Denotational Correctness of Forward-Mode Automatic Differentiation for Iteration and Recursion

MATTHIJS VÁKÁR, Utrecht University, Netherlands

We present semantic correctness proofs of forward-mode Automatic Differentiation (AD) for languages with sources of partiality such as partial operations, lazy conditionals on real parameters, iteration, and term and type recursion. We first define an AD macro on a standard call-by-value language with some primitive operations for smooth partial functions and constructs for real conditionals and iteration, as a unique structure preserving macro determined by its action on the primitive operations. We define a semantics for the language in terms of diffeological spaces, where the key idea is to make use of a suitable partiality monad. A semantic logical relations argument, constructed through a subsconing construction over diffeological spaces, yields a correctness proof of the defined AD macro. A key insight is that, to reason about differentiation at sum types, we work with relations which form sheaves. Next, we extend our language with term and type recursion. To model this in our semantics, we introduce a new notion of space, suitable for modeling both recursion and differentiation, by equipping a diffeological space with a compatible o-cpo-structure. We demonstrate that our whole development extends to this setting. By making use of a semantic, rather than syntactic, logical relations argument, we circumvent the usual technicalities of logical relations techniques for type recursion.

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

Additional Key Words and Phrases: automatic differentiation, semantic correctness, sconing

ACM Reference Format:
Matthijs Vákár. 2018. Denotational Correctness of Forward-Mode Automatic Differentiation for Iteration and Recursion. Proc. ACM Program. Lang. 1, CONF, Article 1 (January 2018), 29 pages.

1 INTRODUCTION

Virtually every application of machine learning [Abadi et al. 2016], computational statistics [Carpenter et al. 2017] and scientific computing [Hascoët and Pascual 2013] requires efficient calculation of derivatives, as derivatives are used in optimization, Markov integration and simulation algorithms. Automatic Differentiation (AD) is typically the method of choice for algorithmically computing derivatives of programs operating between high-dimensional spaces, because of its efficiency and numerical stability. In essence, AD calculates the derivative of a function implemented by a program by applying the chain rule across the program code. This paper contributes a step towards making that informal statement precise, extending the work of [Huot et al. 2020] to account for various sources of partiality, such as partial operations like log, iteration, and recursion.

Roughly speaking, AD comes in two main flavours: forward-mode and reverse-mode. In their naive implementation, reverse-mode outperforms forward-mode when calculating derivatives of functions \( \mathbb{R}^n \rightarrow \mathbb{R}^m \) when \( n \gg m \) and the other way around if \( n \ll m \). This makes reverse-mode the tool of choice, for example, when optimizing a real-valued objective function such as the loss of a neural network. However, recently, [Shaikhha et al. 2019] showed that simple forward-mode implementations can outperform state-of-the-art reverse-mode implementations even on such optimization tasks, when they are combined with standard compiler optimization techniques. Moreover, forward-mode AD is easier to phrase and implement, and understanding how it operates on language features can be an important stepping stone for later grasping the complexities of...
advanced reverse-mode algorithms. Finally, there are applications where forward-mode AD is the algorithm of choice, like in calculating dense Jacobians or Jacobian-vector products, e.g. for use in Newton-Krylov methods [Knoll and Keyes 2004]. These methods are popular techniques for solving systems of non-linear algebraic equations, a problem that is ubiquitous in computational physics.

In this paper, we focus on how forward-mode AD should operate on code involving the fundamental programming techniques of lazy conditionals, iteration, and (term and type) recursion. Our analysis works in the presence of further features of higher-order functions and product and sum types. We phrase forward AD as a source-code transformation on a language with these features and give a proof that this transformation computes the derivatives in the usual mathematical sense. Our work answers a call by the machine learning community for better developed and understood AD techniques for expressive programming languages with features like higher-order functions and recursion [Jeong et al. 2018; van Merrienboer et al. 2018]. In response, we provide an understanding of forward AD on a large fragment of real-world functional languages such as Haskell and O’Caml.

Conditionals on real numbers are useful for pasting together functions implemented by language primitives. In order to use such functions in, for example, gradient-based optimization algorithms, we need to know how to perform AD on these pasted functions. For example, the ReLU function

\[ \text{ReLU}(x) \overset{\text{def}}{=} (x < 0) \text{ to cond. if cond then return } 0 \text{ else return } x \]

is frequently used in the construction of neural networks. The question of how to Automatically Differentiate such functions with “kinks” has long been studied [Beck and Fischer 1994]. The current solution, like the one employed in [Abadi and Plotkin 2020], is to treat such functions as undefined at their kink (in this case at \( x = 0 \)). It is then up to the consumer of the differentiated code to ensure that this undefined behaviour does not cause problems. This technique is used, for example, in probabilistic programming to paste together different approximations to a statistically important density function, to achieve numerical stability in different regimes [Betancourt 2019].

Similarly, iteration constructs, or while-loops, are necessary for implementing iterative algorithms with dynamic stopping criteria. Such algorithms are frequently used in programs that need to be differentiated. For example, iteration can be used to implement differential equation solvers, which are routinely used (and AD’ed) in probabilistic programs for modelling pharmacokinetics [Tsiros et al. 2019]. Other frequently used examples of iterative algorithms that need to be AD’ed are eigen-decompositions and algebraic equation solvers, such as those employed in Stan [Carpenter et al. 2017]. Furthermore, iteration is a popular technique for achieving numerically stable approximations to statistically important density functions, such as that of the Conway-Maxwell-Poisson distribution [Goodrich 2017], where one implements the function using a Taylor series, which is truncated once the next term in the series causes underflow. For example, if we have a function whose \( i \)-th terms in the Taylor expansion can be represented by computations \( i : \text{nat}, x : \text{real} \overset{\text{def}}{\mapsto} t(i, x) : \text{real} \), we would define the underflow-truncated Taylor series by

\[
\begin{align*}
\text{case } x \text{ of } \langle x_1, x_2 \rangle & \mapsto \\
\text{iterate } t(x_1, x_2) \text{ to } y. & \text{ from } x = \langle 0, 0 \rangle, \\
& \text{ if } z \text{ then } (\text{return } (\text{inr } x_2)) \text{ else } (\text{return } (\text{inl } (x_1 + 1, x_2 + y))) \\
\end{align*}
\]

where \( \xi \) is a cut-off for underflow.

Next, as a use case of AD applied to recursive programs, recursive neural networks [Tai et al. 2015] are often mentioned. While basic Child-Sum Tree-LSTMs can also be implemented with primitive recursion (a fold) over an inductively defined tree, there are other related models such
as Top-Down-Tree-LSTMs which require an iterative or general recursive approach [Zhang et al. 2016], where Jeong et al. 2018 has shown that a recursive approach is preferable as it naturally exposes the available parallelism in the model.

Finally, we imagine that coinductive types like streams of real numbers, which can be encoded using recursive types as \( \mu x.1 \rightarrow (\text{real} \times \alpha) \), provide a useful API for on-line machine learning applications [Shalev-Shwartz et al. 2012], where data is processed in real time as it becomes available. For all aforementioned applications, we need an understanding of how to perform AD on recursive programs. This paper provides such an understanding for forward-mode AD.

2 KEY IDEAS

In this section, we give a brief conceptual summary of the key ideas presented in the paper.

We start off by considering a standard higher-order (fine-grain) call-by-value language with product and sum types over a ground type \( \text{real} \) of real numbers and collections \( (\text{Op}_n)_{n \in \mathbb{N}} \) of \( n \)-ary basic operations. We think of these operations as partial functions \( \text{domain} \rightarrow \text{codomain} \). In this section, we give a brief conceptual summary of the key ideas presented in the paper.

We then extend these definitions to a unique structure preserving macro, which acts as partial functions \( \text{domain} \rightarrow \text{codomain} \). This paper provides such an understanding for forward-mode AD.

Let us choose, for all \( n \in \mathbb{N} \), for all \( 1 \leq i \leq n \), computations \( x_1 : \text{real} \), \ldots, \( x_n : \text{real} \) of \( \text{domain} \rightarrow \text{codomain} \). We can then define, using fresh identifiers for all newly introduced variables, type-respecting forward-mode AD macros \( \overrightarrow{D}(\text{real}) \) on values and \( \overrightarrow{D}(\text{computation}) \) on computations, which agree on their action \( \overrightarrow{D}(\text{domain}) \) on types:

\[
\overrightarrow{D}(\text{real}) = \text{real} \times \text{real}
\]

\[
\overrightarrow{D}(\text{op}(v_1, \ldots, v_n)) = \begin{cases} \text{case } \overrightarrow{D}(\text{op}(v_1)) & \text{of } (x_1, x'_1) \rightarrow \ldots \rightarrow \text{case } \overrightarrow{D}(\text{op}(v_n)) & \text{of } (x_n, x'_n) \rightarrow \text{op}(x_1, \ldots, x_n) & \text{to } y. \\
\partial_1 \text{op}(x_1, \ldots, x_n) & \text{to } z_1. \ldots \partial_n \text{op}(x_1, \ldots, x_n) & \text{to } z_n. \\
\text{return } (y, x'_1 * z_1 + \ldots + x'_n * z_n). \end{cases}
\]

\[
\overrightarrow{D}(\text{sign}(v)) = \text{case } \overrightarrow{D}(v) & \text{of } (x, \_ ) \rightarrow \text{sign}(x).
\]

We then extend these definitions to a unique structure preserving macro, which acts as \( \overrightarrow{D}(\text{domain}) \) on values and \( \overrightarrow{D}(\text{computation}) \) on computations. For the cognoscenti, \( (\overrightarrow{D}(\text{domain}), \overrightarrow{D}(\text{computation})) \) is structure preserving in the sense that it is an endomorphism of distributive-closed Freyd categories with iteration on the syntactic category \( \text{Syn}_V \leftrightarrow \text{Syn}_C \) of our language (which acts on iteration as \( \overrightarrow{D}(\text{iterate}_{\text{domain}}(t \text{from } x = v)) = \text{iterate}_{\overrightarrow{D}(C)}(t \text{from } x = \overrightarrow{D}(V)(v)) \)). We see that the induced rule for differentiating real conditionals is \( \overrightarrow{D}(\text{case } \overrightarrow{D}(V)(v) & \text{of } (x, \_ ) \rightarrow \text{if } x \text{ then } \overrightarrow{D}(C)(t) \text{ else } \overrightarrow{D}(C)(s)). \)

The first-order fragment of our language has a natural semantics \( [-] \) in terms of plain multivariate calculus once we choose interpretations \( \text{op} : \mathbb{R}^n \rightarrow \mathbb{R} \) for each \( \text{op} \in \text{Op}_n \). We interpret:

- types \( \tau \) as countable disjoint unions of Euclidean spaces, \( [\tau] = \bigsqcup_{i \in I} \mathbb{R}^{n_i} \) (certain very simple manifolds of varying dimension);
- values \( x_1 : \tau_1, \ldots, x_n : \tau_n \vdash \sigma \) as (total) smooth functions \( [\tau_1] \times \ldots \times [\tau_n] \rightarrow [\sigma] \) between these spaces, where smoothness means that the restriction to any connected component is differentiable in the usual calculus sense;
• computations \( x_1 : \tau_1, \ldots, x_n : \tau_n \vdash^e t : \sigma \) as partial functions \( \llbracket \tau_1 \rrbracket \times \ldots \times \llbracket \tau_n \rrbracket \rightarrow \llbracket \sigma \rrbracket \) between these spaces, which have an open domain of definition on which they are smooth.

We can now state correctness of the macro, where we write \( \mathcal{T}_x f u \) for the usual multivariate calculus derivative of \( f \) at \( x \), evaluated on a tangent vector \( u \).

**Theorem (Correctness of Fwd AD, Thm. 6.2).** For any \( x_1 : \tau_1, \ldots, x_n : \tau_n \vdash^e t : \sigma \), where \( \tau_i, \sigma \) are first-order types, we have that \( \llbracket D_C(t) \rrbracket(x, u) = (\llbracket t \rrbracket(x), \mathcal{T}_x t \circ u) \), for all \( x \) in the domain of \( \llbracket t \rrbracket \) and tangent vectors \( u \) at \( x \). Moreover, \( \llbracket D_C(t) \rrbracket(x, u) \) is defined iff \( \llbracket t \rrbracket(x) \) is.

The proof follows by a straightforward induction on the structure of values and computations when we only consider the first-order fragment of our language. However, we establish this theorem as well for programs between first-order types which may include higher-order subprograms.

To do so, we must extend our semantics \([-]\) to account for higher-order programs, which we achieve by using diffeological spaces [Iglesias-Zemmour 2013]. Diffeological spaces form a conservative extension of the usual setting of multivariate calculus and manifold geometry that models richer types, such as higher-order types. There are many other such convenient settings for differential geometry such as Frölicher spaces [Frölicher 1982] and synthetic differential geometry [Kock 2006], but diffeological spaces to us seems like the simplest suitable setting for our purposes.

The structure of a diffeological space \( X \) is a set \(|X|\) together with a set \( \mathcal{P}^U_X \) of functions \( U \rightarrow X \) for any open subset \( U \) of \( \mathbb{R}^n \) for some \( n \), called the plots, which we think of as "smooth functions into the space". Thus, we determine the geometry of the spaces by choosing the plots. These plots need to satisfy three axioms: (1) any constant function is a plot, (2) precomposition with any smooth function \( f : U' \rightarrow U \) in the usual calculus sense sends plots to plots, (3) we can glue compatible families of plots along open covers. A homomorphism of diffeological spaces \( X \rightarrow Y \), also called a smooth function, is a function \( f : |X| \rightarrow |Y| \) such that postcomposition with \( f \) maps plots to plots.

Any open subset of a Euclidean space, and more generally, any manifold, defines a diffeological space by taking the usual smooth functions as plots. The smooth functions between such spaces considered as manifolds coincide with the diffeological space homomorphisms.

Next, we demonstrate how smooth partial functions with a open domain of definition are captured by an easy-to-define partiality monad \((-)_\perp\) on the category \( \text{Diff} \) of diffeological spaces, which lifts the usual partiality monad on the category of sets and functions: define \( |X|_\perp \) and and

\[
\mathcal{P}^U_{|X|_\perp} \overset{\text{def}}{=} \left\{ \alpha : U \rightarrow |X| + \{\perp\} \mid \alpha^{-1}(X) \subseteq \text{open } U \right\}.
\]

Indeed, total functions \( M \rightarrow N_\perp \) in case \( M \) and \( N \) are manifolds correspond precisely to partial functions \( M \rightarrow N \) that have an open domain of definition in the Euclidean topology and that are smooth on that domain. We show that on general diffeological spaces, this monad classifies smooth partial functions that have a domain of definition that is open in the well-studied D-topology [Christensen et al. 2014]. Moreover, we show that this is a commutative strong monad that models iteration: it is a complete Elgot monad in the sense of [Goncharov et al. 2015]. The idea is to interpret \( \text{iterate } t \) from \( x = y \) as the union (lub) over \( i \) of the \( i \)-fold "self-compositions" of \( \llbracket t \rrbracket \). This monad is also easily seen to interpret \( \text{sign} \) as the smooth partial function \( \llbracket \text{sign} \rrbracket : \mathbb{R} \rightarrow \mathbb{1} + \mathbb{1} \) that sends the positive reals to the left copy of \( \mathbb{1} \) and the negative reals to the right. As diffeological spaces form a bicartesian closed category, we now obtain a canonical interpretation \(-\) of our entire language. We interpret

• types \( \tau \) as diffeological spaces;
• values \( x_1 : \tau_1, \ldots, x_n : \tau_n \vdash^o \sigma \) as smooth functions \( \llbracket \tau_1 \rrbracket \times \ldots \times \llbracket \tau_n \rrbracket \rightarrow \llbracket \sigma \rrbracket \).
• computations \( x_1 : \tau_1, \ldots, x_n : \tau_n \vdash^C t : \sigma \) as smooth functions \( \llbracket \tau_1 \rrbracket \times \cdots \times \llbracket \tau_n \rrbracket \to \llbracket \sigma \rrbracket_\perp \), or, equivalently, as partial functions \( \llbracket \tau_1 \rrbracket \times \cdots \times \llbracket \tau_n \rrbracket \to \llbracket \sigma \rrbracket \) that, on their domain, restrict to smooth functions \( U \to \llbracket \sigma \rrbracket \) where \( U \) is an open subset in the D-topology of \( \llbracket \tau_1 \rrbracket \times \cdots \times \llbracket \tau_n \rrbracket \).

To establish the correctness theorem for the full language, we use a logical relations argument over the semantics in diffeological spaces, where we maintain a binary relation that relates smooth curves \( \mathbb{R} \to \llbracket \tau \rrbracket \) to their tangent curve \( \mathbb{R} \to \llbracket \mathfrak{D}(\tau) \rrbracket \). We derive this argument by using a subconing construction diffeological spaces, like the one that is employed in [Huot et al. 2020]. The key step is to find a suitable definition of the partiality monad \( (\sim)_\perp \) on relations as discussed in [Goubault-Larrecq et al. 2002]. This lifting can be achieved by working with relations that are local in the sense that global membership of the relation can be restricted to membership on subsets of the domain. Conversely, if we establish local membership of the relation, we can derive global membership by gluing. Put differently, we work with relations that are sheaves over open subsets of \( \mathbb{R} \). This approach is justified because differentiation is local operation, and we can glue smooth functions and their derivatives. Once we work with such a relation \( (R^U \subseteq (U \to X) \times (U \to Y))_{U \subseteq \text{open } \mathbb{R}} \), we can simply define the relation \( R^U_{\perp} \subseteq (U \to X_\perp) \times (U \to Y_\perp) \) as containing those pairs \( (y, y') \) of partially defined curves that have the same domain of definition \( V \subseteq \text{open } U \) and which are in the relation on this domain: \( (y|_V, y'|_V) \in R^V \). The correctness theorem then follows by standard logical relations (subconing) techniques. We note that working with relations that are sheaves is particularly important to establish correctness for sum types and if \( \sim \) then \( \sim \) else \( \sim \).

While category theory helped us find this proof, it can be phrased entirely in elementary terms. Indeed, we define, for each open \( U \subseteq \mathbb{R} \), relations \( R^U_{\perp} \subseteq (U \to \llbracket \tau \rrbracket) \times (U \to \llbracket \mathfrak{D}(\tau) \rrbracket)_\perp \) and \( (R^U_{\perp})_\perp \subseteq (U \to \llbracket \tau \rrbracket)_\perp \times (U \to \llbracket \mathfrak{D}(\tau) \rrbracket)_\perp \) using induction on the types \( \tau \) of our language:

\[
R^U_{\text{real}} \overset{\text{def}}{=} \left\{ (y, y') \mid \forall x \in U, y'(x) = \left( y(x), \frac{d}{dt}|_{t=x} y'(t) \right) \right\}
\]

\[
R^U_{\tau_1 \ast \tau_2} \overset{\text{def}}{=} \left\{ (y, y') \mid (y, \pi_1, y', \pi_1) \in R^U_{\tau_1} \text{ and } (y, \pi_2, y', \pi_2) \in R^U_{\tau_2} \right\}
\]

\[
R^U_{\tau_1 + \tau_2} \overset{\text{def}}{=} \left\{ (y, y') \mid \forall i = 1, 2, (y|_{\tau_i}^{y'(1(\tau_i))}, y'|_{\tau_i}^{y'(1(\tau_i))}) \in R^{y'(1(\tau_i))}_{\tau_i} \right\}
\]

\[
R^U_{\text{if} \sim \text{then } \sim \text{else } \sim} \overset{\text{def}}{=} \left\{ (y, y') \mid \forall (\delta, \delta') \in R^U_{\tau_1}(x \mapsto y(x)(\delta(x)), x \mapsto y'(x)(\delta'(x))) \in (R^U_{\tau_2})_\perp \right\}
\]

\[
(R^U_{\tau})_\perp \overset{\text{def}}{=} \left\{ (y, y') \mid y^{-1}(\llbracket \tau \rrbracket) = y'^{-1}(\llbracket \mathfrak{D}(\tau) \rrbracket) \text{ and } (y|_{\mathfrak{D}(\tau)}^{y^{-1}(\tau)}, y'|_{\mathfrak{D}(\tau)}^{y^{-1}(\tau)}) \in R^{y^{-1}(\tau)} \right\}
\]

We then establish the following “fundamental lemma”:

If \( x_1 : \tau_1, \ldots, x_n : \tau_n \vdash^C v : \sigma \) (resp. \( x_1 : \tau_1, \ldots, x_n : \tau_n \vdash^C t : \sigma \)) and, for \( 1 \leq i \leq n \), \((f_i, g_i) \in R^U_{\tau_i}\) for \( U \subseteq \text{open } \mathbb{R} \), then we have that \( \left( (f_1, \ldots, f_n); [v], (g_1, \ldots, g_n); [\mathfrak{D}(\tau)] \right) \in R^U_{\tau} \) (resp. \( \left( (f_1, \ldots, f_n); [t], (g_1, \ldots, g_n); [\mathfrak{D}(\tau)] \right) \in (R^U_{\tau})_\perp \)).

