A Differential-form Pullback Programming Language for Higher-order Reverse-mode Automatic Differentiation

Carol Mak
Luke Ong

Abstract
Building on the observation that reverse-mode automatic differentiation (AD) — a generalisation of backpropagation — can naturally be expressed as pullbacks of differential 1-forms, we design a simple higher-order programming language with a first-class differential operator, and present a reduction strategy which exactly simulates reverse-mode AD. We justify our reduction strategy by interpreting our language in any differential λ-category that satisfies the Hahn-Banach Separation Theorem, and show that the reduction strategy precisely captures reverse-mode AD in a truly higher-order setting.

1 Introduction
Automatic differentiation (AD) [34] is widely considered the most efficient and accurate algorithm for computing derivatives, thanks largely to the chain rule. There are two modes of AD:

- **Forward-mode AD** evaluates the chain rule from inputs to outputs; it has time complexity that scales with the number of inputs, and constant space complexity.
- **Reverse-mode AD** — a generalisation of backpropagation — evaluates the chain rule (in dual form) from outputs to inputs; it has time complexity that scales with the number of outputs, and space complexity that scales with the number of intermediate variables.

In machine learning applications such as neural networks, the number of input parameters is usually considerably larger than the number of outputs. For this reason, reverse-mode AD has been the preferred method of differentiation, especially in deep learning applications. (See Baydin et al. [5] for an excellent survey of AD.)

The only downside of reverse-mode AD is its rather involved definition, which has led to a variety of complicated implementations in neural networks. On the one hand, TensorFlow [1] and Theano [3] employ the define-and-run approach where the computational graph is constructed dynamically during the execution.

Can we replace the traditional graphical representation of reverse-mode AD by a simple yet expressive framework? Indeed, there have been calls from the neural network community for the development of differentiable programming [14, 19, 24], based on a higher-order functional language with a built-in differential operator that returns the derivative of a given program via reverse-mode AD. Such a language would free the programmer from implementational details of differentiation. Programmers would be able to concentrate on the construction of machine learning models, and train them by calling the built-in differential operator on the cost function of their models.

The goal of this work is to present a simple higher-order programming language with an explicit differential operator, such that its reduction semantics is exactly reverse-mode AD, in a truly higher-order manner.

The syntax of our language is inspired by Ehrhard and Regnier [15]’s differential λ-calculus, which is an extension of simply-typed λ-calculus with a differential operator that mimics standard symbolic differentiation (but not reverse-mode AD). Their definition of differentiation via a linear substitution provides a good foundation for our language.

The reduction strategy of our language uses differential λ-category [11] (the model of differential λ-calculus) as a guide. Differential λ-category is a Cartesian closed differential category [9], and hence enjoys the fundamental properties of derivatives, and behaves well with exponentials (curry).

Contributions. Our starting point (Section 2.2) is the observation that the computation of reverse-mode AD can naturally be expressed as a transformation of pullbacks of differential 1-forms. We argue that this viewpoint is essential for understanding reverse-mode AD in a functional setting. Standard reverse-mode AD (as presented in [4, 5]) is only defined in Euclidean spaces.

We present (in Section 3) a simple higher-order programming language, extending the simply-typed λ-calculus [12]
with an explicit differential operator called the *pullback*, $(\Omega \cdot \lambda x. \mathcal{P}) \cdot \mathcal{S}$, which serves as a reverse-mode AD simulator.

Using differential $\lambda$-category [11] as a guide, we design a reduction strategy for our language so that the reduction of the application, $((\Omega \cdot \lambda x. \mathcal{P}) \cdot (\lambda x. \epsilon_p^x)) \cdot \mathcal{S}$, mimics reverse-mode AD in computing the $p$-th row of the Jacobian matrix (derivative) of the function $\lambda x. \mathcal{P}$ at the point $\mathcal{S}$, where $\epsilon_p$ is the column vector with 1 at the $p$-th position and 0 everywhere else. Moreover, we show how our reduction semantics can be adapted to a continuation passing style evaluation (Section 3.5).

Owing to the higher-order nature of our language, standard differential calculus is not enough to model our language and hence cannot justify our reductions. Our final contribution (in Section 4) is to show that any differential $\lambda$-category [11] that satisfies the Hahn-Banach Separation Theorem is a model of our language (Theorem 4.6). Our reduction semantics is faithful to reverse-mode AD, in that it is exactly reverse-mode AD when restricted to first-order; moreover we can perform reverse-mode AD on any higher-order abstraction, which may contain higher-order terms, duals, pullbacks, and free variables as subterms (Corollary 4.8).

Finally, we discuss related works in Section 5 and conclusion and future directions in Section 6.

Throughout this paper, we will point to the attached Appendix for additional content. All proofs are in Appendix E, unless stated otherwise.

### 2 Reverse-mode Automatic Differentiation

We introduce forward- and reverse-mode automatic differentiation (AD), highlighting their respective benefits in practice. Then we explain how reverse-mode AD can naturally be expressed as the pullback of differential 1-forms. (The examples used to illustrate the above methods are collated in Figure 4).

#### 2.1 Forward- and Reverse-mode AD

Recall that the Jacobian matrix of a smooth real-valued function $f : \mathbb{R}^n \to \mathbb{R}^m$ at $x_0 \in \mathbb{R}^n$ is

$$
\mathcal{J}(f)(x_0) := \begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x_0) & \frac{\partial f_1}{\partial x_2}(x_0) & \cdots & \frac{\partial f_1}{\partial x_n}(x_0) \\ \frac{\partial f_2}{\partial x_1}(x_0) & \frac{\partial f_2}{\partial x_2}(x_0) & \cdots & \frac{\partial f_2}{\partial x_n}(x_0) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1}(x_0) & \frac{\partial f_m}{\partial x_2}(x_0) & \cdots & \frac{\partial f_m}{\partial x_n}(x_0) \end{bmatrix}
$$

where $f_j := \pi_j \circ f : \mathbb{R}^n \to \mathbb{R}$. We call the function $\mathcal{J} : C^\infty(\mathbb{R}^n, \mathbb{R}^m) \to C^\infty(\mathbb{R}^n, \mathbb{L}(\mathbb{R}^n, \mathbb{R}^m))$ the *Jacobian*. \footnote{$C^\infty(A, B)$ is the set of all smooth functions from $A$ to $B$, and $\mathbb{L}(A, B)$ is the set of all linear functions from $A$ to $B$, for Euclidean spaces $A$ and $B$.}

**Symbolic Differentiation** Numerical derivatives are standardly computed using *symbolic differentiation*: first compute $\frac{df_i}{dx_j}$ for all $i, j$ using rules (e.g. product and chain rules), then substitute $x_0$ for $x$ to obtain $\mathcal{J}(f)(x_0)$.

For example, to compute the Jacobian of $f : \langle x, y \rangle \mapsto ((x + 1)(2x + y^2))^2$ at $(1, 3)$ by symbolic differentiation, first compute $\frac{df_1}{dx} = 2(x + 1)(2x + y^2)(2x + 2y^2 + 2(x + 1))$ and $\frac{df_2}{dy} = 2(x + 1)(2x + y^2)(2y(x + 1))$. Then, substitute 1 for $x$ and 3 for $y$ to obtain $\mathcal{J}(f)(1, 3) = [660 \ 528]$.

Symbolic differentiation is accurate but inefficient. Notice that the term $(x + 1)$ appears twice in $\frac{df}{dx}$, and $(1 + 1)$ is evaluated twice in $\frac{df}{dx}|_{x=1}$ (because for $h : \langle x, y \rangle \mapsto (x + 1)(2x + y^2)$, both $h(x, y)$ and $\frac{dh}{dx}$ contain the term $(x + 1)$, and the product rule tells us to calculate them separately). This duplication is a cause of the so-called *expression swell problem*, resulting in exponential time-complexity.

**Automatic Differentiation** Automatic differentiation (AD) avoids this problem by a simple divide-and-conquer approach: first arrange $f$ as a composite of elementary functions, $g_1, \ldots, g_k$ (i.e. $f = g_k \circ \cdots \circ g_1$), then compute the Jacobian of each of these elementary functions, and finally combine them via the chain rule to yield the desired Jacobian of $f$.

**Forward-mode AD** Recall the chain rule:

$$
\mathcal{J}(f)(x_0) = \mathcal{J}(g_k)(x_{k-1}) \times \cdots \times \mathcal{J}(g_2)(x_1) \times \mathcal{J}(g_1)(x_0)
$$

for $f = g_k \circ \cdots \circ g_1$, where $x_i := g_i(x_{i-1})$. Forward-mode AD computes the Jacobian matrix $\mathcal{J}(f)(x_0)$ by calculating $a_i := \mathcal{J}(g_i)(x_{i-1}) \times a_{i-1}$ and $x_i := g_i(x_{i-1})$, with $a_0 := \mathbb{I}$ (identity matrix) and $x_0$. Then, $a_k = \mathcal{J}(f)(x_0)$ is the Jacobian of $f$ at $x_0$. This computation can neatly be presented as an iteration of the $\langle \cdot, \cdot \rangle$-reduction, $\langle x \mid \alpha \rangle \overset{g}{\rightarrow} \langle g(x) \mid \mathcal{J}(g)(x) \times \alpha \rangle$, for $g = g_1, \ldots, g_k$, starting from the pair $(x_0 \mid \mathbb{I})$. Besides being easy to implement, forward-mode AD computes the new pair from the current pair $\langle x \mid \alpha \rangle$, requiring no additional memory.

To compute the Jacobian of $f : \langle x, y \rangle \mapsto ((x + 1)(2x + y^2))^2$ at $(1, 3)$ by forward-mode AD, first decompose $f$ into...
elementary functions as \( \mathbb{R}^2 \xrightarrow{g} \mathbb{R}^2 \xrightarrow{\cdot f} \mathbb{R} \), where \( g(x, y) := (x + 1, 2x + y^2) \). Then, starting from \( \langle (3, 1) | 1 \rangle \), iterate the \( \langle \cdot | \cdot \rangle \)-reduction

\[
\langle (1, 3) | \begin{bmatrix} 1 \\ 0 \end{bmatrix} \rangle \xrightarrow{g} \langle (2, 11) | \begin{bmatrix} 1 \\ 2 \end{bmatrix} \rangle \xrightarrow{\cdot f} \langle 484 | [660 \ 528] \rangle
\]

yielding \([660 \ 528] \) as the Jacobian of \( f \) at \( (1, 3) \). Notice that \( (1 + 1) \) is only evaluated once, even though its result is used in various calculations.

In practice, because storing the intermediate matrices \( \alpha_i \) can be expensive, the matrix \( J(f)(x_0) \) is computed column-by-column, by simply changing the starting pair from \( (x_0 | 1) \) to \( (x_0 | e_p) \), where \( e_p \in \mathbb{R}^n \) is the column vector with 1 at the \( p \)-th position and 0 everywhere else. Then, the computation becomes a reduction of a vector-vector pair, and \( \alpha_k = J(f)(x_k) \times e_p \) is the \( p \)-th column of the Jacobian matrix \( J(f)(x_k) \). Since \( J(f)(x_k) \) is a \( m \)-by-\( n \) matrix, \( n \) runs are required to compute the whole Jacobian matrix.

For example, if we start from \( \langle (1, 3) | \begin{bmatrix} 1 \\ 0 \end{bmatrix} \rangle \), the reduction

\[
\langle (1, 3) | \begin{bmatrix} 1 \\ 0 \end{bmatrix} \rangle \xrightarrow{g} \langle (2, 11) | \begin{bmatrix} 1 \\ 2 \end{bmatrix} \rangle \xrightarrow{\cdot f} \langle 484 | [660 \ 528] \rangle
\]

gives us the first column of the Jacobian matrix \( J(f)(1, 3) \).

**Reverse-mode AD** By contrast, reverse-mode AD computes the dual of the Jacobian matrix, \( (J(f)(x_0))^* \), using the chain rule in dual (transpose) form

\[
(J(f)(x_0))^* = (J(g_1)(x_0))^* \times \cdots \times (J(g_k)(x_k-1))^*
\]

as follows: first compute \( x_i := g_i(x_{i-1}) \) for \( i = 1, \ldots, k-1 \) (Forward Phase); then compute \( \beta_i := (J(g_i)(x_i-1))^* \times \beta_{i+1} \) for \( i = k-1 \) with \( \beta_{k+1} := 1 \) (Reverse Phase).

For example, the reverse-mode AD computation on \( f \) is as follows.

**Forward Phase:** \( \langle (1, 3) \rangle \xrightarrow{g} \langle (2, 11) \rangle \xrightarrow{\cdot f} \langle 484 \rangle \)

**Reverse Phase:** \( \langle 484 \rangle \xrightarrow{\cdot f} \langle [44] \rangle \xrightarrow{\cdot f} \langle 1 \rangle \)

In practice, like forward-mode AD, the matrix \( (J(f)(x_0))^* \) is computed column-by-column, by simply setting \( \beta_{k+1} := \pi_p \), where \( \pi_p \in L(\mathbb{R}^m, \mathbb{R}) \) is the \( p \)-th projection. Thus, a run (comprising Forward and Reverse Phase) computes \( (J(f)(x_0))^* (\pi_p) \), the \( p \)-th row of the Jacobian of \( f \) at \( x_0 \). It follows that \( m \) runs are required to compute the \( m \)-by-\( n \) Jacobian matrix.

In many machine learning (e.g. deep learning) problems, the functions \( f : \mathbb{R}^n \to \mathbb{R}^m \) we need to differentiate have many more inputs than outputs, in the sense that \( n \gg m \). Whenever this is the case, reverse-mode AD is more efficient than forward-mode.

**Remark 2.1.** Unlike forward-mode AD, we cannot interleave the iteration of \( x_i \) and the computation of \( \beta_i \). In fact, according to Hoffmann [18], nobody knows how to do reverse-mode AD using pairs \( \langle \cdot | \cdot \rangle \), as employed by forward-mode AD to great effect. In other words, reverse-mode AD does not seem presentable as an *in-place* algorithm.

### 2.2 Geometric Perspective of Reverse-mode AD

Reverse-mode AD can naturally be expressed using pullbacks and differential 1-forms, as alluded to by Betancourt [7] and discussed in [26].

