \vdash \sigma)_1 \equiv \overline{\delta}(\tau)_1 \vdash (\overline{\delta}(\sigma)_1 \ast \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\sigma)_2)) \quad \overline{\delta}(\tau \vdash \sigma)_2 \equiv \overline{\delta}(\tau)_1 \vdash \overline{\delta}(\sigma)_2
\]

On programs, we define it as

\[
\overline{\delta}(\text{op})_{1,2} \equiv \text{op} \quad \overline{\delta}(\text{idr})_{1,2} \equiv x \vdash \text{Dop}(x) \quad \overline{\delta}(\text{lfst})_{1,2} \equiv x \vdash \overline{\delta}(\tau)_1 \vdash x : \overline{\delta}(\tau)_1 \quad \overline{\delta}(\text{idr})_{2,2} \equiv \text{lid}
\]

where \( x : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_1 : \overline{\delta}(\sigma)_1 \) and \( y : \overline{\delta}(\sigma)_1 \vdash \overline{\delta}(s)_1 : \overline{\delta}(\rho)_1 \)

\[
x_1 : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_2 : \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\sigma)_2) \text{ and } y_1 : \overline{\delta}(\sigma)_1 \vdash \overline{\delta}(s)_2 : \text{LFun}(\overline{\delta}(\sigma)_2, \overline{\delta}(\rho)_2)
\]

\[
\overline{\delta}(\text{idr})_{1,2} \equiv \overline{\delta}(\rho)_1 \ast \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\rho)_2)
\]

For reverse AD, we translate each type \( \tau \) into a pair of types \((\overline{\delta}(\tau)_1, \overline{\delta}(\tau)_2)\). We also translate each term \( x : \tau \vdash t : \sigma \) into a pair of terms \( x : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_1 : \overline{\delta}(\tau)_1 \) and \( x : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_2 : \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\sigma)_2) \). We define \( \overline{\delta}(-) \) on types as

\[
\overline{\delta}(\text{real}^n)_{1,2} \equiv \text{real}^n \quad \overline{\delta}(1)_{1,2} \equiv 1 \quad \overline{\delta}(\tau \ast \sigma)_{1,2} \equiv \overline{\delta}(\tau)_1 \ast \overline{\delta}(\sigma)_1 \quad \overline{\delta}(\tau \ast \sigma)_{2,2} \equiv \overline{\delta}(\tau)_2 \ast \overline{\delta}(\sigma)_2
\]

\[
\overline{\delta}(\tau \vdash \sigma)_1 \equiv \overline{\delta}(\tau)_1 \vdash (\overline{\delta}(\sigma)_1 \ast \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\sigma)_2)) \quad \overline{\delta}(\tau \vdash \sigma)_2 \equiv \overline{\delta}(\tau)_1 \vdash \overline{\delta}(\sigma)_2
\]

On programs, we define it as

\[
\overline{\delta}(\text{op})_{1,2} \equiv \text{op} \quad \overline{\delta}(\text{idr})_{1,2} \equiv x \vdash \text{Dop}(x) \quad \overline{\delta}(\text{lfst})_{1,2} \equiv x \vdash \overline{\delta}(\tau)_1 \vdash x : \overline{\delta}(\tau)_1 \quad \overline{\delta}(\text{idr})_{2,2} \equiv \text{lid}
\]

where \( x : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_1 : \overline{\delta}(\sigma)_1 \) and \( y : \overline{\delta}(\sigma)_1 \vdash \overline{\delta}(s)_1 : \overline{\delta}(\rho)_1 \)

\[
x_1 : \overline{\delta}(\tau)_1 \vdash \overline{\delta}(t)_2 : \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\sigma)_2) \text{ and } y_1 : \overline{\delta}(\sigma)_1 \vdash \overline{\delta}(s)_2 : \text{LFun}(\overline{\delta}(\sigma)_2, \overline{\delta}(\rho)_2)
\]

\[
\overline{\delta}(\text{idr})_{1,2} \equiv \overline{\delta}(\rho)_1 \ast \text{LFun}(\overline{\delta}(\tau)_2, \overline{\delta}(\rho)_2)
\]
\[ x_1 : \overrightarrow{D}(\tau) \vdash \overrightarrow{D}(t_2) : \text{LFun}(\overrightarrow{D}(\sigma_2), \overrightarrow{D}(\tau_2)) \quad \text{and} \quad y_1 : \overrightarrow{D}(\sigma_1) \vdash \overrightarrow{D}(s_2) : \text{LFun}(\overrightarrow{D}(\rho_2), \overrightarrow{D}(\sigma_2)) \]

\[ \overrightarrow{D}(\langle \tau \rangle_1) \overset{\text{def}}{=} \langle \rangle \quad \overrightarrow{D}((\langle \tau \rangle_2) \overset{\text{def}}{=} \emptyset \quad \overrightarrow{D}((t, s))_1 \overset{\text{def}}{=} (\overrightarrow{D}(t), \overrightarrow{D}(s))_1 \quad \overrightarrow{D}((t, s))_2 \overset{\text{def}}{=} \text{fst} ; \overrightarrow{D}(t) + \text{lsnd} ; \overrightarrow{D}(s)_2 \]

where \( x_1 : \overrightarrow{D}(\tau) \vdash \overrightarrow{D}(t_2) : \text{LFun}(\overrightarrow{D}(\sigma_2), \overrightarrow{D}(\tau_2)) \) and \( y_1 : \overrightarrow{D}(\sigma_1) \vdash \overrightarrow{D}(s_2) : \text{LFun}(\overrightarrow{D}(\rho_2), \overrightarrow{D}(\tau_2)) \)

\[ \overrightarrow{D}(\text{fst}_{\tau, \sigma})_1 \overset{\text{def}}{=} x : \overrightarrow{D}(\tau)_1 * \overrightarrow{D}(\sigma)_1 \quad \text{fst} : \overrightarrow{D}(\tau)_1 \quad \overrightarrow{D}(\text{fst}_{\tau, \sigma})_2 \overset{\text{def}}{=} \text{lpair}(\text{lid}, \emptyset) \]

\[ \overrightarrow{D}(\text{snd}_{\tau, \sigma})_1 \overset{\text{def}}{=} x : \overrightarrow{D}(\tau)_1 * \overrightarrow{D}(\sigma)_1 \quad \text{snd} : \overrightarrow{D}(\sigma)_1 \quad \overrightarrow{D}(\text{snd}_{\tau, \sigma})_2 \overset{\text{def}}{=} \text{lpair}(\emptyset, \text{lid}) \]

\[ \overrightarrow{D}(\text{ev}_{\tau, \sigma})_1 \overset{\text{def}}{=} x : (\overrightarrow{D}(\tau)_1 \to (\overrightarrow{D}(\sigma)_1 * \text{LFun}(\overrightarrow{D}(\tau_2), \overrightarrow{D}(\sigma_2)))) * \overrightarrow{D}(\tau)_1 \to \text{fst} ((\text{fst} x)(\text{snd} x)) : \overrightarrow{D}(\sigma)_1 \]

\[ \overrightarrow{D}(\text{ev}_{\tau, \sigma})_2 \overset{\text{def}}{=} x_1 : (\overrightarrow{D}(\tau)_1 \to (\overrightarrow{D}(\sigma)_1 * \text{LFun}(\overrightarrow{D}(\tau_2), \overrightarrow{D}(\sigma_2)))) * \overrightarrow{D}(\tau)_1 \to \text{let} \ y = \text{snd} \ x_1 \text{ in} \]

\[ \text{lpair}(\langle \langle y, - \rangle \rangle), \text{snd} ((\text{fst} x_1) y) : \text{LFun}(\overrightarrow{D}(\tau_2), \text{Tens}(\overrightarrow{D}(\tau_1), \overrightarrow{D}(\sigma)_1) * \overrightarrow{D}(\tau)_2) \]

\[ \overrightarrow{D}(\text{L}_1, \cdot, \cdot, \cdot) \overset{\text{def}}{=} x : \overrightarrow{D}(\tau)_1 \to \lambda y. (\overrightarrow{D}(t_1), \overrightarrow{D}(t_2)) * \text{lsnd}[\langle x, y \rangle_2] : \overrightarrow{D}(\sigma)_1 \to (\overrightarrow{D}(\rho)_1 * \text{LFun}(\overrightarrow{D}(\tau_2), \overrightarrow{D}(\sigma_2))) \]

\[ \overrightarrow{D}(\text{L}_2, \cdot, \cdot, \cdot) \overset{\text{def}}{=} x : \overrightarrow{D}(\tau)_1 \to \text{lcur}^{-1}(\lambda y. \overrightarrow{D}(t_2)[\langle x, y \rangle_2]) \quad \text{lsnd} : \text{LFun}(\text{Tens}(\overrightarrow{D}(\sigma_1), \overrightarrow{D}(\tau_2)), \overrightarrow{D}(\tau_2)) \]

where \( z : \overrightarrow{D}(\tau)_1 * \overrightarrow{D}(\sigma)_1 + \overrightarrow{D}(t_1 : \overrightarrow{D}(\rho)_1), \quad z : \overrightarrow{D}(\tau)_1 * \overrightarrow{D}(\sigma)_1 + \overrightarrow{D}(t_2 : \text{LFun}(\overrightarrow{D}(\rho_2), \overrightarrow{D}(\tau_2)) * \overrightarrow{D}(\sigma)_2) \)

We emphasise that this generated code is intended to be compiled by an optimizing compiler. Indeed, leveraging such existing compiler toolchains is one of the prime motivations for this work.

### 9.3 Denotational Semantics for the Applied Target Language

Let us write \( \text{Diff}_{\text{CM}}^{\text{non-lin}} \) for the category whose objects are commutative diffeological monoids \( X \), and whose morphisms \( X \to Y \) are functions \( |X| \to |Y| \) that are diffeological space morphisms, but that may fail to be monoid homomorphisms.

We can give a denotational semantics \( \llbracket - \rrbracket \) to the applied target language in this category by interpreting types \( \tau \) as objects \( \llbracket \tau \rrbracket \) in \( \text{Diff}_{\text{CM}}^{\text{non-lin}} \) and terms \( \Gamma \vdash t : \tau \) as morphisms \( \llbracket t \rrbracket \) in \( \text{Diff}_{\text{CM}}^{\text{non-lin}}(\llbracket \Gamma \rrbracket, \llbracket \tau \rrbracket) \). We interpret types by making use of the categorical constructions on objects in \( \text{Diff}_{\text{CM}} \) described in §5:

\[
\llbracket \text{real}^m \rrbracket \overset{\text{def}}{=} \mathbb{R}^m \\
\llbracket 1 \rrbracket \overset{\text{def}}{=} 1 \\
\llbracket \tau \times \sigma \rrbracket \overset{\text{def}}{=} \llbracket \tau \rrbracket \times \llbracket \sigma \rrbracket \\
\llbracket \tau \to \sigma \rrbracket \overset{\text{def}}{=} (\llbracket \tau \rrbracket, \mathcal{P}_{\llbracket \tau \rrbracket}) \to (\llbracket \sigma \rrbracket)
\]

\[
\llbracket \text{LFun}(\tau, \sigma) \rrbracket \overset{\text{def}}{=} (\llbracket \tau \rrbracket \to \llbracket \sigma \rrbracket) \\
\llbracket \text{Tens}(\tau, \sigma) \rrbracket \overset{\text{def}}{=} (\llbracket \tau \rrbracket, \mathcal{P}_{\llbracket \tau \rrbracket}) \otimes (\llbracket \sigma \rrbracket)
\]

Here, we use the commutative monoid structure on the homomorphism spaces \( \llbracket \tau \rrbracket \to \llbracket \sigma \rrbracket \), which we described in Ex. 5.14. We extend the semantics of \( \text{Syn}'s \) terms to the applied target language (noting that the interpretation \( \llbracket - \rrbracket \) of \( \text{Syn}'s \) terms as \( \text{Diff} \)-morphisms can also serve as a well-typed interpretation in \( \text{Diff}_{\text{CM}}^{\text{non-lin}} \), given our chosen interpretation of objects):

\[
\llbracket (t + s)(v) \rrbracket \overset{\text{def}}{=} \llbracket t(v) \rrbracket + \llbracket s(v) \rrbracket \\
\llbracket \text{id}(v)(x) \rrbracket \overset{\text{def}}{=} x \\
\llbracket (t; s)(v)(x) \rrbracket \overset{\text{def}}{=} \llbracket t(v) \rrbracket(\llbracket t(v)(x) \rrbracket)
\]

\[
\llbracket \text{app}(t, s)(v) \rrbracket \overset{\text{def}}{=} \llbracket t(v) \rrbracket(\llbracket s(v) \rrbracket) \\
\llbracket \text{lswap t}(v)(x)(y) \rrbracket \overset{\text{def}}{=} \llbracket t(v)(y) \rrbracket(x)
\]

\[
\llbracket \text{leval}_1 f \rrbracket(v)(f) \overset{\text{def}}{=} f(\llbracket t(v) \rrbracket) \\
\llbracket (t, -) \rrbracket(t)(v)(x) \overset{\text{def}}{=} (\llbracket t \rrbracket)(v)(x)
\]

\[
\llbracket \text{lcur}^{-1} \rrbracket(t)(v)(y) \overset{\text{def}}{=} \sum_{i=1}^{n}(x \otimes y) \\
\llbracket \text{fst} \rrbracket(v)(x, y) \overset{\text{def}}{=} x \\
\llbracket \text{lsnd} \rrbracket(v)(x, y) \overset{\text{def}}{=} y
\]

\[
\llbracket \text{lpair} \rrbracket(s)(v)(x) \overset{\text{def}}{=} (\llbracket t \rrbracket(v)(x), \llbracket s \rrbracket(v)(x)) \\
\llbracket \lambda \text{lop} : \text{real}^m \rrbracket \overset{\text{def}}{=} \llbracket \Gamma ; y : \text{LDom}(\text{lop}) \vdash \text{lop}(t ; y) : \text{real}^m \rrbracket
\]

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The interpretation of $\text{ln}\, \text{cur}^{-1} t$ is well-defined, for two reasons: first, $\{t\}$ is linear in its last argument by its type; second, $+$ is commutative and associative.