The proof follows by induction on the typing derivation of \( v \) and \( t \), where the only non-trivial step is to show that each basic operation \( \text{op} \) respects the relations (and the other steps follow by standard results about logical relations/subconing). This basic step follows from the chain rule for differentiation, provided that the derivatives of the basic operations are correctly implemented:

\[
[\partial_i \text{op}(x_1, \ldots, x_n)] = \nabla_i \left[ \text{op}(x_1, \ldots, x_n) \right],
\]

where we write \( \nabla_i f \) for the usual calculus partial derivative of a function \( f \) in the direction of the \( i \)-th standard basis vector of \( \mathbb{R}^n \). The correctness result is a straightforward corollary of this lemma.
Next, we extend our language with term and type recursion, in the sense of FPC [Fiore and Plotkin 1994]. To apply the AD macro to recursive types, we first need to define its action on type variables $\alpha \mapsto \mathcal{D}(\alpha) \overset{\text{def}}{=} \alpha$. Next, we can define its action on recursive types, the corresponding values and computations, as well as the induced action on term recursion $\mu x.t$, which can be seen as sugar:

$\mathcal{D}(\mu \alpha.\tau) \overset{\text{def}}{=} \mu \alpha.\mathcal{D}(\tau) \quad \mathcal{D}_V(\text{roll } v) \overset{\text{def}}{=} \text{roll } \mathcal{D}_V(v) \quad \mathcal{D}_C(\mu x.t) \overset{\text{def}}{=} \mu x.\mathcal{D}_C(t)$.

Our semantics in diffeological spaces appears not to suffice to model recursion, for the same reason that sets and partial functions do not. Therefore, we follow the steps taken in [Vákár et al. 2019] and introduce a new notion of space, suitable for modelling both recursion and differentiation: we equip the diffeological spaces with a compatible $\omega$-cpo (chain-complete partial order) structure.

**Definition.** An $\omega$-diffeological space comprises a set $|X|$ with the following structure:

- a diffeology, i.e. specified sets of functions $P^U_X \subseteq U \to |X|$ for $U \subseteq_{\text{open}} \mathbb{R}^n$ subject to the three conditions discussed above: to enforce differentiability;
- a partial order $\leq$ on $|X|$ such that least upper bounds (lubs) of $\omega$-chains exist: to model recursion, such that each $P^U_X$ is closed under pointwise lubs of pointwise $\omega$-chains.

Equivalently, we can define them as $\omega$-cpos internal to $\text{Diff}$. We write $\omega\text{Diff}$ for the category of $\omega$-diffeological spaces and diffeological space homomorphisms that are, additionally, $\omega$-continuous in the sense of preserving lubs of $\omega$-chains. $\omega\text{Diff}$ is again a bicartesian closed category.

We can observe that our previous definition of the partiality monad on $\text{Diff}$ lifts to give a partiality monad on $\omega\text{Diff}$: interpret $\bot$ as a new least element in the order. Again, we obtain a semantics $\llbracket - \rrbracket$ of our original language in $\omega\text{Diff}$, where we equip $\mathbb{R}$ with the discrete order structure, in which all elements are only comparable to themselves. Moreover, we can show that the Kleisli adjunction $\omega\text{Diff} \dashv \omega\text{Diff}_{\bot}$ has sufficient structure to interpret term and type recursion. Indeed, it gives rise to a so-called bilimit compact expansion [Levy 2012], which follows from a development of axiomatic domain theory, similar to that in [Vákár et al. 2019]. As a consequence, we can extend the semantics of our original language to one that also accounts for term and type recursion.

Finally, we extend our logical relations proof to apply to recursive structures. Proving the existence of logical relations defined using type recursion is notoriously difficult and much advanced machinery was developed to accomplish this feat [Pitts 1996]. Much of the difficulty is caused by the fact that one customarily considers logical relations over the syntax, which is not chain-complete. Here, however, we consider relations over a chain-complete semantics. As a consequence, we can circumvent many of the usual technicalities. In particular, our previous logical relations proof extends if we work, instead, with relations that are internal $\omega$-cpos in the category of sheaves on open subsets of $\mathbb{R}$. We show that this category of logical relations lifts the bilimit compact expansion structure of $\omega\text{Diff}$, meaning that the interpretation of recursive types lifts. Stated in elementary terms, we can define logical relations $\left( R^U \subseteq (U \to \llbracket \tau \rrbracket) \times (U \to \llbracket \mathcal{D}(\tau) \rrbracket) \right)_{U \subseteq_{\text{open}} \mathbb{R}}$ using type recursion, as along as we work only with relations for which each $R^U$ is closed under lubs of $\omega$-chains of its elements $(\gamma, \gamma')$. In the end, once we have suitably extended the definition of our logical relations, we establish the same fundamental lemma and the same correctness theorem follows, but now for our more expressive language, in which “first-order types” include algebraic data types like lists and trees.
3 AN AD TRANSLATION FOR ITERATION AND REAL CONDITIONALS

3.1 A simple call-by-value language

We consider a standard fine-grain call-by-value language over a ground type real of real numbers, real constants $c \in \text{Op}_0$ for $c \in \mathbb{R}$, and certain basic operations $\text{op} \in \text{Op}_n$ for each natural number $n \in \mathbb{N}$. We will later interpret these operations as partial functions $\mathbb{R}^n \rightarrow \mathbb{R}$ with domains of definition that are (topologically) open in $\mathbb{R}^n$ on which they are smooth ($C^\infty$) functions. These operations include, for example, unary operations on reals like $\text{exp, log}$, $\zeta \in \text{Op}_1$ (where we mean the mathematical sigmoid function $\zeta(x) \overset{\text{df}}{=} \frac{1}{1 + e^{-x}}$), binary operations on reals like $(+, -, \ast, (/)) \in \text{Op}_2$.

We treat this operations in a schematic way as this reflects the reality of practical AD libraries which are constantly being expanded with new primitive operations. We consider a fine-grain CBV language mostly because it makes the proofs more conceptually clean, but we could have equally worked with a standard coarse-grain CBV language which can be faithfully embedded in our language. We discuss the implied differentiation rules for such a language in Appx. A, which inherit the correctness results that we will prove for the fine-grain language.

The types $\tau, \sigma, \rho$, values $v, w, u$, and computations $t, s, r$ of our language are as follows.

\[ \begin{array}{lll} 
\tau, \sigma, \rho & ::= & \text{types} \\
\mid \text{real} & \mid \text{numbers} & \mid 1 & \mid \tau \times \sigma & \mid \tau \rightarrow \sigma & \mid \tau \rightarrowD \sigma & \mid 1 \mid \tau \times \tau \mid \tau \rightarrowD \sigma \\
\mid 0 & \mid \tau + \sigma & \mid \tau \rightarrowD \sigma & \mid \tau \rightarrowD \sigma & \mid \tau \rightarrowD \sigma & \mid \tau \rightarrowD \sigma & \mid \tau \rightarrowD \sigma \\
\end{array} \]

\[ \begin{array}{lll} 
v, w, u & ::= & \text{values} \\
\mid x, y, z & \mid \langle \rangle & \mid \langle v, w \rangle & \mid \langle v \rangle & \mid \langle v \rangle & \mid \langle v \rangle & \mid \langle v \rangle \\
\mid \epsilon & \mid \text{constant} & \mid \lambda x.t & \mid \text{abstractions} \\
\end{array} \]

\[ \begin{array}{lll} 
t, s, r & ::= & \text{computations} \\
\mid t \text{ to } x.s & \mid \text{sequencing} & \mid \langle \rangle \text{ of } \langle \rangle \rightarrow t & \mid \text{product match} \\
\mid \text{return } v & \mid \text{pure comp.} & \mid \langle v \rangle \text{ of } \langle x, y \rangle \rightarrow t & \mid \text{product match} \\
\mid \text{op}(v_1, \ldots, v_n) & \mid \text{operation} & \mid \text{iterate } t \text{ from } x = v & \mid \text{iteration} \\
\mid \text{case } v \text{ of } \{ \} & \mid \text{sum match} & \mid \text{sign } u & \mid \text{sign function} \\
\mid \text{case } v \text{ of } \{ \text{ inl } x \rightarrow t \} & \mid \text{sum match} & \mid \text{inl } y \rightarrow s & \mid \text{sum match} \\
\end{array} \]

We will use sugar $\text{let } x = v \text{ in } w \overset{\text{df}}{=} w[v/x]$. Let $x = v \text{ in } t \overset{\text{df}}{=} (\lambda x.t) \ v$, and if $v \text{ then } t \text{ else } s \overset{\text{df}}{=} \text{sign } (v) \text{ to } x. \text{case } x \text{ of } \{ \text{ _ } \rightarrow s \} \mid \text{ _ } \rightarrow r \}$. The typing rules are in Figure 1.

3.2 A translation for forward-mode Automatic Differentiation

Let us fix, for all $n \in \mathbb{N}$, for all $\text{op} \in \text{Op}_n$, for all $1 \leq i \leq n$, computations $x_1 : \text{real}, \ldots, x_n : \text{real}$, and $\text{op} \overset{\text{c}}{=} \partial \text{op}(x_1, \ldots, x_n) : \text{real}$, which represent the partial derivatives of $\text{op}$. For example, we can choose $\partial_1(+)(x, y) \overset{\text{df}}{=} \partial_2(+)(x, y) \overset{\text{df}}{=} \text{return } 1, \partial_1(*)(x, y) \overset{\text{df}}{=} \text{return } y$ and $\partial_2(*)(x, y) \overset{\text{df}}{=} \text{return } x, \partial_1 \log(x) \overset{\text{df}}{=} 1/x$ and $\partial_1 \zeta(x) \overset{\text{df}}{=} \zeta(x) / y, \partial_2 \zeta(x) \overset{\text{df}}{=} \text{to } y, \partial_1 y \overset{\text{df}}{=} y \ast z$. Using these terms for representing partial derivatives, we define, in Fig. 2, a structure preserving macro $\overrightarrow{D}$ on the types, values, and computations of our language for performing forward-mode AD. We observe that this induces the following AD rule for our sugar: $\overrightarrow{D}_C(\text{if } v \text{ then } t \text{ else } s) = \text{case } D(v) \text{ of } \langle x, \_ \rangle \rightarrow \text{ if } x \text{ then } D(t) \text{ else } D(s)$. 

3.3 Equational theory

We consider our language up to the usual $\beta\eta$-equational theory for fine-grain CBV, which is displayed in Fig. 3. We could impose further equations for the iteration construct as is done in e.g.
Similarly, real category with iteration generated by $\varnothing$.

Indeed, we can define categories $\text{Syn}_V$ and $\text{Syn}_C$ which both have types as objects. $\text{Syn}_V(\tau, \sigma)$ consists of $(\alpha)\beta\eta$-equivalence classes of values $x : \tau \vdash^\alpha v : \sigma$, where identities are $x : \tau \vdash^\alpha x : \sigma$ and composition of $x : \tau \vdash^\alpha v : \sigma$ and $y : \sigma \vdash^\alpha w : \rho$ is given by $x : \tau \vdash^\alpha \text{let } y = v \text{ in } w : \rho$. Similarly, $\text{Syn}_C(\tau, \sigma)$ consists of $(\alpha)\beta\eta$-equivalence classes of computations $x : \tau \vdash^\alpha t : \sigma$, where identities are $x : \tau \vdash^\alpha \text{return } x : \sigma$ and composition of $x : \tau \vdash^\alpha t : \sigma$ and $y : \sigma \vdash^\alpha s : \rho$ is given by $x : \tau \vdash^\alpha \text{let } y = v \text{ in } s : \rho$. $\text{Syn}_V \hookrightarrow \text{Syn}_C : v \mapsto \text{return } v$ is the free distributive-closed Freyd category with iteration generated by real, the constants $\varnothing$ and operations $\text{op}$ and $\text{sign}$. It has the universal property that for any other distributive-closed Freyd category $\text{[Levy et al. 2003]}$ with iteration $\mathcal{V} \hookrightarrow C$, we obtain a unique structure preserving functor $(F_V, F_C) : (\text{Syn}_V \hookrightarrow \text{Syn}_C) \rightarrow (\mathcal{V} \hookrightarrow C)$ once we fix an object $F(\text{real})$ and compatibly typed morphisms $F_V(\varnothing) \in \mathcal{V}(\varnothing, F(\text{real}))$, $F_C(\text{op}) \in C(F(\text{real})^n, F(\text{real}))$ and $F_C(\text{sign}) \in C(F(\text{real}), \top + \bot)$.

![Typing rules for the our fine-grain CBV language with iteration and real conditionals. We use a typing judgement $\vdash^\alpha$ for values and $\vdash^\gamma$ for computations.](image)

Proc. ACM Program. Lang., Vol. 1, No. CONF, Article 1. Publication date: January 2018.
4 A DENOTATIONAL SEMANTICS VIA DIFFEOLOGICAL SPACES

4.1 Preliminaries

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

- unary, binary, and $I$-ary products as $1, X_1 \times X_2$, and $\prod_{i \in I} X_i$, writing $\pi_i$ for the projections and $()$, $(x_1, x_2)$, and $(x_i)_{i \in I}$ for the tupling maps;

\[
\begin{align*}
\vec{D}(\text{real}) & \overset{\text{def}}{=} \text{real} & \vec{D}(0) & \overset{\text{def}}{=} 0 & \vec{D}(\tau + \sigma) & \overset{\text{def}}{=} \vec{D}(\tau) + \vec{D}(\sigma) \\
\vec{D}(1) & \overset{\text{def}}{=} 1 & \vec{D}(\tau \to \sigma) & \overset{\text{def}}{=} \vec{D}(\tau) \to \vec{D}(\sigma) & \vec{D}(\tau \ast \sigma) & \overset{\text{def}}{=} \vec{D}(\tau) \ast \vec{D}(\sigma) \\
\vec{D}_V(x) & \overset{\text{def}}{=} x & \vec{D}_V(c) & \overset{\text{def}}{=} \langle c, 0 \rangle & \vec{D}_V(\text{inl } v) & \overset{\text{def}}{=} \text{inl } \vec{D}_V(v) \\
\vec{D}_V(\text{inr } v) & \overset{\text{def}}{=} \text{inr } \vec{D}_V(v) & \vec{D}_V(\langle \rangle) & \overset{\text{def}}{=} \langle \rangle & \vec{D}_V(\langle v, w \rangle) & \overset{\text{def}}{=} \langle \vec{D}_V(v), \vec{D}_V(w) \rangle \\
\vec{D}_V(\lambda x.t) & \overset{\text{def}}{=} \lambda x.\vec{D}_V(t) & \vec{D}_C(t \to x. s) & \overset{\text{def}}{=} \vec{D}_C(t) \to x. \vec{D}_C(s) & \vec{D}_C(\text{return } v) & \overset{\text{def}}{=} \text{return } \vec{D}_V(v) \\
\vec{D}_C(\text{case } v \text{ of } \{ \}) & \overset{\text{def}}{=} \vec{D}_C(\text{case } v \text{ of } \{ \text{inl } x \to t \mid \text{inr } y \to s \}) & \vec{D}_C(\text{case } v \text{ of } \{ \text{inl } x \to \vec{D}_C(t) \mid \text{inr } y \to \vec{D}_C(s) \}) \\
\vec{D}_C(\text{case } v \text{ of } \langle \rangle \to t) & \overset{\text{def}}{=} \vec{D}_C(\text{case } v \text{ of } \langle x, y \to t \rangle) & \vec{D}_C(\text{iterate } t \text{ from } x = v) & \overset{\text{def}}{=} \text{iterate } \vec{D}_C(t) \text{ from } x = \vec{D}_V(v) \\
\vec{D}_C(t \, v) & \overset{\text{def}}{=} \vec{D}_C(t) \, \vec{D}_V(v) & \vec{D}_C(\text{sign } v) & \overset{\text{def}}{=} \text{sign } \vec{D}_V(v) \\
\vec{D}_C(\text{op}(v_1, \ldots, v_n)) & \overset{\text{def}}{=} \text{case } \vec{D}_V(v_1) \text{ of } \langle x_1, x'_1 \rangle \to \cdots \to \text{case } \vec{D}_V(v_n) \text{ of } \langle x_n, x'_n \rangle \to \text{op}(x_1, \ldots, x_n) \to y. \\
& \quad \partial_1 \text{op}(x_1, \ldots, x_n) \to z_1 \ldots \partial_n \text{op}(x_1, \ldots, x_n) \to z_n. \\
& \quad \text{return } \langle y, x'_1 * z_1 + \cdots + x'_n * z_n \rangle
\end{align*}
\]

Fig. 2. A forward-mode AD macro defined on types as $\vec{D}(-)$, values as $\vec{D}_V(-)$, and computations as $\vec{D}_C(-)$. All newly introduced variables are chosen to be fresh. We single out the rule for primitive operations op, as this is where the interesting work specific to differentiation happens.

\[
\begin{align*}
\text{return } v \text{ to } x. t & = t^{\langle v \rangle_x} \\
(t \text{ to } x. s) \text{ to } y. r & = t \text{ to } x. (s \text{ to } y. r) \\
\text{case } \text{inl } v \text{ of } \text{inl } x \to t \mid \text{inr } y \to s & = t^{\langle v \rangle_x} \\
\text{case } \text{inr } v \text{ of } \text{inl } x \to t \mid \text{inr } y \to s & = s^{\langle v \rangle_y} \\
\text{case } \langle v, w \rangle \text{ of } \langle x, y \to t \rangle & = t^{\langle v \rangle_x}_{\langle w \rangle_y} \\
\langle \lambda x.t \rangle v & = t^{\langle v \rangle_x}
\end{align*}
\]

Fig. 3. Standard $\beta\eta$-laws for fine-grain CBV. We write $^{\langle x_1, \ldots, x_n \rangle}$ to indicate that the variables are fresh in the left hand side. In the top right rule, $x$ may not be free in $r$. Equations hold on pairs of terms of the same type.
We write $\text{dst} / \text{u1D44B}, / \text{u1D44C}$ for the cotupling maps; $\Sigma_{i \in I} X_i$, writing $u_i$ for the injections and $\llbracket \cdot \rrbracket$, $[x_1, x_2]$, and $[x_i]_{i \in I}$ for the currying maps.

**Monads.** A strong monad $T$ over a cartesian closed category $C$ is a triple $(T, \text{return}, \approx)$ consisting of an assignment of an object $TX$ and a morphism $\text{return}_X : X \to TX$ for every object $X$, and an assignment of a morphism $(\approx_{X,Y}) : TX \times (TY)^X \to TY$, satisfying the monad laws below, expressed in the cartesian closed internal language:

$$((\text{return} x) \approx f) = f(x) \quad (a \approx \text{return}) = a \quad ((a \approx f) \approx g) = (a \approx \lambda x.f(x) \approx g)$$

Every monad yields an endofunctor $T$ on $\text{C}$-morphisms: $T(f) := \text{id} \approx^T (f; \text{return}T)$. The Kleisli category $C_T$ consists of the same objects as $C$, but morphisms are given by $C_T(X,Y) \defeq C(X,TY)$. Identities are return and composition $f \approx g$ is given by $\lambda x.f(x) \approx g$. A strong monad $T$ is commutative when, for every pair of objects $X, Y$:

$$a : TX, b : TY \vdash a \approx \lambda x.b \approx \lambda y.\text{return}(x, y) = b \approx \lambda y.a \approx \lambda x.\text{return}(x, y)$$

We write $\text{dst}_{X,Y}$ for this morphism and call it the double strength.

**Semantics of fine-grain CBV.** Generally, fine-grain call-by-value languages like ours can be interpreted in distributive-closed Freyd categories (with additional support for interpreting iteration, in our case). However, we do not need this level of generality. Instead, we focus on the more specific semantic settings of bicartesian closed categories equipped with suitable partial monads.

Given a bicartesian closed category $C$ and a strong monad $(T, \text{return}, \approx)$, we have a sound interpretation $\llbracket - \rrbracket$ of fine-grain CBV with its $\beta\eta$-equational theory (see [Levy et al. 2003], for details):

$$\llbracket 0 \rrbracket \defeq 0 \quad \llbracket \tau + \sigma \rrbracket \defeq \llbracket \tau \rrbracket + \llbracket \sigma \rrbracket \quad \llbracket 1 \rrbracket \defeq 1 \quad \llbracket \tau \star \sigma \rrbracket \defeq \llbracket \tau \rrbracket \times \llbracket \sigma \rrbracket \quad \llbracket \tau \rightarrow \sigma \rrbracket \defeq T[\llbracket \sigma \rrbracket][\llbracket \tau \rrbracket]$$

$$\llbracket x_1 : \tau_1, \ldots, x_n : \tau_n \rrbracket \defeq \llbracket \tau_1 \rrbracket \times \cdots \times \llbracket \tau_n \rrbracket$$

$$\llbracket \text{return} v \rrbracket(\rho) \defeq \text{return}(\llbracket v \rrbracket(\rho)) \quad \llbracket \text{case } v \text{ of } \{ \} \rrbracket(\rho) \defeq \llbracket \{ \} \rrbracket(\rho)$$

$$\llbracket \text{inl} v \rrbracket(\rho) \defeq \text{inl}(\llbracket v \rrbracket(\rho)) \quad \llbracket \text{inr} v \rrbracket(\rho) \defeq \text{inr}(\llbracket v \rrbracket(\rho))$$

$$\llbracket \text{case } v \text{ of } (\text{inl } x \rightarrow t \mid \text{inr } y \rightarrow s) \rrbracket(\rho) \defeq \llbracket t \rrbracket(\rho, \text{id}) + \llbracket s \rrbracket(\rho, \text{id})$$

$$\llbracket \langle v, w \rangle \rrbracket(\rho) \defeq (\llbracket v \rrbracket(\rho), \llbracket w \rrbracket(\rho))$$

$$\llbracket \lambda x : \tau.t \rrbracket(\rho)(a) \defeq \llbracket t \rrbracket(\rho, a) \quad (a \in \llbracket \tau \rrbracket)$$

$$\llbracket \lambda x : \tau.t \rrbracket(\rho)(a) \defeq \llbracket t \rrbracket(\rho, a) \quad (a \in \llbracket \tau \rrbracket)$$

To interpret the constructions for iteration, we need a chosen family of functions $\text{iterate}_{C,A,B} : C_T(C \times A, A+B) \to C_T(C \times A, B)$ such that the following naturality condition holds with respect to morphisms $f : C \to C'$ in $C$: $(f \times \text{id}_A)_{\text{iterate}_{C',A,B}(g)} = \text{iterate}_{C,A,B}(f \times \text{id}_A)(g)$. Then, we define,

$$\llbracket \tau : \sigma \vdash t : \sigma + \tau \text{ and } \Gamma \vdash v : \sigma, \text{iterate } t \text{ from } x = v \rrbracket(\rho) \defeq \text{iterate}_{\llbracket \tau \rrbracket, \llbracket \sigma \rrbracket, \llbracket \tau \rrbracket}(\llbracket t \rrbracket(\rho), \llbracket v \rrbracket(\rho))$$

We say that a functor $F$ between two categories which support iteration preserves iteration if $\text{iterate}(F(f)) = F(\text{iterate}(f))$.