Let \( E := \mathbb{R}^n \) and \( F := \mathbb{R}^m \). A *differential 1-form* of \( E \) is a smooth map \( \omega \in C^\infty(E, \Lambda(E, \mathbb{R})) \). Denote the set of all differential 1-forms of \( E \) as \( \Omega(E) \). E.g. \( \lambda \times \pi_p \in \Omega(E) \). (Henceforth, by 1-form, we mean differential 1-form.) The pullback (of a 1-form \( \omega \in \Omega(F) \) along a smooth map \( f : E \to F \)) is a 1-form \( \Omega(f)(\omega) \in \Omega(E) \) where

\[
\Omega(f)(\omega) : \quad E \longrightarrow L(E, \mathbb{R})
\]

\[
x \longmapsto (J(f)(x))^* (\omega(f(x)))
\]

Notice the result of an iteration of reverse-mode AD \( (J(f)(x_0))^* (\pi_p) \) can be expressed as \( \Omega(f)(\lambda \times \pi_p)(x_0) \), which can be expanded to \( (\Omega(g_1) \circ \cdots \circ \Omega(g_k)) (\lambda \times \pi_p)(x_0) \). Hence, reverse-mode AD can be expressed as: first iterate the reduction of 1-forms, \( \omega \xrightarrow{g} \Omega(g)(\omega) \), for \( g = g_k, \ldots, g_1 \), starting from the 1-form \( \lambda \times \pi_p \); then compute \( \omega_0(x_0) \), which yields the \( p \)-th row of \( J(f)(x_0) \).

Returning to our example,

\[
\Omega(f)(\lambda \times [1])(1, 3) = (\Omega(g) \circ \Omega(\ast) \circ \Omega((\ast)^\dagger))(\lambda \times [1]^\dagger)(1, 3)
\]

\[
= (J(f)(\ast))(1, 3)((\ast)^\dagger)(\lambda \times [1]^\dagger)(2, 11)
\]

\[
= (J(f)(\ast))(1, 3)((\ast)^\dagger)(2, 11)\rangle(\lambda \times [1]^\dagger)(22)
\]

\[
= (J(f)(\ast))(1, 3)((\ast)^\dagger)(2, 11)\rangle(\lambda \times [1]^\dagger)(484)
\]

\[
= (J(f)(\ast))(1, 3)((\ast)^\dagger)(2, 11)\rangle(\lambda \times [1]^\dagger)(484)^\dagger
\]

\[
= [660 \ 528]^\dagger
\]

which is the Jacobian \( J(f)(1, 3) \).

The pullback-of-1-forms perspective gives us a way to perform reverse-mode AD beyond Euclidean spaces (for example on the function sum: \( L(\mathbb{R}) \to \mathbb{R} \), which returns the sum of the elements of a list); and it shapes our language and reduction presented in Section 3. (Example 3.2 shows how sum can be defined in our language and Appendix A.2 shows how reverse-mode AD can be performed on sum.)
Simple terms $S ::= x \mid \lambda x.S \mid S P \mid \pi_{i}(S) \mid (S, S) \mid \text{lin}(S)$

Pullback terms $P ::= 0 \mid S \mid S + P$

**Figure 1.** Grammar of simple terms $S$ and pullback terms $P$. Assume a collection $\mathcal{V}$ of variables (typically $x, y, z, \omega$), and a collection $\mathcal{F}$ (typically $f, g, h$) of easily-differentiable real-valued functions, in the sense that the Jacobian of $f$, $\mathcal{J}(f)$, can be called by the language, $r$ and $r$ range over $\mathbb{R}$ and $\mathbb{R}^n$ respectively.

**Remark 2.2.** Pullbacks can be generalised to arbitrary $p$-forms, using essentially the same approach. However the pullbacks of general $p$-forms no longer resemble reverse-mode AD as it is commonly understood.

### 3 A Differential-form Pullback Programming Language

#### 3.1 Syntax

Figure 1 presents the grammar of simple terms $S$ and pullback terms $P$, and Figure 2 presents the type system. While the definition of simple terms $S$ is relatively standard (except for the new constructs which will be discussed later), the definition of pullback terms $P$ as sums of simple terms is not.

#### 3.1.1 Sum and Linearity

The idea of sum is important since it specifies the “linear positions” in a simple term, just as it specifies the algebraic notion of linearity in Mathematics. For example, $x(y + z)$ is a term but $(x + y)z$ is not. This is because $(x + y)z$ is the same as $xz + yz$, but $x(y + z)$ cannot. Hence in $S P$, $S$ is in a linear position but not $P$. Similarly, in Mathematics $(f_1 + f_2)(x_1) = f_1(x_1) + f_2(x_1)$ but in general $f_1(x_1 + x_2) \neq f_1(x_1) + f_1(x_2)$ for smooth functions $f_1, f_2$ and $x_1, x_2$. Hence, the function $f$ in an application $f(x)$ is in a linear position while the argument $x$ is not.

Formally we define the set $\text{lin}(S)$ of linear variables in a simple term $S$ by $y \in \text{lin}(S)$ if, and only if, $y$ is in a linear position in $S$.

$$\begin{align*}
\text{lin}(x) &= \{ x \} \\
\text{lin}(\lambda x. S) &= \text{lin}(S) \setminus \{ x \} \\
\text{lin}(S P) &= \text{lin}(S) \setminus \text{FV}(P) \\
\text{lin}(\pi_i(S)) &= \text{lin}(S) \\
\text{lin}(S_1 + S_2) &= \text{lin}(S_1) \cap \text{lin}(S_2) \\
\text{lin}(\mathcal{J} f \cdot S) &= \text{lin}(S) \\
\text{lin}((\lambda x. S_1) \cdot S_2) &= (\text{lin}(S_1) \setminus \text{FV}(S_2)) \cup (\text{lin}(S_2) \setminus \text{FV}(S_1))
\end{align*}$$

$\text{lin}(S) := \varnothing$ otherwise.

For example, $\text{lin}(x z (y z)) = \{ x \}$.

#### 3.1.2 Dual Type, Jacobian, Dual Map and Pullback

Any term of the dual type $\sigma^*$ is considered a linear functional of $\sigma$. For example, $\varepsilon_P^*$ has the dual type $\mathbb{R}^n$. Then the term $\varepsilon_P^*$ mimics the linear functional $\varepsilon_P \in L(\mathbb{R}^n, \mathbb{R})$

The Jacobian $\mathcal{J} f \cdot S$ is considered as the Jacobian of $f$ along $S$, which is a smooth function. For example, let $f : \mathbb{R}^m \rightarrow \mathbb{R}^n$ be “easily differentiable”, then $\mathcal{J} f : v$ mimics the Jacobian $\lambda\mathcal{J} f \cdot v$, i.e. the function $\lambda x. \mathcal{J}(f)(x)(v)$.

The dual map $(\lambda \lambda x. S_1^* \cdot S_2)$ is considered the dual of the linear functional $\lambda x. S_1$, along the function $\lambda x. S_1$, where $x \in \text{lin}(S_1)$. For example, let $r \in \mathbb{R}^m$. The dual map $(\lambda v. (\mathcal{J} f \cdot v) r^* \cdot \varepsilon_P^*$ mimics $(\mathcal{J}(f)(r))^*(\varepsilon_P) \in L(\mathbb{R}^m, \mathbb{R})$, which is the dual pullback of $\varepsilon_P$ along the Jacobian $\mathcal{J}(f)(r)$.

The pullback $(\lambda \lambda x. \mathcal{P}) \cdot S$ is considered the pullback of the 1-form $S$ along the function $\lambda x. P$. For example, $(\lambda \lambda x. S_1^* \cdot P_2) \equiv (\lambda x. S_1^* \cdot P_2)$ mimics $(\lambda x. P)(\lambda x. S_1^* \cdot P_2) \in \Omega(\mathbb{R}^n)$, which is the pullback of the 1-form $\lambda x. \mathcal{P}$ along $f$.

Hence, to perform reverse-mode AD on a term $\lambda x. P$ at $P'$ with respect to $\omega$, we consider the term $((\lambda \lambda x. P) \cdot \omega)P'$.

#### 3.1.3 Notations

We use syntactic sugars to ease a writing. For $n \geq 1$ and $z$ a fresh variable.

$$R_{n+1}^n \equiv R^n \times R$$

$\Omega \mathcal{P} \equiv \sigma \Rightarrow \sigma^*$

$S_{\mathcal{P}} \equiv \pi_{i}(S)$

$\lambda x. P^*$ Let $x = t$ in $S \equiv (\lambda x. S) t$

$\Omega \equiv \lambda x. P^*$

$\lambda x. y, S \equiv \lambda x. S[z_{i} \leftarrow x][z_{n+2} / y]$

Capture-free substitution is applied recursively, e.g.

$((\lambda x. S_1) \cdot S_2)[P/\omega] \equiv ((\lambda x. S_1)[P/\omega]) \cdot (S_2[P/\omega])$ and $((\Omega \lambda x. P) \cdot S)[P/\omega] \equiv (\Omega (\lambda x. P)[P/\omega]) \cdot (S[P/\omega])$. We treat 0 as the unit of our sum terms, i.e. $0 \equiv 0 + 0, S \equiv 0 + S$ and $S \equiv S + 0$; and consider $+_{a}$ as a associative and commutative operator. We also define $S[S_1 + S_2 / y] \equiv S[S_1 / y] + S[S_2 / y]$ if and only if $y \in \text{lin}(S)$. For example, $(S_1 + S_2)P \equiv S_1 P + S_2 P$.

We finish this subsection with some examples that can be expressed in this language.

**Example 3.1.** Consider the running example in computing the Jacobian of $f : (x, y) \mapsto ((x + 1)(2x + y^2))^2$ at $(1, 3)$. Assume $g((x, y)) := (x + 1, 2x + y^2)$, mult and pow2 are in the set of easily differentiable functions, i.e. $g$, mult, pow2 $\in \mathcal{F}$.

The function $f$ can be presented by the term $f((x, y)) = \lambda x. P^*$ $\equiv \text{pow2(mult(g((x, y))))) : R}$. More interestingly, the Jacobian $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$ can be computed in a single pass over the field.
of \( f \) at \((1, 3)\), i.e. \( \mathcal{J}(f)((1, 3)) \), can be presented by the term

\[ \Gamma \vdash ((\Omega \lambda x. y. \text{pow2}(\text{mult}(g(x, y)))))) \cdot (\Omega \left[1\right]) \langle (1, 3) \rangle : \mathbb{R}^{\ast} \]

This is the application of the pullback \( \Omega(f)(\lambda x. [1]^{*}) \) to the point \((1, 3)\), which we saw in Subsection 2.2 is the Jacobian of \( f \) at \((1, 3)\).

**Example 3.2.** Consider the function that takes a list of real numbers and returns the sum of the elements of a list. Using the standard Church encoding of List, i.e. \( \text{List}(X) \equiv (X \rightarrow D \rightarrow D) \rightarrow (D \rightarrow D) \), and \([x_1, x_2, \ldots, x_n] \equiv \lambda f d f x_0 (\ldots (f x_2 (f x_1 d)) \ldots) \) for some dummy type \( D \), sum : \( \text{List}(\mathbb{R}) \rightarrow \mathbb{R} \) is defined to be \( \lambda l l. \lambda x. y. \chi_{\mathbb{R}} \). Hence the Jacobian of sum at a list \([z_0, \ldots, z_n]\) can be expressed as

\[ \omega : (\Omega(\text{List}(\mathbb{R}))) \vdash ((\Omega(\text{sum})) \cdot \omega) \langle [z_0, \ldots, z_n] \rangle : \mathbb{R}^{\ast} \]

Now the question is how we could perform reverse-mode AD on this term. Recall the result of a reverse-mode AD on a function \( f : \mathbb{R}^{p} \rightarrow \mathbb{R}^{m} \) at \( x \in \mathbb{R}^{p} \), i.e. the \( p \)-th row of the Jacobian matrix of \( f \) at \( x \), can be expressed as \( \Omega(f)(\lambda x. \pi_{p}(x)) \), which is \( (\mathcal{J}(f)(x))^{\ast}\langle (\lambda x. \pi_{p}(x)) \rangle = (\mathcal{J}(f)(x))^{\ast} \cdot \pi_{p} \).

In the rest of this Section, we consider how the term \( ((\Omega \lambda y. \mathcal{F}^{\ast}) \cdot \omega) \mathcal{P} \), which mimics \( \Omega(f)(\omega)(x) \), can be reduced. To avoid expression swell, we first perform A-reduction: \( \mathcal{P} \rightarrow_{A}^{\ast} \mathcal{L} \) which decompose a term into a series of "smaller" terms, as explained in Subsection 3.2. Then, we reduce \( ((\Omega \lambda y. \mathcal{L}) \cdot \omega) \mathcal{P} \) by induction on \( \mathcal{L} \), as explained in Subsection 3.3. Lastly, we complete our reduction strategy in Subsection 3.4.

We use the term in Example 3.1 as a running example in our reduction strategy to illustrate that this reduction is faithful to reverse-mode AD (in that it is exactly reverse-mode AD when restricted to first-order). The reduction of the term in Example 3.2 is given in Appendix A.2. It illustrates how reverse-mode AD can be performed on a higher-order function.

### 3.2 Divide: Administrative Reduction

We use the administrative reduction (A-reduction) of Sabry and Felleisen [28] to decompose a pullback term \( \mathcal{P} \) into a let series \( \mathcal{L} \) of elementary terms, i.e.

\[ \mathcal{P} \rightarrow_{A}^{\ast} \text{let } x_1 = \mathbb{E}; \ldots; x_n = \mathbb{E} \text{ in } x_n, \]

where elementary terms \( \mathbb{E} \) and let series \( \mathcal{L} \) are defined as

\[ \mathbb{E} := 0 \mid z_1 + z_2 \mid z \mid \lambda x. \mathcal{L} \mid \lambda z_1 z_2 \mid z \mid (z_1, z_2) \mid \lambda x | f(x) | \mathcal{L} \mid \mathcal{J} f : z | (\lambda x. \mathcal{L})^{\ast} \cdot z | (\Omega \lambda y. \mathcal{L}) \cdot z | \mathcal{F} \mid \mathcal{L} \mid \text{let } z = \mathbb{E} \text{ in } \mathcal{L} \mid \text{let } z \in \mathbb{E} \text{ in } z. \]

Note that elementary terms \( \mathbb{E} \) should be "fine enough" to avoid expression swell. The complete set of A-reductions on \( \mathcal{P} \) can be found in Appendix B. We write \( \rightarrow_{A}^{\ast} \) for the reflexive and transitive closure of \( \rightarrow_{A} \).