### 9.4 A Correctness Proof of AD for the Applied Target Language

With a semantics in place, we can again give a correctness proof of AD. This time, we write out the logical relations proof by hand. It is essentially the unraveling of the categorical subconing argument of §8. Appx. B contains the full proof. Here, we outline the structure.

**Correctness of Forward AD.** By induction on the structure of types, we construct a logical relation $P_\tau \subseteq (\mathbb{R} \Rightarrow \{\tau\}) \times ((\mathbb{R} \Rightarrow \{\overline{\Omega}(\tau)\}) \times (\mathbb{R} \Rightarrow \mathbb{R} \rightarrow \{\overline{\Omega}(\tau)\}))$.

$P_{\text{real}^n} \overset{\text{def}}{=} \{(f, (g, h)) \mid g = f \text{ and } h = Df\}$

$P_1 \overset{\text{def}}{=} \{(((), (x \mapsto r \mapsto ()))\}$

$P_{\tau \times \sigma} \overset{\text{def}}{=} \{(((f, f'), ((g, g'), x \mapsto r \mapsto (h(x)(r), h'(x)(r)))) \mid (f, (g, h)) \in P_\tau, (f', (g', h')) \in P_\sigma\}$

$P_{\tau \rightarrow \sigma} \overset{\text{def}}{=} \{((f, (g, h)) \mid \forall (f', (g', h')) \in P_\tau \cdot \forall x \mapsto f(x)(f'(x)), \forall x \mapsto \pi_1(g(x)g'(x)), x \mapsto r \mapsto h(x)(r)(g'(x)))\}$

Then, we establish the following fundamental lemma.

**Lemma 9.1.** If $t \in \text{Syn}(\tau, \sigma)$ and $f : \mathbb{R} \rightarrow \{\tau\}, g : \mathbb{R} \rightarrow \{\overline{\Omega}(\tau)\}, h : \mathbb{R} \rightarrow \mathbb{R} \rightarrow \{\overline{\Omega}(\tau)\}$ are such that $(f, (g, h)) \in P_\tau$, then $(f; \{t\}, (g; \{\overline{\Omega}(\tau)\}, x \mapsto r \mapsto \{\overline{\Omega}(\tau)\}(g(x))(h(x)(r)))) \in P_\sigma$.

The proof goes via induction on the typing derivation of $t$.

Next, the correctness theorem follows by exactly the argument in the proof of Thm. 8.1.

**Theorem 9.2 (Correctness of Forward AD).** For any typed term $x : \tau + t : \sigma$ in $\text{Syn}$, where $\tau$ and $\sigma$ are first-order types, we have that $\{\overline{\Omega}(\tau)\} = \{t\}$ and $\{\overline{\Omega}(\tau)\} = D\{t\}$.

**Correctness of Reverse AD.** We define, by induction on the structure of types, a logical relation $P_\tau \subseteq (\mathbb{R} \Rightarrow \{\tau\}) \times ((\mathbb{R} \Rightarrow \{\overline{\Omega}(\tau)\}) \times (\mathbb{R} \Rightarrow \mathbb{R} \rightarrow \{\overline{\Omega}(\tau)\}))$.

$P_{\text{real}^n} \overset{\text{def}}{=} \{(f, (g, h)) \mid g = f \text{ and } h = Df\}$

$P_1 \overset{\text{def}}{=} \{(((), (x \mapsto r \mapsto ()))\}$

$P_{\tau \times \sigma} \overset{\text{def}}{=} \{(((f, f'), ((g, g'), x \mapsto r \mapsto (h(x)(r), h'(x)(r)))) \mid (f, (g, h)) \in P_\tau, (f', (g', h')) \in P_\sigma\}$

$P_{\tau \rightarrow \sigma} \overset{\text{def}}{=} \{((f, (g, h)) \mid \forall (f', (g', h')) \in P_\tau \cdot \forall x \mapsto f(x)(f'(x)), \forall x \mapsto \pi_1(g(x)g'(x)), x \mapsto r \mapsto h(x)(r)(g'(x)))\}$

Then, we establish the following fundamental lemma.

**Lemma 9.3.** If $t \in \text{Syn}(\tau, \sigma)$ then $f : \mathbb{R} \rightarrow \{\tau\}, g : \mathbb{R} \rightarrow \{\overline{\Omega}(\tau)\}, h : \mathbb{R} \rightarrow \mathbb{R} \rightarrow \{\overline{\Omega}(\tau)\} \rightarrow \mathbb{R}$ are such that $(f, (g, h)) \in P_\tau$, then $(f; \{t\}, (g; \{\overline{\Omega}(\tau)\}, x \mapsto r \mapsto h(x)((\overline{\Omega}(\tau)\)(g(x))(h(x)(r)))) \in P_\sigma$.

The proof goes via induction on the typing derivation of $t$.

Again, the correctness theorem then follows by exactly the argument in the proof of Thm. 8.1.

**Theorem 9.4 (Correctness of Reverse AD).** For any typed term $x : \tau + t : \sigma$ in $\text{Syn}$, where $\tau$ and $\sigma$ are first-order types, we have that $\{\overline{\Omega}(\tau)\} = \{t\}$ and $\{\overline{\Omega}(\tau)\} = D\{t\}$.

### 9.5 How to Implement the API of the Applied Target Language

We observe that we can implement the API of our applied target language, as follows, in a language that extends the source language with types $\text{List}(\tau)$ of lists of elements of type $\tau$ and a mechanism for creating abstract types, such as a basic module system as found in Haskell (or, a
fortiori, O’Caml). Indeed, we implement $\text{LFun}(\tau, \sigma)$ under the hood, for example, as $\tau \to \sigma$ and $\text{Tens}(\tau, \sigma)$ as $\text{List}(\tau*\sigma)$. The idea is that $\text{LFun}(\tau, \sigma)$, which arose as a right adjoint in our linear language, is essentially a subtype of $\tau \to \sigma$. On the other hand, $\text{Tens}(\tau, \sigma)$, which arose as a left adjoint, is a quotient type of $\text{List}(\tau*\sigma)$. We achieve the desired subtyping and quotient typing by exposing only the API of Fig. 5 and hiding the implementation. We can then implement this interface as follows.

Here, we write $[]$ for the empty list, $t : s$ for the list consisting of $s$ with $t$ prepended on the front, and $\text{fold } t \text{ over } x \text{ in } s \text{ from } acc = init$ for (right) folding an operation $t$ over a list $s$, starting from $init$. Further, the implementer of the AD library can determine which linear operations to include within the implementation of $\text{LFun}$. We expect these linear operations to include various forms of dense and sparse matrix-vector multiplication as well as code for computing Jacobian-vector and Jacobian-adjoint products for the operations op that avoids having to compute the full Jacobian.

This implementation shows that the applied target language is pure and terminating, as is standard for a $\lambda$-calculus extended with lists and some total primitive operations. For completeness, we describe, in Appx. C, the implied big-step operational semantics and prove its adequacy with respect to the denotational semantics $\{\}$. In a principled approach to building a define-then-run AD library, we would shield this implementation using the abstract data types $\text{Tens}(\tau, \sigma)$ and $\text{LFun}(\tau, \sigma)$ as we describe, both for reasons of type safety and because it conveys the intuition behind the algorithm and its correctness. However, nothing stops library implementers from exposing the full implementation. In fact, this seems to be the approach (Vytiniotis et al. 2019) have taken. A downside of this “exposed” approach is that the transformations then no longer respect equational reasoning principles.

9.6 Is this practically relevant? Why exclude map, fold, etc. from your source language?

The aim of this paper is to answer the foundational question of how to perform (reverse) AD at higher types. The problem of how to perform AD of evaluation and currying is highly challenging. For this reason, we have devoted this paper to explaining a solution to that problem in detail, working with a toy language with ground types of black-box, sized arrays $\text{real}^n$ with some first-order operations $\text{op}$. However, many of the interesting applications only arise once we can use higher-order operations such as $\text{map}$ and $\text{fold}$ on $\text{real}^n$.

Our definitions and correctness proofs extend to this setting with higher-order primitives. We plan to discuss and implement them in detail them in an applied follow-up paper. For example, if we add higher-order operations $\text{map } \in \text{Syn}(\text{real } \to \text{real})*\text{real}^n, \text{real}^n$) to the source language, to “map” functions over the black-box arrays, we can define their forward and reverse derivatives as

$$\hat{D}(\text{map})_1(f, v) \equiv \text{map}(f; \text{fst }, v), \quad \hat{D}(\text{map})_2(f, v)(g, w) \equiv \text{map } g + \text{zipWith}(f; \text{snd}) v w,$$

$$\hat{w}(\text{map})_1(f, v) \equiv \text{map}(f; \text{fst }, v), \quad \hat{w}(\text{map})_2(f, v)(w) \equiv \text{zip } w, \text{zipWith } (f; \text{snd}) v w,$$
where we make use of the standard functional programming idiom `zip` and `zipWith`. We assume that we are working internal to the module defining `LFun(τ, σ)` and `Tens(τ, σ)` as we are implementing derivatives of language primitives. As such, we can operate directly on their internal representations which we simply assume to be plain functions and lists of pairs. For a correctness proof, see Appx. D.

Applications frequently require AD of higher-order primitives such as differential and algebraic equation solvers, e.g., for use in pharmacological modelling in Stan (Tsiros et al. 2019). Currently, derivatives of such primitives are derived using the calculus of variations (and implemented with define-by-run AD) (Betancourt et al. 2020; Hannemann-Tamas et al. 2015). Our proof method provides a more lightweight and formal method for calculating, and establishing the correctness of, derivatives for such higher-order primitives. Indeed, most formalizations of the calculus of variations use infinite-dimensional vector spaces and are technically involved (Kriegl and Michor 1997).

10 RELATED WORK

This work is closely related to (Huot et al. 2020), which introduced a similar semantic correctness proof for a version of forward-mode AD, using a subsconing construction. A major difference is that this paper also phrases and proves correctness of reverse-mode AD on a λ-calculus and relates reverse-mode to forward-mode AD. Using a syntactic logical relations proof instead, (Barthe et al. 2020) also proves correctness of forward-mode AD. Again, it does not address reverse AD.

(Cockett et al. 2020) proposes a similar construction to that of §6, and it relates this construction to the differential λ-calculus. This paper develops sophisticated axiomatics for semantic reverse differentiation. However, it neither relates the semantics to a source-code transformation, nor discusses differentiation of higher-order functions.

Importantly, (Elliott 2018) describes and implements what are essentially our source-code transformations, though they were restricted to first-order functions and scalars. (Vytiniotis et al. 2019) sketches an extension of the reverse-mode transformation to higher-order functions in essentially the same way as proposed in this paper. It does not motivate or derive the algorithm or show its correctness. Nevertheless, this short paper discusses important practical considerations for implementing the algorithm, and it discusses a dependently typed variant of the algorithm.

Next, there are various lines of work relating to correctness of reverse-mode AD, which we consider less similar to our work. For example, (Mak and Ong 2020) define and prove correct a formulation of reverse-mode AD on a higher-order language that depends on a non-standard operational semantics, essentially a form of symbolic execution. (Abadi and Plotkin 2020) defines something similar for reverse-mode AD on a first-order language extended with conditionals and iteration. (Brunel et al. 2020) defines an AD algorithm in a simply typed λ-calculus with linear negation and proves it correct using operational techniques. Further, they show that this algorithm corresponds to reverse-mode AD if one uses a non-standard operational semantics. These formulations of reverse-mode AD all depend on non-standard run-times and hence fall into the category of “define-then-run” formulations of reverse-mode AD. Meanwhile, we are concerned with “define-by-run” formulations: source-code transformations producing differentiated code at compile-time, which can then by optimized during compilation with existing compiler tool-chains.

