\( \lambda_S \): Computable semantics for differentiable programming with higher-order functions and datatypes

BENJAMIN SHERMAN, MIT, USA
JESSE MICHEL, MIT, USA
MICHAEL CARBIN, MIT, USA

Deep learning is moving towards increasingly sophisticated optimization objectives that employ higher-order functions, such as integration, continuous optimization, and root-finding. Since differentiable programming frameworks such as PyTorch and TensorFlow do not have first-class representations of these functions, developers must reason about the semantics of such objectives and manually translate them to differentiable code.

We present a differentiable programming language, \( \lambda_S \), that is the first to deliver a semantics for higher-order functions, higher-order derivatives, and Lipschitz but nondifferentiable functions. Together, these features enable \( \lambda_S \) to expose differentiable, higher-order functions for integration, optimization, and root-finding as first-class functions with automatically computed derivatives. \( \lambda_S \)'s semantics is computable, meaning that values can be computed to arbitrary precision, and we implement \( \lambda_S \) as an embedded language in Haskell.

We use \( \lambda_S \) to construct novel differentiable libraries for representing probability distributions, implicit surfaces, and generalized parametric surfaces – all as instances of higher-order datatypes – and present case studies that rely on computing the derivatives of these higher-order functions and datatypes. In addition to modeling existing differentiable algorithms, such as a differentiable ray tracer for implicit surfaces, without requiring any user-level differentiation code, we demonstrate new differentiable algorithms, such as the Hausdorff distance of generalized parametric surfaces.

CCS Concepts: • Mathematics of computing → Arbitrary-precision arithmetic; Continuous functions;
Point-set topology; • Theory of computation → Categorical semantics.

Additional Key Words and Phrases: Constructive Analysis, Diffeological Spaces, Automatic Differentiation

1 INTRODUCTION

Deep learning is centered on optimizing objectives \( \ell : \Theta \rightarrow \mathbb{R} \) over some parameter space \( \Theta \) by gradient descent, following the derivative of \( \ell \) at some particular value \( \theta \in \Theta \) to move in a direction that decreases \( \ell(\theta) \). Before deep-learning practitioners adopted frameworks like TensorFlow and PyTorch, creating a new model (i.e., parameter space and objective) was a laborious and error-prone endeavor, since it involved manually determining and computing the derivative of the objective. The advent of deep-learning frameworks that provide automatic differentiation (AD)—the automated computation of derivatives of a function given just the definition of the function itself—has made creating and modifying models much easier: a user simply writes the objective and its derivative is computed automatically. As a result, progress in deep learning has rapidly accelerated – a testament to the value of programming-language abstractions.

However, the creativity of deep-learning practitioners has exceeded the capabilities of current AD frameworks: practitioners have devised objectives that current AD frameworks cannot handle directly. A simple example is an objective including an expectation over a probability distribution whose parameters may vary, like this:

\[
\ell(\theta) = \mathbb{E}_{x \sim \mathcal{N}(\mu(\theta), \sigma^2(\theta))}[f(x)].
\]

If this \( \ell \) is translated naively to PyTorch, by approximating the expectation with Monte Carlo sampling, the automatically generated derivative will be incorrect. Numerous algorithms have been

Authors’ addresses: Benjamin Sherman, MIT, USA, sherman@csail.mit.edu; Jesse Michel, MIT, USA, jmmichel@mit.edu; Michael Carbin, MIT, USA, mcarbin@csail.mit.edu.
proposed to compute the derivatives of objectives that average over parameterized probability distributions [Figurnov et al. 2018; Jang et al. 2017; Jankowiak and Obermeyer 2018; Naesseth et al. 2017]. How does one compute derivatives of objectives like these in general? No existing differentiable-programming semantics has tackled the problem of differentiating through expectations such as these.

Other objectives are sufficiently complex that they do not even beg an incorrect naive implementation. Objectives that optimize over compact sets

\[ \ell(\theta) = \max_{\delta \in \Delta} f(\theta, \delta) \]

arise in adversarial contexts, including adversarial training and generative adversarial networks (GANs). Conceptually, optimizing this objective with gradient-based techniques requires a semantics for a differentiable max operation over a compact set, which, to date, has not been covered in the literature on the semantics of differentiable programs. Devising the appropriate derivative for these kinds of objectives is an object of current study [Lorraine et al. 2019; Wang et al. 2020].

Sometimes, an objective involves root-finding,

\[ \ell(\theta) = \text{let } x \text{ be such that } g(\theta, x) = 0 \text{ in } f(\theta, x). \]

This arises in learning implicit surfaces, with applications both to learning the decision boundaries of classifiers as well as to reconstructing surfaces from point-cloud data or other visual data. How to compute the derivative of objectives like this is a key contribution of several papers [Atzmon et al. 2019; Bai et al. 2019; Niemeyer et al. 2020].

What do these objectives all have in common? They all involve higher-order functions: their definitions introduce variables that are subject to integration, optimization, or root-finding. Not only are these three operations troublesome in practice, but no semantics of differentiable programming has yet addressed them.