**Example 3.3.** We decompose the term considered in Example 3.1, \( \text{pow2}(\text{mult}(g(x, y)))) \), via administrative reduction.

\[ \text{let } z_1 = (x, y); \]
\[ \text{z}_{2} = \text{g}(z_{1}); \]
\[ z_{3} = \text{mult}(z_{2}); \]
\[ z_{4} = \text{pow2}(z_{3}) \text{ in } z_{4}. \]

This is reminiscent of the decomposition of \( f \) into \( \mathbb{R}^{2} \rightarrow \mathbb{R}^{2} \rightarrow \mathbb{R} \) before performing AD.

### 3.3 Conquer: Pullback Reduction

**3.3.1 Let Series**

After decomposing \( \mathcal{P} \) to a let series \( \mathcal{L} \) of elementary terms via A-reductions in \( ((\Omega \lambda y. \mathcal{F}^{\ast}) \cdot \omega) \), we reduce \( (\Omega \lambda y. \mathcal{L}) \cdot \omega \) by induction on \( \mathcal{L} \) as shown in Figure 3 (Let series). Reduction 7 is the base case and reduction 8 expresses the contra-variant property of pullbacks.

**Example 3.4.** Take \( (\Omega \lambda (x, y). \text{pow2}(\text{mult}(g(x, y)))) \cdot (\Omega [1]) \) discussed in Example 3.1, as when applied to the point \((1, 3)\) is the Jacobian \( \mathcal{J}(f)((1, 3)) \) where \( f((x, y)) = (x + 1)(2x + y^{2})^{2} \). In Example 3.3, we showed that \( \text{pow2}(\text{mult}(g(x, y))) \) is A-reduced to a let series \( \mathcal{L} \). Now via reduction 7 and 8, \( (\Omega \lambda (x, y). \mathcal{L}) \cdot \omega \) is reduced to a
Let Series: $(\Omega \lambda y. \text{let } x = \mathbb{E} \text{ in } x)) \cdot \omega \xrightarrow{(7)} (\Omega \lambda y. \mathbb{E}) \cdot \omega$

$(\Omega \lambda y. \text{let } x = \mathbb{E} \text{ in } \mathbb{L})) \cdot \omega \xrightarrow{(8)} (\Omega \lambda y. \langle y, \mathbb{E} \rangle) \cdot ((\Omega \lambda y. \langle y, x \rangle. \mathbb{L}) \cdot \omega)$

Constant Functions: 

$((\Omega \lambda y. \mathbb{E}) \cdot \omega) \xrightarrow{(9)} 0 \text{ for } y \not\in \text{FV(}\mathbb{E})\text{.}$

Linear Functions:

$((\Omega \lambda y. z + y_{\pi_1}) \cdot \omega) \xrightarrow{(10a)} (\lambda v. v_{\pi_1})^* \cdot (\omega (z + \langle v_{\pi_1} \rangle))$

$((\Omega \lambda y. y_{\pi_1} + y_{\pi_1}) \cdot \omega) \xrightarrow{(10b)} (\lambda v. v_{\pi_1} + v_{\pi_1})^* \cdot (\omega (\langle v_{\pi_1} \rangle + \langle v_{\pi_1} \rangle))$

$((\Omega \lambda y. y_{\pi_1}) \cdot \omega) \xrightarrow{(11)} (\lambda v. v)^* \cdot (\omega \mathbb{V})$

Function Symbols:

$((\Omega \lambda y. y_{\pi_1}, \cdot \omega) \xrightarrow{(12)} (\lambda v. v_{\pi_1})^* \cdot (\omega \langle v_{\pi_1} \rangle)$

Dual Maps:

$((\Omega \lambda y. (\lambda x. \mathbb{L})^* \cdot y_{\pi_1}) \cdot \omega) \xrightarrow{(16a)} (\lambda v. (\lambda x. \mathbb{L})^* \cdot v_{\pi_1})^* \cdot (\omega ((\lambda x. \mathbb{L})^* \cdot \langle v_{\pi_1} \rangle))$ for $y \not\in \text{FV(}\lambda x. \mathbb{L})\text{.}$

Pullback Terms:

$((\Omega \lambda y. (\lambda x. \mathbb{L}) \cdot z) \cdot \omega) \xrightarrow{(17)} ((\Omega \lambda y. \lambda a. (\lambda v. v)^* \cdot (z \mathbb{L}[a/x])) \cdot \omega) \xrightarrow{(\omega \mathbb{L}[a/x])} x \not\in \text{FV(}\mathbb{V})\text{.}$

Abstraction:

$((\Omega \lambda y. \lambda a. \mathbb{L}. (\lambda v. v)^* \cdot (z \mathbb{L}[a/x])) \cdot \omega) \xrightarrow{(18)} (\lambda v. (\lambda v. (\lambda x. \mathbb{L})^* \cdot \langle v_{\pi_1} \rangle) \cdot \langle \lambda x. \mathbb{L}[a/x] \rangle \cdot \omega^* (\lambda v. v)^* \cdot (\omega (z \mathbb{L}[a/x])) \cdot \omega)$

Application:

$((\Omega \lambda y. y_{\pi_1} \cdot z) \cdot \omega) \xrightarrow{(19a)} (\lambda v. v_{\pi_1} z^* \cdot (\omega (\lambda x. \mathbb{L}[a/x])))$

$((\Omega \lambda x. \mathbb{P})^* \cdot \omega) \xrightarrow{(20a)} (\lambda v. v^* \cdot \lambda v. v_{\pi_1} z^* \cdot (\omega (\lambda x. \mathbb{L}[a/x])))$

Pair:

$((\Omega \lambda y. \langle y, \mathbb{E} \rangle) \cdot \omega) \xrightarrow{(20a)} (\lambda v. (\lambda v. \mathbb{E})^* \cdot (\omega (\lambda v. \mathbb{E}[a/x])))$

$((\Omega \lambda y. \langle y, \mathbb{E} \rangle) \cdot \omega) \xrightarrow{(20b)} (\lambda v. (\lambda v. \mathbb{E})^* \cdot (\omega (\lambda v. \mathbb{E}[a/x])))$

$((\Omega \lambda y. \langle y, \mathbb{E} \rangle) \cdot \omega) \xrightarrow{(20b)} (\lambda v. (\lambda v. \mathbb{E})^* \cdot (\omega (\lambda v. \mathbb{E}[a/x])))$ for $y \not\in \text{FV(}\mathbb{E})\text{.}$

Figure 3. Pullback Reductions
series of pullback along elementary terms.

\[
\text{let } z_1 = (x, y); \\
\lambda (x, y). \quad z_2 = g(z_1); \\
(\Omega \lambda (x, y). \quad z_3 = \text{mult}(z_1); \\
\quad z_4 = \text{pow}2(z_3) \text{ in } z_4
\]

\[
\rightarrow^\ast
\]

Via A-reductions and reductions 7 and 8, \((\Omega \lambda y.E)^* \cdot \omega)\) is reduced to a series of pullback along elementary terms \((\Omega \lambda y,E)_1 \cdot \ldots \cdot ((\Omega \lambda y,E_n) \cdot \omega)).\) Now, we define the reduction of pullback along elementary terms when applied to a value\(^5\) \(V\), i.e. \((\Omega \lambda y.E) \cdot \omega)V\).

Recall the pullback of a 1-form \(\omega \in \Omega(F)\) along a smooth function \(f : E \rightarrow F\) is defined to be

\[
\Omega(f)(\omega) : \quad x \mapsto (\mathcal{J}(f)(x))^*(\omega(f(x))
\]

Hence, we have the following pullback reduction

\[
((\Omega \lambda y.E) \cdot \omega) V \rightarrow (\lambda v.S)^* \cdot (\omega(\mathbb{E}[V/y]))
\]

of the application \((\Omega \lambda y.E) \cdot \omega) V\) which mimics the pullback of a variable \(\omega:\) along an abstraction \(\lambda y.E\) at term \(V\).

But how should one define the simple term \(S\) in \((\lambda v.S)^* \cdot (\omega(\mathbb{E}[V/y]))\) so that \(\lambda v.S\) mimics the Jacobian of \(f\) at \(x\), i.e. \(\mathcal{J}(f)(x)\)? We do so by induction on the elementary terms \(E\), shown in Figure 3 Reductions 9-20.

Remark 3.5. For readers familiar with differential \(\lambda\)-
calculus [15], \(S\) is the result of substituting a linear occurrence of \(y\) by \(v\), and then substituting all free occurrences of \(y\) by \(V\) in the term \(E\). Our approach is different from differential \(\lambda\)-calculus in that we define a reduction strategy instead of a substitution. A comprehensive comparison between our language and differential \(\lambda\)-calculus is given in Section 5.

3.3.2 Constant Functions

If \(y\) is not a free variable in \(E\), \(\lambda y.E\) is mimicking a constant function. The Jacobian of a constant function is 0, hence we reduce \((\Omega \lambda y.E) \cdot \omega) V\) to \((\lambda v.0)^* \cdot (\omega(\mathbb{E}[V/y]))\), which is the sugar for 0 as shown in Figure 3 (Constant Functions) Reduction 9. The redexes \((\Omega \lambda y.0) \cdot \omega) V\), \((\Omega \lambda y.E) \cdot \omega) V\) and \((\Omega \lambda y.x)^* \cdot \omega) V\) all reduce to 0.

Henceforth, we assume \(y \in \text{FV}(E)\).

3.3.3 Linear Functions

We consider the redexes where \(y \in \text{lin}(E)\). Then \(\lambda y.E\) is mimicking a linear function, whose Jacobian is itself. Hence

\[(\Omega \lambda y.E \cdot \omega) V\] is reduced to \((\lambda v.S)^* \cdot (\omega(\mathbb{E}[V/y]))\) where \(S\) is the result of substituting \(y\) by \(v\) in \(E\). Figure 3 (Linear Functions) Reductions 10-14 shows how they are reduced.

3.3.4 Smooth Functions

Now consider the redexes where \(y\) might not be a linear variable in \(E\). All reductions are shown in Figure 3.

Function Symbols Let \(f\) be “easily differentiable”. Then, \(\lambda y.f(y_{\pi}\iota)\) is mimicking \(f \circ \pi_i\), whose Jacobian at \(x\) is \(\mathcal{J}(f)(\pi_i(x)) \circ \pi_i\). Hence the Jacobian of \(\lambda y.f(y_{\pi}\iota)\) is \(\lambda v.\mathcal{J}(f \circ \pi_i)(V)(\pi_i)\) and \((\lambda \lambda y.f(y_{\pi}\iota) \cdot \omega) V\) is reduced to \((\lambda v.\mathcal{J}(f \circ \pi_i)(V)(\pi_i))^* \cdot (\omega(f(V(\pi_i))))\) as shown in Reduction 15.

Dual Maps Consider the Jacobian of \(\lambda y.(\lambda x.L)^* \cdot z\) at \(V\). It is easy to see that the result varies depending on where the variable \(y\) is located in the dual map \((\lambda x.L)^* \cdot z\). We consider three cases.

First, if \(y \notin \text{FV}(\lambda x.L)\), we must have \(z \equiv y_{\pi}\iota\). Then \(y\) is a linear variable in \((\lambda x.L)^* \cdot y_{\pi}\iota\), and so the Jacobian of \(\lambda y.(\lambda x.L)^* \cdot y_{\pi}\iota)\) at \(V\) is \(\lambda v.(\lambda x.L)^* \cdot y_{\pi}\iota\). Hence, we have Reduction 16a.

Second, say \(y \notin \text{FV}(z)\). Since dual and abstraction are both linear operations, and \(y\) is only free in \(L\), the Jacobian of \(\lambda y.(\lambda x.L)^* \cdot z\) at \(V\), should be \(\lambda v.(\lambda x.S')^* \cdot z\) where \(\lambda v.S'\) is the Jacobian of \(\lambda y.L\) at \(V\). To find the Jacobian of \(\lambda y.L\) at \(V\), we reduce \((\lambda \lambda y.L \cdot \omega) V\) to \((\lambda v.S')^* \cdot (\omega L(V/y))\). Then \(\lambda v.S'\) is the Jacobian of \(\lambda y.L\) at \(V\). The reduction is given in Reduction 16b. Note that this reduction avoids expression swell, as we are reducing the let series \(L\) in \((\lambda y.(\lambda x.L)^* \cdot z)\) using our pullback reductions, which does not suffer from expression swell.

Finally, for \(y \in \text{FV}(\lambda x.L) \cap \text{FV}(z)\), the Jacobian of \((\lambda y.(\lambda x.L)^* \cdot z)\) at \(V\) is the “sum” of the results we have for the two cases above, i.e. \(\lambda v.(\lambda x.L)^* \cdot y_{\pi}\iota + (\lambda v.S')^* \cdot y_{\pi}\iota\), where the remaining free occurrences of \(y\) are substituted by \(V\), since the Jacobian of a bilinear function \(l : X_1 \times X_2 \rightarrow Y\) is \(\mathcal{J}(l)(x_1, x_2)(v_1, v_2) = l(x_1, v_2) + l(v_1, x_2)\). Hence, we have Reduction 16c.

Pullback Terms Consider \((\Omega \lambda y.(\lambda x.L) \cdot z) \cdot \omega) V\).

Instead of reducing it to some \((\lambda v.S)^* \cdot (\omega ((\Omega \lambda y.\Omega x.L) \cdot z) \cdot \omega)(V/y))\) like the others, here we simply reduce \((\Omega \lambda x.L) \cdot z\) to \((\lambda v.S)^* \cdot (z \mathbb{L}[a/x])\), where \(a\) is a fresh variable and \(z \neq x\), and replace \(\lambda y.(\lambda x.L) \cdot z\) by \(\lambda y.\mathbb{L}[a/x]\) in \((\Omega \lambda y.\Omega x.L) \cdot z) \cdot \omega) V\) as shown in Reduction 17.

Abstraction Consider the Jacobian of \(\lambda y.\lambda x.L\) at \(V\).
We follow the treatment of exponentials in differential λ-category [11] where the (D-curry) rule states that for all $f : Y \times X \rightarrow A$, $D[cur(f)] = D[\text{cur}(f)] = D[f \circ (\pi_1 \times \pi_2 \times \text{Id}_X)]$, which means $J(cur(f))(y) = \lambda u. J(f(-, x))(y(u))$.