Finally, there is a very long history of work on reverse-mode AD, though almost none of it applies the technique to higher-order functions. A notable exception is (Pearlmutter and Siskind 2008), which gives an impressive implementation of reverse AD as a source-code transformation in Scheme. While very efficient, this implementation crucially uses mutation. Moreover, the transformation is complex and correctness is not considered. More recently, (Wang et al. 2019) describes a
much simpler implementation of a reverse AD code transformation, again very performant. However, the transformation is quite different from the one considered in this paper as it relies on a combination of delimited continuations and mutable state. Correctness is not considered, perhaps because of the semantic complexities introduced by impurity.

Our work adds to the existing literature by presenting (to our knowledge) the first principled and pure define-then-run reverse AD algorithm for a higher-order language, by arguing its practical applicability, and by proving semantic correctness of the algorithm.

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A DEFINING THE CORE ALGORITHMS: AD SOURCE-CODE TRANSFORMATIONS

In particular, $\Sigma_{\text{LSyn}}\Sigma_{\text{LSyn}^\text{op}}$ are both Cartesian closed categories. Hence, by the universal property of $\Sigma_{\text{Syn}}$, we obtain unique structure-preserving macros $\overrightarrow{\mathcal{D}}(\cdot) : \Sigma_{\text{Syn}} \rightarrow \Sigma_{\text{LSyn}}$ (forward AD) and $\overleftarrow{\mathcal{D}}(\cdot) : \Sigma_{\text{Syn}} \rightarrow \Sigma_{\text{LSyn}^\text{op}}$ (reverse AD) once we fix a compatible definition on basic types $\text{real}^n$ and on basic operations $\text{op}$. That is, we need to choose suitable terms $\text{Dop}(x;y)$ and $\text{Dop}'(x;y)$ below to represent to the forward and reverse-mode derivatives of the basic operations $\in \text{Op}_{n_1,\ldots,n_k}$. We choose these representations of derivatives as they allow for efficient Jacobian-vector and Jacobian-adjoint products, which are known to be important to achieve performant AD implementations.

$$\overrightarrow{\mathcal{D}}(\text{real}^n_1)_{\cdot 1} = \overrightarrow{\text{real}}_n \quad \overrightarrow{\mathcal{D}}(\text{real}_n)_{\cdot 2} = \overrightarrow{\text{real}}_n$$

$$\overrightarrow{\mathcal{D}}(\text{op})_{\cdot 1} = \text{op} \quad \overrightarrow{\mathcal{D}}(\text{op})_{\cdot 2} \triangleq x : \text{real}^{n_1} \ldots \text{real}^{n_k} ; y : \text{real}^{m_1} \ldots \text{real}^{m_k} \vdash \text{Dop}(x;y) : \text{real}^m$$

$$\overrightarrow{\mathcal{D}}(\text{real}^n_1)_{\cdot 1} = \overrightarrow{\text{real}}_n \quad \overrightarrow{\mathcal{D}}(\text{real}_n)_{\cdot 2} = \overrightarrow{\text{real}}_n$$

$$\overrightarrow{\mathcal{D}}(\text{op})_{\cdot 1} = \text{op} \quad \overrightarrow{\mathcal{D}}(\text{op})_{\cdot 2} \triangleq x : \text{real}^{n_1} \ldots \text{real}^{n_k} ; y : \text{real}^m + \text{Dop}'(x;y) : \text{real}^{n_1} \ldots \text{real}^{n_k}$$

For the AD transformations to be correct, it is important that these derivatives of language primitives are implemented correctly in the sense that

$$[x;y \vdash \text{Dop}(x;y)] = D[\text{op}] \quad [x;y \vdash \text{Dop}'(x;y)] = D[\text{op}]'.$$

The implementation of such derivatives for language primitives is a subtle task that is constantly undertaken in practice by AD library developers, whenever a new primitive operation is added to the library.

The extension of the AD macros $\overrightarrow{\mathcal{D}}$ and $\overleftarrow{\mathcal{D}}$ to the full source language are now determined canonically as the unique Cartesian closed functor extending the previous definitions. However, because of the counter-intuitive nature of the Cartesian closed structures on $\Sigma_{\text{LSyn}}\Sigma_{\text{LSyn}^\text{op}}$, we still consider it worthwhile to list the resulting definitions here, particularly as these transformations lend themselves well to implementation and are highly practically relevant.

A.1 Forward-Mode AD

We define $\overrightarrow{\mathcal{D}}(\cdot)$ on types as

$$\overrightarrow{\mathcal{D}}(\text{1})_{\cdot 1} = 1 \quad \overrightarrow{\mathcal{D}}(\text{1})_{\cdot 2} = 1$$

$$\overrightarrow{\mathcal{D}}(\tau \bullet \sigma)_{\cdot 1} = \overrightarrow{\mathcal{D}}(\tau)_{\cdot 1} \bullet \overrightarrow{\mathcal{D}}(\sigma)_{\cdot 1} \quad \overrightarrow{\mathcal{D}}(\tau \bullet \sigma)_{\cdot 2} = \overrightarrow{\mathcal{D}}(\tau)_{\cdot 2} \bullet \overrightarrow{\mathcal{D}}(\sigma)_{\cdot 2}$$

$$\overrightarrow{\mathcal{D}}(\tau \rightarrow \sigma)_{\cdot 1} = \overrightarrow{\mathcal{D}}(\tau)_{\cdot 1} \rightarrow (\overrightarrow{\mathcal{D}}(\sigma)_{\cdot 1} \bullet \overrightarrow{\mathcal{D}}(\tau)_{\cdot 2} \rightarrow \overrightarrow{\mathcal{D}}(\sigma)_{\cdot 2}) \quad \overrightarrow{\mathcal{D}}(\tau \rightarrow \sigma)_{\cdot 2} = \overrightarrow{\mathcal{D}}(\tau)_{\cdot 1} \rightarrow \overrightarrow{\mathcal{D}}(\sigma)_{\cdot 2}.$$
Correct Reverse AD at Higher Types

A.2 Reverse-Mode AD

We define $\overrightarrow{D}(-)$ on types as

$\overrightarrow{D}(\mathbf{1})_1 \overset{\Delta}{=} \mathbf{1}$

$\overrightarrow{D}(\mathbf{1})_2 \overset{\Delta}{=} \mathbf{1}$

$\overrightarrow{D}(\tau * \sigma)_1 \overset{\Delta}{=} \overrightarrow{D}(\tau)_1 \cdot \overrightarrow{D}(\sigma)_1$

$\overrightarrow{D}(\tau * \sigma)_2 \overset{\Delta}{=} \overrightarrow{D}(\tau)_2 \cdot \overrightarrow{D}(\sigma)_2$

$\overrightarrow{D}(\tau \rightarrow \sigma)_1 \overset{\Delta}{=} \overrightarrow{D}(\tau)_1 \cdot \overrightarrow{D}(\sigma)_1 * \overrightarrow{D}(\tau)_2 \rightarrow \overrightarrow{D}(\sigma)_2$

$\overrightarrow{D}(\tau \rightarrow \sigma)_2 \overset{\Delta}{=} \overrightarrow{D}(\tau)_2 \cdot \overrightarrow{D}(\sigma)_2$

On programs, we define it as

$\overrightarrow{D}(\text{id}_\tau)_1 \overset{\Delta}{=} x: \overrightarrow{D}(\tau)_1 \vdash x: \overrightarrow{D}(\tau)_1$

$\overrightarrow{D}(\text{id}_\tau)_2 \overset{\Delta}{=} x_1: \overrightarrow{D}(\tau)_1; x_2: \overrightarrow{D}(\tau)_2 \vdash x_2: \overrightarrow{D}(\tau)_2$

$\overrightarrow{D}(\text{snd}_\tau)_1 \overset{\Delta}{=} x: \overrightarrow{D}(\tau)_1 \vdash \text{snd} x: \overrightarrow{D}(\tau)_1$

$\overrightarrow{D}(\text{snd}_\tau)_2 \overset{\Delta}{=} x: \overrightarrow{D}(\tau)_1 \vdash \text{snd} x: \overrightarrow{D}(\tau)_2$

$\overrightarrow{D}(\text{ev}_\tau)_1 \overset{\Delta}{=} x: \overrightarrow{D}(\tau)_1 \vdash \lambda y. \overrightarrow{D}(\text{snd}_\tau)_1 \cdot \overrightarrow{D}(\tau)_2 \cdot \overrightarrow{D}(\tau)_2 \vdash \text{snd} x: \overrightarrow{D}(\tau)_2$

$\overrightarrow{D}(\text{ev}_\tau)_2 \overset{\Delta}{=} x_1: \overrightarrow{D}(\tau)_1 \vdash (\overrightarrow{D}(\tau)_1 \cdot \overrightarrow{D}(\tau)_2 \cdot \overrightarrow{D}(\tau)_2) \vdash \text{snd} x_1: \overrightarrow{D}(\tau)_2$

let $y = \text{snd} x_1 \in (\text{snd} x_2) + (\text{snd} (\text{snd} x_1)) \cdot \text{snd} x_2: \overrightarrow{D}(\tau)_2$

$\overrightarrow{D}(\Lambda_{\tau, \sigma, \rho}(t))_1 \overset{\Delta}{=} x: \overrightarrow{D}(\tau)_1 \rightarrow \text{snd} x: \overrightarrow{D}(\tau)_2$

$\overrightarrow{D}(\Lambda_{\tau, \sigma, \rho}(t))_2 \overset{\Delta}{=} x_1: \overrightarrow{D}(\tau)_1 \vdash \lambda y_1. \overrightarrow{D}(\tau)_2 \cdot \overrightarrow{D}(\tau)_2 \cdot \overrightarrow{D}(\tau)_2 \vdash \text{snd} x_1: \overrightarrow{D}(\tau)_2$

where $z: \overrightarrow{D}(\tau)_1 \cdot \overrightarrow{D}(\tau)_1 \vdash t: \overrightarrow{D}(\rho)_1 \cdot z_1: \overrightarrow{D}(\tau)_1 \cdot \overrightarrow{D}(\tau)_1 \cdot \overrightarrow{D}(\tau)_2 + \overrightarrow{D}(\tau)_2: \overrightarrow{D}(\rho)_2$

$\overrightarrow{D}(\Lambda_{\tau, \sigma, \rho}(t))_2 \overset{\Delta}{=} x_1: \overrightarrow{D}(\tau)_1 \vdash \lambda y_1. \overrightarrow{D}(\tau)_2 \cdot \overrightarrow{D}(\tau)_2 \cdot \overrightarrow{D}(\tau)_2 \vdash \text{snd} x_1: \overrightarrow{D}(\tau)_2$

where $x : \overrightarrow{D}(\tau)_1 \vdash \overrightarrow{D}(\tau)_1 \cdot \overrightarrow{D}(\tau)_1 \cdot \overrightarrow{D}(\tau)_1$ and $y : \overrightarrow{D}(\tau)_1 \vdash \overrightarrow{D}(\tau)_1 \cdot \overrightarrow{D}(\tau)_1$