Given bicartesian closed category $C$ with a strong monad $T$ such that $C_T$ supports iteration, therefore, we obtain a canonical interpretation $\llbracket - \rrbracket$ of our full language, once we choose an interpretation of $\text{real}, \text{sign}$, constants $c$ and operations $\text{op}$.
with chosen morphisms \([\text{sign}] \in C_T([\text{real}], \mathbb{1} + \mathbb{1})\), \([c] \in C(\mathbb{1}, [\text{real}])\) and chosen morphisms \([\text{op}] \in C_T([\text{real}]^n, [\text{real}])\) for each \(n \in \mathbb{N}\). We then interpret 
\([c](\rho) \overset{\text{def}}{=} [c]\ [\text{op}(v_1, \ldots, v_n)](\rho) \overset{\text{def}}{=} [\text{op}](\{v_1(\rho), \ldots, v_n(\rho)\}) \overset{\text{def}}{=} [\text{sign}](\{v\}(\rho)).\)

A categorically inclined reader might want to note that \([-\ ]\) is canonical as the uniquely determined structure preserving functor \((\text{Syn}_Y \hookrightarrow \text{Syn}_X) \to (C \hookrightarrow C_T)\) of distributive-closed Freyd categories with iteration, which we discussed in Sec. 3.

\(\omega\text{-cpos.}\) We recall some basic domain theory. Let \(\omega = \{0 \leq 1 \leq \ldots\}\) be the ordinary linear order on the naturals. An \(\omega\text{-chain}\) in a poset \(P = (|P|, \leq)\) is a monotone function \(a_\omega : \omega \to P\). A poset \(P\) is an \(\omega\text{-cpo}\) when every \(\omega\text{-chain} (a_n)_{n \in \mathbb{N}}\) has a least upper bound (lub) \(\bigvee_{n \in \mathbb{N}} a_n\) in \(P\).

**Example 4.1.** Each set \(X\) equipped with the discrete partial order forms an \(\omega\text{-cpo} (X, =)\), e.g., the discrete \(\omega\text{-cpo} \mathbb{R}\) over the real line. For any \(\omega\text{-cpo} X\), we can form a new \(\omega\text{-cpo} X_\bot\) by adding a new element \(\bot\) which will be the least element in the order. \((-\bot)\) lifts the partiality monad on \(\text{Set}\).

For \(\omega\text{-cpos} P\) and \(Q\), an \(\omega\text{-continuous}\) function \(f : P \to Q\) is a monotone function \(f : |P| \to |Q|\) such that for every \(\omega\text{-chain} a\_\omega\), we have: \(f(\bigvee_a a_n) = \bigvee_a f(a_n)\). Such a function \(f : P \to Q\) is a full mono when, for every \(a, b \in |P|\), we have \(f(a) \leq f(b) \implies a \leq b\). Recall that the category \(\omega\text{CPO}\) of \(\omega\text{-cpos}\) and \(\omega\text{-continuous}\) functions is bicartesian closed: coproducts are disjoint unions on both the carrier and order, products are taken componentwise and the exponential \(Q^P\) has carrier \(\omega\text{CPO}(P, Q)\) and order \(f \leq_{Q^P} g\ iff \forall p \in |P|, f(p) \leq_Q g(p)\). A pointed \(\omega\text{-cpo}\) is an \(\omega\text{-cpo}\) with a least element \(\bot\). A strict function is an \(\omega\text{-continuous}\) function that preserves the least elements. The Kleisli category \(\omega\text{CPO}_\bot\) is equivalent to the category of \(\omega\text{-cpos}\) and strict \(\omega\text{-continuous}\) functions.

An \(\omega\text{CPO}(\text{-enriched})\) category \(C\) consists of a locally-small category \(C\) together with an assignment of an \(\omega\text{-cpo} C(A, B)\) to every \(A, B \in \text{ob} C\) whose carrier is the set \(C(A, B)\) such that composition is \(\omega\text{-continuous}\). An \(\omega\text{CPO}\text{-functor},\) a.k.a. a \(\omega\text{-continuous}\) functor, \(F : C \to \mathcal{D}\) between two \(\omega\text{CPO}\)-categories is an ordinary functor \(F : C \to \mathcal{D}\) between the underlying categories, such that every morphism map \(F_{AB} : C(A, B) \to \mathcal{D}(FA, FB)\) is \(\omega\text{-continuous}\). We call such a category \(\omega\text{CPO}_\bot\)-enriched if all homsets has a least element and composition is strict in both arguments.

**Example 4.2.** Every locally-small category is an \(\omega\text{CPO}\)-category whose hom-\(\omega\text{-cpos}\) are discrete. The category \(\omega\text{CPO}\) itself is an \(\omega\text{CPO}\)-category. If \(C\) is an \(\omega\text{CPO}\)-category, its categorical dual \(C^{\text{op}}\) is an \(\omega\text{CPO}\)-category. The category of locally-continuous functors \(C^{\text{op}} \to \omega\text{CPO}\), with the componentwise order on natural transformations \(\alpha : F \to G\), is an \(\omega\text{CPO}\)-category when \(C\) is.

By the Knaster-Tarski theorem, an \(\omega\text{-continuous}\) function \(f : X \to X\) on a pointed \(\omega\text{-cpo}\) \(X\) has a least fixed-point, i.e. a least \(x\) such that \(x = f(x)\). This is given by the lub of the \(\omega\text{-chain} (f^n(\bot))_{n \in \mathbb{N}}\).

**Manifolds.** For our purposes, a smooth manifold \(M\) is a second-countable Hausdorff topological space with a smooth atlas: an open cover \(\mathcal{U}\) together with homeomorphisms \((\varphi_U : U \to \mathbb{R}^n(U))_{U \in \mathcal{U}}\) (called charts) such that \(\varphi_U^{-1}\); \(\varphi_V\) is smooth on its domain of definition for all \(U, V \in \mathcal{U}\). A function \(f : M \to N\) between manifolds is smooth if \(\varphi_U^{-1} f \varphi_V\) is smooth for all charts \(\varphi_U\) and \(\varphi_V\) of \(M\) and \(N\), respectively. Let us write \(\text{Man}\) for the category of smooth manifolds and smooth functions. We are primarily interested in manifolds that are isomorphic to \(\bigsqcup_{i \in I} \mathbb{R}^{n_i}\) for countable \(I\), as they will form the interpretation of our first-order types.

Note that different charts in the atlas of our manifolds may have different finite dimension \(n(U)\). Thus we consider manifolds with dimensions that are potentially unbounded, albeit locally finite. This non-constant dimension does not affect the theory of differential geometry as far as we need it.
Diffeological spaces. We consider a rich notion of differential geometry for our semantics, based on diffeological spaces [Iglesias-Zemmour 2013; Souriau 1980]. The key idea is that a higher-order function is called smooth if it sends smooth functions to smooth functions, meaning that we can never use it to build non-smooth first-order functions. This is reminiscent of a logical relation.

Definition 4.3. A diffeological space \( X = (|X|, \mathcal{P}_X) \) consists of a set \(|X|\) together with, for each \( n \in \mathbb{N} \) and each open subset \( U \) of \( \mathbb{R}^n \), a set \( \mathcal{P}_X^U \) of functions \( U \to |X| \), called plots, such that

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

We call a function \( f : X \to Y \) between diffeological spaces smooth if, for all plots \( p \in \mathcal{P}_X^U \), we have that \( p \circ f \in \mathcal{P}_Y^U \). We write \( \text{Diff}(X,Y) \) for the set of smooth maps from \( X \) to \( Y \). Smooth functions compose, and so we have a category \( \text{Diff} \) of diffeological spaces and smooth functions. We give some examples of such spaces.

Example 4.4 (Manifold diffeology). Given any open subset \( X \) of a cartesian space \( \mathbb{R}^n \) (or, more generally, a smooth manifold \( X \)). We can take the set of smooth \( (C^\infty) \) functions \( U \to X \) in the traditional sense as \( \mathcal{P}_X^U \). Given another such space \( X' \), then \( \text{Diff}(X,X') \) coincides precisely with the set of smooth functions \( X \to X' \) in the traditional sense of calculus and differential geometry.

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

Example 4.5 (Subspace diffeology). Given a diffeological space \( X \) and a subset \( |Y| \subseteq |X| \), we can equip it with the subspace diffeology \( \mathcal{P}^Y_X \overset{\text{def}}{=} \{ \alpha : U \to |Y| \mid \alpha \in \mathcal{P}_X^U \} \).

Example 4.6 (Coproduct diffeology). Given diffeological spaces \( (X_i)_{i \in I} \), we can define \( \coprod_{i \in I} |X_i| \) the coproduct diffeology: \( \mathcal{P}^U_{\coprod_{i \in I} X_i} \overset{\text{def}}{=} \left\{ U \to \coprod_{i \in I} |X_i| \mid \forall i \in I, V_i \overset{\text{def}}{=} \alpha^{-1}|X_i| \subseteq \text{open} \ U \text{ and } \alpha|_{V_i} \in \mathcal{P}_X^{V_i} \right\} \).

Example 4.7 (Product diffeology). Given diffeological spaces \( (X_i)_{i \in I} \), we can equip \( \prod_{i \in I} |X_i| \) with the product diffeology: \( \mathcal{P}^U_{\prod_{i \in I} X_i} \overset{\text{def}}{=} \left\{ (\alpha_i)_{i \in I} \mid \alpha_i \in \mathcal{P}_X^{U_i} \right\} \).

Example 4.8 (Functional diffeology). Given diffeological spaces \( X, Y \), we can equip \( \text{Diff}(X,Y) \) with the functional diffeology \( \mathcal{P}^U_{YX} \overset{\text{def}}{=} \{ \Lambda(\alpha) \mid \alpha \in \text{Diff}(U \times X,Y) \} \).

These examples give us the categorical (co)product and exponential objects, respectively, in \( \text{Diff} \). The embeddings of \( \text{CartSp} \) and \( \text{Man} \) into \( \text{Diff} \) preserve products and coproducts. Further, \( \text{Diff} \) is, in fact, complete and cocomplete (and even is a Grothendieck quasi-topos [Baez and Hoffnung 2011]).

Finally, it is well-known that the Euclidean topology that is induced on manifolds by their atlas has a canonical extension to diffeological spaces, named the \( D \)-topology [Christensen et al. 2014]. It is defined by \( O_X = \{ U \subseteq |X| \mid \forall n \in \mathbb{N}, V \subseteq \text{open} \ \mathbb{R}^n, \alpha \in \mathcal{P}_X^V, \alpha^{-1}U \subseteq \text{open} \ V \} \). This \( D \)-topology defines an (identity on morphisms) adjunction \( O \dashv R : \text{Top} \to \text{Diff} \) from the category \( \text{Top} \) of topological spaces and continuous functions to diffeological spaces, where \( |RS| \overset{\text{def}}{=} |S| \) and \( \mathcal{P}^U_{RS} \overset{\text{def}}{=} \text{Top}(U,S) \).
4.2 Partiality in Diff

We call two partial functions compatible if they agree on the intersection of their domains. A partiality monad on $\text{Diff}$. On the other hand, we have a natural partiality monad on $\text{Diff}$. Ultimately, we are interested in interpreting the first-order fragment of our language in the category $\text{pMan}$ of manifolds and partial functions defined on an open domain on which they are smooth. We are therefore looking for a higher-order extension of $\text{pMan}$. As the D-topology simply reduces to the Euclidean topology on manifolds, it is natural to define a category $\text{Diff}$ of diffeological spaces and partial functions which restrict to a smooth function of diffeological spaces on their domain (equipped with the subspace diffeology), which is D-open in $X$. Then, $\text{pMan}(M, N) \equiv \text{pDiff}(M, N)$ for any two manifolds $M, N$, so that $\text{pDiff}$ can be seen as a higher-order extension of $\text{pMan}$.

A partiality monad. On the other hand, we have a natural partiality monad on $\text{Diff}$. 

Definition 4.9. Given a diffeological space $X$, we equip the set $|X| + \{\perp\}$ with the partiality diffeology: $\mathcal{P}_X^{\perp} \defeq \{\alpha : U \rightarrow |X| + \{\perp\} | V \defeq \alpha^{-1}|X| \subseteq \text{open} U$ and $\alpha|_V \in \mathcal{P}_V\}$. 

This definition is easily seen to give a well-defined diffeology. Note that it is qualitatively different from the coproduct $X + \bot$ in $\text{Diff}$, as $\alpha^{-1}(\{\perp\})$ need not be open.

Proposition 4.10. The partiality monad structure (return, $\Rightarrow$) from $\text{Set}$ lifts to $\text{Diff}$ to make $(-)_\bot$ into a commutative strong monad.

To be explicit, we define return $(x) \defeq x, \bot \Rightarrow f \defeq \bot$ and $x \Rightarrow f \defeq f(x)$ (for $x \neq \bot$).

It turns out that both natural notions of partiality coincide.

Proposition 4.11. We have an equivalence of categories between $\text{pDiff}$ and the Kleisli category $\text{Diff}_\bot$ of $(-)_\bot$.

Indeed, D-open subsets $U \subseteq X$ are precisely those that arise as $\chi_U^{-1}(\star)$ for a smooth characteristic function $X \xrightarrow{\chi_U} \bot$. In particular, $\text{Diff}_\bot(M, N) \equiv \text{pMan}(M, N)$ for any two manifolds $M, N$.

Interpreting operations. We have designed our language such that we have a smooth partial function $\llbracket\text{op}\rrbracket \in \text{pMan}(\mathbb{R}^n, \mathbb{R})$ in mind for any operation symbol $\text{op} \in \text{Op}_n$. As a result, the interpretation of each operation is fixed. Later, we will see that, to establish correctness of our AD macro, we need to have chosen each $\partial_\text{op}(x_1, \ldots, x_n)$ such that $\llbracket\partial_\text{op}(x_1, \ldots, x_n)\rrbracket = \nabla_i[\text{op}]$, where we write $\nabla_i$ for the usual calculus partial derivative along the $i$-th coordinate on $\mathbb{R}^n$.

Next, observe that we have an obvious choice of $\llbracket\text{sign}\rrbracket \in \text{pMan}(\mathbb{R}, \mathbb{R} + \mathbb{1})$. Indeed, we choose the smooth partial function, defined on $\mathbb{R} \setminus \{0\}$, which sends $\mathbb{R}^+$ to $i_1\star$ and $\mathbb{R}^-$ to $i_2\star$.

Interpreting iteration. Observe that we can glue matching families of morphisms in $\text{Diff}$, by axiom (gluing) of a diffeology, and that the union of any collection of D-opens is D-open, by the axioms of a topology. As a consequence, lubs of compatible families of morphisms in $\text{pDiff}$ exist, where we call two partial functions compatible if they agree on the intersection of their domains.

Proposition 4.12. Any compatible family $(f_i)_{i \in I}$ of smooth partial functions $f_i \in \text{pDiff}(X, Y)$ has a least upper bound in $\text{pDiff}(X, Y)$:

\[
\left(\bigvee_{i \in I} f_i\right)(x) \defeq \begin{cases} f_i(x) & \exists i \in I, f_i(x) \in Y \\
\bot & \text{else.} \end{cases}
\]
Moreover, composition in $\text{pDiff}$ respects these lubs: $\left(\bigvee_{i \in I} f_i\right); \left(\bigvee_{j \in J} g_j\right) = \bigvee_{i \in I} \bigvee_{j \in J} f_i; g_j$. Homsets have a least element, the partial function with domain $\emptyset$, and composition is strict in both arguments.

In particular, $\text{pDiff} \cong \text{Diff}^\perp_\perp$ (whose equivalence respects the natural orders) is $\omega$-$\text{CPO}^\perp_\perp$-enriched.

**Lemma 4.13.** The monad $(-)_\perp$ on $\text{Diff}$ has the properties that

- the strength is $\omega$-continuous: $(\text{id} \times \bigvee f_i); s; t = \bigvee_i (\text{id} \times f_i); s; t$;
- copairing in $\text{Diff}^\perp_\perp$ is $\omega$-continuous in both arguments: $\bigvee f_i; \bigvee g_i = \bigvee [f_i; g_i]$;
- the strength and by postcomposition in $\text{Diff}^\perp_\perp$ are strict: $(\text{id} \times \perp); s = \perp$ and $\perp \gg f = \perp$,

where we write $s$ for the strength $s(a, b) = b \gg (\beta \mapsto (a, \text{return}(\beta)))$.

Indeed, all these facts follow from the corresponding facts for the category of sets and partial functions once we observe that we have a forgetful functor $\text{Diff} \to \text{Set}$ which sends $(-)_\perp$ to the usual (strong) partiality monad.

Given $f \in \text{Diff}^\perp_\perp(A, A + B)$, we can observe that the map $\text{Diff}^\perp_\perp(A, B) \to \text{Diff}^\perp_\perp(A; B); h \mapsto f \gg [h, \text{return}_B]$ is $\omega$-continuous. As a consequence, we can define iterate($f$) as the least fixpoint of this map. As shown in Thm. 5.8 of [Goncharov et al. 2015], this determines a complete Elgot monad structure for $(-)_\perp$. Therefore, we can interpret iteration constructs $\text{iterate}_{C,A,B} : \text{Diff}^\perp_\perp(C \times A, A + B) \to \text{Diff}^\perp_\perp(C \times A, B)$ which are natural in $C$. Indeed, iterate_{C,A,B}(f) gets interpreted as the least fixed-point of the $\omega$-continuous map $\text{Diff}^\perp_\perp(C \times A, B) \to \text{Diff}^\perp_\perp(C \times A, B); h \mapsto (\text{diag} \times \text{id}_A); a_{C,C,A}; (\text{id}_C \times f); s; \text{iterate}_{C,A,B} \gg (\text{dist}_{C,A,B}; [h, \pi_2; \text{return}_B])$, where $\text{diag}$ is the diagonal of the cartesian structure, $a$ is the associator of $\times$, and $\text{dist}$ is the distributor of $\times$ over $\perp$.

In sum, we obtain a canonical denotational semantics $[\cdot]$ of our full language, interpreting values $\Gamma \vdash^0 \nu : \tau$ as morphisms $\text{Diff}(\Gamma, [\tau])$ and computations $\Gamma \vdash^\omega t : \tau$ as morphisms $\text{pDiff}(\Gamma, [\tau]) \cong \text{Diff}^\perp_\perp(\Gamma, [\tau])$. In particular, any computation $\Gamma \vdash^\omega t : \tau$ between first-order types is interpreted as a smooth partial function $\text{pMan}(\Gamma, [\tau])$ in the usual calculus sense, as $\text{pMan}(M, N) \cong \text{pDiff}(M, N)$ for manifolds $M, N$.

## 5 Logical Relations and Correct AD for Iteration

Using the same strategy as [Huot et al. 2020], we prove the correctness of AD by employing a logical relations proof over the semantics. We interpret each type $\tau$ as the pair $([\tau], [\text{diff}\tau])$ of diffeological spaces, together with a suitable binary relation $R$ relating curves in $[\tau]$ to their tangent curves in $[\text{diff}\tau]$. Such proofs can be cleanly stated in terms of subsconing, which we recall now.

### 5.1 Preliminaries

**Artin glueing/sconing.** Given a functor $F : C \to D$, the comma category $D/F$ is also known as the *scone* or *Artin glueing* of $F$. Explicitly, it has objects $(D, f, C)$ which are triples of an object $D$ of $D$, an object $C$ of $C$ and a morphism $f : D \to FC$ of $D$. Its morphisms $(D, f, C) \to (D', f', C')$ are pairs $(g, h)$ of morphisms such that $f; F(h) = g; f'$. Under certain conditions, $D/F$ inherits much of the structure present in $C$ and $D$, letting us build new categorical models from existing ones. Indeed, $D/F$ lifts any coproducts that exist in $C$ and $D$ [Rydeheard and Burstall 1988]. Moreover, if $C$ and $D$ are cartesian closed, $D$ has pullbacks, and $F$ preserves finite products, $D/F$ is cartesian closed [Carboni and Johnstone 1995; Johnstone et al. 2007]. Note that we have canonical projection functors $D/F \to C$ and $D/F \to D$. Those preserve the bicartesian closed structure.