**Approach.** We present λS, a differentiable programming language that includes higher-order functions for integration, optimization, and root-finding. A key technical challenge is that these functions are higher-order and our semantic approach must wed higher-order functions with higher-order derivatives and nonsmooth functions to encompass these and other modern deep learning objectives. As a toy example, consider computing the derivative \( f'(0.6) \) of the function

\[ f(c) = \int_0^1 \text{ReLU}(x - c) \, dx, \]

where \( \text{ReLU}(x) = \max(0, x) \). We can compute \( f'(0.6) = -0.4 \) with the \( \lambda_S \) expression

```
eps=1e-2> deriv (λ c ⇒ integral01 (λ x ⇒ relu (x - c)))
0.6
```

where there is a type \( \mathbb{R} \) for real numbers, a function \( \text{relu} : \mathbb{R} \to \mathbb{R} \) for ReLU, a higher-order function \( \text{integral01} : (\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \) for integration over the unit interval \([0,1]\), and a higher-order function for differentiation of real-valued functions \( \text{deriv} : (\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \to \mathbb{R} \). The result can be queried to any precision, returning an interval guaranteed to include the true answer. Here, the precision is specified in the prompt as \( \text{eps}=1e-2 \).

\( \lambda_S \) is the first language that gives semantics to such an operation and moreover is the first to support its computation to arbitrary precision. Note that, in order to determine this derivative, we
must evaluate the derivative of the ReLU function everywhere from -0.6 to 0.4, which includes 0, where ReLU is not (classically) differentiable.

**Contributions.** We present λS, a differentiable programming language whose types are (generalized) smooth spaces and whose functions are (generalized) smooth maps. Our contributions are:

1. The first semantics for a differentiable programming language that admits all of the following: 1) higher-order functions (§5), 2) higher-order derivatives (§4), and 3) Lipschitz but nonsmooth functions, such as min, max, and ReLU (§4).
2. The first semantics for differentiable integration, optimization, and root-finding (§5), enabled by the features above.
3. An implementation of this semantics, including implementations for higher-order functions such as integration (§6). Our implementation is based directly on a constructive categorical semantics that demonstrates how these constructs can be computed to arbitrary precision.
4. New smooth libraries for constructing and computing on three higher-order datatypes: probability distributions, implicit surfaces, and generalized parametric surfaces (§7).

λS’s semantics allows computation with and reasoning about the derivatives of higher-order functions, such as integration, optimization, and root-finding. λS elucidates foundational principles for how to program with smooth values in a sound, arbitrarily precise manner, including which operations are possible to compute soundly and which are not. While in many cases λS is not practically efficient, in some cases, programs can serve as executable specifications to guide programming in other frameworks, to validate separately developed systems, and to suggest new functionality that could be added to other differentiable programming frameworks.

2 AN INTRODUCTION TO λS

We demonstrate λS’s core functionality by implementing a simple differentiable ray tracer, an algorithm that generates an image of a scene as viewed by a camera by tracing how rays of light emanate from a light source, bounce off the scene, and then enter the camera’s aperture. Differentiable ray tracing is a new technique in deep learning that propagates derivatives through image rendering algorithms, permitting the use of inverse graphics to solve computer-vision tasks [Li et al. 2018; Niemeyer et al. 2020]. These techniques optimize the parameters of a scene representation to make the image generated by the ray tracer more closely match a target image.

As a simple example, consider computing the brightness of a particular scene at a particular direction, using the λS library for representing scenes and a function for performing ray tracing, both of which we present in Fig. 1:

```plaintext
eps=1e-5> raytrace (circle (1, -3/4) 1) (1, 1) (1, 0)
[2.587289, 2.587299]
```

Fig. 1a depicts the computation at hand. The camera is located at the origin (0, 0), the circle is centered at (1, -3/4) and has radius 1, the light source is at (1, 1), and we consider a ray pointing horizontally to the right from the camera, in the direction (1, 0). The computation returns an interval and the eps=1e-5 specifies the precision tolerance, such that the interval-valued result, [2.587289, 2.587299], has a width at most 10^-5. Our implementation guarantees that whenever it returns a finite-width interval, the true, real-valued result is contained within that interval.
type Surface $A = A \to \mathbb{R}$

firstRoot $: (\mathbb{R} \to \mathbb{R}) \to \mathbb{R}$ ! language primitive

let dot $(x y : \mathbb{R}^2) : \mathbb{R} = x[0] * y[0] + x[1] * y[1]$
let scale $(c : \mathbb{R}) (x : \mathbb{R}^2) : \mathbb{R}^2 = (c * x[0], c * x[1])$
let norm2 $(x : \mathbb{R}^2) : \mathbb{R} = x[0]^2 + x[1]^2$
let normalize $(x : \mathbb{R}^2) : \mathbb{R}^2 = scale (1 / sqrt (norm2 x)) * x$

deriv $: (\mathbb{R} \to \mathbb{R}) \to (\mathbb{R} \to \mathbb{R})$ ! library function

let gradient $(f : \mathbb{R}^2 \to \mathbb{R}) (x : \mathbb{R}^2) : \mathbb{R}^2 =$
  (deriv $\lambda z : \mathbb{R} \Rightarrow f (z, x[1])$) $x[0]$,
  (deriv $\lambda z : \mathbb{R} \Rightarrow f (x[0], z)$) $x[1]$

(b) Basic definitions used in raytrace below.