$\overrightarrow{D}(\langle \rangle)_1 \overset{\Delta}{=} \mathbf{1}$

$\overrightarrow{D}(\langle \rangle)_2 \overset{\Delta}{=} \mathbf{1}$
\[\tilde{\mathcal{D}}((t,s))_1 \overset{\text{def}}{=} \langle \tilde{\mathcal{D}}(t)_1, \tilde{\mathcal{D}}(s)_1 \rangle\]
\[\tilde{\mathcal{D}}((t,s))_2 \overset{\text{def}}{=} x_1 : \tilde{\mathcal{D}}(\tau)_1; x_2 : \tilde{\mathcal{D}}(\sigma)_2 \triangleleft \tilde{\mathcal{D}}(t)_{\text{fst}}(x_1/x_2) + \tilde{\mathcal{D}}(s)_{\text{snd}}(x_2/x_2) : \tilde{\mathcal{D}}(\tau)_2\]
where \(y_1 : \tilde{\mathcal{D}}(\tau)_1; y_2 : \tilde{\mathcal{D}}(\sigma)_2 \triangleleft \tilde{\mathcal{D}}(t)_2 : \tilde{\mathcal{D}}(\tau)_2\) and \(z_1 : \tilde{\mathcal{D}}(\tau)_1; z_2 : \tilde{\mathcal{D}}(\sigma)_2 + \tilde{\mathcal{D}}(s)_2 : \tilde{\mathcal{D}}(\tau)_2\)

\[\tilde{\mathcal{D}}(\text{fst}, \sigma)_1 \overset{\text{def}}{=} x : \tilde{\mathcal{D}}(\tau)_1 \triangleleft \tilde{\mathcal{D}}(\sigma)_1 + \text{fst } x : \tilde{\mathcal{D}}(\tau)_1\]
\[\tilde{\mathcal{D}}(\text{fst}, \sigma)_2 \overset{\text{def}}{=} \langle : \tilde{\mathcal{D}}(\tau)_1 \triangleleft \tilde{\mathcal{D}}(\sigma)_1; y : \tilde{\mathcal{D}}(\tau)_2 \triangleleft \langle y, y \rangle : \tilde{\mathcal{D}}(\tau)_2 \triangleleft \tilde{\mathcal{D}}(\sigma)_2\]

\[\tilde{\mathcal{D}}(\text{snd}, \sigma)_1 \overset{\text{def}}{=} x : \tilde{\mathcal{D}}(\tau)_1 \triangleleft \tilde{\mathcal{D}}(\sigma)_1 + \text{snd } x : \tilde{\mathcal{D}}(\sigma)_1\]
\[\tilde{\mathcal{D}}(\text{snd}, \sigma)_2 \overset{\text{def}}{=} \langle : \tilde{\mathcal{D}}(\tau)_1 \triangleleft \tilde{\mathcal{D}}(\sigma)_1; y : \tilde{\mathcal{D}}(\tau)_2 \triangleleft \langle y, y \rangle : \tilde{\mathcal{D}}(\tau)_2 \triangleleft \tilde{\mathcal{D}}(\sigma)_2\]

\[\tilde{\mathcal{D}}(\text{ev}, \sigma)_1 \overset{\text{def}}{=} x : (\tilde{\mathcal{D}}(\tau)_1 \rightarrow (\tilde{\mathcal{D}}(\sigma)_1 \triangleleft \tilde{\mathcal{D}}(\tau)_2)) \triangleleft \tilde{\mathcal{D}}(\sigma)_2 + \text{ev } x : \tilde{\mathcal{D}}(\sigma)_2\]

\[\tilde{\mathcal{D}}(\text{ev}, \sigma)_2 \overset{\text{def}}{=} x_1 : (\tilde{\mathcal{D}}(\tau)_1 \rightarrow (\tilde{\mathcal{D}}(\sigma)_1 \triangleleft \tilde{\mathcal{D}}(\tau)_2)) \triangleleft \tilde{\mathcal{D}}(\tau)_2 \triangleleft \tilde{\mathcal{D}}(\sigma)_2\]

\[\tilde{\mathcal{D}}(\Lambda, \rho)(t) \overset{\text{def}}{=} \text{let } y : \text{snd } x_1 \text{ in } \langle !y \otimes x_2, \text{snd } ((\text{fst } x_1 y) \{x_2\}) : \langle !\tilde{\mathcal{D}}(\tau)_1 \triangleleft \tilde{\mathcal{D}}(\tau)_2 \triangleleft \tilde{\mathcal{D}}(\sigma)_2\]

\[\tilde{\mathcal{D}}(\Lambda, \rho)(t) \overset{\text{def}}{=} x_1 : \tilde{\mathcal{D}}(\tau)_1; x_2 : !\tilde{\mathcal{D}}(\tau)_1 \triangleleft \tilde{\mathcal{D}}(\sigma)_2 + \text{case } x_2 \text{ of } !y \otimes z_2 \rightarrow \text{fst } \text{ev } \langle x_1, y \rangle \{z_1\} : \tilde{\mathcal{D}}(\tau)_2\]

where \(z_1 : \tilde{\mathcal{D}}(\tau)_1 \triangleleft \tilde{\mathcal{D}}(\tau)_2 \triangleleft \tilde{\mathcal{D}}(\sigma)_2; z_2 : \tilde{\mathcal{D}}(\sigma)_2 \triangleleft \tilde{\mathcal{D}}(\tau)_2 \triangleleft \tilde{\mathcal{D}}(\sigma)_2\)

### B A MANUAL CORRECTNESS PROOF OF AD THROUGH SEMANTIC LOGICAL RELATIONS

**Correctness of Forward AD.** By induction on the structure of types, we construct a logical relation \(P_t \subseteq (\mathbb{R} \rightarrow \{|\tau|\}) \times ((\mathbb{R} \rightarrow \{\tilde{\mathcal{D}}(\tau)_1\}) \times (\mathbb{R} \rightarrow \mathbb{R} \rightarrow \{\tilde{\mathcal{D}}(\tau)_2\}))\).

\(P_{t^\text{real}} \overset{\text{def}}{=} \{ (f, (g, h)) \mid g = f \text{ and } h = Df \} \quad P_1 \overset{\text{def}}{=} \{ (((), (), x \mapsto r \mapsto r)) \}

\(P_{t^\sigma} \overset{\text{def}}{=} \{ (((f, f'), (g, g')), x \mapsto r \mapsto (h(x)(r), h'(x)(r))) \mid (f, (g, h)) \in P_r, (f', (g', h')) \in P_{\sigma} \}

\(P_{t^\rightarrow \sigma} \overset{\text{def}}{=} \{ ((f, (g, h)) \mid \forall (f', (g', h')) \in P_r. (x \mapsto f(x)(f'(x)), (x \mapsto \pi_1(g(x)(g'(x))))),
\quad x \mapsto r \mapsto (\pi_2(g(x)(g'(x)))(h'(x)(r) + h(x)(r)(g'(x)))) \in P_{\sigma} \}\}

Then, we establish the following fundamental lemma.

**Lemma B.1.** If \(t \in \text{Syn}(\tau, \sigma)\) and \(f : \mathbb{R} \rightarrow \{|\tau|\}, g : \mathbb{R} \rightarrow \{\tilde{\mathcal{D}}(\tau)_1\}, h : \mathbb{R} \rightarrow \mathbb{R} \rightarrow \{\tilde{\mathcal{D}}(\tau)_2\}\) are such that \((f, (g, h)) \in P_r\), then \((f; \{t\}, (g; \tilde{\mathcal{D}}(t)_1), x \mapsto r \mapsto \langle \tilde{\mathcal{D}}(t)_2 \rangle(g(x))(h(x)(r))) \in P_{\sigma}\)

**Proof.** We prove this by induction on the typing derivation of well-typed terms. We start with the cases of ev and \(\Lambda(t)\) as they are by far the most interesting. Consider \(ev \in \text{Syn}((\tau \rightarrow \sigma)*r, \sigma)\). Then

\[\tilde{\mathcal{D}}(\text{ev})_1 \in \text{Syn}((\tilde{\mathcal{D}}(\tau)_1 \rightarrow (\tilde{\mathcal{D}}(\sigma)_1 \triangleleft \tilde{\mathcal{D}}(\tau)_2)) \triangleleft \tilde{\mathcal{D}}(\sigma)_2)\]

\[\tilde{\mathcal{D}}(\text{ev})_2 \in \text{Syn}(((\tilde{\mathcal{D}}(\tau)_1 \rightarrow (\tilde{\mathcal{D}}(\sigma)_1 \triangleleft \tilde{\mathcal{D}}(\tau)_2)) \triangleleft \tilde{\mathcal{D}}(\sigma)_2) \triangleleft \tilde{\mathcal{D}}(\tau)_1)_1\]

\[\text{LFun}((\tilde{\mathcal{D}}(\tau)_1 \rightarrow \tilde{\mathcal{D}}(\tau)_2) \triangleleft \tilde{\mathcal{D}}(\tau)_2, \tilde{\mathcal{D}}(\sigma)_2))\]
Then
\[
\|ev\|(f, x) = f x
\]
\[
\|\overline{\exists}(ev)_1\|(f, x) = \pi_1(f x)
\]
\[
\|\overline{\exists}(ev)_2\|(f, x)(g, y) = (\pi_2(f x)) y + g x.
\]
Suppose that \((f, (g, h)) \in P_{(\tau \to \sigma)\rightarrow \rho}\). That is, \(f = (f_1, f_2), g = (g_1, g_2)\) and \(h(x)(r) = (h_1(x)(r), h_2(x)(r))\) for \((f_1, (g_1, h_1)) \in P_{\tau \to \sigma}\) and \((f_2, (g_2, h_2)) \in P_{\tau}\). Then, we want to show that
\[
((f_1, f_2), \|ev\|, ((g_1, g_2); \|\overline{\exists}(ev)_1\|), x \mapsto r \mapsto \|\overline{\exists}(ev)_2\|((g_1(x), g_2(x))(h_1(x)(r), h_2(x)(r)))) \in P_{\sigma}
\]
which is to say that
\[
(x \mapsto f_1(x)(f_2(x)),
(x \mapsto \pi_1(g_1(x))(g_2(x)),
(x \mapsto r \mapsto (\pi_2(g_1(x))(g_2(x)))(h_2(x)(r)) + h_1(x)(r)(g_2(x)))) \in P_{\sigma}.
\]
This holds because \((f_1, (g_1, h_1)) \in P_{\tau \to \sigma}\) by definition of \(P_{\tau \to \sigma}\).
Suppose that the fundamental lemma holds for \(t \in \text{Syn}(\tau \ast \sigma, \rho)\). We then have that
\[
\overline{\exists}(t)_1 \in \text{Syn}(\overline{\exists}(\tau)_1 \ast \overline{\exists}(\sigma)_1, \overline{\exists}(\rho)_1)
\]
\[
\overline{\exists}(t)_2 \in \text{Syn}(\overline{\exists}(\tau)_1 \ast \overline{\exists}(\sigma)_1, \text{LFun}(\overline{\exists}(\tau)_2 \ast \overline{\exists}(\sigma)_2, \overline{\exists}(\rho)_2)).
\]
Then, we show that \(\Lambda(t) \in \text{Syn}(\tau, \sigma \to \rho)\) does as well. Now,
\[
\overline{\exists}(\Lambda(t))_1 \in \text{Syn}(\overline{\exists}(\tau)_1, \overline{\exists}(\sigma)_1 \to (\overline{\exists}(\rho)_1 \ast (\overline{\exists}(\sigma)_2 \to \overline{\exists}(\rho)_2)))
\]
\[
\overline{\exists}(\Lambda(t))_2 \in \text{Syn}(\overline{\exists}(\tau)_1, \text{LFun}(\overline{\exists}(\tau)_2, \overline{\exists}(\sigma)_1 \to \overline{\exists}(\rho)_2)).
\]
Then
\[
\|\Lambda(t)\|((x)(y) = \|t\|(x, y)
\]
\[
\|\overline{\exists}(\Lambda(t))_1\|((x)(y) = (\|\overline{\exists}(t)\|((x, y), w \mapsto \|\overline{\exists}(t)_2\|((x, y), (0, w))))
\]
\[
\|\overline{\exists}(\Lambda(t))_2\|((x)(v) = \|\overline{\exists}(t)_2\|((x, v), (0, v), 0).
\]
Suppose that \((f, (g, h)) \in P_{\tau}\). We need to show that \((f; \|\Lambda(t)\|, (g; \|\overline{\exists}(\Lambda(t))_1\|), x \mapsto r \mapsto \|\overline{\exists}(\Lambda(t))_2\|((g(x))(h(x)(r)))) \in P_{\sigma \to \rho}\). That is, that
\[
(x \mapsto (y \mapsto \|t\|(f(x), y)),
(x \mapsto (y \mapsto (\|\overline{\exists}(t)\|(g(x), y), w \mapsto \|\overline{\exists}(t)_2\|((g(x), y)(0, w)))),
(x \mapsto r \mapsto (y \mapsto \|\overline{\exists}(t)_2\|((g(x), y)(h(x)(r), 0)))) \in P_{\sigma \to \rho}.
\]
This requirement is equivalent to the statement that for all \((f', (g', h')) \in P_{\sigma}\),
\[
(x \mapsto \|t\|(f(x), f'(x)),
(x \mapsto \|\overline{\exists}(t)\|(g(x), g'(x)),
(x \mapsto r \mapsto \|\overline{\exists}(t)_2\|((g(x), g'(x))(0, h'(x), r)) + \|\overline{\exists}(t)_2\|((g(x), g'(x))(h(x)(r), 0))) \in P_{\rho}
\]
As \(w \mapsto \|\overline{\exists}(t)_2\|((g(x), g'(x))(w))\) is linear in \(w\) by virtue of its type, it is enough to show that
\[
(x \mapsto \|t\|(f(x), f'(x)),
(x \mapsto \|\overline{\exists}(t)\|(g(x), g'(x)),
\]
(x, r) \mapsto [\overrightarrow{D}(t)_{2}](g(x), g'(x))(h(x)(r), h'(x)(r))) \in P_{\rho}

which is true as \((f, (g, h)) \in P_{\tau} and (f', (g', h')) \in P_{\sigma}\) by assumption while \([t]\) respects the logical relation by our induction hypothesis.