**Factorization systems.** Recall that an orthogonal factorisation system on a category $C$ is a pair $(E, M)$ consisting of two classes of morphisms of $C$ such that:

- Both $E$ and $M$ are closed under composition, and contain all isomorphisms.
- Every morphism $f : X \to Y$ in $C$ factors into $f = e; m$ for some $m \in M$ and $e \in E$. 

Proc. ACM Program. Lang., Vol. 1, No. CONF, Article 1. Publication date: January 2018.
• Functoriality: for each situation as on the left, there is a unique \( h : A \to A' \) as on the right:

\[
\begin{array}{cccc}
X & e \in E & A & m \in M \\
\downarrow & = & \downarrow g & \implies \\
X' & e' \in E & A' & m' \in M \\
\end{array}
\]

In case \( C \) is \( \omega \text{CPO-} \)enriched, we call \((E, M)\) an \( \omega \text{CPO-} \)enriched factorization system in case the assignment \((f, g) \mapsto h\) in the diagram above is \( \omega \)-continuous.

**Subsconing.** Suppose that \( D \) is equipped with some orthogonal factorization system \((E, M)\) and that we are given a functor \( F : C \to D \). We call the full subcategory \( D//F \) of \( D/F \) on the objects \((D, f, C)\) where \( f \in M \) the subscone of \( F \). Often, \( M \) will consist exclusively of monos, in which case we can think of the objects of \( D//F \) as objects \( C \) of \( C \) together with a predicate \( m : D \to FC \) (in \( M \)) on \( FC \). Then, morphisms are simply morphisms \( h \) in \( C \) such that \( Fh \) respects the predicate. \( D//F \) is easily seen to be a reflective subcategory of \( D/F \), hence its products are computed as in \( D/F \) and it inherits the existence of coproducts from \( D/F \). If \( M \) is closed under \( I \)-ary coproducts, \( I \)-ary coproducts are computed in \( D//F \) as in \( D/F \). Finally, if \( M \) is closed under exponentiation (or, equivalently, \( E \) is closed under binary products), the exponentials of \( D/F \) also give exponentials in \( D//F \), making \( D//F \) cartesian closed.

In case we specialize to the case of \( D = \text{Set} \) and \( F = C(\bot, -) \) and we work with the usual epimono factorization system, we see that the bicartesian closed structure of \( D//F \) precisely yields the usual formulas of logical predicates over \( C \) [Mitchell and Scedrov 1992]. We can thus see (the interpretation of a language) in a subscone as a generalized logical relations argument.

For \( \omega \text{CPO-} \)enriched categories \( C \) and \( D \) and a locally continuous functor \( F : C \to D \), \( D//F \) is a reflective subcategory of \( D/F \) in the \( \omega \text{CPO-} \)enriched sense in case \((E, M)\) is an \( \omega \text{CPO-} \)enriched factorization system.

**Sheaves.** Given a topological space \( X = (|X|, O_X) \), a presheaf on the open subsets \( O_X \) is a contravariant functor \( F \) from the poset \( O_X \) to \( \text{Set} \). Given an open cover \( \mathcal{U} \) of \( W \in O_X \), a matching family of \( F \) for \( \mathcal{U} \) is a tuple \((x_U \in F(U))_{U \in \mathcal{U}} \) such that \( F(V \subseteq U)(x_U) = F(V \subseteq U')(x_{U'}) \) for all \( U, U' \in \mathcal{U} \) and \( V \subseteq \text{open} U \cap U' \). An amalgamation of such a matching family is an element \( x \in FW \) such that \( F(U \subseteq W)(x) = x_U \), for all \( U \in \mathcal{U} \). A presheaf \( F \) on \( O_X \) is called a sheaf if every matching family has a unique amalgamation. Sheaves and natural transformations form a cartesian closed category \( \text{Sh}(O_X) \) with all small limits and colimits. (In fact, they form a Grothendieck topos.) Further, epis and monos (i.e. componentwise injective natural transformations) form an orthogonal factorization system on \( \text{Sh}(O_X) \). By a subsheaf \( G \) of a sheaf \( F \), we mean a sheaf \( G \) such that \( GU \subseteq FU \) for all \( U \in O_X \) and \( G(U \subseteq U') \) is the restriction of \( F(U \subseteq U') \) for all \( U \subseteq U' \in O_X \).

**5.2 Subsconing for correctness of AD**

In [Huot et al. 2020], the idea is to build an interpretation \( \llbracket - \rrbracket \) of the language in the subscone \( \text{Diff} \times \text{Diff}//\text{Diff} \times \text{Diff}((\mathbb{R}, \mathbb{R}), -) \), where we interpret each \( \tau \) as the pair \( (\llbracket \tau \rrbracket, \llbracket D(\tau) \rrbracket) \) together with the relation which relates each curve in \( \llbracket \tau \rrbracket \) to its tangent curve in \( \llbracket D(\tau) \rrbracket \). This category almost has enough structure to lift the interpretation of our language: it is bicartesian closed. All that is missing is a lifting of the partiality monad \( (-) \perp \). One may try to define a lifting \( (-) \perp \) sending relations \( R \) on \( (\mathbb{R} \to X) \times (\mathbb{R} \to Y) \) to relations \( (\mathbb{R} \to X \perp) \times (\mathbb{R} \to Y \perp) \). A natural definition states that \( R \perp \) contains those pairs \((y, y')\) of partially defined curves in \( X \) and \( Y \), such that they have the same domain and are in \( R \) when restricted to their domain. Indeed, to prove AD correctness, we want the relation \( R \) of \( \llbracket \text{real} \rrbracket \) to say that the second curve has the same domain as the first and is the derivative of the first on its domain. However, a priori, we cannot make sense of the statement.
that \((y, y') \in R\) on their domain, as \(R\) only tracks curves with domain \(\mathbb{R}\)!
Therefore, we need to generalize to relations which track arbitrary partially defined curves. It turns out that it is best to treat such relations on partially defined curves as sheaves of relations over \(O_R\) (rather than as mere tuples or presheaves of relations) if we want the proof apply to sum types.

Thus, using the fact that one-dimensional plots form a sheaf over \(O_R\) by the (rearrangement) and (gluing) axioms, we consider the subcone \(\mathrm{Gl}\) of the functor

\[
F_{\mathrm{Gl}} : \mathbf{Diff} \times \mathbf{Diff} \to \mathbf{Sh}(O_R) \quad (X, Y) \mapsto \mathcal{P}_X \times \mathcal{P}_Y,
\]

where we work with the epi-mono factorization system on \(\mathbf{Sh}(O_R)\). Concretely, objects of \(\mathrm{Gl}\) are triples \((X, Y, R)\) of two diffeological spaces \(X, Y\) and a subshf \(R \subseteq \mathcal{P}_X \times \mathcal{P}_Y\).

Unroll the latter further: \(R\) gives for every \(U \subseteq \text{open } \mathbb{R}\) a relation \(R_U \subseteq \mathcal{P}^U \times \mathcal{P}^U\) such that relations restrict and glue in the sense that

- if \(V \subseteq \text{open } U\) and \((y, y') \in R^U\), then \((y|_V, y'|_V) \in R^V\);
- if \(y \in \mathcal{P}^W_X\) and \(y' \in \mathcal{P}^W_Y\) and \(U\) is an open cover of \(W\) such that \((y|_U, y'|_U) \in R^U\) for all \(U \in \mathcal{U}\), then also \((y, y') \in R^W\).

Morphisms \((X, Y, R) \to (X', Y', R')\) in \(\mathrm{Gl}\) are pairs \((X \xrightarrow{g} X', Y \xrightarrow{h} Y')\) of diffeological space morphisms such that, for any \(U \in O_R\), \((y, y') \in R_U^U\) implies that \((y; g; y'; h) \in R_\mathcal{U}^U\). By the general theory for subconing discussed above, \(\mathrm{Gl}\) lifts the bicartesian closed structure of \(\mathbf{Diff} \times \mathbf{Diff}\) along the obvious forgetful functor \(\mathrm{Gl} \to \mathbf{Diff} \times \mathbf{Diff}\).

To lift \((-)_{\times} \times (-)_{\times}\) to \(\mathrm{Gl}\), we define, given \((X, Y, R)\),

\[
R^U_{\perp} \overset{\text{def}}{=} \left\{ \left( (y, y') \in \mathcal{P}^U_X \times \mathcal{P}^U_Y \mid y^{-1}(X) = y'^{-1}(Y) \text{ and } (y|_{y^{-1}(X)}; y'|_{y^{-1}(X)}) \in R^U_{y^{-1}(X)} \right) \right\}.
\]

This definition is easily seen to give a subshf of \(\mathcal{P}_\perp \times \mathcal{P}_\perp\).

**Proposition 5.1.** The strong monad operations of \((-)_{\times} \times (-)_{\times}\) lift to \(\mathrm{Gl}\), turning \((-)_{\perp}\) into a commutative strong monad.

One can either verify this proposition by hand or observe that it follows from the general theory of logical relations for monadic types of [Goubault-Larrecq et al. 2002], if we work with the partiality monad \((\mathcal{U}_f)U \overset{\text{def}}{=} \{(V, x) \mid V \in O_U \text{ and } x \in FV\}\), return \(U(x) \overset{\text{def}}{=} (U, x)\), \((V, x) \xrightarrow{\alpha_U} (U, x)\) on \(\mathbf{Sh}(O_R)\) together with the obvious distributive law \(F_{\mathrm{Gl}} : T \to \mathcal{P}_X \times \mathcal{P}_Y\).

**Corollary 5.2.** The lifted monad \((-)_{\perp}\) lifts the interpretation of iteration in \((-)_{\times} \times (-)_{\times}\).

**Proof.** Indeed, the interpretation of iteration is constructed entirely out of the structure of the strong monad, the bicartesian closed structure, and the \(\text{poCPO}\)-enrichment of \(\mathbf{Diff} \times \mathbf{Diff}_{\perp}\). Seeing that \(\mathrm{Gl}_{\perp}\) lifts all of this structure, it lifts the interpretation of iteration as well. \(\Box\)

### 5.3 Correctness of Forward AD

Next, we build an interpretation \(\{-\}\) of our language in \(\mathrm{Gl}\) lifting the interpretation \(\left[ - \right], \left[ \overline{D}(-) \right]\) of our language in \(\mathbf{Diff} \times \mathbf{Diff}\) and show that correctness of forward AD follows. If we unwind all the definitions of the categorical structure of \(\mathrm{Gl}\), the subconing argument can be seen as the elementary logical relations proof described in section 2.

Suppose we are given a smooth partial function \(f : U \to V\) between open subsets \(U \subseteq \mathbb{R}^n\) and \(V \subseteq \mathbb{R}^m\) and a vector \(v \in \mathbb{R}^m\). We write \(\nabla_{\alpha} f\) for the smooth partial function \(U \to \mathbb{R}^m\) which has the same (open) domain \(D\) as \(f\) and calculates the directional derivative of \(f|D\) in direction \(v\) on \(D\). We will slightly abuse notation and write \(\nabla f\) for some \(1 \leq i \leq n\) to mean \(\nabla e_i f\) where \(e_i\) is the \(i\)-th standard basis vector of \(\mathbb{R}^n\). Similarly, in case \(U\) is one-dimensional, we write \(\nabla f\) for \(\nabla e_i f\).
To establish correctness of \( \overline{\mathcal{B}}(-) \) with respect to the semantics \([-]\), it is important to note that
\[
(\text{real})^V \overset{\text{def}}{=} \{(f, (f, \nabla f)) \mid f \in \mathcal{P}^V \} \subseteq \mathcal{P}^V \times \mathcal{P}^{V\times\mathbb{R}}
\]
forms a sheaf on \( \mathcal{O}_\mathbf{R} \), hence an object in \( \mathbf{Gl} \). It forms a sheaf because differentiation is a local operation, in the sense that (1) derivatives restrict to open subsets \( U - [\nabla (f|_U) = (\nabla f)_U] \) and (2) derivatives glue along open covers \( U - [\nabla \text{glue} (f|_U)_{U \in \mathcal{U}} = \text{glue} (\nabla f|_U)_{U \in \mathcal{U}}] \).

Observe that \((\text{sign } \mathbf{I}, \overline{\mathcal{B}}(\text{sign } \mathbf{I})) = (\text{sign } \mathbf{I}, (\pi_1; \text{sign } \mathbf{I})) \in \mathbf{Gl}(\{\text{real}, \{1|+\}\})\): Indeed, assume that \((\alpha, \alpha') \in \{\text{real}\}^U\). That is, \(\alpha = (\alpha; \nabla \alpha)\). We show that \((\alpha; \text{sign } \mathbf{I}, \alpha; \text{sign } \mathbf{I}) = (\alpha, \alpha')\): \((\text{sign } \mathbf{I}, \overline{\mathcal{B}}(\text{sign } \mathbf{I})) \in \mathbf{Gl}(\{1|+\})\); using the definition of the coproduct in \( \mathbf{Gl} \), we have that
\[
\{(1|+)^U \} = \{(\beta, \beta') \mid (\beta^{-1}(1 + 1) = \beta^{-1}(1 + 1)) \text{ and } (\beta|_{\beta^{-1}(1+1)}, \beta'|_{\beta^{-1}(1+1)}) \in (1|+)\}\}
\[
= \{(\beta, \beta') \mid (\beta^{-1}(1 + 1) = \beta'^{-1}(1 + 1)) \text{ and } \beta|_{\beta^{-1}(1+1)} = \beta'|_{\beta^{-1}(1+1)}\}
\]
\[
= \{(\beta, \beta) \mid \beta \in \mathbf{Diff}(U, (1 + 1))\}\).
\]

For these equalities to hold, it is important that we work with sheaves and not mere presheaves.

Then, as long as the operations respect the relation, which follows if \( \delta_0 \text{op}(x_1, \ldots, x_n) = \nabla_0 \text{op}(x_1, \ldots, x_n) \), for all \( n \)-ary operations \( \text{op} \) and all \( 1 \leq i \leq n \), it follows immediately that \((-)\) extends uniquely to the full language to lift the interpretation \([-][-] [\overline{\mathcal{B}}(-)]\). (This equation is precisely the criterion that \( \delta_0 \text{op} \) is a correct implementation of the \( i \)-th partial derivative of \( \text{op} \).) Indeed, observe that \((-)\) and the projection functor \( \text{proj} : \mathbf{Gl} \rightarrow \mathbf{Diff} \times \mathbf{Diff} \) are structure preserving, as are \((\text{id}, \overline{\mathcal{B}}(-))\) and \([-] \times [-]\). Meanwhile, \((\text{id}, \overline{\mathcal{B}}(-)); [-] \times [-]\) and \((-); \text{proj} \) agree on \( \text{real} \) and all operations \( \text{op} \) and \( \text{sign} \). By the universal property of the syntax, therefore, \((-); \text{proj} = ([-], \overline{\mathcal{B}}(-))\).

In particular, for any computation \( x_1 : \text{real}, \ldots, x_n : \text{real} \vdash^c t : \text{real} \), we have that \((\llbracket t \rrbracket, \llbracket \overline{\mathcal{B}}(t) \rrbracket) \in (\mathbf{Gl})_{\downarrow}((\text{real})^n, (\text{real}))\). Given a point \( x \in \mathbb{R}^n \) and a tangent vector \( v \in \mathbb{R}^n \), there exists some smooth curve \( y : \mathbb{R} \rightarrow \mathbb{R}^n \) such that \( y(0) = x \) and \( \nabla y(0) = v \). Now, by the chain rule, \((y, (y, \nabla y)) \in \mathbf{Gl}((\text{real}), (\text{real})^n)\). Therefore, \((y; \llbracket t \rrbracket, (y, \nabla y); \llbracket \overline{\mathcal{B}}(t) \rrbracket) \in \mathbf{Gl}((\text{real}), (\text{real}))\). That is, \((y, \nabla y); \llbracket \overline{\mathcal{B}}(t) \rrbracket = (y; [t], \nabla y; [t])\) and so, in particular, evaluating at 0, \( \llbracket \overline{\mathcal{B}}(t) \rrbracket(x, v) \) is defined iff \( [t](x) \) is defined and in that case \( \llbracket \overline{\mathcal{B}}(t) \rrbracket(x, v) = ([t](x), \nabla x; [t](x))\).

**Corollary 5.3 (Semantic Correctness of \( \overline{\mathcal{B}} \) (Limited)).** For any \( x_1 : \text{real}, \ldots, x_n : \text{real} \vdash^c t : \text{real} \), we have that \( \llbracket \overline{\mathcal{B}}_C(t) \rrbracket(x, v) = ([t](x), \nabla x; [t](v)) \), for all \( x \) in the domain of \([t]\) and \( v \) tangent vectors at \( x \). Moreover, \( \llbracket \overline{\mathcal{B}}_C(t) \rrbracket(x, v) \) is defined iff \([t](x)\) is.

### 6 Correctness of Forward AD at First-Order Types

We can extend this correctness result to functions between arbitrary first-order types.

#### 6.1 Preliminaries

**Tangent bundles.** We recall that the derivative of any smooth function \( f : M \rightarrow N \) between manifolds is given as follows. For each point \( x \) in a manifold \( M \), define the tangent space \( T_x M \) to be the set \( \{y \in \text{Man}(\mathbb{R}, M) \mid y(0) = x\}/\sim \) of equivalence classes \( [y] \) of smooth curves \( y \) in \( M \) based at \( x \), where we identify \( y_1 \sim y_2 \) iff \( \nabla_y y_1; f(0) = \nabla_y y_2; f(0) \) for all smooth \( f : M \rightarrow \mathbb{R} \). The tangent bundle of \( M \) is the set \( T(M) \defeq \bigcup_{x \in M} T_x M \). The charts of \( M \) equip \( T(M) \) with a canonical manifold structure. Then for smooth \( f : M \rightarrow N \), the derivative \( T(f) : T(M) \rightarrow T(N) \) is defined as \( T(f)(x, [y]) \defeq (f(x), [y; f]) \). By the chain-rule, \( T \) is a functor \( \text{Man} \rightarrow \text{Man} \). As is well-known, we can understand the tangent bundle of a composite space in terms of that of its parts.

**Lemma 6.1 (Tangent Bundles of (Co)Products).** For countable \( I \) and \( n \in \mathbb{N} \), there are canonical isomorphisms \( T(\bigcup_{i \in I} M_i) \cong \bigcup_{i \in I} T(M_i) \) and \( T(M_1 \times \ldots \times M_n) \cong T(M_1) \times \ldots \times T(M_n) \).
6.2 Correctness at first-order types

We define a canonical isomorphism \( \varphi^\mathcal{B}_\tau : \llbracket \mathcal{B}(\tau) \rrbracket \rightarrow \mathcal{T}(\llbracket \tau \rrbracket) \) for every type \( \tau \), by induction on the structure of types. We let \( \varphi^\mathcal{B}_\tau : \llbracket \mathcal{B}(\text{real}) \rrbracket \rightarrow \mathcal{T}(\llbracket \text{real} \rrbracket) \) be given by \( \varphi^\mathcal{B}_\tau(x, x') \triangleq (x, \{t \mapsto x + x't\}) \). For the other types, we use Lem. 6.1.

Next, we note that the tangent bundle functor \( \mathcal{T} : \text{Man} \rightarrow \text{Man} \) extends to a functor \( \mathcal{T} \) on the category of manifolds and partial maps \( \text{pMan} \rightarrow \text{pMan} \). Indeed, given a smooth partial function \( f : M \rightarrow N \) between manifolds, we define \( \mathcal{T}(f) : \mathcal{T}(M) \rightarrow \mathcal{T}(N) \) to have domain \( \mathcal{T}(f^{-1}(N)) \subseteq \mathcal{T}(M) \) and definition \( \mathcal{T}(f)(\mathcal{T}(\mathcal{T}(f^{-1}(N)))) \).

This extension lets us extend the correctness result of Cor. 5.3 to functions between arbitrary first-order types, i.e. types which do not contain any function type constructors.

**Theorem 6.2 (Semantic correctness of \( \mathcal{B} \) (full)).** For any first-order type \( \tau \), any first-order context \( \Gamma \) and any computation \( \Gamma \vdash^c t : \tau \), the syntactic translation \( \mathcal{B} \) coincides with the tangent bundle functor, modulo these canonical isomorphisms: \( \llbracket \mathcal{B}_\mathcal{C}(t) \rrbracket ; \varphi^\mathcal{B}_\tau = \varphi^\mathcal{B}_\tau ; \mathcal{T}(\llbracket t \rrbracket) \).

**Proof.** For any partial curve \( y \in \text{pMan}(\mathbb{R}, M) \), let \( \tilde{y} \in \text{pMan}(\mathbb{R}, \mathcal{T}(M)) \) be the tangent curve, given by \( \tilde{y}(x) = (y(x), \{t \mapsto y(x + t)\}) \), which has the same domain as \( y \).