! camera assumed to be at the origin

let raytrace $(s : Surface (\mathbb{R}^2)) (lightPos : \mathbb{R}^2)$ (rayDirection : $\mathbb{R}^2$) $: \mathbb{R} =$
  let t_star = firstRoot $(\lambda t : \mathbb{R} \Rightarrow s (scale t rayDirection))$ in
  let y = scale t_star rayDirection in
  let normal : $\mathbb{R}^2 = - gradient s y$ in
  let lightToSurf = y - lightPos in
  max 0 (dot (normalize normal) (normalize lightToSurf)) /
  (norm2 y * norm2 lightToSurf)

(c) A $\lambda_S$ function for differentiable ray tracing of implicit surfaces.

Fig. 1. A library for differentiable ray tracing and scene representation.

$\lambda_S$ permits differentiation of any functions in the language, so we can compute how the brightness would change if the circle were moved up by an infinitesimal amount:

eps=1e-3> deriv $(\lambda y : \mathbb{R} \Rightarrow raytrace (circle (0, y) 1) (1, 1) (1, 0)) (-3/4)$
[1.3477, 1.3484]

The $\lambda_S$ function deriv $: (\mathbb{R} \to \mathbb{R}) \to (\mathbb{R} \to \mathbb{R})$ computes the derivative of a scalar-valued real function. The result indicates that when the circle is moved up infinitesimally from its current location, the brightness increases infinitesimally at a rate of $\sim 1.35$ units brightness per unit distance the circle is moved up.

Several changes occur when the circle is moved up that affect the image brightness. The point at which the light ray bounces off the circle moves closer to the camera, decreasing the distance from the camera to the circle (increasing brightness) but increasing the distance from the light to the camera (decreasing brightness). Both the direction of the surface normal of the circle at the point where the light deflects and the direction from the light source to that point change, increasing the angle between the surface normal of the circle and the light ray (decreasing brightness). Automatic differentiation automatically takes all of these effects into account.

Figure 1c shows the implementation of the differentiable ray tracing in $\lambda_S$. The function firstRoot $: (\mathbb{R} \to \mathbb{R}) \to \mathbb{R}$ in the definition of raytrace computes the distance that the light travels from the scene to the camera. Given a function $f : \mathbb{R} \to \mathbb{R}$, firstRoot $f$ performs root finding, computing min${\{x \in [0, 1] \mid f(x) = 0\}}$. $\lambda_S$’s higher-order functions for root
finding are novel, and accordingly, λS’s ability to express differentiable ray tracing of implicit surfaces (embodied in raytrace) without needing any custom code for specifying derivatives.

The differentiable ray tracer raytrace critically depends on λS’s unique support for higher-order functions, higher-order derivatives, and Lipschitz but nondifferentiable functions like min, max, and ReLU. We now provide a brief introduction to these three features.

2.1 Higher-order functions

The raytrace function must compute the distance the ray of light travels from the scene to the camera, represented by the let-definition \( t_{\text{star}} \) in raytrace. When applied to the scene circle \((1, y)\), the definition reduces to

\[
\text{let } t_{\text{star}} y = \text{firstRoot } (\lambda t : \mathbb{R} \Rightarrow 1 - y^2 - (t - 1)^2)
\]

The function firstRoot : \((\mathbb{R} \rightarrow \mathbb{R}) \rightarrow \mathbb{R}\) is a higher-order function since it takes a function as input. In order to admit a function like this in a differentiable programming language, the language must be able to compute how the result of firstRoot changes when there is an infinitesimal perturbation to its input function. In this example, we want to know how \( t_{\text{star}} \) changes when \( y \) changes? To answer this, define \( f t y = 1 - y^2 - (t - 1)^2 \). Then \( t_{\text{star}} \) finds a solution for the variable \( t \) to the equation \( f t y = 0 \). So whatever change is induced by changing \( y \) must be counterbalanced by changing \( t_{\text{star}} \). λS’s semantics validate the equation (for values of \( y \) giving well-defined roots)

\[
\text{deriv } t_{\text{star}} y = - \text{deriv } (\lambda y_0 : \mathbb{R} \Rightarrow f (t_{\text{star}} y) y_0) y / \text{deriv } (\lambda t : \mathbb{R} \Rightarrow f t y) (t_{\text{star}} y)
\]

This equation for the derivative of root finding is known as the implicit function theorem. By the rules of calculus, we can further simplify this to

\[
\text{deriv } t_{\text{star}} y = - y / (t_{\text{star}} y - 1).
\]

Note that the semantics of λS ensures that these equations are indeed program equivalences: one can substitute one expression for the other within the context of a larger expression without affecting its meaning. Indeed, taking \( y = -3/4 \), and evaluating both sides of the expression above in λS produces compatible answers, roughly \(-1.1\), which indicates that moving the circle up decreases the distance that the light travels from the circle to the camera.