Consider \(\mathsf{fst} \in \text{Syn}(\tau \ast \sigma, \tau)\) (the case for \(\mathsf{snd}\) will be almost identical so we omit it). Then

\[
\overrightarrow{D}(\mathsf{fst})_{1} \in \text{Syn}(\overrightarrow{D}(\tau)_{1} \ast \overrightarrow{D}(\sigma)_{1}, \overrightarrow{D}(\tau)_{1})
\]

\[
\overrightarrow{D}(\mathsf{fst})_{2} \in \text{Syn}(\overrightarrow{D}(\tau)_{1} \ast \overrightarrow{D}(\sigma)_{1}, \text{LFun}(\overrightarrow{D}(\tau)_{2} \ast \overrightarrow{D}(\sigma)_{2}, \overrightarrow{D}(\tau)_{2}))
\]

and

\[
\begin{align*}
[\mathsf{fst}](x, y) &= x \\
[\overrightarrow{D}(\mathsf{fst})_{1}](x, y) &= x \\
[\overrightarrow{D}(\mathsf{fst})_{2}](x, y)(v, w) &= v.
\end{align*}
\]

Suppose that \((f, (g, h)) \in P_{\tau \ast \sigma}\). That is, \(f = (f_{1}, f_{2}), g = (g_{1}, g_{2})\) and \(h(x)(r) = (h_{1}(x)(r), h_{2}(x)(r))\) for some \((f_{1}, (g_{1}, h_{1})) \in P_{\tau}\) and \((f_{2}, (g_{2}, h_{2})) \in P_{\sigma}\). Then, we need to show that

\[
(f; [\mathsf{fst}], (g; [\overrightarrow{D}(\mathsf{fst})_{1}]), x \mapsto r \mapsto [\overrightarrow{D}(\mathsf{fst})_{2}](g(x))(h(x)(r))) \in P_{\tau}
\]

i.e.

\[
(f_{1}, (g_{1}, h_{1})) \in P_{\tau}.
\]

But that’s true by assumption!

Suppose that \(t \in \text{Syn}(\tau, \sigma)\) and \(s \in \text{Syn}(\tau, \rho)\) respect the logical relation. Then, we want to show that \(\langle t, s \rangle \in \text{Syn}(\tau, \sigma \ast \rho)\) does as well. Now,

\[
[\overrightarrow{D}(\langle t, s \rangle)_{1}] \in \text{Syn}(\overrightarrow{D}(\tau)_{1}, \overrightarrow{D}(\sigma)_{1} \ast \overrightarrow{D}(\rho)_{1})
\]

\[
[\overrightarrow{D}(\langle t, s \rangle)_{2}] \in \text{Syn}(\overrightarrow{D}(\tau)_{1}, \text{LFun}(\overrightarrow{D}(\tau)_{2} \ast \overrightarrow{D}(\rho)_{2}, \overrightarrow{D}(\tau)_{2}))
\]

and

\[
\begin{align*}
[\langle t, s \rangle](x) &= ([t](x), [s](x)) \\
[\overrightarrow{D}(\langle t, s \rangle)_{1}](x) &= (\overrightarrow{D}(t)_{1}(x), \overrightarrow{D}(s)_{1}(x)) \\
[\overrightarrow{D}(\langle t, s \rangle)_{2}](x)(v) &= (\overrightarrow{D}(t)_{2}(x)(v), \overrightarrow{D}(s)_{2}(x)(v)).
\end{align*}
\]

Suppose that \((f, (g, h)) \in P_{\tau}\. We want to show that

\[
(f; [\langle t, s \rangle], (g; [\overrightarrow{D}(\langle t, s \rangle)_{1}]), x \mapsto r \mapsto [\overrightarrow{D}(\langle t, s \rangle)_{2}](g(x))(h(x)(r))) \in P_{\sigma \ast \rho}
\]

i.e.

\[
((f; [t]), f; ([s]), (g; [\overrightarrow{D}(t)_{1}]), g; [\overrightarrow{D}(s)_{1}]),
\]

\[
x \mapsto r \mapsto ([\overrightarrow{D}(t)_{2}](g(x))(h(x)(r)), [\overrightarrow{D}(s)_{2}](g(x))(h(x)(r))) \in P_{\sigma \ast \rho}.
\]

Which holds by definition of \(P_{\sigma \ast \rho}\) as \(t\) and \(s\) respect the logical relation by assumption.

Consider \(\langle \rangle \in \text{Syn}(\tau, 1)\). Observe that

\[
\overrightarrow{D}(\langle \rangle)_{1} \in \text{Syn}(\overrightarrow{D}(\tau)_{1}, 1)
\]

\[
\overrightarrow{D}(\langle \rangle)_{2} \in \text{Syn}(\overrightarrow{D}(\tau)_{1}, \text{LFun}(\overrightarrow{D}(\tau)_{2}, 1))
\]

and

\[
\begin{align*}
[\langle \rangle](x) &= () \\
[\overrightarrow{D}(\langle \rangle)_{1}](x) &= () \\
[\overrightarrow{D}(\langle \rangle)_{2}](x)(v) &= ()
\end{align*}
\]
Correct Reverse AD at Higher Types

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Suppose that \((f, (g, h)) \in P_r\). Then, we need to show that
\[
(f; \{\{\}\}, \{\langle g, \{\{D(\{\} )\}_1\}_1\}\}, x \mapsto r \mapsto \{\{D(\{\} )\}_2\}_1(g(x)(h(x)(r)))) \in P_1.
\]
That is, we need to show that \((\langle \rangle, (\langle \rangle, (\langle \rangle))) \in P_1\), but that holds by definition of \(P_1\).

Consider \(id \in \text{Syn}(\tau, \tau)\). Observe that
\[
\{\{id\}_1\}_1 \in \text{Syn}(\{\{D\}_1\}_1, \{\{D\}_1\}_1)
\]
and
\[
\{\{id\}_2\}_1 \in \text{Syn}(\{\{D\}_2\}_1, \text{LFun}(\{\{D\}_2\}_2, \{\{D\}_2\}_2)).
\]

Suppose that \((f, (g, h)) \in P_r\). Then, we need to show that
\[
(f; \{\{id\}_1\}, \{\langle g, \{\{D\}_1\}_1\}\}_1\}, x \mapsto r \mapsto \{\{D\}_2\}_1((g(x)(h(x)(r)))) \in P_r.
\]
That is, we need to show that \((f, (g, h)) \in P_r\), but that holds by assumption.

Consider composition: suppose that \(t \in \text{Syn}(\tau, \sigma)\) and \(s \in \text{Syn}(\sigma, \rho)\) both respect the logical relation. Then, \(t; s \in \text{Syn}(\tau, \rho)\). Further,
\[
\{\{t; s\}_1\}_1(x) = \{\{s\}_1\}_1(\{\{t\}_1\}_1(x))
\]
\[
\{\{t; s\}_2\}_1(x)(v) = \{\{t\}_1\}_1(\{\{s\}_2\}_1(\{\{t\}_1\}_1(x))(\{\{s\}_2\}_1(x)(v))
\]
\[
\{\{t; s\}_2\}_2(x)(v) = \{\{t\}_1\}_2(\{\{s\}_2\}_2(\{\{t\}_1\}_2(x))(\{\{s\}_2\}_2(x)(v)).
\]

Suppose that \((f, (g, h)) \in P_r\). We need to show that
\[
(f; \{\{t; s\}_1\}, \{\langle g, \{\{D\}_1\}_1\}\}_1\}, x \mapsto r \mapsto \{\{D\}_2\}_1((g(x)(h(x)(r)))) \in P_\rho.
\]
That is,
\[
(f; \{\{t\}_1\}, \{\{g\}_1\}_1\}_1\),
\[
\{\{D(t)\}_1\}_1; \{\{D(s)\}_1\}_1\},
\]
\[
x \mapsto r \mapsto \{\{D(t)\}_2\}_1(\{\{D(t)\}_1\}_1(x))(\{\{D(s)\}_2\}_1(\{\{D(t)\}_2\}_1(g(x)(h(x)(r)))) \in P_\rho.
\]
But that follows from the fact that \(s\) respects the logical relation as
\[
(f; \{\{t\}_1\},
\[
\{\{g\}_1\}_1\}_1\},
\]
\[
x \mapsto r \mapsto \{\{D(t)\}_2\}_1(g(x)(h(x)(r)))) \in P_\rho.
\]
since \(t\) respects the logical relation.

The base cases of operations hold by the chain rule. Indeed, consider \(op \in \text{Syn}(\text{real}^{n_1} \cdots \text{real}^{n_k}, \text{real}^{m})\). Note that \(op = \{\{D\}_1\}_1 \in \text{Syn}(\text{real}^{n_1} \cdots \text{real}^{n_k}, \text{real}^{m})\) and \(Dop = \{\{D\}_2\}_2 \in \text{Syn}(\text{real}^{n_1} \cdots \text{real}^{n_k}, \text{LFun}(\text{real}^{n_1} \cdots \text{real}^{n_k}, \text{real}^{m}))\). We have that
\[
\{\{op\}_1\}_1(x) = \{\{D\}_1\}_1(\{\{op\}_1\}_1(x))
\]
\[
\{\{D\}_2\}_2(x)(v) = \{\{Dop\}_1\}_1(x)(v) = D\{\{op\}_1\}_1(x)(v),
\]
where we use the crucial assumption that the derivatives of primitive operations are implemented correctly. Then, let \((f, (g, h)) \in P_{\text{real}^{n_1} \cdots \text{real}^{n_k}}\). That is, \((f, (g, h)) = ((f_1, \ldots, f_k), ((g_1, \ldots, g_k), x \mapsto\).
r \mapsto (h_1(x)(r), \ldots, h_k(x)(r)))$, for $(f_i, (g_i, h_i)) \in P_{\text{real}}^{\nu_i}$, for $1 \leq i \leq k$. We want to show that $(f; \{g\}; \{\overline{D}(\sigma)\}_1)^{(x)(r) \mapsto r} \in P_{\text{real}}^m$. That is,

\[
(f; \{g\}; \{\overline{D}(\sigma)\}_x \mapsto r \mapsto D\{g\}(g(x))(h(x)(r))) \in P_{\text{real}}^m.
\]

That is,

\[
((f_1, \ldots, f_k); \{g\}; (g_1, \ldots, g_k); \{\overline{D}(\sigma)\}, x \mapsto r \mapsto D\{g\}(g(x))(h_1(x)(r), \ldots, h_k(x)(r))) \in P_{\text{real}}^m.
\]

By the assumption that $(f, (g, h_i)) \in P_{\text{real}}^{\nu_i}$, we have that $g_i = f_i$ and $h_i = Df_i$. Therefore, we need to show that

\[
((f_1, \ldots, f_k); \{g\}; (f_1, \ldots, f_k); \{\overline{D}(\sigma)\}, x \mapsto r \mapsto D\{g\}(f_1(x)(r), \ldots, Df_k(x)(r))) \in P_{\text{real}}^m.
\]

Using the chain rule for multivariate differentiation (and a little bit of linear algebra), this is equivalent to,

\[
((f_1, \ldots, f_k); \{g\}; (f_1, \ldots, f_k); \{\overline{D}(\sigma)\}, D((f_1, \ldots, f_k); \{\overline{D}(\sigma)\})) \in P_{\text{real}}^m.
\]

Therefore, the fundamental lemma follows.

Next, the correctness theorem follows by exactly the argument in the proof of Thm. 8.1.

**Theorem B.2 (Correctness of Forward AD).** For any typed term $x : \tau + t : \sigma$ in $\text{Syn}$, where $\tau$ and $\sigma$ are first-order types, we have that

\[
\{\overline{D}(\tau)_1\} = \{t\} \quad \text{and} \quad \{\overline{D}(\tau)_2\} = D\{t\}.
\]

**Correctness of Reverse AD.** We define, by induction on the structure of types, a logical relation

\[
P_{\tau} \subseteq (\mathbb{R} \to \{\tau\}) \times ((\mathbb{R} \to \{\overline{D}(\tau)_1\}) \times (\mathbb{R} \to \{\overline{D}(\tau)_2\} \to \mathbb{R})).
\]

\[
P_{\text{real}}^{\nu_1} \overset{\text{def}}{=} \{(f, (g, h)) \mid g = f \quad \text{and} \quad h = (Df)^f\}
\]

\[
P_{\tau} \times \sigma \overset{\text{def}}{=} \{((f, f'), ((g, g'), x \mapsto \tau \mapsto h(x)(\pi_1)) \wedge h'(x)(\pi_2)) \mid (f, (g, h)) \in P_{\tau}, (f', (g', h')) \in P_{\sigma}\}
\]

\[
P_{\tau \to \sigma} \overset{\text{def}}{=} \{(f, (g, h)) \mid \forall (f', (g', h')) \in P_{\tau}, (x \mapsto f(x)(f'(x)), (x \mapsto \pi_1(g)(g'(x))))\}
\]

\[
x \mapsto \tau \mapsto h(x)((g'(x) \otimes \tau) + h'(x)((\pi_2(g)(g'(x))))(\pi_2)) \in P_{\sigma}\}
\]

Then, we establish the following fundamental lemma.