First, we note that a smooth partial map \( h \in \text{pMan}(\mathcal{T}(M), \mathcal{T}(N)) \) is of the form \( \mathcal{T}(g) \) for some \( g \in \text{pMan}(M, N) \) if for all smooth partial curves \( y \in \text{pMan}(\mathbb{R}, M) \) we have \( \tilde{y} ; h = (y; g) \in \text{pMan}(\mathbb{R}, \mathcal{T}(N)) \). Therefore, it is enough to show that \( \tilde{y} ; \varphi^\mathcal{B}_\tau ; \mathcal{T}(\llbracket t \rrbracket) = \tilde{y} ; \llbracket \mathcal{B}_\mathcal{C}(t) \rrbracket ; \varphi^\mathcal{B}_\tau \) for all smooth partial curves \( y \in \text{pMan}(\mathbb{R}, \llbracket \mathcal{B}(\Gamma) \rrbracket) \), where \( \tilde{y} \) is the unique smooth partial curve in \( \text{pMan}(\mathbb{R}, \llbracket \mathcal{B}(\Gamma) \rrbracket) \) such that \( \tilde{y} ; \varphi^\mathcal{B}_\tau = \tilde{y} \).

Second, for any first-order type \( \tau \), \( \llbracket \tau \rrbracket \subseteq \{((f, \tilde{f}) | f : \mathbb{R} \rightarrow \llbracket \tau \rrbracket) \}. \) This equation is shown by induction on the structure of types. For this result to hold at sum types, it is important that our logical relations are sheaves (and not mere presheaves). Moreover, for such \( \tau \), \( \llbracket \tau \rrbracket \subseteq \{((f, \tilde{f}) | f : \mathbb{R} \rightarrow \llbracket \tau \rrbracket) \} \).

We conclude the theorem by combing these two observations:

\[
\tilde{y} ; \varphi^\mathcal{B}_\tau ; \mathcal{T}(\llbracket t \rrbracket) = \tilde{y} ; \mathcal{T}(\llbracket \llbracket t \rrbracket \rrbracket) = \tilde{y} ; \llbracket \mathcal{B}_\mathcal{C}(t) \rrbracket ; \varphi^\mathcal{B}_\tau = \tilde{y} ; \llbracket \mathcal{B}_\mathcal{C}(t) \rrbracket ; \varphi^\mathcal{B}_\tau,
\]

where in the last step, we use the fact that \( \llbracket \llbracket t \rrbracket, \mathcal{B}_\mathcal{C}(t) \rrbracket \) respects the logical relation. \( \square \)

7 A LANGUAGE WITH TERM AND TYPE RECURSION

We extend our language of Sec. 3 with term and type recursion. We work with iso-recursive types. That is, we add the following types \( \tau, \sigma, \rho \), values \( v, w, u \), and computations \( t, s, r \).

\[
\begin{align*}
\tau, \sigma, \rho & ::= \text{types} \quad | \quad \alpha, \beta, \gamma \quad \text{type variables} \\
& \quad | \quad \ldots \quad \text{as before} \quad | \quad \mu \alpha. \tau \quad \text{recursive types} \\
v, w, u & ::= \text{values} \quad | \quad \text{roll } v \quad \text{recursive type constructors} \\
& \quad | \quad \ldots \quad \text{as before} \\
t, s, r & ::= \text{computations} \quad | \quad \text{case } v \text{ of } \text{roll } x \rightarrow t \quad \text{recursive type match} \\
& \quad | \quad \ldots \quad \text{as before}
\end{align*}
\]

We extend the type system with the rules of Fig. 4. Every typing judgement should now be read relative to a kinding context \( \Delta = \alpha_1, \ldots, \alpha_n \) which contains the free type variables used in the judgement, where \( \mu \alpha. \) binds the right-most type variable in the kinding context. As this kind-system is standard (see e.g. [Vákár et al. 2019]), we leave it implicit for ease of notation.

Proc. ACM Program. Lang., Vol. 1, No. CONF, Article 1. Publication date: January 2018.
As is well-known, at this point, iteration and term recursion can be defined as sugar in terms of the primitives for type recursion (and their typing rules become derivable) [Abadi and Fiore 1996]:

\[
\mu z.t \triangleq \text{let \ } body = (\lambda x.\lambda y.\text{case \ } x \text{ \ of \ roll \ } x' \rightarrow (\text{return } x')x \text{ to } z \ y \ \text{in} \ (\text{return \ body})(\text{roll body)}\
\]

iterate \( t \) from \( x = v \triangleq (\mu z.\lambda x.t \ \text{to} \ y. \text{case} \ y \ \text{of} \ \{ \text{inl} \ x' \rightarrow (\text{return } z)x' \ \mid \ \text{inr} \ x'' \rightarrow \text{return } x'' \} \) \( v \).

We extend the forward AD macro in the unique structure preserving way:

\[
\begin{align*}
\overline{\mathcal{D}}(\alpha) & \triangleq \alpha \\
\overline{\mathcal{D}}(\mu x.\tau) & \triangleq \mu x.\overline{\mathcal{D}}(\tau) \\
\overline{\mathcal{D}}(\text{case } v \text{ of } \text{roll } x \rightarrow t) & \triangleq \text{case } \overline{\mathcal{D}}(v) \text{ of } \text{roll } x \rightarrow \overline{\mathcal{D}}(t).
\end{align*}
\]

Lemma 3.1 is easily seen to continue to hold on this extended language, when we add the \( \beta\eta \)-rules of Fig. 5. We can observe that the AD rules for iteration and term recursion can be derived from those for type recursion.

8 \( \omega \)-DIFFEIOLOGICAL SPACES AND DIFFERENTIABLE SEMANTICS OF RECURSION

8.1 Preliminaries

Bilimit compact expansions. We recall some basic machinery for solving recursive domain equations [Levy 2012]. Recall that an embedding-projection-pair (ep-pair) \( u : A \Rightarrow B \) in an \( \omega \text{-CPO-enriched category} \mathcal{B} \) is a pair consisting of a \( \mathcal{B} \)-morphism \( u^e : A \rightarrow B \), the embedding, and a \( \mathcal{B} \)-morphism \( u^p : B \rightarrow A \), the projection, such that \( p; e \leq \text{id} \) and \( e; p = \text{id} \). An embedding \( u : A \Rightarrow B \) is the embedding part of some ep-pair \( A \leftarrow B \).

An \( \omega \)-chain of ep-pairs \( (u_n)_{n \in \mathbb{N}} \) in \( \mathcal{B} \) consists of a countable sequence of objects \( A_n \) and a countable sequence of ep-pairs \( a_n : A_n \Rightarrow A_{n+1} \). A bilimit \((D, d)\) of such an \( \omega \)-chain consists of an object \( D \) and a countable sequence of ep-pairs \( d_n : A_n \Rightarrow D \) such that, for all \( n \in \mathbb{N} \), \( a_n; d_{n+1} = d_n \), and \( \bigvee_{n \in \mathbb{N}} d_n = \text{id}_D \). The celebrated limit-colimit coincidence [Smyth and Plotkin 1982] states that the bilimit structure is equivalent to a colimit structure \((D, d^\oplus)\) for \((\langle A_n \rangle, \langle a_n^\sigma \rangle)\), in which case \( d_n^\oplus \) are uniquely determined, and similarly equivalent to a limit structure \((D, d^\cap)\) for \((\langle A_n \rangle, \langle a_n^\cap \rangle)\), in which case \( d_n^\cap \) are uniquely determined.

A zero object is an object that is both initial and terminal. A zero object in an \( \omega \text{-CPO-category} \) is an ep-zero object if every morphism into it is a projection and every morphism out of it is an embedding.

A bilimit compact category is an \( \omega \text{-CPO-category} \mathcal{B} \) with an ep-zero and ep-pair \( \omega \)-chain bilimits. When \( \mathcal{A}, \mathcal{B} \) are bilimit compact, every locally continuous, mixed-variance functor \( F : \mathcal{A}^{\text{op}} \times \mathcal{B}^{\text{op}} \times \mathcal{A} \times \mathcal{B} \rightarrow \mathcal{B} \) has a parameterised solution to the recursive equation \( \text{roll} : F(A, X, A', X) \rightarrow X \).

\[
\begin{array}{c}
\frac{\Gamma, x : \tau \vdash t : \tau}{\Gamma \vdash \mu x.t : \tau} \\
\frac{\Gamma \vdash \alpha : \tau}{\Gamma \vdash \mu x.\alpha : \tau} \\
\frac{\Gamma \vdash v : \mu x.\tau}{\Gamma \vdash \text{roll } v : \mu x.\tau} \\
\frac{\Gamma \vdash \text{case } v \text{ of } \text{roll } x \rightarrow t : \tau}{\Gamma \vdash \text{case } v \text{ of } \text{roll } x \rightarrow t : \tau}
\end{array}
\]

Fig. 4. Typing rules for term and type recursion. As usual, we treat \( \mu x. \) as a type level variable binder.

\[
\text{case } \text{roll } v \text{ of } \text{roll } x \rightarrow t = t^{\langle \text{roll } v \rangle} \\
\text{case } v \rightarrow t = t^{\langle \text{roll } v \rangle}
\]

Fig. 5. Standard \( \beta\eta \)-laws for recursive types (which imply rules for term recursion and iteration.).
every \( A, A' \) in \( \mathcal{A} \), qua the bilimit \((\mu B.F(A, B, A', B), d_{F,A,A'})\) of

\[
F^{op}(A, \iff, A'; \iff) \iff F(A, F(A, 0, A', 0), A', F(A, 0, A', 0)) \iff \cdots \iff F^n(A, A') \iff \cdots
\]

The solution is minimal in the sense of Pitts [1996]. The assignments \( \mu B.F(A, B, A', B) \) extend to a mixed-variance functor \( \mu B.F(-, B, -): \mathcal{A}^{op} \times \mathcal{A} \to \mathcal{B} \) by \( \mu B.F(f, b, g, B) := \bigvee_n d^n_{\alpha}; F^n(f, g); d^n_{\alpha}. \)

Finally, a bilimit compact expansion \( J : C \to \mathcal{B} \) is a triple consisting of an \( \omega \text{-CPO}\)-category \( C \), a bilimit compact category \( \mathcal{B} \); and an identity-on-objects, locally continuous, order respecting functor \( J : C \to \mathcal{B} \) such that, for every ep-pair \( (A, a), (B, b) \) in \( \mathcal{B} \), their bilimits \((D, d), (E, e)\), and countable collection of \( C\)-morphisms \((\alpha_n : A_n \to B_n)_{n \in \mathbb{N}}\) such that for all \( n \):

\[
a^e_n; j_{\alpha_n+1} = j_{\alpha_n}; b^e_n, \quad d^p_n; j_{\alpha_n} = j_{\alpha_n+1}; b^p_n
\]

(i.e., \( J\alpha : (A, a^e) \to (B, b^e) \) and \( J\alpha : (A, a^p) \to (B, b^p) \) are natural transformations), there is a \( C\)-morphism \( f : D \to E \) such that \( Jf = \bigvee_n d^n_{\alpha}; \alpha_n; e^e_n. \) The motivation for this definition: given two bilimit compact expansions \( I : D \to \mathcal{A}, J : C \to \mathcal{B} \), and two locally continuous functors

\[
F : D^{op} \times C^{op} \times D \times C \to C \quad G : \mathcal{A}^{op} \times \mathcal{B}^{op} \times \mathcal{A} \times \mathcal{B} \to \mathcal{B} \quad \text{s.t. } I^{op} \times J^{op} \times I \times J; G = F; J
\]

the functor \( \mu B.G(-, B, -) : \mathcal{A}^{op} \times \mathcal{A} \to \mathcal{B} \) restricts to \( \mu B.G(I^{op}, B, J, B) : D^{op} \times D \to C \). Bilimit compact expansions are closed under small products, opposites, and exponentiation with small categories [Levy 2012].

**Semantics of recursion.** We again restrict our attention to monad models as considered in Sec. 4. Suppose that we are given a bicartesian closed category \( C \) with a strong monad \( T \) such that the Kleisli adjunction gives rise to a bilimit compact expansion \( J : C \to C_T. \) Suppose further that the copairing \([-,-]\) and the exponential adjunction \(- \times A \to (-)^A\) in \( C \) are locally continuous. As the left adjoint \((-) \times A\) preserves all colimits, hence lubs, it follows that \((-) \times (-), (-) + (-)\) and \((T)^{(-)}\) extend to locally continuous bifunctors \((-) \otimes (-), (-) \oplus (-), (-) \mapsto (-)\) on \( C_T:\)

\[
f \otimes f \overset{\text{def}}{=} (f \times f'); \text{dst } f \oplus f' \overset{\text{def}}{=} (f + f'); [\text{Tinl}, \text{Tinr}] f \overset{\text{def}}{=} f' \overset{\text{def}}{=} \Lambda((\text{id}, A, \text{snd}; f'); \iff)); \text{return.}
\]

We describe how to extend the interpretation of Sec. 4 to the full language of Sec. 7 in a category with such structure. We write \([\Delta]_{\forall} \overset{\text{def}}{=} \prod_{\alpha \in \Delta} C\) and \([\Delta]_{c} \overset{\text{def}}{=} \prod_{\alpha \in \Delta} C_T\) for a kinding context \( \Delta. \) We interpret types in context \( \Delta \) as locally continuous functors \([\Delta]^{c}_{op} \times [\Delta]_{c} \to C_T\) which restrict to \([\Delta]^{c}_{op} \times [\Delta]_{o} \to C. \) We interpret values and computations as corresponding natural transformations. We extend \([-\cdot]-\) of Sec. 4 to apply componentwise, using \( \otimes, \oplus, \mapsto \) to interpret product, sum and function types as locally continuous functors on \( C_T.; \) and we interpret

\[
[\alpha] \overset{\text{def}}{=} \pi_{2}; \pi_{\alpha} \quad [\mu X.] \overset{\text{def}}{=} \mu X.; [r](-, \ldots, -, \alpha, \ldots, -, \alpha) \\
[\Delta|\Gamma \vdash^c \tau] \overset{\text{def}}{=} C[\Delta]^{c}_{c}([\Gamma], [\Gamma]) \quad [\Delta|\Gamma \vdash^e \tau] \overset{\text{def}}{=} C[\Delta]^{e}_{c}([\Gamma], [\Gamma]) \\
[\text{roll } v](\rho) \overset{\text{def}}{=} \text{roll}(v)(\rho)) \quad [\text{case } v \text{ of } \text{roll } x \to t](\rho) \overset{\text{def}}{=} [t](\text{roll}^{-1}(v)(\rho))).
\]

**Scott topology.** Given an \( \omega\text{-cpo} \([|\cdot|], \leq_{\omega}\)\), there is a canonical topology on \(|\cdot|\) called the Scott topology. A subset \( U \subseteq |\cdot|\) is Scott-open iff it is arises as \( \chi_{U}^{-1}(\star)\) for some \( \omega\text{-continuous characteristic function } X \overset{\text{--}}{\to} 1.\) In explicit terms, Scott open subsets are precisely those for which

- \( x \leq y \) and \( x \in U \) implies \( y \in U \) (upwards closure);
- \( x = \bigvee_{i \in \mathbb{N}} x_i \) and \( \forall i \in \mathbb{N}, x_i \notin U \) implies \( x \notin U \) (\( \omega\)-chain inaccessibility).

Let us write \( \omega\text{-CPO} \) for the category of \( \omega\text{-cpos} \) and partial functions with a Scott open domain on which they are \( \omega\text{-continuous}. \) Then, we have an equivalence \( \omega\text{-CPO} \cong \omega\text{-CPO}_{\perp}. \)
8.2 $\omega$-diffeological spaces

As far as we are aware, no established mathematical theory is suitable for describing both differentiation and recursion. For this reason, we introduce a new notion of an $\omega$-diffeological space, or, briefly, $\omega$-ds.

Definition 8.1. An $\omega$-ds consists of a triple $([X], P_X, \leq_X)$ such that $([X], P_X)$ is a diffeological space and $([X], \leq_X)$ is an $\omega$-cpo satisfying the additional condition that $(\bigvee_{i \in \mathbb{N}} a_i)(x) \overset{def}{=} \bigvee_{i \in \mathbb{N}} (a_i(x))$ defines a plot $\bigvee_{i \in \mathbb{N}} a_i \in P_X^U$, for any $\omega$-chain $(a_i \in P_X^U)_{i \in \mathbb{N}}$ in the pointwise order. Homomorphisms $X \to Y$ of such structures are defined to be functions $f : |X| \to |Y|$, such that $f : ([X], P_X) \to ([Y], P_Y)$ is a morphism of diffeological spaces and $f : ([X], \leq_X) \to ([Y], \leq_Y)$ is $\omega$-continuous. We write $\omega$Diff for the category of $\omega$-dses and their homomorphisms.

Example 8.2. Any diffeological space $X$ can be interpreted as an $\omega$-ds by taking $\leq_X$ as the discrete order $=_{\text{X}}$. In particular, this is true for any Cartesian space or manifold.

Example 8.3. Let $X$ be an $\omega$-ds. Any subset $A \subseteq |X|$ which is an $\omega$-cpo under the induced order from $X$ is an $\omega$-ds under the subspace diffeology.

Example 8.4. Given a family $(X_i)_{i \in I}$ of $\omega$-dses, we can form their product by equipping $\prod_{i \in I} |X_i|$ with the product diffeology and product order.

Example 8.5. Given a family $(X_i)_{i \in I}$ of $\omega$-dses, we can form their coproduct by equipping $\bigsqcup_{i \in I} |X_i|$ with the coproduct diffeology and coproduct order.

Example 8.6. Given $\omega$-dses $X, Y$, we can equip $\omega$Diff$(X, Y)$ with the pointwise order and diffeology $P_{XY}^U \overset{def}{=} \{ \Lambda(\alpha) \mid \alpha \in \omega$Diff$(U \times X, Y) \}$.

These examples give us the categorical (co)product and exponential objects, respectively, in $\omega$Diff. In fact, in Appx. C we give various characterizations of $\omega$Diff, which, in particular, show that the category is locally presentable, hence complete and cocomplete.

Next, we turn to the interpretation of partiality in $\omega$Diff. Let us call subsets D-Scott open if they are both D-open and Scott open. There is a natural notion of partial function $X \to Y$ in $\omega$Diff: partial functions $|X| \to |Y|$ which are defined on a D-Scott open subset $D \subseteq |X|$ on which they restrict to an $\omega$-ds morphism $D \to Y$ (using the subspace order and diffeology). Let us write $\text{poDiff}$ for the category of $\omega$-dses and such partial functions. As we interpret first-order types as manifolds with the discrete order in $\omega$Diff, the semantics of computations between first-order types again lies in the full subcategory $\text{pMan}$ of $\text{poDiff}$.

Alternatively, we have a natural partiality monad $(\bot)_\bot$ on $\omega$Diff. Indeed, for an $\omega$-ds $X$, we use $X_\bot$ as having underlying diffeological space $(|X|, P_X)_\bot$ and underlying $\omega$-cpo $(|X|, \leq_X)_\bot$, where we use the previously defined partiality monads $(\bot)_\bot$ on Diff and $\omega$CPO.

Proposition 8.7. $(\bot)_\bot$ defines a locally continuous commutative strong monad on $\omega$Diff. Moreover, its Kleisli category $\omega$Diff$\bot$ is equivalent to $\text{poDiff}$.

Again, the important observation is that D-Scott open subsets in $X$ are precisely those subsets with a characteristic function $X \to 1_\bot$ which is an $\omega$-ds morphism.

This category of partial maps has sufficient structure to interpret term and type recursion.

Proposition 8.8. $\omega$Diff $\hookrightarrow$ poDiff forms a bilimit compact expansion.

The proof goes via a development of axiomatic domain theory [Fiore 2004] in $\omega$Diff that is entirely analogous to that given in [Vákár et al. 2019, Sec. 5] for $\omega$-quasi-Borel spaces. The only difference are that we work with
• the category of ω-dses instead of ω-quasi-Borel spaces;
• the domain structure consisting of (the isomorphism closure of) inclusions of D-Scott open subsets with the subspace order and diffeology instead of Borel-Scott open monos (in fact, just like in [Vákár et al. 2019], these are precisely the monos that arise as the pullback of \( \text{return}_\perp \) along some “characteristic function” \( X \to \perp_\perp \));
• \( T \) equal to \( (-)_\perp \) as we are not interested in modelling probability.

With these minor changes, we can inline Sec. 5 of loc. cit. here to derive bilimit compactness. We therefore refer the reader to [Vákár et al. 2019, Sec. 5] for this development.

**Corollary 8.9.** We obtain a canonical interpretation \([-\, -]\) of the full language of Sec. 7 in \( \omega \text{Diff} \).

This corollary follows once we note that \([-\, -]\) and the exponential adjunction are locally continuous as they lift the corresponding locally continuous structures in \( \omega \text{CPO} \). We have extended our previous semantics for the limited language, if we forget about the \( \omega \)-cpo-structure on objects.