We implement the firstRoot function as a language primitive by specifying not only how firstRoot acts on values but also how derivatives propagate through it, via the implicit function theorem (see §5.1 for more detail).

2.2 Higher-order derivatives

The brightness of the image computed by the raytrace function depends on the angle at which the ray of light deflects as it bounces off the circle, so we need to know which direction the circle faces where the light hits it, which is known as the surface normal. In the code for raytrace, the surface normal is computed as

\[
\text{let } \text{normal} : \mathbb{R}^2 = - \text{gradient } s y
\]
Consider, for instance, the unit circle centered at \((0, 0)\), i.e., \(\text{circle} (0, 0) 1\), given by the function \(f(x, y) = 1 - x^2 - y^2\). The surface normal is given by the negative gradient,

\[-\nabla f(x, y) = -\left( \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right) = (2x, 2y)\]

So, for instance, the point \((1/\sqrt{2}, 1/\sqrt{2})\) on the upper-right of the circle has a surface normal that points up and to the right, in the direction \((2/\sqrt{2}, 2/\sqrt{2})\).

Note that, in the raytrace code itself, this gradient computation requires the computation of derivatives of the implicitly defined surface in order to compute the image brightness. Accordingly, computing the derivative of the image brightness with respect to an infinitesimal perturbation in the scene requires computing the second derivatives of the implicitly defined surface with respect to its arguments. Thus, higher-order differentiation is a valuable language feature.

In \(\lambda_S\), differentiation is a first-class programming construct, so higher-order differentiation is naturally supported, as we can compute higher-order derivatives by applying the \(\text{deriv} : (\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \to \mathbb{R}\) function multiple times. Note that some approaches to differentiable programming do not support higher-order differentiation (see Table 1) and thus do not have differentiation as a first-class construct. Higher-order derivatives are also used for numerical-integration, in optimization algorithms, and in other contexts.

The requirement to support higher-order derivatives means that language primitives, such as \(\text{firstRoot}\), must specify not only how they act on values but also how derivatives of all orders propagate through them.

### 2.3 Nondifferentiability

Note that the raytrace code uses the built-in function \(\text{max} : \mathbb{R} \to \mathbb{R} \to \mathbb{R}\) in computing the image brightness. If the light source is behind the scene, the dot product of the surface normal and the vector from the light to the surface will be negative, but the brightness should be 0, rather than this negative value. Hence, we clamp the value to be at least zero by applying \(\text{max} 0\). Note that this function is exactly the rectified linear unit (ReLU) that is common in deep learning:

\[
\text{let relu} (x : \mathbb{R}) : \mathbb{R} = \text{max} 0 x
\]

ReLU is not differentiable at 0. When we compute its derivative at 0 in \(\lambda_S\), we get a nonmaximal result. That means that, for sufficiently fine (\(\leq 1\)) precision tolerances, we get nontermination:

\[
\text{eps=}1e-1> \text{deriv relu} 0 \quad \text{eps=}2> \text{deriv relu} 0
\]

\[(\text{nontermination}) \quad [0.0, 1.0] \]

The interval approximations never converge to intervals smaller than \([0, 1]\). The type \(\mathbb{R}\) contains, in addition to the real numbers, nonmaximal elements like this one, which we name \([0, 1]\), i.e., \(\text{ReLU}'(x) = [0, 1]\).

Differentiable programming frameworks such as PyTorch admit min and max operations, but they are unsound, in the sense that one can define \(f(x) = \text{max}(x, 0) + \text{min}(0, x)\), which is the identity function, but compute in PyTorch that \(f'(0) = 2\), whereas it should be \(f'(0) = 1\). Because of this issue, most differentiable programming semantics leave the derivative of max undefined at 0.

However, \(\lambda_S\)’s interval-valued semantics for functions like max enables productive computational functionality that the partiality approach would not permit. For instance, suppose rather than having a point light source for ray-tracing, we instead have a line light source, so we integrate
over the entire line, using the primitive higher-order function \( \text{integral01} : (\mathbb{R} \to \mathbb{R}) \to \mathbb{R} \), where for \( f : \mathbb{R} \to \mathbb{R} \), \( \text{integral01} f \) computes the integral of \( f \) over the unit interval, \( \int_{0}^{1} f(x) \, dx \). For simplicity, consider a camera located at \((0, 1)\) pointing downwards at a flat surface that stretches from \((-1, y)\) to \((1, y)\), with a light source stretching from \((1, 0)\) to \((1, 1)\). Furthermore, let us disregard the effect of brightness decreasing when the light travels longer distances, such that the brightness is

\[
\text{let brightness} \ (y : \mathbb{R}) : \mathbb{R} = \\
\text{integral01} (\lambda y0 : \mathbb{R} \Rightarrow \max \ 0 \ ((y0 - y) / \sqrt{1 + (y0 - y)^2}))
\]