**Lemma B.3.** If $t \in \text{Syn}(\tau, \sigma)$ then $f : \mathbb{R} \to \{\tau\}$, $g : \mathbb{R} \to \{\overline{D}(\tau)_1\}$, $h : \mathbb{R} \times \{\overline{D}(\tau)_2\} \to \mathbb{R}$ are such that $(f, (g, h)) \in P_{\tau}$, then $(f; \{t\}, (g; \{\overline{D}(t)_1\}, x \mapsto \tau \mapsto h(x)(\{\overline{D}(t)_2\}(g(x))(\pi_2)) \in P_{\sigma}$.

**Proof.** The proof goes by induction on the typing derivation of well-typed terms $t \in \text{Syn}$. Indeed, we first consider the cases of evaluation and currying, as they are the most interesting. Consider $\text{ev} \in \text{Syn}((\tau \rightarrow \sigma) \times \tau, \sigma)$. Then

\[
\overline{D}(\text{ev})_1 \in \text{Syn}((\overline{D}(\tau)_1) \rightarrow (\overline{D}(\sigma)_1) \times (\overline{D}(\tau)_2) \rightarrow \overline{D}(\tau)_1) \times (\overline{D}(\sigma)_1) \times (\overline{D}(\tau)_2) \rightarrow \overline{D}(\tau)_1) \rightarrow \overline{D}(\tau)_1)
\]

\[
\overline{D}(\text{ev})_2 \in \text{Syn}((\overline{D}(\tau)_1) \rightarrow (\overline{D}(\sigma)_1) \times (\overline{D}(\tau)_2) \rightarrow \overline{D}(\tau)_2) \rightarrow \overline{D}(\tau)_2)
\]

\[
\overline{D}(\text{ev})_2 \times \sigma = (\overline{D}(\tau)_1 \times (\overline{D}(\sigma)_1) \times (\overline{D}(\tau)_2) \rightarrow \overline{D}(\tau)_1 \times (\overline{D}(\sigma)_1) \times (\overline{D}(\tau)_2) \rightarrow \overline{D}(\tau)_1)\}
\]

\[
\text{LFun}(\overline{D}(\sigma)_1, \text{Tens}(\overline{D}(\tau)_1, \overline{D}(\sigma)_1))\}
\]

Then

\[
\{\text{ev}\}(f, x) = f x
\]

\[
\{\text{ev}\}(\text{ev})_1(f, x) = \pi_1(f x)
\]
\[
\llbracket D(\text{ev})_2\rrbracket (f, x)(v) = (x \otimes v, (\pi_2(f, x))(v)).
\]

Suppose that \((f’, (g’, h’)) \in P_{(r \to \sigma)_r}\). That is, \((f’, (g’, h’)) = ((f_1, f_2), ((g_1, g_2), x \mapsto v \mapsto h_1(x)(\pi_1 v) + h_2(x)(\pi_2 v)))\) for some \((f_1, (g_1, h_1)) \in P_{r \to \sigma}\) and \((f_2, (g_2, h_2)) \in P_r\). We want to show that
\[
(x \mapsto \llbracket \text{ev} \rrbracket (f_1(x), f_2(x)),
(x \mapsto \llbracket D(\text{ev})_1 \rrbracket (g_1(x), g_2(x)),

x \mapsto v \mapsto h_1(x)(\pi_1(\llbracket D(\text{ev})_2 \rrbracket (g_1(x), g_2(x))(v)) + h_2(x)(\pi_2(\llbracket D(\text{ev})_2 \rrbracket (g_1(x), g_2(x))(v)))))) \in P_{\sigma}.
\]

That is,
\[
(x \mapsto f_1(x)(f_2(x)),
(x \mapsto \pi_1(\llbracket D(\text{ev})_2 \rrbracket (g_1(x), g_2(x)))),

x \mapsto v \mapsto h_1(x)(\pi_1(!g_2(x) \otimes v, (\pi_2(g_1(x)g_2(x)))(v))) + h_2(x)(\pi_2(!g_2(x) \otimes v, (\pi_2(g_1(x)g_2(x)))(v)))))) \in P_{\sigma}.
\]

Now, this is precisely the condition that \((f_1, (g_1, h_1)) \in P_{r \to \sigma}\).

Suppose that \(t \in \text{Syn}(r \to \sigma, \rho)\) is such that \(\llbracket D(t) \rrbracket\) respects the logical relation. Observe that \(\llbracket D(t) \rrbracket_1 \in \text{Syn}(\llbracket D(\pi) \rrbracket_1 * \llbracket D(\sigma) \rrbracket_1, \llbracket D(\rho) \rrbracket_1)\) and \(\llbracket D(t) \rrbracket_2 \in \text{Syn}(\llbracket D(\pi) \rrbracket_2 * \llbracket D(\sigma) \rrbracket_2, \llbracket D(\rho) \rrbracket_2)\).

We show that \(\llbracket D(\Lambda(t)) \rrbracket_1\) also respects the relation. Observe that \(\Lambda(t) \in \text{Syn}(r, \sigma \to \rho)\) and \(\llbracket D(\Lambda(t)) \rrbracket_1 \in \text{Syn}(\llbracket D(\pi) \rrbracket_1, \llbracket D(\sigma) \rrbracket_1 \to (\llbracket D(\rho) \rrbracket_1 * \llbracket D(\sigma) \rrbracket_2), \llbracket D(\rho) \rrbracket_2)\) and \(\llbracket D(\Lambda(t)) \rrbracket_2 \in \text{Syn}(\llbracket D(\pi) \rrbracket_2, \llbracket D(\sigma) \rrbracket_2, \llbracket D(\rho) \rrbracket_2)\). We have that
\[
\llbracket D(\Lambda(t)) \rrbracket_1(t)(x)(y) = (\llbracket D(t) \rrbracket_1(t)(x, y), v \mapsto \pi_2(\llbracket D(t) \rrbracket_2(t)(x, y, v)))
\]

\[
\llbracket D(\Lambda(t)) \rrbracket_2(t)(x)(\prod_{i=1}^n y_i \otimes v_i) = \sum_{i=1}^n \pi_1(\llbracket D(t) \rrbracket_2(t)(x, y_i)(v_i)).
\]

Suppose that \((f, (g, h)) \in P_r\). We want to show that
\[
(x \mapsto \llbracket \Lambda(t) \rrbracket(f(x)),
(x \mapsto \llbracket D(\Lambda(t)) \rrbracket_1(g(x)),

x \mapsto v \mapsto h(x)(\llbracket D(\Lambda(t)) \rrbracket_2(g(x))(v)))) \in P_{\sigma \to \rho}.
\]

That is, we want to establish that for all \((f’, (g’, h’)) \in P_{\sigma}\), we have that
\[
(x \mapsto \llbracket \Lambda(t) \rrbracket(f_1(x))(f_2(x)),
(x \mapsto \pi_1(\llbracket D(\Lambda(t)) \rrbracket_1(g(x)))(g’(x))

x \mapsto v \mapsto h(x)(\llbracket D(\Lambda(t)) \rrbracket_2(g(x))(g’(x))(v)) + h’(x)((\pi_2(\llbracket D(\Lambda(t)) \rrbracket_1(g(x))(g’(x)))v)))) \in P_{\rho}.
\]

That is,
\[
(x \mapsto t(f(x), f’(x)),
(x \mapsto \llbracket D(t) \rrbracket_1(g(x), g’(x))

x \mapsto v \mapsto h(x)(\pi_1(\llbracket D(t) \rrbracket_2(g(x), g’(x))(v)) + h’(x)((\pi_2(\llbracket D(t) \rrbracket_2(g(x), g’(x)))v)))) \in P_{\rho}.
\]
Now, we have that \(((f, f'), ((g, g'), \sigma), x \mapsto v \mapsto h(x)(\pi_1 v) + h'(x)(\pi_2 v)) \in P_{\tau \sigma}\). Moreover, \(\llbracket \overline{D}(t) \rrbracket\) respects the logical relation, meaning that

\[
\begin{align*}
& (x \mapsto \llbracket t \rrbracket (f(x), f'(x)),
& (x \mapsto \llbracket \overline{D}(t_1) \rrbracket (g(x), g'(x)),
& x \mapsto v \mapsto h(x)(\pi_1 \llbracket \overline{D}(t_2) \rrbracket (g(x), g'(x))(v)) + h'(x)(\pi_2 \llbracket \overline{D}(t_2) \rrbracket (g(x), g'(x))(v))) \in P_p,
\end{align*}
\]

which is what we wanted to show!

Next, we turn to product projections. We consider \(\text{fst}\). The other projection is analogous. We have that \(\text{fst} \in \text{Syn}(\tau \times \sigma, \tau)\). Therefore, \(\overline{D}((\text{fst})_1) \in \text{Syn}(\overline{D}(\tau) \times \overline{D}(\sigma), \overline{D}(\tau)_1)\) and \(\overline{D}((\text{fst})_2) \in \text{Syn}(\overline{D}(\tau)_2 \times \overline{D}(\sigma)_2, \overline{D}(\tau)_2 \times \overline{D}(\sigma)_2)\). We have that

\[
\begin{align*}
\llbracket (\text{fst})_1 \rrbracket \llbracket (x, y) \rrbracket &= x \\
\llbracket (\text{fst})_2 \rrbracket \llbracket (x, y)(v) \rrbracket &= (v, 0).
\end{align*}
\]

Suppose that \((f, (g, h)) \in P_{\tau \sigma}\). That is, \(((f, f'), ((g, g'), \sigma), x \mapsto v \mapsto h_1(x)(\pi_1 v) + h_2(x)(\pi_2 v))\) for \((f_1, (g_1, h_1)) \in P_{\tau}\) and \((f_2, (g_2, h_2)) \in P_{\sigma}\). We have to show that

\[
\begin{align*}
& (x \mapsto \llbracket \text{fst} \rrbracket (f_1(x), f_2(x)),
& (x \mapsto \llbracket \overline{D}((\text{fst})_1) \rrbracket (g_1(x), g_2(x)),
& x \mapsto v \mapsto h_1(x)(v) + h_2(x)(v)) \in P_{\tau}.
\end{align*}
\]

That is,

\[
\begin{align*}
& (x \mapsto f_1(x)) \\
& (x \mapsto g_1(x),
& x \mapsto v \mapsto h_1(x)(v) + h_2(x)(0))) \in P_{\tau}.
\end{align*}
\]

By linearity of \(h_2\) in its second argument which holds by virtue of its type, it is enough to show that

\[
\begin{align*}
& (x \mapsto f_1(x)) \\
& (x \mapsto g_1(x),
& x \mapsto v \mapsto h_1(x)(v))) \in P_{\tau},
\end{align*}
\]

which is true by assumption.

Further, suppose that \(t \in \text{Syn}(\tau, \sigma)\) and \(s \in \text{Syn}(\tau, \rho)\) and assume that \(\llbracket \overline{D}(t) \rrbracket\) and \(\llbracket \overline{D}(s) \rrbracket\) respect the logical relation. We will show that \(\llbracket \overline{D}((t, s)) \rrbracket\) also respects the logical relation. Observe that \((t, s) \in \text{Syn}(\tau, \sigma \times \rho)\). Therefore, \(\overline{D}((\overline{D}(t), s)_1) \in \text{Syn}(\overline{D}(\tau)_1 \times \overline{D}(\sigma)_1 \times \overline{D}(\rho)_1)\) and \(\overline{D}((\overline{D}(t), s)_2) \in \text{Syn}(\overline{D}(\tau)_2 \times \overline{D}(\sigma)_2 \times \overline{D}(\rho)_2)\). We have that

\[
\begin{align*}
\llbracket (\overline{D}(t), s)_1 \rrbracket \llbracket (x) \rrbracket &= (\llbracket (\overline{D}(t)_1) \rrbracket \llbracket (x) \rrbracket, \llbracket (\overline{D}(s) \rrbracket \llbracket (x) \rrbracket) \\
\llbracket (\overline{D}(t), s)_2 \rrbracket \llbracket (x)(v) \rrbracket &= \llbracket (\overline{D}(t)_2) \rrbracket \llbracket (x)(\pi_1 v) \rrbracket + \llbracket (\overline{D}(s)_2) \rrbracket \llbracket (x)(\pi_2 v) \rrbracket.
\end{align*}
\]

Suppose that \((f, (g, h)) \in P_{\tau}\). We need to show that

\[
\begin{align*}
& (x \mapsto \llbracket (t, s) \rrbracket (f(x))) \\
& (x \mapsto \llbracket (\overline{D}((t, s)_1) \rrbracket, \\
& x \mapsto v \mapsto h(x)(\llbracket (\overline{D}((t, s)_2) \rrbracket (g(x))(v)))) \in P_{\sigma \times \rho}.
\end{align*}
\]
That is,
\[
(x \mapsto (\|t\| (f(x)), \|s\| (f(x)))) \\
(x \mapsto (\|\overline{D}(t)\| (f(x)), \|\overline{D}(s)\| (f(x)))),
\]
\[
x \mapsto v \mapsto h(x)(\|\overline{D}(t)\| (g(x))(\pi_1 v) + \|\overline{D}(s)\| (g(x))(\pi_2 v))) \in P_{\sigma \rho}.
\]
By linearity of \(h\) in its second argument, it is enough to show that
\[
(x \mapsto (\|t\| (f(x)), \|s\| (f(x)))) \\
(x \mapsto (\|\overline{D}(t)\| (f(x)), \|\overline{D}(s)\| (f(x)))),
\]
\[
x \mapsto v \mapsto h(x)(\|\overline{D}(t)\| (g(x))(\pi_1 v) + h(x)(\|\overline{D}(s)\| (g(x))(\pi_2 v))) \in P_{\sigma \rho},
\]
which is true by the assumption that \(\|\overline{D}(t)\|\) and \(\|\overline{D}(s)\|\) respect the logical relation and \((f, (g, h)) \in P_T\).