We conclude this section by noting that the semantics we have constructed is canonical in the following two senses. First, it is a conservative extension to the full language of Sec. 7, respecting all \( \text{βη}\)-laws, of the canonical semantics of the first-order fragment of our language in \text{Man} and \( \text{pMan} \). Stronger still: even the semantics of programs involving recursion and higher-order functions lie in the two canonical categories \text{Man} and \( \text{pMan} \) for differential geometry, as long as their types are first-order. Second, this denotational semantics satisfies an adequacy theorem with respect to the (completely uncontroversial) operational semantics of our language (see Appx. B), showing that our interpretation is a sound means for establishing contextual equivalences of the operational semantics. We hope that these two facts convince the reader of the canonical status of our semantics and that they add weight to the correctness theorem of AD with respect to the semantics, which we prove in the next section.

**9 LOGICAL RELATIONS AND CORRECT AD FOR RECURSION**

**9.1 Preliminaries**

**Distributive and codistributive laws of monads.** Suppose we are given two categories each equipped with a monad, \( (C, S, \text{return}^S, \mu^S) \) and \( (D, T, \text{return}^T, \mu^T) \), together with a functor \( F : C \to D \). Then, a natural transformation \( \sigma : F; T \to S; F \) is called a **distributive law** if it satisfies \( \text{return}^T; \sigma = \text{return}^S; \mu^T; \sigma \) and \( \mu^T; \sigma = T; \sigma; \text{return}^S; \mu^S \).

Similarly, \( \tau : S; F \to F; T \) is called a **co-distributive law** if it satisfies \( \text{return}^T; \tau = \text{return}^T; \mu^T; \tau \) and \( F; \mu^S; \tau = \tau; \text{return}^S; \mu^S; \tau \).

(Co)distributive laws naturally arise for the following reason [Appelgate 1965; Mulry 1993].

**Distributive** laws \( \sigma : F; T \to S; F \) are in 1-1 correspondence with liftings of \( F : C \to D \) to a functor between the Eilenberg-Moore categories: \( G : C^S \to D^T \) such that the left diagram below commutes. Co-distributive laws \( \tau : S; F \to F; T \) are in 1-1 correspondence with extensions of \( F : C \to D \) to a functor between the Kleisli categories: \( H : C_S \to D_T \) such that the right diagram below commutes. Here, we have that \( H(A \xrightarrow{F} SB) \overset{\text{def}}{=} FA \xrightarrow{Ff} F(SB) \xrightarrow{\tau} T(FB) \).

\[
\begin{array}{ccc}
C & \xrightarrow{F} & D \\
\uparrow & & \uparrow \\
C^S & \xrightarrow{G} & D^T \\
\downarrow & & \downarrow \\
C_S & \xrightarrow{H} & D_T.
\end{array}
\]

**Monad liftings.** We discussed in Sec. 5 how to lift most categorical structure to (sub)scones. Here, we recall a more systematic way of lifting monads due to [Goubault-Larrecq et al. 2002]. Suppose we have monads \( (C, S, \text{return}^S, \mu^S) \), \( (D, T, \text{return}^T, \mu^T) \), a functor \( F : C \to D \) and a distributive
law $\sigma : F; T \to S; F$. Then, we obtain a monad $\tilde{T}$ (which lifts $S$ and $T$) on the scone $D/F$ by defining

$$\tilde{T}(D, f, C) \overset{\text{def}}{=} (TD, Tf; \sigma, SC) \quad \text{return}_{(D,f,C)} \overset{\text{def}}{=} (\text{return}_T, \text{return}_S) \quad \tilde{\mu}_{(D,f,C)} \overset{\text{def}}{=} (\mu^T, \mu^S).$$

Given an orthogonal factorization system $(E, M)$ on $D$ such that $M$ is closed under $T$ and contains $\sigma$, $\tilde{T}$ restricts to a monad on $D/F$. Suppose that $S$ and $T$ are strong monads with strengths $\text{st}^S$ and $\text{st}^T$, respectively, such that $(\text{id} \times \sigma); F(\text{st}^S) = \text{st}^T; \sigma$. In case $C$ and $D$ have finite products and $F$ preserves them, $\tilde{T}$ gives a strong monad on $D/F$. If we further assume that $M$ is closed under finite products, $\tilde{T}$ gives a strong monad on $D//F$. The strength of $\tilde{T}$ is given by the pair $(\text{st}^T, \text{st}^S)$.

### 9.2 Logical relations over $\omega$-dse

We extend our previous logical relations argument of Sec. 5 to apply to the semantics of recursion in $\omega\text{Diff}$. To do so, we extend our definition of the relation to recursive types as

$${R^U}_{\mu, \tau} \overset{\text{def}}{=} \{(y, y') \mid (y'; \text{roll}^{-1}, y'; \text{roll}^{-1}) \in {R^U}_{\tau[\mu \mapsto \tau]}\}.$$ 

That is, we would like to define the relation itself using type recursion. Using this definition of the relation, it is not hard to prove the fundamental lemma we need for the correctness of AD. The challenge, however, is to show that it is in fact possible to define the relation using recursion. Usually, one shows this using the complicated recipes of [Pitts 1996]. However, it is not clear that they apply to the situation we are interested in. Luckily, however, we are in a situation that is, in some ways, much simpler than that of [Pitts 1996]: we are considering relations over an $\omega\text{CPO}$-enriched semantics, rather than the non-chain-complete syntax of a language. As a consequence, it is enough to show that the natural category of logical relations $\omega\text{Gl}$ over $\omega\text{Diff} \times \omega\text{Diff}$ has a bilimit compact expansion $\omega\text{Gl} \rightarrow \omega\text{Gl}_{\perp}$, where the bilimits in $\omega\text{Gl}_{\perp}$ lift those in $\omega\text{Diff} \times \omega\text{Diff}_{\perp}$. Then, it automatically follows that our interpretation $([\cdot], [\vec{T}(\cdot)])$ of our language in $\omega\text{Diff} \times \omega\text{Diff} \rightarrow \omega\text{Diff}_{\perp} \times \omega\text{Diff}_{\perp}$ lifts to $\omega\text{Gl}$, showing the correctness of AD.

A first attempt might be to define $\omega\text{Gl}$ as the subscone of the functor $\omega\text{Diff} \times \omega\text{Diff} \rightarrow \text{Sh}(O_R)$; $(X, Y) \mapsto P_X \times P_Y$. However, the resulting category does not (obviously) give a bilimit compact expansion. Instead, we change the codomain of the functor above with the category $\text{Sh}_{\omega\text{CPO}}(O_R)$ of internal $\omega$-cpos in $\text{Sh}(O_R)$, called $\omega$-cpo-sheaves from now, and componentwise $\omega$-continuous natural transformations. We can characterise these as follows:

**Lemma 9.1.** An $\omega$-cpo-sheaf $([X], \leq_X)$ in $\text{Sh}(O_R)$ is the data of a sheaf $[X] \in \text{Sh}(O_R)$ together with a subsheaf $\leq_X$ of $[X] \times [X]$ such that $(|X|U, (\leq_X)U)$ forms an $\omega$-cpo and $|X|(U \subseteq V) : |X|V \rightarrow |X|U$ is $\omega$-continuous for each $U \subseteq_{\text{open}} V \subseteq_{\text{open}} R$.

$\text{Sh}_{\omega\text{CPO}}(O_R)$ is $\omega\text{CPO}$-enriched by using the order $\alpha \leq \beta \overset{\text{def}}{=} \forall U \in O_R, x \in U. \alpha_U(x) \leq \beta_U(x)$ on the homsets. Further, 

**Proposition 9.2.** $\text{Sh}_{\omega\text{CPO}}(O_R)$ is a bicartesian closed category.

Indeed, we can show that it is locally presentable, as the category of models of an essentially algebraic theory like that of $\omega$-cpos in any locally presentable category, e.g. any Grothendieck topos like $\text{Sh}(O_R)$, is locally presentable [Adámek et al. 1994, Proposition 1.53]. Its products are simply taken as the componentwise product in $\omega\text{CPO}$. Its coproducts are more complicated, but we shall not need them in generality. Its exponentials are defined by $[Y^X]; C \overset{\text{def}}{=} \text{Sh}_{\omega\text{CPO}}(O_R)(YC \times X, Y)$, where we write $y$ for the Yoneda embedding, which we equip with the pointwise order.

To construct a subscone of a functor valued in this category, we observe that we have a suitable orthogonal factorization system. First, we note that we have a closure operator $\text{Cl}$ on subsheaves $A$ of $|X|$ for an object $X$ of $\text{Sh}_{\omega\text{CPO}}(O_R)$: $\text{Cl} A$ is defined by the smallest chain-complete
subsheaf of \(|X|\) containing \(A\). We can give a predicative construction of \(\mathcal{C}L\mathcal{A}\) using transfinite induction: iterate the closure of \(A\) in \(|X|\) under both lubs of existing \(\omega\)-chains and amalgamations in \(|X|\) of existing matching families in \(A\) transfinately often (potentially creating new \(\omega\)-chains and matching families at each step). This iteration defines an ordinal-indexed increasing chain and it must stabilize as it is bounded by the cardinality of \(|X|\). Let us call a subsheaf \(A \subseteq |X|\) \(\mathrm{Cl}\)-closed if \(\mathrm{Cl}\, A = A\) and let us call a morphism \(A \to B\) in \(\mathbf{Sh}_{\omega\mathrm{CPO}}(\mathcal{O}_R)\) \(\mathrm{Cl}\)-dense if its componentwise image is a \(\mathrm{Cl}\)-closed subsheaf of \(|B|\).

**Lemma 9.3.** Taking \(\mathcal{M}\) to consist of morphisms which are componentwise full monos (i.e. \(\mathrm{Cl}\)-closed monos) and \(\mathcal{E}\) to consist of \(\mathrm{Cl}\)-dense morphisms gives an \(\omega\mathrm{CPO}\)-enriched orthogonal factorization system on \(\mathbf{Sh}_{\omega\mathrm{CPO}}(\mathcal{O}_R)\). Further, \(\mathcal{E}\) and \(\mathcal{M}\) are closed under products.

The latter statement follows because \(\mathrm{Cl}\) respects products as a consequence of lubs and amalgamations both being taken componentwise in a product.

This factorization system lets us consider the subscone of functors valued in \(\mathbf{Sh}_{\omega\mathrm{CPO}}(\mathcal{O}_R)\). We have a locally continuous functor \(\mathcal{F}_{\omega\mathrm{Gl}}: \omega\text{Diff} \times \omega\text{Diff} \to \mathbf{Sh}_{\omega\mathrm{CPO}}(\mathcal{O}_R)\); \((X, Y) \mapsto (U \mapsto \mathcal{P}^U_X \times \mathcal{P}^U_Y)\) which preserves finite products. We write \(\omega\text{Gl}\) for its subscone, which has triples \((X, Y, R)\) as objects: two \(\omega\)-dses \(X, Y\) and a componentwise fully included sub-\(\omega\)-cpo-sheaf \(R\) of \(\mathcal{P}^X_X \times \mathcal{P}^Y_Y\). Put simply, we work with pairs \(X, Y\) of \(\omega\)-dses with relations \(R^U \subseteq \mathcal{P}^U_X \times \mathcal{P}^U_Y\) for each \(U \subseteq \text{open } \mathbb{R}\) such that

- the relations \(R^U\) restrict to open subsets and glue along open covers, as before in Sec. 9;
- each \(R^U\) is chain-complete: for an \(\omega\)-chain \((y_i, y'_i)\) in \((y, y')\) in \(\mathcal{P}^U_X \times \mathcal{P}^U_Y\) such that \(\forall i \in \mathbb{N}, (y_i, y'_i) \in R^U\), we also have \((y, y') \in R^U\).

Morphisms \((X, Y, R) \to (X', Y', R')\) in \(\omega\text{Gl}\) are pairs \((X \xrightarrow{g} X', Y \xrightarrow{h} Y')\) of \(\omega\)-ds morphisms such that, for any \(U \subseteq \mathcal{O}_R\), \((y, y') \in R^U\) implies that \((y; g, y'; h) \in R'^U\).

**Proposition 9.4.** \(\omega\text{Gl}\) is a bicartesian closed category. Further, the copairing and the exponential adjunction are locally continuous.

The first statement follows from the general theory of subsconing from Sec. 5. The second statement follows as the \(\omega\text{CPO}\)-enrichment as well as the coproducts and exponential adjunction are lifted from \(\omega\text{Diff} \times \omega\text{Diff}\), where we have already established this result. A quick verification shows that the explicit formulae for the logical relation at sum and product types given in Sec. 2 stay valid. To see the formula for coproducts stays valid, we can note that this particular coproduct is straightforward because it is a coproduct of subsheaves of sheaves of continuous functions.

Next, we lift the monad \((-) \perp \times (-) \perp\) on \(\omega\text{Diff} \times \omega\text{Diff}\) to a monad \((-) \perp\) on \(\omega\text{Gl}\), using the same definition as before:

\[
R^U_\perp \overset{\text{def}}{=} \{(y, y') \in \mathcal{P}^U_X \times \mathcal{P}^U_Y \mid y^{-1}(X) = y'^{-1}(Y) \text{ and } (y|_{y^{-1}(X)}, y'|_{y'^{-1}(X)}) \in R'^{-1}(X)\}.
\]

**Proposition 9.5.** The strong monad operations of \((-) \perp \times (-) \perp\) lift to \(\omega\text{Gl}\), turning \((-) \perp\) into a locally continuous commutative strong monad.

Again, we can verify this proposition by hand or appeal to the general results of [Goubault-Larrecq et al. 2002], which we recalled in Sec. 9.1. We discuss the latter option as it will be of further interest.

We have a locally continuous commutative strong monad \((-) \perp\) on \(\mathbf{Sh}_{\omega\text{CPO}}(\mathcal{O}_R)\):

\[
F_\perp U \overset{\text{def}}{=} \{((V, x) \mid V \in \mathcal{O}_U \text{ and } x \in FV), ((V, x) \leq (V', x')) \overset{\text{def}}{=} (V \subseteq V' \text{ and } x \leq F(V \subseteq V')(x'))\}
\]

\[
\text{return}_U(x) \overset{\text{def}}{=} (U, x) \quad (V, x) \Rightarrow_U \alpha_U \overset{\text{def}}{=} \alpha_V(x).
\]

**Proposition 9.6.** \(\mathbf{Sh}_{\omega\text{CPO}}(\mathcal{O}_R) \hookrightarrow \mathbf{Sh}_{\omega\text{CPO}}(\mathcal{O}_R) \perp\) is a bilitlimit compact expansion.
Again, the proof goes via a development of axiomatic domain theory [Fiore 2004] in $\text{Sh}_{\omega\text{CPO}}(O_{\boxtimes})$ that is entirely analogous to that given in [Vákár et al. 2019, Sec. 5] for $\omega$-quasi-Borel spaces. The only difference are that we work with

- the category of $\omega$-cps-sheaves instead of $\omega$-quasi-Borel spaces;
- the domain structure consisting of the monos that arise as the pullback of return$_{\perp}$ along some “characteristic function” $X \rightarrow \mathbb{1}_{\perp}$;
- $T$ equal to the partiality monad $(\cdot )_{\perp}$ as we are not interested in modelling probability.

With these minor changes, we can inline Sec. 5 of loc. cit. here to derive bilimit compactness.

Further, we can observe that we have a distributive law $\sigma : F_{\omega \text{Gl}}; (\cdot )_{\perp} \rightarrow (\cdot )_{\perp}; F_{\omega \text{Gl}}$ defined by

$$(V, (y, y')) \mapsto \begin{cases} y(x) & x \in V \\ \perp & \text{else} \end{cases}, \begin{cases} y'(x) & x \in V \\ \perp & \text{else} \end{cases}.$$ 

Moreover, we can note that $\sigma$ is a full mono and $(\cdot )_{\perp}$ preserves full monos. As a consequence, we obtain a canonical monad lifting $(\cdot )_{\perp}$ of $(\cdot )_{\perp}$ to the subscone $\omega \text{Gl}$, by Sec. 9.1. Again, the resulting formulas for $(R_{T})_{\perp}$ and $R_{T;\sigma}$ remain the same as those from Sec. 2.

We derive a technical lemma to show that the subscone has a bilimit compact expansion.

**Lemma 9.7.** Given locally continuous monads $S$ and $T$ on $\omega\text{CPO}$-categories $C$ and $D$, a locally continuous functor $F : C \rightarrow D$ and a distributive law $\sigma : F; T \rightarrow S; F$, giving rise to a monad lifting $\tilde{T}$ to the scone $D//F$. Suppose that $C \hookrightarrow C_{S}$ and $D \hookrightarrow D_{T}$ are bilimit compact expansions. Further assume that

1. every embedding $\alpha \in C_{S}$ is a morphism in $C$ (factors over return);
2. $F(\perp^{P}) = \perp^{P}; T([[F_{0}]); \sigma]$;
3. $\sigma$ is a split mono with right inverse $\tau$ which is a codistributive law $S; F \rightarrow F; T$.

And suppose that $C \hookrightarrow C_{S}$ and $D \hookrightarrow D_{T}$ give bilimit compact expansions. Then, the Kleisli adjunction $D//F \leftrightarrow (D//F)_{\tilde{T}}$ also gives a bilimit compact expansion.

Further, if we are given a $\omega\text{CPO}$-enriched factorization system $(E, M)$ on $D$ such that $\sigma \in M$ and $M$ is closed under $T$, we have seen that $\tilde{T}$ restricts to the subscone $D//F$. Then $D//F \leftrightarrow (D//F)_{\tilde{T}}$ also gives a bilimit compact expansion.

In the lemma above, the bilimits in $(D//F)_{\tilde{T}}$ lift those in $C_{S}$ and $D_{T}$. Explicitly, $(D//F)_{\tilde{T}}$, the ep-zero object is $(\emptyset_{D_{T}}, [[F_{0}]), 0_{C_{S}})$ and the bilimit of an ep-pair-$\omega$-chain $((D_{n}, f_{n}, C_{n}), (g_{n}, h_{n}))_{n \in \mathbb{N}}$ is

$$(D_{\omega}, f_{\omega}, C_{\omega}), (d_{n}, d'_{n})_{n \in \mathbb{N}},$$

where $(D_{\omega}, (d_{n})_{n \in \mathbb{N}})$ is the bilimit of $(D_{n}, d_{n})_{n \in \mathbb{N}}$ in $D_{T}$, $(C_{\omega}, (d'_{n})_{n \in \mathbb{N}})$ is the bilimit of $(C_{n}, h_{n})_{n \in \mathbb{N}}$ in $C_{S}$, and $f_{\omega}$ is the unique $D$-morphism such that $f_{\omega}; \text{return}^{T} = \bigvee_{n \in \mathbb{N}} d_{n}^{T}; T(f_{n}; F(d'_{n})).$ Remembering that $(D//F)$ is a $\omega\text{CPO}$-enriched-reflective subcategory of $D/F$ (as $(E, M)$ is an $\omega\text{CPO}$-enriched factorization system), we can construct bilimits in $(D//F)_{\tilde{T}}$ by applying the locally continuous reflector $(D//F) \rightarrow (D//F)$ to the corresponding bilimits in $(D//F)_{\tilde{T}}$.

We observe that in our setting $\sigma$ does have a right inverse $\tau$ which defines a codistributive law:

$$(\cdot , \alpha') \mapsto (\text{Dom}(\alpha) \cap \text{Dom}(\alpha'), (\alpha|_{\text{Dom}(\alpha) \cap \text{Dom}(\alpha')}, \alpha'|_{\text{Dom}(\alpha) \cap \text{Dom}(\alpha')}).$$

The other conditions of the lemma are also easily seen to be satisfied. As a consequence, we conclude the following.

**Corollary 9.8.** $\omega \text{Gl} \hookrightarrow \omega \text{Gl}_{\perp}$ is a bilimit compact expansion, and it lifts the bilimits of $\omega \text{Diff} \hookrightarrow \omega \text{Diff}_{\perp}$.

We can finally conclude that we can interpret our full language in $\omega \text{Gl}$.  

Proc. ACM Program. Lang., Vol. 1, No. CONF, Article 1. Publication date: January 2018.
Corollary 9.9. The interpretation \( \llbracket - \rrbracket, \llbracket \mathcal{B}(-) \rrbracket \) in \( \omega \text{Diff} \times \omega \text{Diff} \) of the language with type recursion lifts to an interpretation \( \llbracket - \rrbracket \) in \( \omega \text{Gl} \).

In particular, we can define the relation \( R^{U}_{\mu r r} \) above using type recursion as a part of the interpretation \( \llbracket - \rrbracket \) of our language in \( \omega \text{Gl} \).

By repeating the argument of Sec. 5.3 and 6, the general correctness theorem 6.2 for forward AD now extends to the full language with term and type recursion. We note that it holds for first-order types, which are arbitrary types that do not contain any function type constructors. These are all interpreted as objects of \( \omega \text{Diff} \) which are isomorphic to manifolds. In particular, they include algebraic data types such as lists \( \mu \text{a.1}+\text{real} \alpha \) and trees \( \mu \text{a.1}+\text{real} \alpha \star \text{real} \alpha \) holding real numbers.

10 RELATED WORK AND CONCLUDING REMARKS

This work extends the semantics and correctness proofs of AD developed in [Huot et al. 2022, 2020] to apply to languages with partial features such as recursion. We model recursion by borrowing techniques developed by [Vákár et al. 2019] for combining probability and recursion, and we apply them to the combination of differentiation and recursion, instead. [Nunes and Vákár 2022a,b] present a simplified account of the proofs in the present paper. The algorithms discussed in the present paper can lead to efficient reverse AD algorithms, as shown in [Smeding and Vákár 2023, 2024b].