When \( 0 \leq y \leq 1 \), the integrand will be nondifferentiable with respect to \( y \) at the point where \( y0 = y \). For instance, taking \( y0 = y = 1/2 \), we find that the derivative of the integrand is

\[
\text{deriv} (\lambda y : \mathbb{R} \Rightarrow \max \ 0 \ ((1/2 - y) / \sqrt{1 + (1/2 - y)^2})) (1/2) = [-1, 0].
\]

When \( y0 \) is just greater than \( y \), the derivative will be near \(-1\), but when \( y0 \) is just less than \( y \) is just less than \( y \), the derivative will be near \(0\). Because the derivative at this point is a bounded interval, rather than a completely undefined result, it ends up being soundly neglected when it is integrated over:

\[
\text{eps}=1e-3> \text{deriv brightness} (1/2) = [-0.4476, -0.4469]
\]

The expression \( \text{deriv brightness} (1/2) \) is indeed maximal, meaning that it can be evaluated to arbitrary precision. Were the derivative of the integrand to be undefined rather than interval-valued, \( \text{deriv brightness} (1/2) \) would necessarily need to be undefined as well, but with these semantics, we can soundly compute the correct derivative.

This generalized notion of derivative that works for ReLU is based on Clarke’s generalized derivative [Clarke 1990]. The basic idea can be motivated by the desire for continuity and robustness in the numerical computation. The derivative of ReLU is 1 for numbers imperceptibly greater than 0, and the derivative is 0 for numbers imperceptibly smaller than 0, so the derivative of ReLU at 0 should be consistent with those nearby answers. The specialization relation \( \sqsubseteq \) on \( \mathbb{R} \) formalizes this notion of compatible behavior, where we have \([0, 1] \sqsubseteq 0 \) and \([0, 1] \sqsubseteq 1 \). We will prove a soundness theorem for our language that says that derivatives are always compatible, i.e., related by \( \sqsubseteq \), with the infinitesimal rates of change indicated by its value-level operation.

### 3 SYNTAX AND SEMANTICS OF \( \lambda S \)

\(+\), \(-\), \(*\), \(/\) : \( \mathbb{R} \to \mathbb{R} \to \mathbb{R} \)

\(\text{tangent A B} : (A \to B) \to \text{Tan} A \to \text{Tan} B\)

\(\text{tangentValue A} : \text{Tan} A \to A\)

\(\text{record} (\equiv) A B = \{ \text{to} : A \to B,\ \text{from} : B \to A \}\)

\(\text{tangent_R} : \text{Tan} \mathbb{R} \equiv \mathbb{R} \times \mathbb{R}\)

\(\text{tangentProd A B} : \text{Tan} (A \times B) \equiv \text{Tan} A \times \text{Tan} B\)

\(\text{tangentTo_R A} : \text{Tan} (A \to \mathbb{R}) \equiv (A \to \mathbb{R}) \times (A \to \mathbb{R})\)

\(\text{argmax01} : (\mathbb{R} \to \mathbb{R}) \to \mathbb{R}\)

\(\lambda S\) is System F with the constants shown in Fig. 2. These include basic operators, such as arithmetic and trigonometric operators, higher-order operators, and primitives to compute derivatives.
Higher-order Operators. The function integral01 gives the Riemannian integral of a function on the interval \([0, 1]\). max01 maximizes a function over the interval \([0, 1]\), and argmax01 finds its maximizing argument. cutRoot finds the root of a function \(f : \mathbb{R} \to \mathbb{R}\), assuming that it has a single root and is negative for smaller values and positive for larger values. firstRoot, on input \(f : \mathbb{R} \to \mathbb{R}\), finds the first root of \(f\) on a region starting at 0.

Derivatives. tangent is a first-class function that computes derivatives, where the type function Tan gives the space of tangent bundles over a space; conceptually, a space of pairs of values and derivatives. The function tangentValue projects the value part of this tangent bundle. The isomorphisms of tangent bundles – i.e., tangent_R, tangentProd, and tangentTo_R – assist with manipulating the information that corresponds to the derivative part of the tangent bundle when it is possible for certain spaces. To concretize the concept behind these isomorphisms, we now present the implementation of deriv from Fig. 1, which uses tangent and these isomorphisms:

```plaintext
let deriv (f : \mathbb{R} \to \mathbb{R}) (x : \mathbb{R}) : \mathbb{R} =
    snd (tangent_R.to (tangent f (tangent_R.from (x, 1))))
```