Next, we consider \((\emptyset) \in \text{Syn}(\tau, 1)\). We have that
\[
\|\overline{D}(\emptyset)\|_1 (x) = () \\
\|\overline{D}(\emptyset)\|_2 (x)(v) = 0.
\]
Therefore, given any \((f, (g, h)) \in P_T\), we need to show that
\[
(x \mapsto \|\emptyset\| (f(x))) \\
(x \mapsto \|\overline{D}(\emptyset)\|_1 (g(x)),
\]
\[
x \mapsto v \mapsto h(x)(\|\overline{D}(\emptyset)\|_2 (g(x))(v))) \in P_T.
\]
That is,
\[
(x \mapsto ()) \\
(x \mapsto ()),
\]
\[
x \mapsto v \mapsto h(x)(0))) \in P_T.
\]
This follows as \(h\) is linear in its second argument by virtue of its type.

Consider identities: \(\text{id} \in \text{Syn}(\tau, \tau)\). Then, \(\overline{D}(\text{id})_1 \in \text{Syn}(\overline{D}(\tau), \overline{D}(\tau))\) and \(\overline{D}(\text{id})_2 \in \text{Syn}((\overline{D}(\tau)\), \text{LFun}(\overline{D}(\tau), \overline{D}(\tau))\)). We have
\[
\|\text{id}\|_1 (x) = x \\
\|\overline{D}(\text{id})\|_1 (x) = x \|\overline{D}(\text{id})\|_2 (x)(v) = v.
\]
Suppose that \((f, (g, h)) \in P_T\). Then, we need to show that \((f; \|\text{id}\|, (g; \|\overline{D}(\text{id})\|_1), x \mapsto v \mapsto h(x)(\|\overline{D}(\text{id})\|_2 (g(x))(v))) \in P_T\). That is, \((f, (g, x \mapsto v \mapsto h(x)(v))) \in P_T\), which is true by assumption.

Consider composition: \(t \in \text{Syn}(\tau, \sigma)\) and \(s \in \text{Syn}(\sigma, \rho)\), which both respect the logical relation in the sense of the fundamental lemma. Then, \(\overline{D}(t)_1 \in \text{Syn}(\overline{D}(\tau), \overline{D}(\sigma))\), \(\overline{D}(s)_1 \in \text{Syn}(\overline{D}(\sigma), \overline{D}(\rho))\), \(\overline{D}(t)_2 \in \text{Syn}((\overline{D}(\tau)\), \text{LFun}(\overline{D}(\tau), \overline{D}(\tau))\)), and \(\overline{D}(s)_2 \in \text{Syn}((\overline{D}(\sigma)\), \text{LFun}(\overline{D}(\sigma), \overline{D}(\sigma))\)). Further, \(\overline{D}(t; s)_1 \in \text{Syn}((\overline{D}(\tau)\), \text{LFun}(\overline{D}(\tau), \overline{D}(\tau))\)) \(\overline{D}(t; s)_2 \in \text{Syn}((\overline{D}(\tau)\), \text{LFun}(\overline{D}(\tau), \overline{D}(\tau))\)). We have that
\[
\|t; s\|_1 (x) = x \\
\|\overline{D}(t; s)_1\|_1 (x) = \|\overline{D}(s)_1\|_1 (\|\overline{D}(t)_1\|_1 (x)) \\
\|\overline{D}(t; s)_2\|_1 (x)(v) = \|\overline{D}(t)_2\|_1 (x)(\|\overline{D}(s)_2\|_1 (\|\overline{D}(t)_1\|_1 (x))(v)).
\]
Suppose that \((f, (g, h)) \in P_T\). We want to show that
\[
(f; \|t; s\|, (g; \|\overline{D}(t; s)_1\|), x \mapsto v \mapsto h(x)(\|\overline{D}(t; s)_2\|_1 (g(x))(v))) \in P_{\rho}.
\]
That is,
\[(f; \{t\}; \{s\}, g; \{\tilde{D}(t)_1\}; \{s\}_1), \]
\[x \mapsto v \mapsto h(x)(\{\tilde{D}(t)_2\}(g(x))(\{\tilde{D}(s)_2\}(\{\tilde{D}(t)_1\}(g(x))(v)))) \in P_{\rho}.\]

Now, as \(t\) respects the logical relation, by our induction hypothesis, we have that
\[(f; \{t\}, g; \{\tilde{D}(t)_1\}; \{s\}_1), \]
\[x \mapsto v \mapsto h(x)(\{\tilde{D}(t)_2\}(g(x))(\{\tilde{D}(s)_2\}(\{\tilde{D}(t)_1\}(g(x))(v)))) \in P_{\sigma}.\]

Therefore, as \(s\) also respects the logical relation, by our induction hypothesis, we have that
\[(f; \{t\}; \{s\}, g; \{\tilde{D}(t)_1\}; \{s\}_1), \]
\[x \mapsto v \mapsto h(x)(\{\tilde{D}(t)_2\}(g(x))(\{\tilde{D}(s)_2\}(\{\tilde{D}(t)_1\}(g(x))(v)))) \in P_{\rho}.\]

The base cases of operations hold by the chain rule. Indeed, consider
\(op \in \text{Syn}(\text{real}^{n_1} \ast \ldots \ast \text{real}^{n_k}, \text{real}^m)\). Note that \(op = \tilde{D}(op)_1 \in \text{Syn}(\text{real}^{n_1} \ast \ldots \ast \text{real}^{n_k}, \text{real}^m)\) and
\((\text{Dop}_i') = \tilde{D}(op)\in \text{Syn}(\text{real}^{n_1} \ast \ldots \ast \text{real}^{n_k}, \text{LFun}(\text{real}^m, \text{real}^{n_1} \ast \ldots \ast \text{real}^{n_k}))\). We have that
\[\{\text{op}\}(x) = \{\tilde{D}(\text{op})_1\}(x)\]
\[\{\tilde{D}(op)_2\}(x)(v) = \{\text{Dop}_i'\}(x)(v) = D\{\text{op}\}^i(x)(v),\]
where we use the crucial assumption that the derivatives of primitive operations are implemented correctly. Then, let \((f, (g, h)) \in P_{\text{real}^{n_1} \ast \ldots \ast \text{real}^{n_k}}\). That is, \((f, (g, h)) = ((f_1, \ldots, f_k), ((g_1, \ldots, g_k) \times x \mapsto v \mapsto h_1(x)(\pi_1 v) + \ldots + h_k(x)(\pi_k v)), (f_i, (g_i, h_i))) \in P_{\text{real}^{n_i}}, \text{for } 1 \leq i \leq k\). We want to show that
\[(f; \{\text{op}\}, (g; \{\tilde{D}(\text{op})_1\}); x \mapsto v \mapsto h(x)(\{\tilde{D}(op)_2\}(g(x))(v))) \in P_{\text{real}^m}.\]

That is,
\[(f; \{\text{op}\}, (g; \{\tilde{D}(\text{op})_1\}), x \mapsto v \mapsto h(x)(D\{\text{op}\}^i(x)(v))) \in P_{\text{real}^m}.\]

That is,
\[((f_1, \ldots, f_k); \{\text{op}\}, ((g_1, \ldots, g_k); \{\text{op}\}), x \mapsto v \mapsto \sum_{i=1}^{k} h_i(x)(\pi_i(D\{\text{op}\}^i(g_i(x))(v))) \in P_{\text{real}^m}.\]

By the assumption that \((f_i, (g_i, h_i)) \in P_{\text{real}^{n_i}},\) we have that \(g_i = f_i\) and \(h_i = Df_i^i\). Therefore, we need to show that
\[((f_1, \ldots, f_k); \{\text{op}\}, ((f_1, \ldots, f_k); \{\text{op}\}), x \mapsto v \mapsto \sum_{i=1}^{k} Df_i^i(x)(\pi_i(\text{D}(\{\text{op}\})^i(f_i(x))(v)))) \in P_{\text{real}^m}.\]

Using the chain rule for multivariate differentiation (and a little bit of linear algebra), this is equivalent to,
\[((f_1, \ldots, f_k); \{\text{op}\}, ((f_1, \ldots, f_k); \{\text{op}\}, D((f_1, \ldots, f_k); \{\text{op}\})(v))) \in P_{\text{real}^m}.\]

Therefore, the fundamental lemma follows. \(\square\)

Again, the correctness theorem then follows by exactly the argument in the proof of Thm. 8.1.

**Theorem B.4 (Correctness of Reverse AD).** For any typed term \(x : \tau \vdash t : \sigma \in \text{Syn}, \) where \(\tau\) and \(\sigma\) are first-order types, we have that
\[\{\tilde{D}(t)_1\} = \{t\} \quad \text{and} \quad \{\tilde{D}(t)_2\} = D\{t\}^i.\]
\section{Operational Semantics and Adequacy for the Applied Target Language}

\subsection{Big-Step Semantics}

For completeness, we describe the big-step operational semantics for the applied target language which is implied by our suggested implementation. Because of purity, the precise evaluation strategy is unimportant. (We use call-by-name evaluation.) We write \( t \Downarrow N \) to indicate that a term \( t \) evaluates to normal form \( N \). If no rule applies to a term \( t \), we intend it to be a normal form (i.e. \( t \Downarrow t \)). As normal forms are unique, we will write \( \Downarrow \) for the unique \( N \) such that \( t \Downarrow N \).

\begin{align*}
\frac{\text{op}(t) \Downarrow \text{op}(c)}{\frac{t \Downarrow c \quad t' \Downarrow c'}{t + t' \Downarrow c + c'}} \\
\frac{\tau \Downarrow N}{\frac{\text{fst} t \Downarrow N_1 \quad \text{snd} t \Downarrow N_2}{s \Downarrow N \quad t \Downarrow \lambda x. t' \quad s \Downarrow N' \quad t'[N'/\lambda x. t'] \Downarrow N}} \\
\frac{s \Downarrow \text{lapp}(s, t) \Downarrow N}{\frac{r \Downarrow \text{lop}(t) \quad t \Downarrow c \quad s \Downarrow c'}{t \Downarrow \text{lapp}(r, s) \Downarrow \text{lop}(\text{op}(c)(c'))}} \\
\frac{\text{fst} t \Downarrow \langle N, N' \rangle \quad \text{lsnd} t \Downarrow \langle N, N' \rangle}{t \Downarrow \text{lapp}(t, s) \Downarrow N} \\
\frac{t \Downarrow \text{lcur}^{-1} s \quad r \Downarrow r_1 + r_2 \quad \text{lapp}(t, r_1) \Downarrow N_1 \quad \text{lapp}(t, r_2) \Downarrow N_2 \quad N_1 + N_2 \Downarrow N}{t \Downarrow \text{lcur}^{-1} s \quad r \Downarrow \text{lapp}(t', s') \quad t' \Downarrow \{ (r', -) \} \quad \text{lapp}(s r', s') \Downarrow N} \\
\end{align*}

\subsection{Adequacy of the Semantics}

Finally, we note that this implementation of the target language is sensible as the denotational semantics \( \Downarrow - \Downarrow \) is adequate with respect to the operational semantics induced by the implementation.

Indeed, define \emph{program contexts} \( C[\_] \) of type \( \sigma \) with a hole of type \( \tau \) to be terms \( \_ : \tau + C[\_] : \sigma \) which use the variable \( \_ \) exactly once. We write \( C[t] \) for the capturing substitution \( C[\_][t/\_] \). We will consider a notion of contextual equivalence in which only the types \text{real}\( ^\sigma \) are observable. We call two closed terms \( + t,s : \tau \) contextually equivalent if, for all program contexts \( C[\_] \) of observable
We claim that the following is a correct implementation of reverse derivatives for zip where we make use of the standard functional programming functions.

We first show two standard lemmas.

**Lemma C.1 (Compositionality of \( \llbracket - \rrbracket \)).** For any two terms \( \Gamma \vdash t, s : \tau \) and any compatible program context \( C[\_] \) we have that \( \llbracket t \rrbracket = \llbracket s \rrbracket \) implies \( \llbracket C[t] \rrbracket = \llbracket C[s] \rrbracket \).