The first other work on formalization and correctness of AD for languages with partiality that we are aware of is [Abadi and Plotkin 2020]. They show semantic correctness for a define-by-run formulation of reverse AD on a first-order language with lazy real conditionals and recursion. In parallel with the present work, [Mazza and Pagani 2021] developed a correctness proof for the reverse AD variant of the algorithm discussed in this paper when applied to the PCF language. Their proofs use operational rather than denotational methods. An alternative, functional approach to AD that is particularly suitable for reverse AD is CHAD [Elliott 2018; Smeding and Vákár 2024a; Vákár 2021; Vytiniotis et al. 2019]. CHAD can be applied to inductive and coinductive types [Nunes and Vákár 2023] and iteration [Nunes et al. 2024], but an account of recursion and recursive types is currently still missing from the literature. We are hopeful that similar proof techniques to those of the present paper should enable a correctness proof of a future CHAD algorithm for recursion and recursive types.

Many popularly used AD systems apply the technique to partially defined programs built using lazy conditionals, iteration and recursion: e.g. Stan [Carpenter et al. 2015], PyTorch [Paszke et al. 2017], TensorFlow Eager [Agrawal et al. 2019], and Lantern [Wang et al. 2019]. This paper makes a contribution towards the mathematical foundations of such systems. In particular, it demonstrates how to correctly perform forward-mode AD on language with partial features. We plan to use the techniques developed in this paper to examine the foundations of reverse-mode AD on iterative and recursive language features in future work.

ACKNOWLEDGMENTS

We have benefited from discussing this work with many people, including Mathieu Huot, Ohad Kammar, Sam Staton, and others. This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 895827.

REFERENCES

Martín Abadi, Paul Barham, Jianmin Chen, Zhifeng Chen, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Geoffrey Irving, Michael Isard, et al. 2016. Tensorflow: A system for large-scale machine learning. In 12th USENIX Symposium on Operating Systems Design and Implementation (OSDI 16). 265–283.
Martin Abadi and Marcelo P. Fiore. 1996. Syntactic considerations on recursive types. In Proceedings 11th Annual IEEE Symposium on Logic in Computer Science. IEEE, 242–252.

Martin Abadi and Gordon D. Plotkin. 2020. A Simple Differentiable Programming Language. In Proc. POPL 2020. ACM.

Jiří Adámek, J. Adamek, J. Rosicky, et al. 1994. Locally presentable and accessible categories. Vol. 189. Cambridge University Press.

Akshay Agrawal, Akshay Naresh Modi, Alexandre Passos, Allen Lavoie, Ashish Agarwal, Asim Shankar, Igor Ganichev, Josh Levenberg, Mingsheng Hong, Rajat Monga, et al. 2019. TensorFlow Eager: A multi-stage, Python-embedded DSL for machine learning. arXiv preprint arXiv:1903.01855 (2019).

Harry Wesley Appelgate. 1965. Acyclic models and resolvent functors. Ph.D. Dissertation. Columbia University.

John Baez and Alexander Hoffnung. 2011. Convenient categories of smooth spaces. Trans. Amer. Math. Soc. 363, 11 (2011), 5789–5825.

Thomas Beck and Herbert Fischer. 1994. The if-problem in automatic differentiation. J. Comput. Appl. Math. 50, 1-3 (1994), 119–131.

Michael Betancourt. 2019. Double-Pareto Lognormal Distribution in Stan. https://bit.ly/2YFRNoV

Stephen L. Bloom and Zoltán Ésik. 1993. Iteration theories. In Iteration Theories. Springer, 159–213.

Aurelio Carboni and Peter Johnstone. 1995. Connected limits, familial representability and Artin gluing. Mathematical Structures in Computer Science 5, 4 (1995), 441–459.

Bob Carpenter, Andrew Gelman, Matthew D. Hoffman, Daniel Lee, Ben Goodrich, Michael Betancourt, Marcus Brubaker, Jiqiang Guo, Peter Li, and Allen Riddell. 2017. Stan: A probabilistic programming language. Journal of statistical software 76, 1 (2017).

Bob Carpenter, Matthew D. Hoffman, Marcus Brubaker, Daniel Lee, Peter Li, and Michael Betancourt. 2015. The Stan math library: Reverse-mode automatic differentiation in C++. arXiv preprint arXiv:1509.07164 (2015).

John Daniel Christensen, Gordon Sinnamon, and Enxin Wu. 2014. The D-topology for diffeological spaces. Pacific J. Math. 272, 1 (2014), 87–110.

Conal Elliott. 2018. The simple essence of automatic differentiation. Proceedings of the ACM on Programming Languages 2, ICFP (2018), 70.

Marcelo P. Fiore. 2004. Axiomatic domain theory in categories of partial maps. Vol. 14. Cambridge University Press.

Marcelo P. Fiore and Gordon D. Plotkin. 1994. An axiomatisation of computationally adequate domain theoretic models of FPC. In Proceedings Ninth Annual IEEE Symposium on Logic in Computer Science. IEEE, 92–102.

Alfred Frölicher. 1982. Smooth structures. In Category theory. Springer, 69–81.

Sergey Goncharov, Christoph Rauch, and Lutz Schröder. 2015. Unguarded recursion on coinductive resumptions. Electronic Notes in Theoretical Computer Science 319 (2015), 183–198.

Ben Goodrich. 2017. Conway-Maxwell-Poisson Distribution. https://bit.ly/2Y8n314

Jean Goubault-Larrecq, Slawomir Lasota, and David Nowak. 2002. Logical relations for monadic types. In International Workshop on Computer Science Logic. Springer, 553–568.

Laurent Hascoet and Valérie Pascual. 2013. The Tapenade automatic differentiation tool: Principles, model, and specification. ACM Transactions on Mathematical Software (TOMS) 39, 3 (2013), 1–43.

Mathieu Huot, Sam Staton, and Matthijs Vákár. 2022. Higher order automatic differentiation of higher order functions. Logical Methods in Computer Science 18 (2022).

Mathieu Huot, Sam Staton, and Matthijs Vákár. 2020. Correctness of Automatic Differentiation via Diffeologies and Categorical Gluing. Full version. arxiv:2001.02209.

Patrick Iglesias-Zemmour. 2013. Diffeology. American Mathematical Soc.

Eunji Jeong, Joo Seong Jeong, Soojeong Kim, Gyeong-In Yu, and Byung-Gon Chun. 2018. Improving the expressiveness of deep learning frameworks with recursion. In Proceedings of the Thirteenth EuroSys Conference. 1–13.

Peter T. Johnstone, Stephen Lack, and P Sobocinski. 2007. Quasitoposes, Quasiadhesive Categories and Artin Glueing. In Proc. CALCO 2007.

Dana A. Knoll and David E. Keyes. 2004. Jacobian-free Newton–Krylov methods: a survey of approaches and applications. J. Comput. Phys. 193, 2 (2004), 357–397.

Anders Kock. 2006. Synthetic differential geometry. Vol. 333. Cambridge University Press.

Paul Blain Levy. 2012. Call-by-push-value: A Functional/imperative Synthesis. Vol. 2. Springer Science & Business Media.

Paul Blain Levy, John Power, and Hayo Thielecke. 2003. Modelling environments in call-by-value programming languages. Information and computation 185, 2 (2003), 182–210.

Damiano Mazza and Michele Pagani. 2021. Automatic differentiation in PCF. Proceedings of the ACM on Programming Languages 5, POPL (2021), 1–27.

John C Mitchell and Andre Seedorf. 1992. Notes on sconing and relators. In International Workshop on Computer Science Logic. Springer, 352–378.

Proc. ACM Program. Lang., Vol. 1, No. CONF, Article 1. Publication date: January 2018.
Eugenio Moggi. 1988. *Computational lambda-calculus and monads*. University of Edinburgh, Department of Computer Science, Laboratory for …

Philip S. Mulry. 1993. *Lifting theorems for Kleisli categories*. In *International Conference on Mathematical Foundations of Programming Semantics*. Springer, 304–319.

Fernando Lucreti Nunes, Gordon Plotkin, and Matthijs Vákár. 2024. Homomorphic Reverse Differentiation of Iteration. *ACM Workshop on Languages for Inference* (LAFI) (2024). https://popl24.sigplan.org/details/lafi-2024-papers/5/Homomorphic-Reverse-Differentiation-of-Iteration

Fernando Lucreti Nunes and Matthijs Vákár. 2022a. Automatic Differentiation for ML-family languages: correctness via logical relations. *arXiv preprint arXiv:2210.07724* (2022).

Fernando Lucreti Nunes and Matthijs Vákár. 2022b. Logical Relations for Partial Features and Automatic Differentiation Correctness. *arXiv preprint arXiv:2210.08530* (2022).

Fernando Lucreti Nunes and Matthijs Vákár. 2023. CHAD for expressive total languages. *Mathematical Structures in Computer Science* 33, 4-5 (2023), 311–426.

Adam Paszke, Sam Gross, Soumith Chintala, Gregory Chanan, Edward Yang, Zachary DeVito, Zeming Lin, Alban Desmaison, Luca Antiga, and Adam Lerer. 2017. Automatic differentiation in pytorch. (2017).

Andrew M. Pitts. 1996. Relational properties of domains. *Inform. Comput.* 127, 2 (1996), 66–90.

David E. Rydeheard and Rod M. Burstall. 1988. *Computational category theory*. Vol. 152. Prentice Hall Englewood Cliffs.

Amir Shaikhha, Andrew Fitzgibbon, Dimitrios Vytiniotis, and Simon Peyton Jones. 2019. Efficient differentiable programing in a functional array-processing language. *Proceedings of the ACM on Programming Languages* 3, ICFP (2019), 97.

Shai Shalev-Shwartz et al. 2012. Online learning and online convex optimization. *Foundations and Trends® in Machine Learning* 4, 2 (2012), 107–194.

Tom J. Smeding and Matthijs Vákár. 2023. Efficient dual-numbers reverse AD via well-known program transformations. *Proceedings of the ACM on Programming Languages* 7, POPL (2023), 1573–1600.

Tom J. Smeding and Matthijs Vákár. 2024a. Efficient CHAD. *Proceedings of the ACM on Programming Languages* 8, POPL (2024), 1060–1088.

Tom J. Smeding and Matthijs Vákár. 2024b. Parallel Dual-Numbers Reverse AD. *arXiv preprint arXiv:2207.03418v3* (2024).

Michael B. Smyth and Gordon D. Plotkin. 1982. The category-theoretic solution of recursive domain equations. *SIAM J. Comput.* 11, 4 (1982), 761–783.

Jean-Marie Souriau. 1980. *Groupes différentiels*. In *Differential geometrical methods in mathematical physics*. Springer, 91–128.

Kai Sheng Tai, Richard Socher, and Christopher D Manning. 2015. Improved semantic representations from tree-structured long short-term memory networks. *arXiv preprint arXiv:1503.00075* (2015).

Periklis Tsiros, Frederic Y Bois, Aristides Dokoumetzidis, Georgia Tsiliki, and Haralambos Sarimveis. 2019. Population pharmacokinetic reanalysis of a Diazepam PBPK model: a comparison of Stan and GNU MCSim. *Journal of Pharmacokinetics and Pharmacodynamics* 46, 2 (2019), 173–192.

Matthijs Vákár. 2021. Reverse AD at Higher Types: Pure, Principled and Denotationally Correct. In *ESOP*. 607–634.

Matthijs Vákár, Ohad Kammar, and Sam Staton. 2019. A domain theory for statistical probabilistic programming. *Proceedings of the ACM on Programming Languages* 3, POPL (2019), 36.

Matthijs Vákár. 2024. Reverse AD at Higher Types: Pure, Principled and Denotationally Correct. In *ESOP*. 607–634.

Matthijs Vákár, Ohad Kammar, and Sam Staton. 2019. A domain theory for statistical probabilistic programming. *Proceedings of the ACM on Programming Languages* 3, POPL (2019), 36.

Bart van Merrienboer, Olivier Breuleux, Arnaud Bergeron, and Pascal Lamblin. 2018. Automatic differentiation in ML: Where we are and where we should be going. In *Advances in neural information processing systems*. 8757–8767.

Dimitrios Vytiniotis, Dan Belov, Richard Wei, Gordon Plotkin, and Martin Abadi. 2019. The differentiable curry. In *Program Transformations for ML Workshop at NeurIPS 2019*.

Fei Wang, Xilun Wu, Gregory Essertel, James Decker, and Tiark Rompf. 2019. Demystifying differentiable programming: Shift/reset the penultimate backpropagator. *Proceedings of the ACM on Programming Languages* 3, ICFP (2019).

Xingxing Zhang, Liang Lu, and Mirella Lapata. 2016. Top-down Tree Long Short-Term Memory Networks. In *Proceedings of NAACL-HLT*. 310–320.
A  FORWARD AD ON COARSE-GRAIN CBV

We recall that standard coarse-grain CBV, also known as the $\lambda_C$-calculus, computational $\lambda$-calculus, or, plainly, CBV, constructs [Moggi 1988] can be faithfully encoded in fine-grain CBV [Levy 2012; Levy et al. 2003]. This translation $(-)^\dagger$ operates on types and contexts as the identity. It translates terms $\Gamma \vdash t : \tau$ of coarse-grain CBV into computations $\Gamma \vdash^{c} t^{\dagger} : \tau$ of fine-grain CBV. This translation illustrates the main difference between coarse-grain and fine-grain CBV: in coarse-grain CBV, values are subset of computations, while fine-grain CBV is more explicit in keeping values and computations separate. This makes it slightly cleaner to formulate an equational theory, denotational semantics, and logical relations arguments.

We list the translation $(-)^\dagger$ below where all newly introduced variables are chosen to be fresh.

| coarse-grain CBV construct $t$ | fine-grain CBV translation $t^{\dagger}$ |
|--------------------------------|---------------------------------|
| $x$                           | return $x$                     |
| $c$                           | return $c$                     |
| $\text{inl } t$               | $t^{\dagger}$ $\to x$. return $\text{inl } x$ |
| $\text{inr } t$               | $t^{\dagger}$ $\to x$. return $\text{inr } x$ |
| $\langle \rangle$             | return $\langle \rangle$       |
| $(t, s)$                      | $t^{\dagger}$ $\to x$. $s^{\dagger}$ $\to y$. return $(x, y)$ |
| $\lambda x.t$                 | return $\lambda x.t^{\dagger}$ |
| $\text{roll } t$              | $x$ $\to t^{\dagger}$. $\text{roll } x$ |
| $\text{op}(t_1, \ldots, t_n)$ | $t^{\dagger}_1$ $\to x_1$. $\ldots$. $t^{\dagger}_n$ $\to x_n$. $\text{op}(x_1, \ldots, x_n)$ |
| $\text{case } t \text{ of } \{ \}$ | $t^{\dagger}$ $\to x$. case $x$ of $\{ \}$ |
| $\text{case } t \text{ of } \{ \text{inl } x \rightarrow s \mid \text{inr } y \rightarrow r \}$ | $t^{\dagger}$ $\to z$. case $z$ of $\{ \text{inl } x \rightarrow s^{\dagger} \mid \text{inr } y \rightarrow r^{\dagger} \}$ |
| $\text{case } t \text{ of } \langle \rangle \rightarrow s$ | $t^{\dagger}$ $\to x$. case $x$ of $\langle \rangle \rightarrow s^{\dagger}$ |
| $t \text{ s}$                 | $t^{\dagger}$ $\to x$. $s^{\dagger}$ $\to y$. $x y$ |
| $\text{iterate } t \text{ from } x = s$ | $s^{\dagger}$ $\to y$. iterate $t^{\dagger}$ from $x = y$ |
| $\text{sign } t$              | $t^{\dagger}$ $\to x$. $\text{sign } x$ |
| $\text{case } t \text{ of } \text{roll } x \rightarrow s$ | $t^{\dagger}$ $\to y$. case $y$ of $\text{roll } x \rightarrow s^{\dagger}$ |
| $\mu x.t$                     | $\mu x.t^{\dagger}$            |
| let $x = t$ in $s$            | $t^{\dagger}$ $\to x$. $s^{\dagger}$. |

This translation induces a semantics $\llbracket (-)^\dagger \rrbracket$ for coarse-grain CBV in $\omega\text{Diff}$, in terms of the semantics $\llbracket - \rrbracket$ of fine-grain CBV.

Moreover, it induces the following forward-mode AD rules for coarse-grain CBV. The macro $\overrightarrow{D}(-)$ on types is as for fine-grain CBV. On terms, we define a single macro $\overrightarrow{D}(-)$ by

$$
\overrightarrow{D}(x) \overset{\text{def}}{=} x
\overrightarrow{D}(c) \overset{\text{def}}{=} (c, \emptyset)
\overrightarrow{D}(\text{inl } t) \overset{\text{def}}{=} \text{inl } \overrightarrow{D}(t)
\overrightarrow{D}(\text{inr } t) \overset{\text{def}}{=} \text{inr } \overrightarrow{D}(t)
\overrightarrow{D}(\langle \rangle) \overset{\text{def}}{=} \langle \rangle
\overrightarrow{D}(\langle t, s \rangle) \overset{\text{def}}{=} (\overrightarrow{D}(t), \overrightarrow{D}(s))
\overrightarrow{D}(\lambda x.t) \overset{\text{def}}{=} \lambda x. \overrightarrow{D}(t)
$$
The value of our correctness proof of forward AD based on a denotational semantics entirely depends on whether the reader believes that the specified semantics is in some sense correct. Recall that our category $\omega\text{Diff}$ forms a conservative extension of the category $\text{Man}$ of manifolds and smooth functions, while $\text{poDiff}$ is a conservative extension of that $\text{pMan}$ of manifolds and smooth partial functions, completing them to bicartesian closed category with a bilimit compact expansion. As such, we can interpret a higher-order language with recursive types, while the first-order fragment of our language gets its standard interpretation in $\text{Man}$ and $\text{pMan}$, possibly the most canonical setting for differential geometry. Note that even programs which contain higher-order sub-programs get interpreted in $\text{Man}$ and $\text{pMan}$, as long as their types are first-order.

Still, however, some readers might be interested to understand the connection with the operational semantics of our language in order to be convinced that the specified denotational semantics is of value. We detail that correspondence here.

As a fine-grain CBV language, we have an uncontroversial operational semantics: as a small-step semantics $t \leadsto s$, we simply use a directed version of the $\beta$-rules of our language, supplemented
with rules which specify how to evaluate basic operations.

\[
\begin{align*}
\text{return } v \text{ to } x & : t \leadsto t[x/v] \\
\text{case } (v, w) \text{ of } (x, y) & \leadsto t[x/v, y/w] \\
(\lambda x . t) & \leadsto t[x/v] \\
op(c_1, \ldots, c_n) & \leadsto \text{return } \|\text{op}\|(c_1, \ldots, c_n) \\
\text{sign } c & \leadsto \text{return } (\langle \rangle) \\
\text{case } \text{inl } v \text{ of } \{ \text{inl } x \rightarrow t \mid \text{inr } y \rightarrow s \} & \leadsto t[x/v] \\
\text{case } \text{inr } v \text{ of } \{ \text{inl } x \rightarrow t \mid \text{inr } y \rightarrow s \} & \leadsto s[y/v] \\
\text{case } \text{roll } v \text{ of } \text{roll } x & \leadsto t[x/v] \\
\end{align*}
\]

Observe that this immediately determines the operational semantics for our sugar if \( v \) then \( t \) else \( s \), iterate \( t \) from \( x = v \), and \( \mu x . t \) as well as for coarse-grain CBV.

From this small-step semantics, we can define a big-step semantics \( t \Downarrow v \stackrel{\text{def}}{=} t \leadsto^* \text{return } v \), where we write \( \leadsto^* \) for the transitive closure of \( \leadsto \).

Program contexts of type \( \sigma \) with a hole \( \_ \) of type \( \Gamma \vdash \_ : \tau \) are terms \( C[\Gamma \vdash - : \tau] \) of type \( \sigma \) with a single variable of type \( \tau \), where this variable \( - \) always occurs inside the term in contexts \( \Gamma' \geq \Gamma \). Write \( C[t] \) for the capturing substitution \( C[\Gamma \vdash - : \tau][t/\_] \).

Two computations \( \Gamma \vdash^c t, s : \tau \) are in the contextual preorder \( t \preceq s \) when for all program contexts \( C[\Gamma \vdash - : \tau] \) of type \( \text{real} \), we have that \( C[t] \Downarrow v \) implies that \( C[s] \Downarrow v \). We say that \( t \) and \( s \) are contextually equivalent, writing \( t \simeq s \), when \( t \preceq s \) and \( s \preceq t \).

We can now state and prove adequacy of our denotational semantics with respect to this operational semantics.

**Theorem B.1 (Adequacy).** Suppose that two computations \( \Gamma \vdash^c t, s : \tau \) are comparable in our denotational semantics in \( \omega\text{Diff} \) in the sense that \( \llbracket t \rrbracket \leq \llbracket s \rrbracket \). Then, \( t \simeq s \) in the observational preorder. In particular, \( \llbracket t \rrbracket = \llbracket s \rrbracket \) implies that \( t \simeq s \).