4.1 Preliminaries

A domain \(D\) is a set with a partial-order structure \(\sqsubseteq\) that supports directed joins \(\bigsqcup_{d \in S} d\), which are just joins of directed subsets \(S \subseteq D\), which are those subsets such that if \(x, y \in D\), then there is some \(z \in D\) such that \(x \sqsubseteq z\) and \(y \sqsubseteq z\). We call the partial-order relation \(\sqsubseteq\) specialization. The
An element may be infinite. The bottom element, and we refer to it with the symbol $\bot$. Note that $\mathbb{R}$ serves as a bottom element, and we refer to it with the symbol $\bot$. Arithmetic operations can be extended from $\mathbb{R}$ to $\mathbb{R}$ (see, e.g., Edalat and Lieutier [2004]). Note that $\mathbb{R}$ serves as a bottom element, and we refer to it with the symbol $\bot$. For any vector space $V$, let $C(V)$ be the set of nonempty convex sets in $V$, with an order relation $\subseteq$ also corresponding to reverse inclusion. Note that $V$ serves as a bottom element, and we refer to it with the symbol $\bot$. Note that $\mathbb{R}^n$ embeds into $C(\mathbb{R}^n)$ by viewing an element $x \in \mathbb{R}^n$ as a (convex) hyperrectangle, where some dimensions of the hyperrectangle may be infinite.

**Syntax**

| variables $x$ | types $\tau ::= * \mid \tau_1 \times \tau_2 \mid [K]$ |
| contexts $\Gamma ::= \cdot \mid \Gamma, x : \tau$ | functions $f \in \text{Arr}(\text{AD})$ |
| expressions $e ::= x \mid [f](e)$ | intuition is that $y$ behaves in a way that is compatible with how $x$ behaves.

An element $x \in D$ is maximal if for any $y \in D$, if $x \leq y$, then $y \leq x$.

Define

$$R \doteq \{[a, b] \mid a, b \in \mathbb{R}, a \leq b\} \cup \{\mathbb{R}\}$$

as the domain of interval reals, partially ordered ($\subseteq$) by reverse set inclusion. Its maximal elements are the intervals of the form $[a, a]$, which we often just write as $a$. Arithmetic operations can be extended from $\mathbb{R}$ to $\mathbb{R}$ (see, e.g., Edalat and Lieutier [2004]). Note that $\mathbb{R}$ serves as a bottom element, and we refer to it with the symbol $\bot$. For any vector space $V$, let $C(V)$ be the set of nonempty convex sets in $V$, with an order relation $\subseteq$ also corresponding to reverse inclusion. Note that $V$ serves as a bottom element, and we refer to it with the symbol $\bot$. Note that $\mathbb{R}^n$ embeds into $C(\mathbb{R}^n)$ by viewing an element $x \in \mathbb{R}^n$ as a (convex) hyperrectangle, where some dimensions of the hyperrectangle may be infinite.

**Fig. 3. Syntax and typing rules for the language for AD.**

| Types | Contexts | Terms |
|-------|----------|-------|
| $\tau$ type | $\Gamma$ context | $[e] : [\Gamma] \leadsto [\tau]$ |
| $[\tau] \in \text{Ob}(\text{AD})$ | $[\Gamma] \in \text{Ob}(\text{AD})$ | $\Gamma \vdash x : \tau$ |
| $[\star] \doteq 1_{\text{AD}}$ | $[\cdot] \doteq 1_{\text{AD}}$ | $[\cdot] : [\Gamma] \leadsto [\tau]$ |
| $[\tau_1 \times \tau_2] \doteq [\tau_1] \times [\tau_2]$ | $[\Gamma, x : \tau] \doteq [\Gamma] \times [\tau]$ | $\Gamma \vdash f : [\tau_1] \leadsto [\tau_2]$ |
| $[\bot] \doteq K$ | $\Gamma \vdash [f](e) : [\tau_2]$ | $\Gamma \vdash \text{let } x \doteq e \text{ in } e_2 : [\tau_2]$ |
| $\Gamma \vdash e_1 : [\tau_1]$ | $\Gamma \vdash \text{let } x \doteq e_1 \text{ in } e_2 : [\tau_2]$ | $\Gamma \vdash \text{let } x \doteq e_1 \text{ in } e_2 : [\tau_2]$ |
| $\Gamma \vdash e_2 : [\tau_1 \times \tau_2]$ | $\Gamma \vdash \text{let } x \doteq e_1 \text{ in } e_2 : [\tau_2]$ | $\Gamma \vdash \text{let } x \doteq e_1 \text{ in } e_2 : [\tau_2]$ |
| $\Gamma \vdash e_3 : [\tau_2]$ | $\Gamma \vdash \frac{\partial e_y}{\partial x} \big|_{x = e_x} : [\tau_2]$ | $\Gamma \vdash \frac{\partial e_y}{\partial x} \big|_{x = e_x} : [\tau_2]$ |

**Fig. 4.** Semantics of the language for AD. We present the semantics of context membership and variable references in Appendix A.
The Clarke derivative. Let $f : \mathbb{R}^n \to \mathbb{R}^m$. If $f$ is locally Lipschitz on $X \subseteq U$, let $Z_f \subseteq X$ be the points of nondifferentiability of $f$. The Bouligand subdifferential of $f$ at $x \in X$ is the set of matrices

$$
\partial_B f(x) \triangleq \left\{ H : \mathbb{R}^{m \times n} \mid H = \lim_{j \to \infty} Jf(x_j) \text{ for some sequence } (x_j)_{j \in \mathbb{N}} \text{ where } x_j \in X \setminus Z_f \text{ for all } j \in \mathbb{N} \text{ and } \lim_{j \to \infty} x_j = x \right\},
$$

where $J$ is the Jacobian operator defining the derivative of a function at a point where it is differentiable. The Clarke Jacobian of $f$ at $x$ is $\partial f(x) \triangleq \operatorname{hull}(\partial_B f(x))$. The Clarke Jacobian $\partial f(x) \in C(\mathbb{R}^{m \times n})$ is always compact.