According to this (D-curry) rule, the Jacobian of $\lambda y. \lambda x. \text{L}$ at $V$ should be $\lambda v. \lambda S \text{L}$ where $\lambda v. \text{L}$ is the Jacobian of $\lambda y. \text{L}$ at $V$. Hence similar to the dual map case, we first reduce $(\lambda \lambda y. \lambda x. \text{L} \cdot \omega) \text{V}$ to $(\lambda \lambda v. \text{L})^* \cdot (\omega \text{L}[\text{V}/y])$ and obtain the Jacobian of $\lambda y. \text{L}$ at $V$, i.e. $\lambda v. \text{L}$ and then reduce $(\lambda \lambda y. \lambda x. \text{L} \cdot \omega) \text{V}$ to $(\lambda v. \text{L})^* \cdot (\omega (\lambda x. \text{L}[\text{V}/y]))$ as shown in Reduction 18.

**Remark 3.6.** Doing induction on elementary terms defined in Subsection 3.2, we can see that there are a few elementary terms $\mathbb{E}$ where $(\lambda \lambda y. \mathbb{E}) \cdot \omega) \text{V}$ is not a redex, namely

value 1: $((\lambda \lambda y. z \cdot \omega) \text{V}$ where $z$ is a free variable,

value 2: $((\lambda \lambda y. y \cdot \omega) \text{V}$ where $\lambda v. \text{V}$ is a constant function, the Jacobian of $\lambda y. y \cdot \omega) \text{V}$ is just $\lambda v. \text{V}$ and we have Reduction 19c.

Having these terms as values makes sense intuitively, since they have “inappropriate” values in positions. Values 1 has a free variable $z$ in a function position. Value 2 substitutes $y_\pi$ by $\forall_\pi$ which is a non-abstraction, to a function position.

**Pair** Last but not least, we consider the Jacobian of $\lambda y. (y, \mathbb{E})$ at $V$. It is easy to see that Jacobian is $\lambda v. (\forall, \mathbb{S})$ where $\lambda v. \mathbb{S}$ is the Jacobian of $\lambda y. \mathbb{E}$, as shown in Reduction 20a and Reduction 20b.

**Example 3.7.** Take our running example. In Examples 3.3 and 3.4 we showed that via A-reductions and Reductions 7 and 8, $(\lambda \lambda x. y. \text{pow}(\text{mult}(g(x, y))) \cdot \omega) \text{V}$ is reduced to

\[
\begin{align*}
(\lambda \lambda \lambda (x, y) \cdot \text{pow}(\text{mult}(g(x, y))))\cdot \omega & \rightarrow (\lambda \lambda \lambda 3) \cdot \omega \\
& \rightarrow (\lambda \lambda \lambda 1) \cdot \omega \\
& \rightarrow (\lambda \lambda \lambda 1) \cdot \omega \\
& \rightarrow (\lambda \lambda \lambda 1) \cdot \omega
\end{align*}
\]

We show how it can be reduced when applied to $(1, 3)$.

\[
\begin{align*}
(\lambda \lambda \lambda (x, y) \cdot \text{pow}(\text{mult}(g(x, y))))\cdot \omega & \rightarrow (\lambda \lambda \lambda 3) \cdot \omega \\
& \rightarrow (\lambda (\lambda 3) \cdot \omega) \\
& \rightarrow (\lambda 3) \\
& \rightarrow (\lambda 1) \\
& \rightarrow (\lambda 1)
\end{align*}
\]

Notice how this is reminiscent of the forward phase of reverse-mode AD performed on $f : \langle x, y \rangle \mapsto \langle (x + 1)(2x + y^2) \rangle^2$ at $(1, 3)$ considered in Subsection 2.1.

Moreover, we used the reduction $f(r) \rightarrow f(r)$ couples of times in the argument position of an application. This is to avoid expression swell. Note 1 + 1 is only evaluated once in (**) even when the result is used in various computations. Hence, we must have a call-by-value reduction strategy as presented below.
3.4 Combine

Reductions in Subsections 3.2 and 3.3 are the most interesting development of the paper. However, they alone are not enough to complete a reduction strategy. In this subsection, we define contexts and redexes so that any non-value term can be reduced.

The definition of context \( C \) is the standard call-by-value context, extended with duals and pullbacks. Notice that the context \((\Omega \lambda y.CA) \cdot \mathbb{S}\) contains a \( C \)-context defined in Subsection 3.2. This follows from the idea of reverse-mode AD to decompose a term into elementary terms before differentiating them.

\[
C ::= [] \mid C + P \mid V + CA \mid CA \mid V \mid \pi_i(C) \mid \langle C, S \rangle \mid \langle V, C \rangle | f(C) | \lbrack f \rbrack \cdot C | (\lambda x.S) \cdot V | \langle (\lambda x.C) \cdot V \rangle \cdot V |
\]

\[
\bar{D}((\lambda y.CA) \cdot \mathbb{S}) \cdot C \mid (\Omega \lambda y.(\mathbb{E} \cdot C) \cdot (\Omega \lambda y.(y, \mathbb{E})) \cdot C)
\]

Our redex \( r \) extend the standard call-by-value redex with four sets of terms.

\[
r ::= (\lambda x.S) \cdot V \mid \pi_i(\langle V, V \rangle) \mid f(P) \mid (\lbrack f \rbrack \cdot C) \cdot V' \\
\mid (\lambda v.(\lbrack f \rbrack \cdot v) y) \cdot V' \cdot V'' \mid (\lambda v_1.V_1) \cdot (\lambda v_2.V_2) \cdot V_3 \\
\mid (\Omega \lambda y.L) \cdot S \mid \langle (\Omega \lambda y.(\mathbb{E} \cdot V_1) \cdot V_2) \rangle \cdot V_2 \mid (\Omega \lambda y.(y, \mathbb{E}) \cdot V_1) \cdot V_2
\]

where either \( V_2 \not\equiv (\lbrack f \rbrack \cdot v) \cdot V_3 \). A value \( V \) is a pullback term \( P \) that cannot be reduced further, i.e. a term in normal form.

The following standard lemma, which is proved by induction on \( P \), tells us that there is at most one redex to reduce.

**Lemma 3.8.** Every term \( P \) can be expressed as either \( C[r] \) for some unique context \( C \) and redex \( r \) or a value \( V \).

Let’s look at the reductions of redexes. (1-4) are the standard call-by-value reductions. (5) reduces the dual along a linear map \( l \) and (6) is the contra-variant property of dual maps.

\[
\begin{align*}
(\lambda x.S) \cdot V &\quad \to \quad \mathbb{S}[V/x] \quad \pi_i(\langle V_1, V_2 \rangle) \quad (\langle V, C \rangle) \\
\lbrack f \rbrack &\quad \to \quad f(P) \quad (\lbrack f \rbrack \cdot C) \\
(\lambda v.(\lbrack f \rbrack \cdot v) y) &\quad \to \quad (\lbrack f \rbrack \cdot (\lbrack f \rbrack \cdot v) y) \\
(\lambda v_1.V_1) &\quad \to \quad (\lambda v_2.V_2) \cdot V_3 \\
\end{align*}
\]

\[
\begin{align*}
(\Omega \lambda y.L) \cdot S &\quad \to \quad \langle (\Omega \lambda y.(\mathbb{E} \cdot V_1) \cdot V_2) \rangle \\
(\Omega \lambda y.(y, \mathbb{E}) \cdot V_1) &\quad \to \quad (\Omega \lambda y.(y, \mathbb{E}) \cdot V_2)
\end{align*}
\]

where either \( V_2 \not\equiv (\lbrack f \rbrack \cdot v) \cdot V_3 \). A value \( V \) is a pullback term \( P \) that cannot be reduced further, i.e. a term in normal form.

3.5 Continuation-Passing Style

Differential 1-forms \( \Omega E := C^\infty(E, \mathbb{L}(E, \mathbb{R})) \) is similar to the continuation of \( E \) with the “answer” \( \mathbb{R} \). We can indeed write our reduction in a continuation passing style (CPS) manner. Let \( \langle P \mid S \rangle_y = (\Omega \lambda y.P) \cdot \mathbb{S} \), then we can treat \( \langle P \mid S \rangle_y \) as a configuration of an element \( \Gamma \uplus \{ y : \sigma \} \rhd \mathbb{P} \cdot \tau \) and a “continuation” \( \Gamma \vdash \mathbb{S} : \Omega \mathbb{R} \). The rules for the redexes \( \langle L \mid S \rangle_y \), \( \langle E \mid V \rangle_y \) and \( \langle y, \mathbb{E} \rangle \mid V \rangle \) were directly converted from Reductions 7-20. For example, Reduction 8 can be written as \( \langle \text{let } x = E \text{ in } L \mid \omega \rangle \to \langle \langle y, \mathbb{E} \rangle \mid L \rangle \mid \omega \rangle \mid \langle x, y \rangle \rangle \).

We prefer to write our language without the explicit mention of CPS since this paper focuses on the syntactic notion of reverse-mode AD using pullbacks and 1-forms. Also, 1-form of the type \( \sigma \) is more precisely described as an element
of the function type $\Omega \sigma \equiv \sigma \Rightarrow \sigma^*$, than of the continuation of $\sigma$, i.e. $\sigma \Rightarrow (\sigma \Rightarrow \mathbb{R})$.

## 4 Model

We show that any differential $\lambda$-category satisfying the Hahn-Banach Separation Theorem can soundly model our language.

### 4.1 Differential Lambda-Category

Cartesian differential category [9] aims to axiomatise fundamental properties of derivative. Indeed, any model of synthetic differential geometry has an associated Cartesian differential category. [13]

**Cartesian differential category** A category $C$ is a Cartesian differential category if

- every homset $C(A, B)$ is enriched with a commutative monoid $(C(A, B), +_{AB}, 0_{AB})$ and the additive structure is preserved by composition on the left. i.e. $(g+h) \circ f = g \circ f + h \circ f$ and $0 \circ f = 0$.
- it has products and projections and pairings of additive maps are additive. A morphism $f$ is additive if it preserves the additive structure of the homset on the right. i.e. $f \circ (g+h) = f \circ g + f \circ h$ and $f \circ 0 = 0$.

and it has an operator $D[-] : C(A, B) \rightarrow C(A \times A, B)$ that satisfies the following axioms:

- $D$ is linear: $D[f + g] = D[f] + D[g]$ and $D[0] = 0$
- $D$ is additive in its first coordinate: $D[f] \circ (h + k, \nu) = D[f] \circ (h, \nu) + D[f] \circ (k, \nu)$, $D[f] \circ (0, \nu) = 0$
- $D$ behaves with projections: $D[\text{Id}] = \pi_1$, $D[\pi_1] = \pi_1 \circ \pi_2$ and $D[\pi_2] = \pi_2 \circ \pi_1$
- $D$ behaves with pairings: $D[(f, g)] = (D[f], D[g])$
- Chain rule: $D[g \circ f] = D[g] \circ D[f] \circ \pi_2$
- $D$ is linear in its first component: $D[D[f]] \circ (g, h, k) = D[D[f]] \circ (g, k)$
- Independence of order of partial differentiation: $D[D[f]] \circ (0, h, k) = D[D[f]] \circ (0, g, k)$

We call $D$ the Cartesian differential operator of $C$.

**Example 4.1.** The category $\text{FVect}$ of finite dimensional vector spaces and differentiable functions is a Cartesian differential category, with the Cartesian differential operator $D[f](v, x) = J(f)(x)(v)$.

Differential $\lambda$-category A Cartesian differential category is a differential $\lambda$-category if

- it is Cartesian closed,
- $\lambda(-)$ preserves the additive structure, i.e. $\lambda(f + g) = \lambda(f) + \lambda(g)$ and $\lambda(0) = 0$,
- $D[-]$ satisfies the (D-curry) rule: for any $f : A_1 \times A_2 \rightarrow B$, $D(\lambda(f)) = \lambda(D[f] \circ (\pi_1 \times x_{A_1}, \pi_2 \times \text{Id}_{A_2}))$

**Linearity** A morphism $f$ in a differential $\lambda$-category is linear if $D[f] = f \circ \pi_1$.

**Example 4.2.** The category $\text{Con}^\omega$ of convenient vector space and smooth maps, considered by [8], is a differential $\lambda$-category with the Cartesian differential operator $D[f](v, x) := \lim_{t \to 0} (f(x + tv) - f(x))/t$, as shown in Lemma E.2.

### 4.2 Hahn-Banach Separation Theorem

We say a differential $\lambda$-category $C$ satisfies Hahn-Banach Separation Theorem if $\mathbb{R}$ is an object in $C$ and for any object $A$ in $C$ and distinct elements $x, y$ in $A$, there exists a linear morphism $l : A \rightarrow \mathbb{R}$ that separates $x$ and $y$, i.e. $l(x) \neq l(y)$.

**Example 4.3.** The category $\text{Con}^\omega$ of convenient vector space and smooth maps satisfies the Hahn-Banach Separation Theorem, as shown in Proposition E.3.

### 4.3 Interpretation

Let $C$ be a differential $\lambda$-category that satisfies Hahn-Banach Separation Theorem. Since $C$ is Cartesian closed, the interpretations for the $\lambda$-calculus terms are standard, and hence omitted. The full set of interpretations can be found in Appendix C.

- $[R] := \mathbb{R}$
- $[\sigma^*] := L([\sigma], \mathbb{R})$
- $[\sigma_1 \times \sigma_2] := C([\sigma_1], [\sigma_2])$

where $L([\sigma], \mathbb{R}) := \{ f \in C([\sigma], \mathbb{R}) | D[f] = f \circ \pi_1 \}$ is the set of all linear morphisms from $[\sigma]$ to $\mathbb{R}$.

- $[0]_{\gamma} := 0$
- $[S + P]_{\gamma} := [S]_{\gamma} + [P]_{\gamma}$
- $[\lambda x. S]_{\gamma} := \lambda x. [S]_{\gamma}$
- $[(\Omega \lambda x.P) \cdot S]_{\gamma} := \lambda x. [S]_{\gamma} \cdot \langle [P]_{\gamma}(y, x) (D[\text{cur}(\mathbb{P})]y) \gamma \rangle$
1. If \( x \in \text{lin}(P_1) \), then \( \text{cur}(P_1)\gamma \) is linear, i.e. \( D[\text{cur}(P_1)\gamma_1] = (\text{cur}(P_1)\gamma_1) \circ \pi_1 \).
2. \([P_2]y\) is linear, i.e. \( D[P_2]y = ([P_2]y) \circ \pi_1 \).

**Lemma 4.5** (Substitution). Let \( \Gamma \vdash S[P/x] : \tau \Rightarrow \Gamma \cup \{ x : \sigma \} \vdash S : \tau \Rightarrow \{ \text{Id}_{\Gamma} \} : \sigma \).