**Proof (Sketch).** It is enough to show the corresponding statement for the induced denotational semantics \( \llbracket - \rrbracket \) of our language in \( \omega\text{CPO} \), if we forget about the diffeology. Indeed, the bicartesian closed structure, as well as the bilimit compact expansion structures of \( \omega\text{Diff} \) lift those in \( \omega\text{CPO} \) while also \( \llbracket t \rrbracket \leq \llbracket s \rrbracket \) iff \( \|\llbracket t \rrbracket\| \leq \|\llbracket s \rrbracket\| \). That is, what we need to do is a standard adequacy over a semantics in \( \omega\text{CPO} \) of a standard CBV language. This is precisely the setting where the traditional methods of [Pitts 1996] apply. Indeed, we can simply use a minor extension of the adequacy proof given in [Pitts 1996]: we define the logical relation at \( \text{real} \) as \( r \leq^\llbracket - \rrbracket \text{real } r \) and we add two more cases to the induction for the fundamental lemma, one for \( \text{sign} \) and one for \( \text{op} \). These two steps in the fundamental lemma go through almost tautologically because of our choice of denotational semantics precisely matches the operational semantics for these constructs. Once the fundamental lemma is established, the adequacy theorem again follows because the interpretation of values in our semantics remains injective (faithful), even once we add the type \( \text{real} \) (indeed, values \( c \) of type \( \text{real} \) are in 1-1-correspondence with real numbers \( c \in \mathbb{R} \)). 

This shows that our denotational semantics is, in particular, a sound method for proving contextual equivalences of the operational semantics.

**C CHARACTERIZING \( \omega\text{Diff} \)**

We describe three additional categories equivalent to \( \omega\text{Diff} \). Each approaches the question of how to combine diffeological and \( \omega\text{CPO} \) structures in a different way. We summarise the characterisations:

**Theorem 7.1.** We have equivalences of categories: \( \omega\text{Diff} \cong \mathcal{E}_{\omega\text{q}} \cong \omega\text{CPO}(\text{Diff}) \cong \omega\text{diff} - \text{Mod} (\text{Set}) \).

We describe these equivalent categories. For our semantics, we only need these consequences:
Corollary 7.2. The category of \( \omega \)-diffeological spaces, \( \omega \text{Diff} \), is locally \( \mathfrak{c}^+ \)-presentable, where \( \mathfrak{c}^+ \) is the successor cardinal of the continuum. In particular, it has all small limits and colimits.

C.1 \( \mathcal{E}_{\omega q} \): a Domain-Theoretic Completion of Multivariate Calculus

Diffeological spaces are a quasi-topos completion of the category \( \text{Open} \) of open subsets of some \( \mathbb{R}^n \) and smooth functions. Indeed \cite{BaezHoffnung2011} establish an equivalence \( -^\# : \mathcal{E}_q \simeq \text{Diff} \), where \( \mathcal{E}_q \) is the full sub-category of presheaves \([\text{Open}^{op}, \mathbf{Set}]\) consisting of those functors \( F : \text{Open}^{op} \to \mathbf{Set} \) that are:

- sheaves with respect to open covers; and
- separated: the functions \( m_F \overset{\text{def}}{=} (Fr)_{r \in U} : FU \to \prod_{r \in U} F \mathbb{1} \) are injective, for all \( U \in \text{Open} \).

This equivalence is given on objects by mapping \( F \) to the diffeological space \( F^\# \) whose carrier is \( F \mathbb{1} \) and whose \( U \)-plots are the image \( m_F[FU] \) under the injection from the separatedness condition. Therefore, \( m_F : FU \to \prod_{r \in U} F \mathbb{1} \) restricts to a bijection \( \xi_F : FU \simeq S_U^{F \mathbb{1}} \). The equivalence is given on morphisms \( \alpha : F \to G \) by \( \alpha^\# \overset{\text{def}}{=} \alpha_\mathbb{1} \). Given any \( \text{Diff} \)-morphism \( f : F^\# \to G^\# \), by setting:

\[
\alpha_U : FU \xrightarrow{\xi_F} S_U^{F \mathbb{1}} \xrightarrow{(-) \circ f} S_U^{G \mathbb{1}} \xrightarrow{\xi_G} GU
\]

we obtain the natural transformation \( \alpha : F \to G \) for which \( \alpha^\# = f \). As an adjoint equivalence to \( -^\# \), we can choose, for every diffeological space \( X \), the separated sheaf \( \mathbb{X} := X^a \) where \( a \) is either an object or a morphism, and the (co)unit of this adjoint equivalence is given by \( \eta_X : X^b \mathbb{1} = X^b \mathbb{1} \to X \mathbb{1} \simeq X \). (See \cite{BaezHoffnung2011} for a more detailed discussion of this equivalence.)

We define a similar category \( \mathcal{E}_{\omega q} \) to be the full subcategory of \([\text{Open}^{op}, \omega \text{CPO}]\) consisting of those functors \( F : \text{Open}^{op} \to \omega \text{CPO} \) that are:

- sheaves; and
- \( \omega \text{CPO} \)-separated: the functions \( m_F \overset{\text{def}}{=} (Fr)_{r \in U} : FU \to \prod_{r \in U} F \mathbb{1} \) are full monos for all \( U \in \text{Open} \).

Post-composing with the forgetful functor \( [-] : \text{Diff} \to \mathbf{Set} \) yields a forgetful functor \( [-] : \mathcal{E}_{\omega q} \to \mathcal{E}_q \), as the underlying function of a full mono is injective.

We equip \( \mathcal{E}_{\omega q} \) with an \( \omega \text{CPO} \)-category structure by setting the order componentwise:

\[
\alpha \leq \beta \iff \forall U \in \text{Open}. \alpha_U \leq \beta_U
\]

Recall that an \( \omega \text{CPO} \)-equivalence is an adjoint pair of locally-continuous functors whose unit and counit are isomorphisms. To specify an \( \omega \text{CPO} \)-equivalence, it suffices to give a fully-faithful locally-continuous essentially surjective functor in either way, together with a choice of sources and isomorphisms for the essential surjectivity.

Proposition 7.3. The equivalence \( -^\# : \mathcal{E}_{\omega q} \simeq \omega \text{Diff} \) of 7.1 is \( \omega \text{CPO} \)-enriched, and given by:

\[
F^\# := ([\mathbb{1}], m_F[F \mathbb{1}], \leq_{F \mathbb{1}}) \quad (\alpha : F \to G)^\# := \alpha_\mathbb{1}
\]

Moreover, the two forgetful functors \( [-] : \mathcal{E}_{\omega q} \to \mathcal{E}_q \) and \( [-] : \omega \text{Diff} \to \text{Diff} \) form a map of adjoints.

C.2 \( \omega \text{CPO}(\text{Diff})\): \( \omega \)-cpos Internal to \( \text{Diff} \)

The category \( \text{Diff} \) is a Grothendieck quasi-topos, which means it has a canonical notion of a sub-space: strong monos. Sub-spaces let us define relations/predicates, and interpret a fragment
of higher-order logic formulae as subspaces. In particular, we can interpret $\omega$-cpos’s definition internally to Diff and Scott-continuous morphisms between such $\omega$-cpos as a subspace of the Diff-function space, to form the category $\omega\text{CPO}(\text{Diff})$. We interpret functional operations, like the sup-operation of a $\omega$-cpo and the homomorphisms of $\omega$-cpos, as internal functions, rather than as internal functional relations, as the two notions differ in a non-topos quasi-topos such as Diff.

C.3 $\omega\text{diff–Mod(}\text{Set})$: Models of an Essentially Algebraic Theory

Both $\omega\text{CPO}$ and Diff are locally presentable categories. Therefore, there are essentially algebraic theories $\omega\text{cpo}$ and qbs and equivalences $\omega\text{cpo–Mod(}\text{Set}) \simeq \omega\text{CPO}$ and qbs–Mod(Set) $\simeq$ Diff of their categories of set-theoretic algebras. We combine these two presentations into a presentation $\omega\text{diff}$ for $\omega$-diffeological space, given in the following subsections, by taking their union, identifying the element sorts and adding a sup operation for $\omega$-chains of the random elements, and a single axiom stating this sup is computed pointwise. Local presentability, for example, implies the existence of all small limits and colimits.

An $\omega$-cpo or a diffeological space are essentially algebraic, in a precise sense [Adámek et al. 1994, Chapter 3.D]. We will use this algebraic nature to analyse the diffeological domains and see how the diffeological structure interacts with the $\omega$-cpo structure.

C.3.1 Presentations. For the following, fix a regular cardinal $\kappa$. Given a set $S$ with cardinality $|S| < \kappa$, whose elements we call sorts, an $S$-sorted ($\kappa$-ary) signature $\Sigma$ is a pair $\Sigma = \langle O, \text{arity} \rangle$ consisting of a set of operations and arity : $O \to \mathcal{S}^{\kappa \times S}$ assigns to each operation $\text{op} \in O$ a sequence $(s_i)_{i \in I}$, indexed by some set $I$ of cardinality $|I| < \kappa$, assigning to each index $i \in I$ its argument sort, together with another result sort $s$. We write $(\text{op} : \prod_{i \in I} s_i \to s) \in \Sigma$ for arity$(\text{op}) = ((s_i)_{i \in I}, s)$.

Given an $S$-sorted signature $\Sigma$, and a $S$-indexed sequence of sets $\mathcal{V} = \langle \mathcal{V}_s \rangle_{s \in S}$ of variables we define the collections of $S$-sorted terms $\text{Term}^S \mathcal{V} = \langle \text{Term}^S_{s} \mathcal{V} \rangle_{s \in S}$ over $\mathcal{V}$ inductively as follows:

$$x \in \text{Term}_s \mathcal{V}$$

for all $i \in I$, $t_i \in \text{Term}_{s_i} \mathcal{V}$

$$\text{op} : \prod_{i \in I} \in \text{Term}_s \mathcal{V}$$

Given a signature $\Sigma$ and a sort $s$, an equation of sort $s$ is a pair of terms $(t_1, t_2) \in \text{Term}_{s} \mathcal{V}$ over some set of variables. As each term must involve less than $\kappa$-many variables, due to $\kappa$’s regularity we may fix the indexed set of variables $\mathcal{V}$ to be any specified collection of sets of cardinality $\kappa$.

**Definition C.1.** An essentially algebraic presentation $P$ is a tuple $(S, \Sigma_t, \Sigma_p, \text{Def}, \text{Eq})$ containing:

- a set $S$ of sorts;
- two $S$-sorted signatures with disjoint sets of operations:
  - a signature $\Sigma_t$ of total operations;
  - a signature $\Sigma_p$ of partial operations;
- we denote their combined signature by $\Sigma \overset{\text{def}}{=} \bigl( \Omega_{\Sigma_t} \cup \Omega_{\Sigma_p}, [\text{arity}_{\Sigma_t}, \text{arity}_{\Sigma_p}] \bigr)$;
- for each $(\text{op} : \prod_{i \in I} s_i \to s) \in \Sigma_p$, a set $\text{Def}(\text{op})$ of $\Sigma_t$-equations over the variables $\langle x_i : s_i | i \in I \rangle$ which we call the assumptions of $\text{op}(x_i)_{i \in I}$; and
- a set $\text{Eq}$ of $\Sigma$-equations which we call the axioms.

The point of this definition is just to introduce the relevant vocabulary. We will only be considering the following presentation for posets, then $\omega$-cpos, then diffeological spaces:

**Example C.2** (poset presentation cf. [Adámek et al. 1994, Examples 3.35(1),(4)]). The presentation of posets, pos, has two sorts:

- element, which will be the carrier of the poset; and
• inequation, which will describe the poset structure.

The total operations are:
• lower : inequation → element, assigning to each inequation its lower element;
• upper : inequation → element, assigning to each inequation its upper element;
• refl : element → inequation, used to impose reflexivity;

The partial operations are:
• irrel : inequation × inequation → inequation, used to impose proof-irrelevance on inequa-

tions, with Def (irrel(e₁, e₂)):
  \[ \text{lower}(e₁) = \text{lower}(e₂) \quad \text{upper}(e₁) = \text{upper}(e₂) \]
• antisym : inequation × inequation → element, used to impose anti-symmetry, with Def (antisym(e, e^{op})):
  \[ \text{lower}(e) = \text{upper}(e^{op}) \quad \text{upper}(e) = \text{lower}(e^{op}) \]
• trans : inequation × inequation → inequation, used to impose transitivity, with Def (trans(e₁, e₂)):
  \[ \text{upper}(e₁) = \text{lower}(e₂) \]

The axioms are:
\[ e₁ = \text{irrel}(e₁, e₂) = e₂ \quad \text{(proof irrelevance)} \]
\[ \text{lower}(\text{refl}(x)) = x = \text{upper}(\text{refl}(x)) \quad \text{(reflexivity)} \]
\[ \text{lower}(e₁) = \text{antisym}(e₁, e₂) = \text{lower}(e₂) \quad \text{(anti-symmetry)} \]
\[ \text{lower}(\text{trans}(e₁, e₂)) = \text{lower}(e₁) \quad \text{upper}(\text{trans}(e₁, e₂)) = \text{upper}(e₂) \quad \text{(transitivity)} \]

Example C.3 (ω-cpo presentation). In addition to the operations and axioms for posets, the pre-

sentation of \( ω \)-cpos includes the following partial operations:
• \( \lor : \prod_{n ∈ N} \text{inequation} → \text{element} \), used to express lbs of \( ω \)-chains, with Def (\( \lor_{n ∈ N} eₙ \)):
  \[ \text{upper}(eₙ) = \text{lower}(e_{n+1}) \text{, for each } n ∈ N \]
• for each \( k ∈ N \), \( \text{ub}ₖ : \prod_{n ∈ N} \text{element} → \text{inequation} \), collectively used to impose the lub being

an upper-bound, with Def (\( \text{ub}ₖ ((eₙ))_{n ∈ N} \)):
  \[ \text{upper}(eₙ) = \text{lower}(e_{n+1}) \text{, for each } n ∈ N \]
• least : \( \text{element} × \prod_{n ∈ N} \text{inequation} × \prod_{n ∈ N} \text{inequation} \rightarrow \text{inequation} \), used to express that

the lub is the least bound, with Def (least(x, (eₙ)_{n ∈ N}, (bₙ)_{n ∈ N})):
  \[ \text{upper}(eₙ) = \text{lower}(e_{n+1}) \quad \text{upper}(bₙ) = x \quad \text{lower}(eₙ) = \text{lower}(bₙ) \text{, for each } n ∈ N \]

The axioms are:
\[ \text{lower}(\text{ub}ₖ (eₙ)) = \text{lower}(eₖ) \quad \text{upper}(\text{ub}ₖ (eₙ)) = \lor_{n ∈ N} (eₙ) \quad \text{(upper bound)} \]
\[ \text{lower}(\text{least}(x, (eₙ), (bₙ))) = \lor_{n ∈ N} (eₙ) \quad \text{upper}(\text{least}(x, (eₙ), (bₙ))) = x \quad \text{(least upper bound)} \]

Example C.4 (diff presentation). The presentation of diffeological spaces, \( \text{diff} \), has continuum

many sorts:
• element, which will be the carrier of the diffeological space; and
• plotₕ, for each \( U ∈ \text{Open} \), which will be the \( U \)-indexed plots.

The total operations are:
There are two partial operations:

- \( \text{ev}_r : \text{plot}_U \rightarrow \text{element} \), for each \( r \in U \), evaluating a plot at \( r \in U \);
- \( \text{const} : \text{element} \rightarrow \text{plot}_U \) assigning to each element \( x \) the constantly-\( x \) plot; and
- \( \text{rearrange}_\varphi : \text{plot}_V \rightarrow \text{plot}_U \), for each smooth \( \varphi : U \rightarrow V \), precomposing plots with \( \varphi \).

There are two partial operations:

- \( \text{ext} : \text{plot}_U \times \text{plot}_U \rightarrow \text{plot}_U \), used for establishing that a plot is uniquely determined extensionally, with Def (ext(\( \alpha, \beta \))) given by
  \[
  \{ \text{ev}_r(\alpha) = \text{ev}_r(\beta) : \text{element}| r \in U \}
  \]
  and
- \( \text{match}_U : \prod_{U \in \mathcal{U}} \text{plot}_U \rightarrow \text{plot}_U \), for each open cover \( \mathcal{U} \) of \( W \), with Def (match\( _U (f_U)_{U \in \mathcal{U}} \))
  given by:
  \[
  \{ \text{ev}_r(f_U)|U, V \in \mathcal{U}, r \in U \cap V \}
  \]
  used for pasting together a \( \mathcal{U} \)-indexed family of compatible plots into a case split.

The axioms are:

\[
\alpha = \text{ext}(\alpha, \beta) = \beta \quad \text{(extensionality)}
\]
\[
\{ \text{ev}_r(\text{const}(x)) = x| r \in U \} \quad \text{(constantly)}
\]
\[
\{ \text{ev}_r(\text{rearrange}_\varphi \alpha) = \text{ev}_{\varphi(r)} \alpha| \varphi : U \rightarrow V \in \text{Open}, r \in U \} \quad \text{(rearrange)}
\]
\[
\{ \text{ev}_r(\text{match}_U (\alpha_U)_{U \in \mathcal{U}}) = \text{ev}_r(\alpha_U)|\mathcal{U} \text{ open cover of } W, U \in \mathcal{U}, r \in U \} \quad \text{(match)}
\]

We can now present \( \omega \)-diffeological spaces:

**Example C.5 (\( \omega \)-diffeological space presentation).** The presentation \( \omega \text{diff} \) of \( \omega \)-diffeological spaces extends the presentations \( \omega \text{copo} \) and \( \text{diff} \), identifying the element sort, with the following additional partial operations, for all \( U \in \text{Open} \):

- \( \bigsqcup : \prod_{n \in \mathbb{N}} \text{plot}_U \times \prod_{n \in \mathbb{N}, r \in U} \text{inequation} \rightarrow \text{plot}_U \), used for establishing that the plots are closed under lubs w.r.t. the pointwise order, with Def \( \bigsqcup((\alpha_n)_{n \in \mathbb{N}}, (e'_n)_{n \in \mathbb{N}, r \in U}) \) given by:
  \[
  \{ \text{lower}(e'_n) = \text{ev}_r(\alpha_n), \text{upper}(e'_n) = \text{ev}_r(\alpha_{n+1}), |n \in \mathbb{N}, r \in U \}
  \]

The additional axioms are:

\[
\{ \text{ev}_r(\bigsqcup((\alpha_n)_{n \in \mathbb{N}}, (e'_n)_{n \in \mathbb{N}, r \in U})) = \bigvee (e'_n)_{n \in \mathbb{N}}| r \in U \} \quad \text{(pointwise lubs)}
\]

**C.3.2 Algebras.** Every essentially algebraic presentation induces a category of set-theoretic models, and this category for the \( \omega \)-cpo presentation is equivalent to \( \omega \text{CPO} \). Moreover, we can interpret such presentations in any category with sufficient structure, namely countable products and equalisers (i.e., countable limits). We briefly recount how to do this.

Let \( C \) be a category with \( \lambda \)-small limits, with \( \lambda \) regular. As usual, if \( \Sigma \) is any \( S \)-sorted \( \lambda \)-ary signature, we define a (multi-sorted) \( \Sigma \)-algebra \( A = ([[s]])_{s \in S}, [-] \) to consist of an \( S \)-indexed family of objects \( ([[s]])_{s \in S} \), the \textit{carrier} of the algebra, and an assignment, to each op : \( \prod_{i \in I} s_i \rightarrow s \) in \( \Sigma \), of a morphism:

\[
\text{[op]} : \prod_{i \in I} [[s_i]] \rightarrow [[s]]
\]

Given such an algebra \( A \), and an \( S \)-indexed set \( \forall \) of variables with \( |\forall_s| < \lambda \) for each \( s \in S \), each term \( t \) in \( \text{Term}_s \), \( \forall \) denotes a morphism:

\[
[t]_s : \prod_{s \in S} [[s]]^{\forall_s} \rightarrow [[s]]
\]
as follows:

\[ [x]_s : \prod_{s \in S} [s]^V s \rightarrow [s] \]

\[ [\text{op} (t_i)_{i \in I}] : \prod_{s \in S} [s]^V s \rightarrow \prod_{i \in I} [s] \]

(When \(|V_s| \geq \lambda\), there are less than \(\lambda\) different variables that actually appear in \(t\), and so we can find a smaller set of sorts and variables for which to define as above.)

A \(\Sigma\)-homomorphism \(h : A \rightarrow B\) between \(\Sigma\)-algebras \(A, B\) is an \(S\)-indexed family of functions \(h_s : A[s] \rightarrow B[s]\) such that, for every operation symbol \(\text{op} : \prod_{i \in I} s_i \rightarrow s\) in \(\Sigma\):

\[
\begin{align*}
\prod_{i \in I} A[s_i] & \xrightarrow{\prod_{i \in I} h_{s_i}} \prod_{i \in I} B[s_i] \\
A[\text{op}] & \quad = \quad B[\text{op}] \\
A[s] & \xrightarrow{h_s} B[s]
\end{align*}
\]

We denote the category of \(\Sigma\)-algebras in \(C\) and their homomorphisms by \(\Sigma-\text{Mod}(C)\).