Given $f : \mathbb{R}^n \to \mathbb{R}^m$, let $U$ be the largest open set on which $f$ is both defined and locally Lipschitz. We can define the partial Clarke Jacobian of $f$ to be

$$
\partial_\perp f(x) = \begin{cases} 
\partial f(x) & x \in U \\
\perp & x \notin U
\end{cases}
$$
such that $\partial_\perp : (\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to C(\mathbb{R}^{n \times m})$. We can map values of $C(A)$ to $A_\perp$ (for any $A$) by mapping maximal elements $\{x\} \in C_\perp(A)$ to $x \in A_\perp$ and everything else to $\perp$. Using this conversion, we can also give the partial Clarke Jacobian the type $\partial_\perp : (\mathbb{R}^n \to C(\mathbb{R}^m)) \to \mathbb{R}^n \to C(\mathbb{R}^{n \times m})$, and thus we can also iterate the partial Clarke Jacobian construction to get higher-order derivatives $\partial_\perp^{k} : (\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to C(\mathbb{R}^{n \times m^k})$.

4.2 Smoothish maps

We will now define AD. The objects of AD are the natural numbers, where $n \in \mathbb{N}$ corresponds to $n$-dimensional Euclidean space. To emphasize that we are thinking of Euclidean space, we write the object $n \in \mathbb{N}$ as $\mathbb{R}^n$. A morphism of AD is a smoothish map; a derivative tower that is consistent. A derivative tower $f$ between spaces $\mathbb{R}^n$ and $\mathbb{R}^m$, $f : \mathbb{R}^n \to \mathbb{R}^m$, is a collection of continuous maps (taking the Scott topology for $\mathcal{R}$)

$$
f^{(k)} : \mathbb{R}^n \times (\mathbb{R}^n)^k \to \mathbb{R}^m
$$

for each $k \in \mathbb{N}$, where $f^{(k)}$ represents the $k$th-order derivative. This defines a smoothish map as a power series, where the first $\mathbb{R}^n$ argument is the point where the map is evaluated, and the remaining $k$ arguments represent the inputs to a multilinear map representing the derivative.\footnote{This representation as derivative towers is largely drawn from [Elliott 2008].}

Given vectors $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^k$, let $x \otimes y \in \mathbb{R}^{n \times k}$ denote the tensor product. Define $\operatorname{Mat}_k : (\mathbb{R}^n \times (\mathbb{R}^n)^k \to \mathbb{R}^m) \to \mathbb{R}^n \to \mathbb{R}^{n \times m^k}$ at a point $x \in \mathbb{R}^n$ such that $\operatorname{Mat}_k(f)(x) = M$ if there is a matrix $M \in \mathbb{R}^{m \times n^k}$ such that for all $dx_1, \ldots, dx_k \in \mathbb{R}^k$, we have

$$
f(x; dx_1, \ldots, dx_k) = M \cdot (dx_1 \otimes \ldots \otimes dx_k),
$$

and $\operatorname{Mat}_k(f)(x) = \perp$ if there is no such matrix.

Definition 4.1. We define a consistency relation $\operatorname{Cons}_k(g, f)$ for a function $g : \mathbb{R}^n \times (\mathbb{R}^n)^k \to \mathbb{R}^m$ and a function $f : \mathbb{R}^n \to C(\mathbb{R}^{n^k \times m})$ to hold if for all $x \in \mathbb{R}^n$ and for all $dx_1, \ldots, dx_k \in \mathbb{R}^n$,

$$
g(x; dx_1, \ldots, dx_k) \subseteq f(x) \cdot (dx_1 \otimes \ldots \otimes dx_k),
$$

implicitly using the embedding of $\mathbb{R}^m$ into $C(\mathbb{R}^m)$ on the left-hand side to make the comparison in $C(\mathbb{R}^m)$. A derivative tower $f$ is consistent if for all $k \in \mathbb{N}$, we have

$$
\operatorname{Cons}_{k+1}(f^{(k+1)}, \partial_\perp \operatorname{Mat}_k(f^{(k)})),
$$

meaning that each successive derivative $f^{(k+1)}$ is consistent with the value-level behavior of $f^{(k)}$.\footnote{This representation as derivative towers is largely drawn from [Elliott 2008].}
A *smoothish map* $f$ is a consistent derivative tower. We call a smoothish map *smooth* if $f^{(k)}$ is maximal for all $k$ (which agrees with the standard definition of a smooth map). We will later show that smoothish maps form a category $\text{AD}$, and then by categorical semantics, that all expressions in the first-order language map to that category.