Any differential \( \lambda \)-category satisfying Hahn-Banach Separation Theorem is a sound model of our language. Note that the Hahn-Banach Separation Theorem is crucial in the proof.

**Theorem 4.6** (Correctness of Reductions). Let \( \Gamma \vdash P : \sigma \).
1. \( P \rightarrow_A P' \) implies \( [P] = [P'] \).
2. \( P \rightarrow P' \) implies \( [P] = [P'] \).

**Proof.** The full proof can be found in Appendix E.

2. Case analysis on reductions of pullback terms. Consider Reduction 16.2.

Let \( y \in \Gamma[1] \). By IH, and \( V_{\pi_1} \equiv \lambda z P' \), we have \([((\Omega A z P') \cdot \omega) V_{\pi_1}] = ([\lambda \omega' S'] \cdot \omega(\langle P' V_{\pi_2} \rangle)]\) which means for any 1-form \( \phi \) and \( v \),
\[
\phi([P'] y, [V_{\pi_1}] y)) = (\text{cur}([P'] y))(D(cur([P'] y))(v, [V_{\pi_1}] y))
\]

Let \( l \) be a linear morphism to \( R \), then \( \lambda x.l \) is a 1-form and hence we have \( l(D[\text{cur}(P') y](v, [V_{\pi_1}] y)) = l([S'] \gamma, v, y) \).

By the contra-positive of the Hahn-Banach Separation Theorem, it implies \( D[\text{cur}(P') y](v, [V_{\pi_1}] y) = [S'] \gamma, v, y) \).

Note that (by D-eval) in [21], \( D[e \circ (\pi_i, \pi_j)](v, x) = \pi_i(v)(\pi_j(x)) + D[\pi_i(x)](\pi_j(v), \pi_j(x)) \).

Hence we have
\[
[\langle \Omega (\lambda y \cdot \pi_1 \cdot \pi_2) \rangle \cdot \omega] y
\]

\[
= \lambda v.[\omega] y ([\langle \pi_1 \pi_2 \rangle y, \langle V \rangle y)] (D[v \circ (\pi_i, \pi_j)](v, \langle V \rangle y))
\]

\[
= \lambda v.[\omega] y ([\langle \pi_1 \pi_2 \rangle y, \langle V \rangle y]) (\langle v_{\pi_1}(\langle V \rangle y) + D[\langle V \rangle y](v_{\pi_2}, \langle V \rangle y)\rangle)
\]

\[
= \lambda v.[\omega] y ([\langle \pi_1 \pi_2 \rangle y, \langle V \rangle y]) (\langle v_{\pi_1}(\langle V \rangle y) + D[\text{cur}(P') y](v_{\pi_2}, \langle V \rangle y)\rangle)
\]

\[
= \lambda v.[\omega] y ([\langle \pi_1 \pi_2 \rangle y, \langle V \rangle y]) (\langle v_{\pi_1}(\langle V \rangle y) + S'(V_{\pi_2} y)\rangle)
\]

The following corollary tells us that our reduction is faithful to reverse-mode AD (in that it is exactly reverse-mode AD when restricted to first-order) and we can perform reverse-mode AD on any abstraction which might contain higher-order terms, duals, pullbacks and free variables.

**Corollary 4.8.** Let \( \Gamma \cup \{ y : \sigma \} \vdash P_1 : \tau, P_2 : \sigma, y \in \Gamma[1] \).
1. Let \( \sigma \equiv R^n, \tau \equiv R^n \). If \( ((\lambda y P_1) \cdot \sigma_\tau) P_2 \rightarrow^\ast \forall V \), then the \( p \)-th row of the Jacobian matrix of \([P_1](y, -) \) at \([P_2]y \) is \( ([V] y) \).
2. Let \( l \) be a linear morphism from \([v] \) to \([P] \). If \( (l P_1) \cdot \omega P_2 \rightarrow^\ast ((\lambda v P') \cdot \omega \omega P') \) for some fresh variable \( \omega \), then the derivative of \( l \circ (P_1)(y, -) \) at \([P_2]y \) along some \( v \in [\sigma] \) is \( l([P_1]'(y, \lambda x.l, v)) \) i.e. \( D[l \circ (P_1)](y, -)(v, P_2) = l(P_1)'(y, \lambda x.l, v) \).

**Example 4.9.** In Example 3.9, we showed that \( ((\lambda x.y.\text{pow}(2\sinh(x, y))) \cdot \pi_1)(1, 3) \rightarrow^\ast \). Note that [660 528] is exactly the Jacobian matrix of \( f : (x, y) \mapsto ((x + 1)2 + y^2)^2 \) at \( (1, 3) \).

5 Related Work

We discuss recent works on calculi / languages that provide differentiation capabilities.

### 5.1 Differential Lambda-Calculus

The standard bearer is none other than differential \( \lambda \)-calculus [15], which has inspired the design of our language.

The implementation guided by differential \( \lambda \)-calculus is a form of symbolic differentiation, which suffers from expression swell. For this reason, Manzyuk [22] introduced the perturbative \( \lambda \)-calculus, a \( \lambda \)-calculus with a forward-mode AD operator. Our language is complementary to these calculi, in that it implements higher-order reverse-mode AD; moreover, it is call-by-value, which is crucial for reverse-mode AD to avoid expression swell, as illustrated in Example 3.7.

What is the relationship between our language and differential \( \lambda \)-calculus? We can give a precise answer via a compositional translation \( (\cdot) \) to a differential \( \lambda \)-calculus extended by real numbers, function symbols, pairs and projections, defined as follows:

\[
s, t ::= x | \lambda x.s | s T | Ds \cdot t | \pi_i(s) | \langle s, t \rangle | r | \text{f}(T) | Df \cdot t \quad S, T ::= 0 | s + T \quad \text{where } r \in \mathbb{R}, f \in \mathbb{F}
\]

The major cases of the definition of \((\cdot) \) are:

\[
(f(S))_i := \sigma_i \Rightarrow R \quad \text{where } \sigma_i = \lambda v. \sum_{i=1}^n f_i(\pi_i(v))
\]
Because differential $\lambda$-calculus does not have linear function type, $(S_1)_f$ is no longer in a linear position in $(\lambda x.S_1)^* \cdot S_2$. Though the translation does not preserve linearity, it does preserve reductions and interpretations (Lemma 5.1).

**Lemma 5.1.** Let $P$ be a term.

1. If $P \rightarrow P'$, then there exists a reduct $s$ of $P$, such that $P_t \rightarrow^* s$ in $L_D$.
2. $[P] = [P_t]$ in C.

A corollary of Lemma 5.1 (1) is that our reduction strategy is strongly normalizing.

**Corollary 5.2 (Strong Normalization).** Any reduction sequence from any term is finite, and ends in a value.

## 5.2 Differentiable Programming Languages

Encouraged by calls [14, 19, 24] from the machine learning community, the development of reverse-mode AD programming language has been an active research problem. Following Pearlmutter and Siskind [27], these languages usually treat reverse-mode AD as a meta-operator on programs.

**First-order** Elliott [16] gives a categorical presentation of reverse-mode AD. Using a functor over Cartesian categories, he presents a neat implementation of reverse-mode AD.

As is well-known, conditional does not behave well with smoothness [6]; nor does loops and recursion. Abadi and Plotkin [2] address this problem via a first-order language with conditionals, recursively defined functions, and a construct for reverse-mode AD. Using real analysis, they prove the coincidence of operational and denotational semantics.

To our knowledge, these treatments of reverse-mode AD are restricted to first-order functions.

**Towards higher-order** The first work that extends reverse-mode AD to higher orders is by Pearlmutter and Siskind [27]; they use a non-compositional program transformation to implement reverse-mode AD.

Inspired by Wang et al. [32, 33], Brunel et al. [10] study a simply-typed $\lambda$-calculus augmented with a notion of linear negation type. Though our dual type may resemble their linear negation, they are actually quite different. In fact, our work can be viewed as providing a positive answer to the last paragraph of [10, Sec. 7], where the authors address the relation between their work and differential lambda-calculus. They describe a “naive” approach of expressing reverse-mode AD in differential lambda-calculus in the sense that it suffers from “expression swell”, which our approach does not (see Example 3.7). Moreover, Brunel et al. use a program transformation to perform reverse-mode AD, whereas we use a first-class differential operator. Brunel et al. [1] prove correctness for performing reverse-mode AD on real-valued functions (Theorem 5.6, Corollary 5.7 in [1]), whereas we allow any (higher-order) abstraction to be the argument of the pullback term and proved that the result of the reduction of such a pullback term is exactly the derivative of the abstraction (Corollary 4.8).

Building on Elliott [16]’s categorical presentation of reverse-mode AD, and Pearlmutter and Siskind [27]’s idea of differentiating higher-order functions, Vytiniotis et al. [31] developed an implementation of a simply-typed differentiable programming language.

However, all these treatments are not purely higher-order, in the sense that their differential operator can only compute the derivative of an “end to end” first-order program (which may be constructed using higher-order functions), but not the derivative of a higher-order function.

As far as we know, our work gives the first implementation of reverse-mode AD in a higher-order programming language that directly computes the derivative of higher-order functions using reverse-mode AD (Corollary 4.8 (2)).

## 6 Conclusion and Future Directions

After outlining the mathematical foundation of reverse-mode AD as the pullback of differential 1-forms (Section 2.2), we presented a simple higher-order programming language with an explicit differential operator, $(\Omega(\lambda x. P)) \cdot S$, (Subsection 3.1) and a call-by-value reduction strategy to divide (A-reductions in Subsection 3.2), conquer (pullback reductions in Subsection 3.3) and combine (Subsection 3.4) the term $((\Omega(\lambda x. P)) \cdot \omega) S$, such that its reduction exactly mimics reverse-mode AD. Examples are given to illustrate that our reduction is faithful to reverse-mode AD. Moreover, we show how our reduction can be adapted to a CPS evaluation (Subsection 3.5).

We showed (in Section 4) that any differential $\lambda$-category that satisfies the Hahn-Banach Separation Theorem is a sound model of our language (Theorem 4.6) and how our reduction precisely captures the notion of reverse-mode AD, in both first-order and higher-order settings (Corollary 4.8).
**Future Directions.** An interesting direction is to extend our language with probability, which can serve as a compiler intermediate representation for “deep” probabilistic frameworks such as Edward [29] and Pyro [30]. Inference algorithms that require the computation of gradients, such as Hamiltonian Monte Carlo and variational inference, which Edward and Pyro rely on, can be expressed in such a language and allows us to prove correctness.

### References

[1] Martín Abadi, Paul Barham, Jianmin Chen, Zhifeng Chen, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Geoffrey Irving, Michael Isard, Manjunath Kudlur, Josh Levenberg, Rajat Monga, Sherry Moore, Derek Gordon Murray, Benjamin Steiner, Paul A. Tucker, Vijay Vasudevan, Peter Warden, Martin Wicke, Yuan Yu, and Xiaoqiang Zheng. 2016. TensorFlow: A System for Large-Scale Machine Learning. In 12th USENIX Symposium on Operating Systems Design and Implementation, OSDI 2016, Savannah, GA, USA, November 2-4, 2016. 265–283. https://www.usenix.org/conference/osdi16/technical-sessions/presentation/abadi

[2] Martin Abadi and Gordon D. Plotkin. 2020. A simple differentiable programming language. *PACMPL* 4 (2020), 38:1–38:28. https://doi.org/10.1145/3371106

[3] Rami Al-Rfou, Guillaume Alain, Amjad Almahairi, Christof Angermüller, Dzmitry Bahdanau, Nicolas Ballas, Frédéric Bastien, Justin Bayer, Anatoly Belikov, Alexander Belopolsky, Yoshua Bengio, Arnaud Bergeron, James Bergstra, Valentin Bisson, Josh Bleecker Snyder, Nicolas Bouchard, Nicolas Boulanger-Lewandowski, Xavier Bouthillier, Alexandre de Brébisson, Olivier Breuleux, Pierre Luc Carrier, Kyunghyun Cho, Jan Chorowski, Paul F. Christiano, Tim Cooijmans, Marc-Alexandre Côté, Myriam Côté, Aaron C. Courville, Yann N. Dauphin, Olivier Delalleau, Julien Demouth, Guillaume Desjardins, Sander Dieleman, Laurent Dinh, Melanie Ducoffe, Vincent Dumoulin, Samira Ehraimi Kahou, Dumitru Erhan, Ziye Fan, Orhan Firat, Mathieu Germain, Xavier Glorot, Ian J. Goodfellow, Matthew Graham, Çağlar Güçlü, Philippe Hamel, Ian Harlouchet, Jean-Philippe Heng, Balázs Hidasi, Sina Honari, Arjun Jain, Sébastien Jean, Kai Jia, Mikhaïl Khanin, Vivek Kulkarni, Alex Larochelle, Pascal Lamblin, Eric Larsen, César Laurent, Seán Lee, Simon Lefrançois, Simon Lemieux, Nicholas Léonard, Zhouhan Lin, Jesse A. Livezey, Cory Lorentz, Jeremiah Lowin, Qianli Ma, Pierre-Antoine Manzagol, Olivier Mastropietro, Robert McGibbon, Roland Memisevic, Bart van Merriënboer, Vincent Michalski, Mehdi Mirza, Alberto Orlandi, Christopher Joseph Pal, Razvan Pascanu, Mohammad Pezeshki, Colin Raffel, Daniel Renshaw, Matthew Rocklin, Adriana Romero, Markus Roth, Peter Sadowski, John Salvatier, François Savard, Jan Schlüter, John Schulman, Gabriel Schwartz, Iulian Vlad Serban, Dmitriy Serdyuk, Samira Shabanian, Étienné Simon, Sigurd Spieckermann, S. Ramana Subramanyam, Jakub Szynkowski, Jérémie Tanguay, Gijs van Tulder, Joseph P. Turian, Sébastien Urban, Pascal Vincent, Francesco Visin, Harm de Vries, David Warde-Farley, Dustin J. Webb, Matthew Wilson, Kelvin Xu, Liujun Xue, Li Yao, Sanjiang Zheng, and Ying Zhang. 2016. Theano: A Python framework for fast computation of mathematical expressions. *CoRR* abs/1605.02688 (2016). arXiv:1605.02688 http://arxiv.org/abs/1605.02688

[4] F. Bauer. 1974. Computational Graphs and Rounding Error. *SIAM J. Numer. Anal.* 11, 1 (1974), 87–96. https://doi.org/10.1137/0711010

[5] Atılım Gunes Baydin, Barak A. Pearlmutter, Alexey Andreyevich Radul, and Jeffrey Mark Siskind. 2017. Automatic Differentiation in Machine Learning: a Survey. *J. Mach. Learn. Res.* 18 (2017), 153:1–153:43. http://jmlr.org/papers/v18/17-468.html

[6] Thomas Beck and Herbert Fischer. 1994. The iF-problem in automatic differentiation. *J. Comput. Appl. Math.* 50, 1 (1994), 119 – 131. https://doi.org/10.1016/0377-0427(94)90294-1

[7] Michael Betancourt. 2018. A geometric theory of higher-order automatic differentiation. arXiv preprint arXiv:1812.11592 (2018).