This is proved by induction on the structure of terms.

**Lemma C.2 (Soundness of \( \llbracket \rrbracket \)).** In case \( t \), we have that \( \llbracket t \rrbracket = \llbracket \llbracket t \rrbracket \rrbracket \).

This is proved by induction on the definition of \( \llbracket \rrbracket \): note that every operational rule is also an equation in the semantics.

Then, adequacy follows.

**Theorem C.3 (Adequacy).** In case \( \llbracket t \rrbracket = \llbracket s \rrbracket \), it follows that \( t \approx s \).

**Proof.** Suppose that \( \llbracket t \rrbracket = \llbracket s \rrbracket \) and let \( C[\_] \) be a compatible program context of ground type. Then, \( \llbracket \llbracket C[t] \rrbracket \rrbracket = \llbracket C[s] \rrbracket = \llbracket \llbracket \llbracket C[t] \rrbracket \rrbracket \rrbracket \) by the previous two lemmas. Finally, as normal forms of type \( \text{real}^n \) are simply constants, which are easily seen to be faithfully interpreted in our semantics, it follows that \( \llbracket C[t] \rrbracket = \llbracket C[s] \rrbracket \). Therefore, \( t \approx s \). \( \square \)

In particular, it follows that the AD correctness proofs of this paper apply to this particular implementation technique.

## D REVERSE AD OF HIGHER-ORDER OPERATIONS SUCH AS MAP

So far, we have considered our arrays of reals to be primitive objects which can only be operated on by first-order operations. Next, we show that our framework also lends itself to treating higher-order operations on these arrays. This is merely a proof of concept and we believe a thorough treatment for such operations – in the form of AD rules with a correctness proof and implementation – deserves a paper of its own. Let us consider, as a case study, what happens when we add the standard functional programming idiom of a higher-order map operation \( \text{map} \in \text{Syn}(\text{real} \to \text{real}^\ast \text{real}^n, \text{real}^n) \) to our source language. We will derive the reverse AD rules for this operation and prove them correct. We observe that according to the rules of this paper

\[
\overrightarrow{\mathcal{D}}(\text{map})_1 \in \text{Syn}((\text{real} \to (\text{real} \ast (\text{LFun}(\text{real}, \text{real})))) \ast \text{real}^n, \text{real}^n)
\]

\[
\overrightarrow{\mathcal{D}}(\text{map})_2 \in \text{Syn}(((\text{real} \to (\text{real} \ast (\text{LFun}(\text{real}, \text{real})))) \ast \text{real}^n), \text{LFun}(\text{real}^n, \text{Tens}(\text{real}, \text{real}) \ast \text{real}^n))
\]

We claim that the following is a correct implementation of reverse derivatives for map:

\[
\overleftarrow{\mathcal{D}}(\text{map})_1(f, v) \overset{\text{def}}{=} \text{map}(f; \text{fst}, v)
\]

\[
\overleftarrow{\mathcal{D}}(\text{map})_2(f, v)(w) \overset{\text{def}}{=} (\text{zip } w, \text{zipWith } (f; \text{snd}) v w),
\]

where we make use of the standard functional programming functions \( \text{zip} \) and \( \text{zipWith} \). We assume that we are working internal to the module defining \( \text{LFun}(\tau, \sigma) \) and \( \text{Tens}(\tau, \sigma) \) as we are implementing derivatives of language primitives. As such, we can operate directly on their internal representations which we simply assume to be plain functions and lists of pairs.

Given this implementation, we have the following semantics:

\[
\llbracket \text{map} \rrbracket (f, v) = (f(\pi_1 v), \ldots, f(\pi_n v))
\]

\[
\llbracket \overleftarrow{\mathcal{D}}(\text{map})_1 \rrbracket (f, v) = (\pi_1(f(\pi_1 v)), \ldots, \pi_1(f(\pi_n v)))))
\]
\[ \{ \tilde{D}(\text{map})_2 \}(f, v)(w) = (\sum_{i=1}^{n} ((\pi_1 v) \otimes (\pi_i w)), ((\pi_2(f(\pi_1 v)))(\pi_1 w), \ldots, (\pi_2(f(\pi_n v)))(\pi_n w)) \]

We show correctness of the suggested derivative implementations by extending our previous logical relations argument of Appx. B with the corresponding case in the induction over terms when proving the fundamental lemma. After the fundamental lemma is established again for this extended language, the previous proof of correctness remains valid. Suppose that \((f, (g, h)) \in P_{\text{real} \rightarrow \text{real}^n \text{real}^n}\). That is, \(f = (f_1, f_2), g = (g_1, g_2)\) and \(h = \pi_1; h_1 + \pi_2; h_2\) for \((f_1, (g_1, h_1)) \in P_{\text{real} \rightarrow \text{real}}\) and \((f_2, (g_2, h_2)) \in P_{\text{real}^n}\). Then, we need to show that
\[
(f; \{\text{map}\}, g; \{\tilde{D}(\text{map})_1\}, x \mapsto v \mapsto h(x)(\{\tilde{D}(\text{map})_2\}(g(x))(v))) \in P_{\text{real}^n}
\]
i.e. (by definition)
\[
(x \mapsto (f_1(x)(\pi_1 f_2(x)), \ldots, f_1(\pi_n f_2(x))),
\)
\[
(x \mapsto (\pi_1(g_1(x)(\pi_1 g_2(x))), \ldots, \pi_1(g_1(x)(\pi_n g_2(x)))))
\]
\[
x \mapsto v \mapsto h_1(x)(\sum_{i=1}^{n} ((\pi_i g_2(x)) \otimes (\pi_i v)) +
\]
\[
h_2(x)((\pi_2 g_1(x)(\pi_1 g_2(x)))(\pi_1 v), \ldots, (\pi_2 g_1(x)(\pi_n g_2(x)))(\pi_n v))) \in P_{\text{real}^n}
\]
i.e. (by linearity of \(v \mapsto h_1(x)(v)\))
\[
(x \mapsto (f_1(x)(\pi_1 f_2(x)), \ldots, f_1(\pi_n f_2(x))),
\)
\[
(x \mapsto (\pi_1(g_1(x)(\pi_1 g_2(x))), \ldots, \pi_1(g_1(x)(\pi_n g_2(x)))))
\]
\[
x \mapsto v \mapsto \left(\sum_{i=1}^{n} h_1(x)((\pi_i g_2(x)) \otimes (\pi_i v)) \right) +
\]
\[
h_2(x)((\pi_2 g_1(x)(\pi_1 g_2(x)))(\pi_1 v), \ldots, (\pi_2 g_1(x)(\pi_n g_2(x)))(\pi_n v))) \in P_{\text{real}^n}
\]
i.e. (by linearity of \(v \mapsto h_2(x)(v)\))
\[
(x \mapsto (f_1(x)(\pi_1 f_2(x)), \ldots, f_1(\pi_n f_2(x))),
\)
\[
(x \mapsto (\pi_1(g_1(x)(\pi_1 g_2(x))), \ldots, \pi_1(g_1(x)(\pi_n g_2(x)))))
\]
\[
x \mapsto v \mapsto \sum_{i=1}^{n} h_1(x)((\pi_i g_2(x)) \otimes (\pi_i v)) +
\]
\[
h_2(x)(0, \ldots, 0, (\pi_2 g_1(x)(\pi_1 g_2(x)))(\pi_1 v), 0 \ldots, 0))) \in P_{\text{real}^n}
\]
Using the fact that \(((f_1^1), \ldots, f^n), ((g_1^1), \ldots, g^n), x \mapsto v \mapsto h^1(x)(\pi_1 v) + \ldots + h^n(x)(\pi_n v))) \in P_{\text{real}^n}\) if \((f^1, (g^1, h^1)) \in P_{\text{real}}\) (this is basic multivariate calculus), it is enough to show that for \(i = 1, \ldots, n\),
\[
(x \mapsto f_1(x)(\pi_i f_2(x)),
\)
\[
(x \mapsto \pi_1(g_1(x)(\pi_i g_2(x))),
\)
\[
x \mapsto v \mapsto h_1(x)((\pi_i g_2(x)) \otimes v) + h_2(x)(0, \ldots, 0, (\pi_2 g_1(x)(\pi_i g_2(x)))(v), 0 \ldots, 0)) \in P_{\text{real}}.
\]
By definition of \(P_{\text{real} \rightarrow \text{real}}\), it is enough to show that
\[
(x \mapsto \pi_i f_2(x),
\)
\[
(x \mapsto \pi_i g_2(x)),
\]
\[
x \mapsto v \mapsto h_2(x)(0, \ldots, 0, v, 0 \ldots, 0) \in P_{\text{real}}.
\]
Now, this follows from basic multivariate calculus as \((f_2, (g_2, h_2)) \in P_{\text{real}^n}\).
We show correctness of this implementation again by extending the proof of our fundamental lemma with the inductive case for map. This leads to the following semantics:

\[ \overline{D}(\text{map})_1(f, v) \triangleq \text{map}(f; \text{fst}, v) \]

\[ \overline{D}(\text{map})_2(f, v)(g, w) \triangleq \text{zipWith}(f; \text{snd}) v w + \text{map} g v. \]

This implementation leads to the following semantics:

\[ \langle \overline{D}(\text{map})_1 \rangle(f, v) = (\pi_1(f(\pi_1 v)), \ldots, \pi_1(f(\pi_n v))) \]

\[ \langle \overline{D}(\text{map})_2 \rangle(f, v)(g, w) = (\pi_2(f(\pi_1 v)))(\pi_1 w), \ldots, (\pi_2(f(\pi_n v)))(\pi_n w)) \]

\[ + (g(\pi_1 v), \ldots, g(\pi_n v)). \]

We show correctness of this implementation again by extending the proof of our fundamental lemma with the inductive case for map. The correctness theorem then follows as before once the fundamental lemma has been extended.

Suppose that \((f, (g, h)) \in P_{(\text{real} \rightarrow \text{real})^n}\). That is, \(f = (f_1, f_2), g = (g_1, g_2)\) and \(h = x \mapsto r \mapsto (h_1(x)(r), h_2(x)(r))\) for \((f_1, (g_1, h_1)) \in P_{\text{real} \rightarrow \text{real}}\) and \((f_2, (g_2, h_2)) \in P_{\text{real}^n}\). Then, we need to show that

\( (f; \langle \text{map} \rangle, (g; \langle \overline{D}(\text{map})_1 \rangle), x \mapsto r \mapsto (\langle \overline{D}(\text{map})_2 \rangle(g(x))(h(x)(r)))) \in P_{\text{real}^n} \)

i.e. (by definition)

\[ (x \mapsto (f_1(x)(\pi_1 f_2(x)), \ldots, f_1(x)(\pi_n f_2(x))), \]

\[ (x \mapsto (\pi_1(g_1(x)(\pi_1 f_2(x))), \ldots, \pi_1(g_1(x)(\pi_n f_2(x)))), \]

\[ x \mapsto r \mapsto ((\pi_2(g_1(x)(\pi_1 g_2(x)))(\pi_1 h_2(x)(r)), \ldots, \]

\[ (\pi_2(g_1(x)(\pi_1 g_2(x)))(\pi_n h_2(x)(r)))) \]

\[ + (h_1(x)(r)(\pi_1 g_2(x), \ldots, h_1(x)(r)(\pi_n g_2(x))))) \in P_{\text{real}^n}. \]

Observing that \((f^i, (g^i, h^i)) \in P_{\text{real}}\) implies that

\[ (x \mapsto (f^1(x), \ldots, f^n(x)), \]

\[ (x \mapsto (g^1(x), \ldots, g^n(x)), \]

\[ x \mapsto r \mapsto (h^1(x)(r), \ldots, h^n(x)(r))))) \in P_{\text{real}}, \]

as derivatives of tuple-valued functions are computed componentwise, it is enough to show that for each \(1 \leq i \leq n\), we have that

\[ (x \mapsto f_1(x)(\pi_1 f_2(x)), \]

\[ (x \mapsto \pi_1(g_1(x)(\pi_1 f_2(x))), \]

\[ x \mapsto r \mapsto (\pi_2(g_1(x)(\pi_1 g_2(x)))(\pi_1 h_2(x)(r)) + h_1(x)(r)(\pi_1 g_2(x)))) \in P_{\text{real}}. \]
By definition of $P_{\text{real}\rightarrow\text{real}}$, as $(f_1, (g_1, h_1)) \in P_{\text{real}\rightarrow\text{real}}$ it is now enough to show that $(f_2; \pi_1, (g_2; \pi_1, x \mapsto r \mapsto \pi_1(h_2(x)(r)))) \in P_{\text{real}}$. This follows as $(f_2, (g_2, h_2)) \in P_{\text{real}}^n$ and derivatives of tuple-valued functions are computed componentwise.

It follows that the proposed implementation of forward AD for \texttt{map} is semantically correct.