[8] Richard Blute, Thomas Ehrhard, and Christine Tasson. 2010. A convenient differential category. *CoRR* abs/1006.3140 (2010). arXiv:1006.3140 http://arxiv.org/abs/1006.3140

[9] Richard F Blute, J Robin B Cockett, and Robert AG Seely. 2009. Cartesian differential categories. *Theory and Applications of Categories 22*, 23 (2009), 622–672.

[10] Alois Brunel, Damiano Mazza, and Michele Pagani. 2019. Back-propagation in the Simply Typed Lambda-calculus with Linear Negation. *CoRR* abs/1909.13768 (2019). arXiv:1909.13768 http://arxiv.org/abs/1909.13768

[11] Antonio Bucciarelli, Thomas Ehrhard, and Giulio Manzonetto. 2010. Categorical Models for Simply Typed Resource Calculi. *Electr. Notes Theor. Comput. Sci.* 265 (2010), 213–230. https://doi.org/10.1016/j.entcs.2010.08.013

[12] Alonzo Church. 1965. *The Calculi of Lambda-Conversion*. New York : Kraus Reprint Corporation.

[13] J. Robin B. Cockett and Geoff S. H. Cruttwell. 2014. Differential Structure, Tangent Structure, and SDG. *Applied Categorical Structures 22*, 2 (2014), 331–417. https://doi.org/10.1007/s10485-013-9312-0

[14] David Dalrymple. 2016. 2016: What do you consider the most interesting recent [scientific] news? What makes it important? https://www.edge.org/response-detail/26794. (2016). Accessed: 2020-01-07.

[15] Thomas Ehrhard and Laurent Regnier. 2003. The differential lambda-calculus. *Theor. Comput. Sci.* 309, 1-3 (2003), 1–41. https://doi.org/10.1016/S0304-3975(03)00392-X

[16] Conal Elliott. 2018. The simple essence of automatic differentiation. *PACMPL* 2, 1CFP (2018), 70:1–70:29. https://doi.org/10.1145/3236765

[17] Alfred Frolicher and Andreas Kriegl. 1988. *Linear spaces and differentiation theory*. Chichester : Wiley.

[18] Philipp H. W. Hoffmann. 2016. A Hitchhiker’s Guide to Automatic Differentiation. *Numerical Algorithms 72*, 3 (01 Jul 2016), 775–811. https://doi.org/10.1007/s11075-015-0067-6

[19] Yann LeCun. 2018. Deep Learning est mort. Vive Differentiable Programming! https://www.facebook.com/yann.lecun/posts/10155003011462143. (2018). Accessed: 2020-01-07.

[20] Dougal Maclaurin, David Duvenaud, and Ryan P. Adams. 2015. AutoGrad: Effortless Gradients in Numpy. Presented in AutoML Workshop, ICML, Cascais, Portugal.

[21] Giulio Manzonetto. 2012. What is a categorical model of the differential and the resource λ-calculi? *Mathematical Structures in Computer Science* 22, 3 (2012), 451–520. https://doi.org/10.1017/S096012951000594

[22] Oleksandr Manzyuk. 2012. A Simply Typed λ-Calculus of Forward Automatic Differentiation. *Electr. Notes Theor. Comput. Sci.* 286 (2012), 257–272. https://doi.org/10.1016/j.entcs.2012.08.017
[23] Peter W. Michor and Andreas Kriegl. 1997. *The convenient setting of global analysis*. Providence, R.I. : American Mathematical Society.

[24] Christopher Olah. 2015. Neural Networks, Types, and Functional Programming. http://colah.github.io/posts/2015-09-NN-Types-FP/. (2015). Accessed: 2020-01-07.

[25] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, Alban Desmaison, Andreas Köpf, Edward Yang, Zach DeVito, Martin Raison, Alykhan Tejani, Sasank Chilamkurthy, Benoit Steiner, Lu Fang, Junjie Bai, and Soumith Chintala. 2019. PyTorch: An Imperative Style, High-Performance Deep Learning Library. CoRR abs/1912.01703 (2019). arXiv:1912.01703 http://arxiv.org/abs/1912.01703

[26] Barak A. Pearlmutter. 2019. A Nuts-and-Bolts Differential Geometric Perspective on Automatic Differentiation. Presented in Languages for Inference Workshop, Cascais, Portugal.

[27] Barak A. Pearlmutter and Jeffrey Mark Siskind. 2008. Reverse-mode AD in a functional framework: Lambda the ultimate backpropagator. ACM Trans. Program. Lang. Syst. 30, 2 (2008), 7:1–7:36. https://doi.org/10.1145/1330017.1330018

[28] Amr Sabry and Matthias Felleisen. 1992. Reasoning About Programs in Continuation-Passing Style. In Proceedings of the Conference on Lisp and Functional Programming, LFP 1992, San Francisco, California, USA, 22-24 June 1992. ACM, 288–298. https://doi.org/10.1145/141471.141563

[29] Dustin Tran, Matthew D. Hoffman, Rif A. Saurous, Eugene Brevdo, Kevin Murphy, and David M. Blei. 2017. Deep Probabilistic Programming. CoRR abs/1701.03757 (2017). arXiv:1701.03757 http://arxiv.org/abs/1701.03757

[30] Uber. 2017. Pyro (Retrieved) Nov 2018. (2017). http://pyro.ai/

[31] Dimitriios Vytiniotis, Dan Belov, Richard Wei, Gordon Plotkin, and Martin Abadi. 2019. The Differentiable Curry. Presented in Program Tranformations for Machine Learning Workshop, NeurIPS, Vancouver, Canada.

[32] Fei Wang, James M. Decker, Xilun Wu, Grégory M. Esertel, and Tiark Rompf. 2018. Backpropagation with Callbacks: Foundations for Efficient and Expressive Differentiable Programming. In *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, 3-8 December 2018, Montréal, Canada*, Samy Bengio, Hanna M. Wallach, Hugo Larochelle, Kristen Grauman, Nicolò Cesa-Bianchi, and Roman Garnett (Eds.). 10201–10212. http://papers.nips.cc/book/advances-in-neural-information-processing-systems-31-2018

[33] Fei Wang, Daniel Zheng, James M. Decker, Xilun Wu, Grégory M. Esertel, and Tiark Rompf. 2019. Demystifying differentiable programming: shift/reset the penultimate backpropagator. PACMPL 3, ICFP (2019), 96:1–96:31. https://doi.org/10.1145/3341700

[34] R. E. Wengert. 1964. A simple automatic derivative evaluation program. Commun. ACM 7, 8 (1964), 463–464. https://doi.org/10.1145/355586.364791
Appendix

A Examples

A.1 Simple Example

We focus on how to compute the derivative of \( f : (x, y) \mapsto ((x + 1)(2x + y^2))^3 \) at \((1, 3)\) by different modes of AD.

First \( f \) is decomposed into elementary functions as
\[
\mathbb{R}^2 \xrightarrow{g} \mathbb{R}^2 \xrightarrow{\ast} \mathbb{R} \xrightarrow{\ast} \mathbb{R},
\]
where \( g(x, y) := (x + 1, 2x + y^2) \).

Then, Figure 4 summarize the iterations of different modes of AD.

Now we show how Section 3 tells us how to perform reverse-mode AD on \( f \).

**Term** Assuming \( g, \text{mult}, \text{pow2} \in \mathcal{F} \), we can define the following term in the language.

\[
\vdash ((\Omega \lambda (x, y). \text{pow2}(\text{mult}(g((x, y))))) \cdot (\Omega \lambda [1])) (1, 3) : \mathbb{R}^n
\]

This term is the application of the pullback \( \Omega(f)\lambda x.[1]^* \) to the point \( (1, 3) \), which is exactly the Jacobian of \( f \) at \((1, 3)\).

**Administrative Reduction** We decompose the term \( \text{pow2}(\text{mult}(g((x, y)))) \), via administrative reduction, into a list of elementary terms.

\[
\text{pow2}(\text{mult}(g((x, y)))) \rightarrow^* A \equiv \frac{\lambda z_1 = (x, y); z_2 = g(z_1); z_3 = \text{mult}(z_2); z_4 = \text{pow2}(z_3) \text{ in } z_4}{z_1 = \langle x, y \rangle; z_2 = g(z_1); z_3 = \text{mult}(z_2); z_4 = \text{pow2}(z_3) \text{ in } z_4}
\]

This is reminiscent of the decomposition of \( f \) into \( \mathbb{R}^2 \xrightarrow{g} \mathbb{R}^2 \xrightarrow{\ast} \mathbb{R} \) before performing AD.

**Splitting the Omega** Now via reduction 7 and 8, \((\Omega \lambda (x, y). \omega)(1, 3) \) is reduced to a series of pullback along elementary terms.

\[
\vdash ((\Omega \lambda (x, y). (\text{pow2}((\text{mult}(g((x, y))))))) \cdot (\Omega \lambda [1])) (1, 3) \equiv \frac{\lambda z_1 = (x, y); z_2 = g(z_1); z_3 = \text{mult}(z_2); z_4 = \text{pow2}(z_3) \text{ in } z_4}{(\Omega \lambda (x, y), (x, y)) \cdot (\Omega \lambda ((x, y), z_1), (x, y), z_1, g(z_1)) \cdot (\Omega \lambda ((x, y), z_1, z_2), (x, y), z_1, z_2, \text{mult}(z_2)) \cdot (\Omega \lambda ((x, y), z_1, z_2, z_3), \text{pow2}(z_3)) \cdot \omega}
\]

**Pullback Reduction** We showed that via A-reductions and Reductions 7 and 8, \((\Omega \lambda (x, y). \text{pow2}(\text{mult}(g((x, y)))))) \cdot \omega \) is reduced to

\[
\vdash ((\Omega \lambda (x, y), (x, y)) \cdot (\Omega \lambda ((x, y), z_1), (x, y), z_1, g(z_1)) \cdot (\Omega \lambda ((x, y), z_1, z_2), (x, y), z_1, z_2, \text{mult}(z_2)) \cdot (\Omega \lambda ((x, y), z_1, z_2, z_3), \text{pow2}(z_3)) \cdot \omega)
\]

We show how it can be reduced when applied to \((1, 3)\).

\[
\begin{align*}
(\Omega \lambda (x, y), (x, y)) \cdot \\
(\Omega \lambda ((x, y), z_1), (x, y), z_1, g(z_1)) \\
(\Omega \lambda ((x, y), z_1, z_2), (x, y), z_1, z_2, \text{mult}(z_2)) \\
(\Omega \lambda ((x, y), z_1, z_2, z_3), \text{pow2}(z_3)) \cdot \omega
\end{align*}
\]

= \[
\begin{align*}
\frac{20.1}{11} \cdot \\
\frac{20.1}{14.3} \cdot \\
\frac{20.1}{14.3} \cdot \\
\frac{20.1}{14.3} \cdot
\end{align*}
\]

Notice how this is reminiscent of the forward phase of reverse-mode AD performed on \( f : (x, y) \mapsto ((x + 1)(2x + y^2))^3 \) at \((1, 3)\) considered in Figure 4.

Moreover, we used the reduction \( f(r) \xrightarrow{3} f(r) \) couples of times in the argument position of an application. This is to avoid expression swell. Note \( 1 + 1 \) is only evaluated once in \((*)\) even when the result is used in various computations.

**Combine** Replacing \( \omega \) by \( \Omega [1] \equiv \lambda x.[1]^* \), we have shown so far that

\[
((\Omega \lambda (x, y). (\text{pow2}(\text{mult}(g((x, y))))))) \cdot (\Omega \lambda [1]) (1, 3)
\]

is reduced to

\[
\begin{align*}
(\lambda (v_1, v_2). ((v_1, v_2), (v_1, v_2))) \\
(\lambda (v_1, v_2), v_3), ((v_1, v_2), v_3, (\text{mult} \cdot v_3)(2, 11))) \\
(\lambda (v_1, v_2), v_3, v_4), ((\text{pow2} \cdot v_3)(22)^* \cdot (\omega 484))
\end{align*}
\]

Now via reduction 5 and \( \beta \) reduction, we further reduce it to

\[
\begin{align*}
\frac{\lambda (v_1, v_2), v_3, v_4), ((\text{pow2} \cdot v_3)(22)^* \cdot (\omega 484))}{\lambda (v_1, v_2), v_3, v_4), ((\text{pow2} \cdot v_3)(22)^* \cdot (\omega 484))}
\end{align*}
\]

\[
\begin{align*}
(\lambda (v_1, v_2), v_3, v_4), ((\text{pow2} \cdot v_3)(22)^* \cdot (\omega 484))
\end{align*}
\]
Naïve Forward Mode: \[
\langle (1, 3) \mid \frac{1}{1} \rangle \xrightarrow{g} \langle (2, 11) \mid \frac{5}{2} \rangle \xrightarrow{\ast} \langle 22 \mid [15, 12] \rangle \xrightarrow{(-)^2} \langle 484 \mid [660, 528] \rangle
\]
Forward Mode: \[
\langle (1, 3) \mid \frac{1}{1} \rangle \xrightarrow{g} \langle (2, 11) \mid \frac{5}{2} \rangle \xrightarrow{\ast} \langle 22 \mid [15] \rangle \xrightarrow{(-)^2} \langle 484 \mid [660] \rangle
\]
Reverse Mode: Forward Phase: \[
\langle (1, 3) \xrightarrow{g} (2, 11) \xrightarrow{\ast} 22 \xrightarrow{(-)^2} 484
\]
Reverse Phase: \[
\langle 660 \xrightarrow{[528]} 484 \xrightarrow{[88]} \ast \xrightarrow{[44]} (-)^2 \xrightarrow{[1]} \rangle
\]
Pullback: \[
\langle \Omega(g) \circ \Omega(+) \circ \Omega((-))^2 \rangle \langle \lambda x. [1] \rangle (1, 3) = \langle \langle J \langle \lambda x. [1] \rangle \rangle \rangle \langle \langle J \langle \lambda x. [1] \rangle \rangle \rangle \langle \langle J \langle \lambda x. [1] \rangle \rangle \rangle
\]
\[
\langle \langle J \langle \lambda x. [1] \rangle \rangle \rangle \langle \langle J \langle \lambda x. [1] \rangle \rangle \rangle \langle \langle J \langle \lambda x. [1] \rangle \rangle \rangle
\]
Notice how this mimics the reverse phase of reverse-mode AD on \( f : \langle x, y \rangle \mapsto ((x + 1)(2x + y^2))^2 \) at \( (1, 3) \) considered in Figure 4.

A.2 Sum Example

Consider the function that takes a list of real numbers and returns the sum of the elements of a list. We show how Section 3 tells us how to perform reverse-mode AD on such a higher-order function.

Term Using the standard Church encoding of List, i.e.

\[
\text{List}(X) \equiv (X \to D \to D) \to (D \to D)
\]

\[
[x_1, x_2, \ldots, x_n] \equiv \lambda f d. f x_0 \cdot \ldots (f x_2 (f x_1 d))
\]

for some dummy type \( D \), \( \text{sum} : \text{List}(R) \to R \) can be expressed in our language in Section 3 to be \( \lambda l. (\lambda x y. x + y) \Omega \). Hence the derivative of sum at a list \( [2, 1] \) can be expressed as

\[
\{ \omega : \Omega(\text{List}(R)) \} \cdot \Omega(\text{sum}) \cdot \omega \mid [2, 1] : R^*.
\]

Administrative Reduction We first decompose the body of the sum: \( \text{List}(R) \to R \) term, considered in Example 3.2, i.e. \( l (\lambda x y. x + y) 0 \) via administrative reduction described in Subsection 3.2.

\[
\begin{align*}
\lambda (\lambda x y. x + y) 0 & \quad \rightarrow_A \langle \langle \text{let} z'_1 = l \rangle (\text{let} z'_2 = x + y \text{ in } z'_2) \rangle \text{ (let } z'_3 = 0 \text{ in } z'_3) \\
\text{let } z_1 &= l; \\
\text{let } z_2 &= \lambda x y. (\text{let } z'_2 = x + y \text{ in } z'_2); \\
\text{let } z_3 &= z_1 z_2 \text{ in } z_3;
\end{align*}
\]

Pullback Reduction First, Figure 5 shows that \( \{ \Omega(\Omega(\lambda l. (\lambda x y. x + y) \Omega)) \} \cdot \omega \) is reduced to \( (\lambda v. v - i \langle \Omega(\lambda l. (\lambda x y. x + y) \Omega) \rangle \rangle) \cdot (\lambda v. v - i \langle \Omega(\lambda l. (\lambda x y. x + y) \Omega) \rangle \rangle) \cdot \omega \)

Splitting the Omega After the A-reductions where \( l (\lambda x y. x + y) 0 \) is A-reduced to a let series, we reduce \( \Omega(\lambda l. (\lambda x y. x + y) \Omega)) \cdot \omega \) via Reductions 7 and 8.

\[
\begin{align*}
\Omega(\lambda l. (\lambda x y. x + y) 0)) \cdot \omega & \quad \rightarrow_A \langle \text{let } z_1 = l; \\
\text{let } z_2 &= \lambda x y. (\text{let } z'_2 = x + y \text{ in } z'_2); \\
\text{let } z_3 &= z_1 z_2 \text{ in } z_3; \\
\text{let } z_4 &= 0; \\
\text{let } z_5 &= z_3 z_4 \text{ in } z_5
\end{align*}
\]
\[
\left(\Omega \ [\begin{array}{c}
\frac{2}{3} \\
\frac{3}{4}
\end{array}] \cdot \omega \right) (\lambda x.y.L) =
\left(\frac{\Omega \lambda f.d. f \cdot \frac{2}{3}}{\frac{3}{4}} (f \ \frac{2}{3} d) \cdot \omega \right) (\lambda x.y.L) \\
\xrightarrow{\ast} \left(\frac{\Omega \lambda f.d. f \cdot \frac{2}{3}}{\frac{3}{4}} (f \ \frac{2}{3} d) \cdot \omega \right) (\lambda x.y.L)
\]

**Figure 5. Reduction of \( (\Omega [\begin{array}{c}
\frac{2}{3} \\
\frac{3}{4}
\end{array}] \cdot \omega ) (\lambda x.y.L) \)**

**B Administrative Reduction**

Elementary terms \( E \), let series \( L \), A-contexts \( C_A \) and A-redexes \( r_A \) are defined as follows.

\[
E := 0 | z_1 + z_2 | z | \lambda x.\underline{L} | z_1 z_2 | z_1 \ \frac{2}{3} (z_1, z_2) \ |
\frac{f}{2} (z) | \frac{f}{{\frac{2}{3}}} \cdot z | (\lambda x.\underline{L}) \ ] z | \frac{2}{3} \\
L := z \in E | L \in E | \underline{L} | E \in E | z \ \frac{2}{3} (L, C_A) | \frac{C_A}{L} \ |
\frac{f(L)}{C_A} \ |
\frac{\lambda x.\underline{L}}{L} | \frac{\lambda x.\underline{L}}{C_A} | \frac{\lambda x.\underline{L}}{\lambda x.C_A} | \frac{\lambda x.\underline{L}}{\lambda x.C_A} | \frac{\lambda x.\underline{L}}{\lambda x.C_A} | L | C_A | \pi_1(C_A)
\]

where \( B \equiv \left(\begin{array}{c}
\frac{2}{3} \\
\frac{3}{4}
\end{array}\right) \), \( \lambda x.y.\underline{L} \), \( \lambda d.+(\frac{2}{3}, +(\frac{3}{4}, d)) \), \( 0, 6 \).

Hence, \( \lambda v.(\lambda x.y.\underline{L}) \ ) is the derivative of sum \( \Omega \lambda L(\lambda x.\underline{L}) \ )

at \( \left[\begin{array}{c}
\frac{2}{3} \\
\frac{3}{4}
\end{array}\right] \).

This sequence of reduction tells us how the derivative of sum at \( \left[\begin{array}{c}
\frac{2}{3} \\
\frac{3}{4}
\end{array}\right] \) can be computed using reverse-mode AD.

Lemma B.1. Every pullback term \( \underline{P} \) can be expressed as either \( C_A[r_A] \) for some unique A-context \( C_A \) and A-redex \( r_A \) or a let series of elementary terms \( L \).

An A-redex \( r_A \) is reduced to a let series \( L \) as follows.

\[
\lambda x.L \xrightarrow{\ast} L_1 + L_2 \xrightarrow{\ast} L_1 \xrightarrow{\ast} L_2 \xrightarrow{\ast} L_3 \xrightarrow{\ast} L_4 \xrightarrow{\ast} L_5
\]

\[
\lambda x.L \xrightarrow{\ast} x_1 = x_1 + x_2 \xrightarrow{\ast} x_1 + x_2 \xrightarrow{\ast} x_1 + x_2 \xrightarrow{\ast} x_1 + x_2
\]

17
\[ \llbracket f \rrbracket (s) = f \circ [s] \]
\[ \llbracket D_f \rrbracket (s) = \lambda y. D(f)(\llbracket s \rrbracket y, x) \]

### Translation to Differential Lambda-Calculus

\[ 0_t := 0 \]
\[ (S + P)_t := S_t + P_t \]
\[ (\langle S_1, S_2 \rangle)_t := \langle S_1,t \rangle, \langle S_2,t \rangle \]
\[ y_t := y \]
\[ (\lambda x.S)_t := \lambda y.S_t \]
\[ f(P)_t := f(P_t) \]
\[ (S P)_t := S_t P_t \]
\[ (\langle f, S \rangle)_t := Df \cdot \llbracket S \rrbracket_t \]

\[ \langle n \rangle_t := \lambda u. \sum_{i=1}^{\lambda \lambda y.t} f_i(u) \]
\[ \langle (\lambda y.S)_t \cdot S_t \rangle_t := \lambda v. \langle (S_1)_t \rangle_t \langle v, v \rangle \]
\[ \langle (\Omega \lambda x.P) \cdot S \rangle_t := \lambda xv. \langle P \rangle_t (\llbracket x, y \rrbracket) (D\llbracket P \rrbracket_t) (\llbracket v, x \rrbracket) \]

where \( f := r_t = -1 \).

### E Proofs

#### Proposition E.1

The derivative of any constant morphism \( f \) in a differential \( \lambda \)-category is 0, i.e. \( D[f] = 0 \).

**Proof.** A constant morphism \( f : A \to B \) that maps all of \( A \) to \( b \in B \) can be written as \( f = (\lambda z.b) \circ 0 \) where \( 0 : A \to B \) and \( \lambda z.b : B \to B \). So by [CD1,2,5] we have \( D[f] = D[(\lambda z.b) \circ 0] = D[\lambda z.b] \circ \langle 0, 0 \circ \pi_2 \rangle = D[\lambda z.b] \circ \langle 0, 0 \pi_2 \rangle = 0 \). \( \square \)

#### Lemma E.2

Con\( \infty \) is a differential \( \lambda \)-category with the differential operator

\[ D[f](\llbracket v, x \rrbracket) := \langle f \rangle (\llbracket x, v \rrbracket) = \lim_{t \to 0} (f(x + tv) - f(x))/t. \]

**Proof.** [17, 23] have shown that Con\( \infty \) is Cartesian closed, and [8] have shown that Con\( \infty \) is a Cartesian differential category. What is left to show is that \( \lambda \) (preserves the additive structure and \( D[-] \) satisfies the (D-curry) rule, i.e.

\[ D[(\lambda f)](x) \circ (\pi_1 \times 0, \pi_2 \times 1d) \]

We first show that \( \lambda \) is additive, i.e. \( \lambda (f + g) = \lambda f + \lambda g \) and \( \lambda (0) = 0 \). Note that for \( f, g, 0 : A \times B \to C \) and \( a \in A, b \in B \), \( \lambda (f + g)(a, b) = (f + g)(a, b) = f(a, b) + g(a, b) = \lambda (f)(a, b) + \lambda (g)(a, b) \) and \( \lambda (0)(a, b) = 0(a, b) = 0 = 0(a, b) \).

Now we show that \( D[-] \) satisfies the (D-curry) rule. Let \( f : A \times B \to C, v, x \in A \) and \( b \in B \).

\[ D[(\lambda f)](\llbracket v, x \rrbracket) b = \left( \lim_{t \to 0} (\lambda f)(x + tv) - \lambda f(x) \right) b \]

\[ = \lim_{t \to 0} \langle f(x + tv, b) - f(x, b) \rangle \]

\[ = \lim_{t \to 0} \langle f(x, b) + l(t, 0), b \rangle \]

\[ = D[f] \circ (\pi_1 \times 0, \pi_2 \times 1d) \rangle (\llbracket v, x \rrbracket, b) \]

\[ = \lambda (D[f] \circ (\pi_1 \times 0, \pi_2 \times 1d)) (\llbracket v, x \rrbracket, b) \]
Proposition E.3. Let $E$ be a convenient vector space and $x, y \in E$ be distinct elements in $E$. Then, there exists a bornological linear map $l : E \to \mathbb{R}$ that separates $x$ and $y$, i.e. $l(x) \neq l(y)$.

Proof. This follows from the fact that convenient vector space is separated.

$x \neq y$ implies that $x - y \neq 0$. Hence by separation, there is a bornological linear map $l : E \to \mathbb{R}$ such that $l(x - y) \neq 0$. Notice that $l$ is linear, so we have $l(x) - l(y) \neq 0$ which implies $l(x) \neq l(y)$.

Lemma 4.4 (Linearity). Let $\Gamma_1 \cup \{x : \sigma_1\} \vdash P_1 : \tau$ and $\Gamma_2 \vdash P_2 : \sigma^*$. Let $y_1 \in \Gamma_1$ and $y_2 \in \Gamma_2$. Then,

1. If $x \in \text{lin}(P_1)$, then $\text{cur}(P_1)\gamma_1$ is linear, i.e. $D[\text{cur}(P_1)\gamma_1] = (\text{cur}(P_1)\gamma_1) \circ \pi_1$.
2. If $\Gamma_2 = \text{lin}(P_2)$, then $\text{cur}(P_2)\gamma$ is linear, i.e. $D[\text{cur}(P_2)\gamma] = (\text{cur}(P_2)\gamma) \circ \pi_1$.

Proof. Induction on the structure of $P$ on the following two statements.

IH.1 If $\Gamma_1 \cup \{x : \sigma_1\} \vdash x : \sigma_1$ and $x \in \text{lin}(P)$, then for any $y_1 \in \Gamma_1$, $\text{cur}(P)\gamma_1$ is linear, i.e. $D[\text{cur}(P)\gamma_1] = (\text{cur}(P)\gamma_1) \circ \pi_1$.

IH.2 If $\Gamma_2 \vdash P : \sigma^*$, then for any $y_2 \in \Gamma_2$, $\text{cur}(P)\gamma$ is linear, i.e. $D[\text{cur}(P)\gamma] = (\text{cur}(P)\gamma) \circ \pi_1$.

(var) Say $P \equiv x$.

(1) If $\Gamma_1 \cup \{x : \sigma_1\} \vdash P : \tau$ and $x \in \text{lin}(x)$, then $D[\text{cur}(x)\gamma_1] = D[\text{Id}] = \pi_1 = \text{Id} \circ \pi_1 = (\text{cur}(x)\gamma_1) \circ \pi_1$.

(2) If $\Gamma_2 \vdash P : \sigma^*$, then for any $y_2 \in \Gamma_2$, $\text{cur}(P)\gamma$ is linear, i.e. $D[\text{cur}(P)\gamma] = (\text{cur}(P)\gamma) \circ \pi_1$.

(dual) Say $P \equiv (\lambda x. S_1)^* \cdot S_2$.

(1) Let $\Gamma_1 \cup \{x : \sigma_1\} \vdash P \equiv (\lambda x. S_1)^* \cdot S_2 : \tau$ and $x \in \text{lin}(\text{term}(\lambda x. S_1)^\gamma \cdot S_2) \equiv \text{lin}(\lambda x. S_1) \setminus \text{FV}(S_2) \cup \text{lin}(S_2) \setminus \text{FV}(S_1)$, then for any $y_1 \in \Gamma_1$ and since $S_2\gamma \equiv x$ is of a dual type, by IH.2,

\[
D[\text{cur}(\lambda x. S_1)^\gamma \cdot S_2\gamma](\nu, x) = \lambda z. (D[S_2\gamma](\nu, x))(g(x, z)) + D[S_2\gamma](\nu, x)(D[g(\nu, z)](\nu, x), g(x, z))
\]

where $g : \langle \nu, x, z \rangle \mapsto [S_2\gamma](\nu, x, z)$. Note that $g$ can only be in either $\text{lin}(S_2)$ \text{FV}(S_2) or $\text{lin}(S_2) \setminus \text{FV}(S_2)$ but not both. Say $x \in \text{lin}(S_2 \setminus \text{FV}(S_2))$, then by Proposition E.1 and IH.1,

\[
D[\text{cur}(\lambda x. S_1)^\gamma \cdot S_2\gamma](\nu, x) = \lambda z. (D[S_2\gamma](\nu, x))(S_2\gamma(\nu, x, z))
\]

Lemma 4.5 (Substitution). $\Gamma \vdash S[P/x : \tau] = \Gamma \cup \{x : \sigma_1 \vdash S : \tau\} \circ (\text{Id}^\gamma, [\Gamma \vdash P : \sigma_1])$

Proof. The only interesting cases are dual and pullback maps.

\[
((\lambda x. S_1)^\gamma \cdot S_2)[P'/y] = (\lambda x. S_1)[P'/y]^\gamma \cdot S_2[P'/y]
\]

\[
(((\lambda x. S_1)^\gamma \cdot S_2)[P'/y])\gamma = (\lambda x. S_1)[P'/y]^\gamma \cdot S_2[P'/y] \circ \text{cur}(S_2)[P'/y] \gamma
\]

\[
(\Omega \lambda x. P)[S/P'] \equiv (\Omega \lambda x. P)[S/P'] \circ \text{cur}(S_2)[P'/y] \gamma
\]

\[
(((\Omega \lambda x. P)[S/P'])\gamma \equiv (\Omega \lambda x. P)[S/P'] \circ \text{cur}(S_2)[P'/y] \gamma
\]

Theorem 4.6 (Correctness of Reductions). Let $\Gamma \vdash P : \sigma$.

1. $P \rightarrow^A P' \equiv \text{fct}(P) = P'$.
2. $P \rightarrow^P P' \equiv \text{fct}(P) = P'$.

Proof. 1. Easy induction on $\rightarrow^A$.

2. Case analysis on reductions of pullback terms. Let $y \in \Gamma$.

(1-4) $\text{cur}(S[V/x]) = S[V_1, V_2]$, $\text{cur}(V_1, V_2) = [V_1, f(r)]$ and $\text{fct}(f') = D(f)(r)$ are easily verified using the Substitution Lemma 4.5.

(5) Let $\text{fct}(f)(r) = [a_{ij}]_{i=1,...,m, j=1,...,n}$ and $r' = [r'_{ij}]_{i=1,...,m}$.

(2) Let $\Gamma_2 \vdash (\lambda x. S_1)^\gamma \cdot S_2 : \sigma^* \gamma (2, \gamma) \in \Gamma_2$. Then, by IH.1 and IH.2,

\[
D[(\lambda x. S_1)^\gamma \cdot S_2]\gamma = (\lambda x. S_1)[P'/y] \circ \text{cur}(S_2)[P'/y] \gamma
\]

\[
((\lambda x. S_1)^\gamma \cdot S_2)[P'/y] = (\lambda x. S_1)[P'/y]^\gamma \cdot S_2[P'/y]
\]

All other cases are straightforward inductive proofs.

\[
((\lambda x. S_1)^\gamma \cdot S_2)[P'/y] = D[(\lambda x. S_1)^\gamma \cdot S_2]_{\gamma}(\lambda x. S_1)[P'/y] \circ \text{cur}(S_2)[P'/y] \gamma
\]

\[
((\lambda x. S_1)^\gamma \cdot S_2)[P'/y] = (\lambda x. S_1)[P'/y] \circ \text{cur}(S_2)[P'/y] \gamma
\]

\[
((\lambda x. S_1)^\gamma \cdot S_2)[P'/y] = D[(\lambda x. S_1)^\gamma \cdot S_2]_{\gamma}(\lambda x. S_1)[P'/y] \circ \text{cur}(S_2)[P'/y] \gamma
\]

\[
((\lambda x. S_1)^\gamma \cdot S_2)[P'/y] = (\lambda x. S_1)[P'/y] \circ \text{cur}(S_2)[P'/y] \gamma
\]

\[
((\lambda x. S_1)^\gamma \cdot S_2)[P'/y] = D[(\lambda x. S_1)^\gamma \cdot S_2]_{\gamma}(\lambda x. S_1)[P'/y] \circ \text{cur}(S_2)[P'/y] \gamma
\]

\[
((\lambda x. S_1)^\gamma \cdot S_2)[P'/y] = (\lambda x. S_1)[P'/y] \circ \text{cur}(S_2)[P'/y] \gamma
\]
\[(\mathcal{J}(f)(r))^\ast (\langle \cdot, \cdot \rangle)(\lambda \nu. \sum_{i=1}^{m} r_i v_i = \lambda \nu. \sum_{j=1}^{n} a_{ij} v_j) = \lambda \nu. \sum_{j=1}^{n} (r_j \cdot a_{ij}) v_j = \lambda \nu. \sum_{j=1}^{n} (\mathcal{J}(f)(r))^\ast \cdot r_j v_j = \left(\left(\mathcal{J}(f)(r)\right)^\ast \times r\right)^\ast \cdot y.\]

(6) Say \( \Gamma \cup \{v_1 : \sigma_1, v_2 : \sigma_2\} \vdash \mathcal{V}_2 : \tau \). Let \( \Gamma \cup \{v_1 : \sigma_1, v_2 : \sigma_2\} \vdash \mathcal{V}_2 : \tau \) where \( v_1 \) is not a free variable in \( \mathcal{V}_2 \).

\[\left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \nu. \sum_{i=1}^{m} \gamma_i v_i).\]

(7) Using the Substitution Lemma 4.5.

\[\left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \nu. \sum_{i=1}^{m} \gamma_i v_i)\right](\lambda \lambda. y. z) = \left[\left[\left[\left[\left[\mathcal{L}(x, z)\right] \mathcal{L}(y, z)\right] \mathcal{L}(z, z)\right] \mathcal{L}(x, z)\right] \mathcal{L}(y, z)\right] \mathcal{L}(z, z)\right] \mathcal{L}(x, z) \Rightarrow \tau.\]

(8) Consider \( \left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \lambda. (x, y))\right](\lambda \lambda. y. z) = \left[\left[\left[\left[\left[\mathcal{L}(x, z)\right] \mathcal{L}(y, z)\right] \mathcal{L}(z, z)\right] \mathcal{L}(x, z)\right] \mathcal{L}(y, z)\right] \mathcal{L}(z, z)\right] \mathcal{L}(x, z) \Rightarrow \tau.\]

(9) Say \( y \) is not free in \( \mathcal{V}_1 \) and \( \left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \lambda. y. z)\right] \Rightarrow 0.\]

Then, \( \left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)\right](\lambda \lambda. y. z) = \left[\left[\left[\left[\left[\mathcal{L}(x, z)\right] \mathcal{L}(y, z)\right] \mathcal{L}(z, z)\right] \mathcal{L}(x, z)\right] \mathcal{L}(y, z)\right] \mathcal{L}(z, z)\right] \mathcal{L}(x, z) \Rightarrow 0.\]

since \( \text{cur}(\mathbb{E})y \) is a constant function and the derivative of any constant function is 0 by Proposition E.1.

(10) We present the proof for (10b).

\[\left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \lambda. y. z)\right] \Rightarrow (\lambda \lambda. v_\pi \ast v_{\pi}).\]

(11) \( \left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \lambda. y. z)\right] \Rightarrow (\lambda \lambda. v_\pi \ast v_{\pi}).\]

(12) \( \left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \lambda. y. z)\right] \Rightarrow (\lambda \lambda. v_\pi \ast v_{\pi}).\]

(13) We prove for (13c).

\[\left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \lambda. y. z)\right] \Rightarrow (\lambda \lambda. v_\pi \ast v_{\pi}).\]

(14) \( \left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \lambda. y. z)\right] \Rightarrow (\lambda \lambda. v_\pi \ast v_{\pi}).\]

Hence, \( \left[\left[\langle \mathcal{V}_1, \mathcal{V}_2 \rangle, \mathcal{V}_3 \rangle \right] (\langle \cdot, \cdot \rangle)(\lambda \lambda. y. z)\right] \Rightarrow (\lambda \lambda. v_\pi \ast v_{\pi}).\]
Differential-form Pullback Programming Language and Reverse-mode AD

\[= (\lambda v. (\int f \cdot v_{\pi_1})) \circ (\omega ((\int f \cdot v_{\pi_1})) \circ (\omega (f (\int v_{\pi_1}))))\]

(15) \( (\Omega \lambda y. (f(y_{\pi_1})) \cdot \omega) \nabla \rightarrow (\lambda v. (\int f \cdot v_{\pi_1})) \circ (\omega (f (\int v_{\pi_1}))) \]

\[= (\lambda x.v. \omega y ((\int f (x_{\pi_1})) \circ (\int f (\int f (x_{\pi_1})))) \circ \omega) \nabla \]

First, note that since \( V_{\pi_1} \) is the dual type, hence by Lemma 4.2, \( D[\int v_{\pi_1}] y = (\int v_{\pi_1}) y \circ \pi_1. \)

\( D\text{cur}((\lambda z.L) \cdot y_{\pi_1}) y) \circ (v, [\int v_{\pi_1}] y) \)

(16) We prove for the most complicated case (16c) which leads to (16a) and (16b).

By IH, \( (\Omega \lambda y. (\nabla L) \cdot \omega) \nabla = (\lambda v. S^* \cdot \omega V^*) \) implies for any 1-form \( \phi, y, x, v. \)

\[\phi((\int L(y, [\int v_{\pi_1}] y, x))(\int [\int v_{\pi_1}] y, y, z)(v, [\int v_{\pi_1}] y))\]

By Hahn-Banach Theorem, we have \( D[\int L(y, ) \cdot (v, [\int v_{\pi_1}] y)] = (S) (y, x, v). \)

First, note that since \( V_{\pi_1} \) is the dual type, hence by Lemma 4.2, \( D[\int v_{\pi_1}] y = (\int v_{\pi_1}) y \circ \pi_1. \)

18) If \( ((\Omega \lambda y. (\nabla L) \cdot \omega) \nabla \rightarrow (\lambda v. S^* \cdot \omega V) \) and \( x \notin FV(V), \) then \( ((\Omega \lambda y. (\nabla L) \nabla) \cdot V) \nabla \rightarrow (\lambda v. S^* \cdot V \lambda x.L V/y). \)

Recall the D-curry rule, \( D\text{cur}(f) = \text{cur}(D[f] \circ (\pi_1 \times 0, \pi_2 \times 1d)). \) By IH, we have \( (\Omega \lambda y. (\nabla L) \cdot \omega) \nabla = (\lambda v. S^* \cdot \omega (L/V/y)), \) which means for any 1-form \( \phi, y, x, v. \)

\[\phi((\int L(y, [\int v_{\pi_1}] y, x))(\int [\int v_{\pi_1}] y, y, z)(v, [\int v_{\pi_1}] y))\]

By Hahn-Banach Theorem, \( D[\int L(y, ) \cdot (v, [\int v_{\pi_1}] y)] = (S) (y, x, v). \) Now

\( D\text{cur}((\lambda x.L) y) \circ (v, [\int v_{\pi_1}] y) \)

where \( f := \text{uncur}(\text{cur}(L))(y, -). \) Hence, we have

\[\((\Omega \lambda y. (\nabla L) \cdot V) \nabla \rightarrow (\lambda v. S^* \cdot V \lambda x.L V/y)((\lambda x.[V/y]) \cdot \pi_1) y)\]

(17) \( ((\Omega \lambda y. (\nabla L) \cdot V) \nabla \rightarrow (\lambda v. S^* \cdot V \lambda x.L V/y)) \)

\( if \ ((\Omega \lambda x.L \cdot z) a \rightarrow (\lambda v. S^* \cdot z \lambda a/x) \) for fresh variable a.

By IH, \( (\Omega \lambda x.L \cdot z) a = (\lambda v. S^* \cdot z \lambda a/x) \) implies for any \( \phi, y, a, v. \)

\[\phi((\int L(y, a, y))(\int [\int v_{\pi_1}] y, a))(\int [\int v_{\pi_1}] y, a, v))\]

By Hahn-Banach Theorem, \( D[\int L(y, ) \cdot (v, [\int v_{\pi_1}] y)] = (S) (y, a, v). \)
\[
\begin{align*}
\gamma &\to \phi\left(\left[\left[\gamma\right]\right],\left[\left[\gamma\right]\right]\right)
= \phi\left(\left[\left[\gamma\right]\right]\right)\left(\left[\left[\gamma\right]\right]\right)
\end{align*}
\]

Lemma 5.1. Let \( P \) be a term.

1. If \( P \rightarrow P' \), then there exists a reduct \( s \) of \( P' \) such that \( P \rightarrow^* s \) in \( L_D \).

2. \( [P] = [P_1] \) in C.

Proof. 1. Easy induction on \( \rightarrow \).

2. We prove by induction on \( P \). Most cases are trivial. Let \( y \in \Gamma \).

\[
\begin{align*}
\left(\left[\left[\left[\gamma\right]\right]\right]\right) &\rightarrow \left(\left[\left[\gamma\right]\right]\right)
\end{align*}
\]

(dual)

\[
\begin{align*}
\left(\left[\left[\left[\gamma\right]\right]\right]\right) &\rightarrow \left(\left[\left[\gamma\right]\right]\right)
\end{align*}
\]

(p)

Corollary 5.2 (Strong Normalization). Any reduction sequence from any term is finite, and ends in a value.

Proof. If \( P \) does not terminates, then we can form a reduction sequence in \( L_D \) that does not terminates using Lemma 5.1 (1) and confluent property of differential \( \lambda \)-calculus, proved in [15]. Then, this contradicts the strong normalization property of differential \( \lambda \)-calculus. \( \square \)