### 4.3 Primitives

Any first-order primitive may be implemented by giving its power-series representation. We use the notation $f^{(k)}(x; \vec{v})$ to denote the $k$th derivative of $f$ at $x$ in directions $\vec{v}$; a smoothish map $f$ is defined by the collection of these functions for all $k \in \mathbb{N}$. These data provide power-series expansions around any input point. There is a map $0 : \Gamma \rightarrow A$ (for any $\Gamma, A \in \text{AD}$) that always returns zero regardless of its input. A linear map $f : A \rightarrow B$ determines a smooth map linear($f$) : $A \rightarrow B$ by

$$
\text{linear}(f)^{(0)}(x) \triangleq f(x)
$$

$$
\text{linear}(f)^{(1)}(x; v) \triangleq f(v)
$$

$$
\text{linear}(f)^{(k+2)}(x; \vec{v}) \triangleq 0
$$

**Derivative-tower construction.** A derivative tower can be viewed as a stream of a function and all of its derivatives. Streams are characterized by the isomorphism

$$
\text{Stream}(A) \equiv A \times \text{Stream}(A)
$$

that says that a stream $s : \text{Stream}(A)$ is exactly composed of its head, head($s$) : $A$, and its tail, tail($s$) : Stream($A$). To construct a derivative tower, we define the map foldDer as an analogue to the *cons* operation on streams. For instance, given value-level definitions of sine and cosine, sin and cos, it is well-founded to define their derivative towers as

$$
\|\sin\|_\text{AD} \triangleq \text{foldDer}(\sin, [x, dx \vdash \cos(x) \times dx]_\text{AD})
$$

$$
\|\cos\|_\text{AD} \triangleq \text{foldDer}(\cos, [x, dx \vdash -\sin(x) \times dx]_\text{AD}),
$$

just as it would be to define two mutually recursive streams evens $=$ cons(0, map($\lambda x. x + 1$, odds)) and odds $=$ cons(1, map($\lambda x. x + 3$, evens))

We define foldDer as follows, where $f : A \rightarrow B$ and $g : A \times A \rightarrow B$, such that foldDer($f, g$) : $A \rightarrow B$.\[
\begin{align*}
\text{foldDer}(f, g)^{(0)}(x) & \triangleq f(x) \\
\text{foldDer}(f, g)^{(k+1)}(x; v_1, \ldots, v_{k+1}) & \triangleq g^{(k)}((x, v_1); (v_2, 0), \ldots, (v_{k+1}, 0)) \quad (k \in \mathbb{N})
\end{align*}
\]

One of the perturbations $v_1$ is passed in as the value to $g$, and then that perturbation is not considered to have any derivatives itself, hence the 0s in the second components of the perturbation passed to $g$.

#### 4.3.1 Arithmetic operations.

The binary arithmetic operations are first-order functions and so can be represented in $\text{AD}$ as functions with the type $\mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$. Addition and subtraction are linear, so their semantics is simply \(\|+\|_\text{AD} \triangleq \text{linear(+)}\) and \(\|-\|_\text{AD} \triangleq \text{linear(-)}\). We define the smooth multiplication operator by

$$
\|\times\|_\text{AD} \triangleq \text{foldDer}(\lambda(x, y), x \times y, [x, y, (dx, dy) \vdash x \times dy + y \times dx]_\text{AD}),
$$

whose derivative is the familiar product rule. Note that our definition of $\|\times\|_\text{AD}$ has two recursive references to multiplication’s own *smooth* map. This recursive reference is well-founded because
the result is used in a way that does not demand any further differentiation. This recursive pattern is similar to defining the stream of natural numbers \( nats : \text{Stream}([\mathbb{N}]) \) by

\[
nats \triangleq \text{cons}(0, \text{map}(\lambda x. \, x + 1) \, nats),
\]

where mapping a function over \( nats \) does not demand any further calls to \( \text{tail} \). Reciprocals \( \text{used for division} \) can be defined using \( \text{foldDer} \) as well, where all \( k \)-th order derivatives will return \( \bot \) when the input is \( 0 \).

### 4.3.2 Lipschitz but nonsmooth functions.

Many functions, like \( \max, \min, \) and \( \text{ReLU} \), are locally Lipschitz but not smooth. These functions are used pervasively in contexts that require differentiation, so their admissibility in a differential-programming semantics is paramount. Whereas most differential-programming semantics say that derivative of \( \max \) is undefined when its arguments are equal, our use of Clarke derivatives permits a non-\( \bot \) result.

We define \( \max \) as follows, where hull computes the interval corresponding to the convex hull of the union of a set of points.

\[
\|\max\|^{(0)}_{\text{AD}}(x, y) \triangleq \max(x, y)
\]

\[
\|\max\|^{(1)}_{\text{AD}}((x, y); (dx, dy)) \triangleq \begin{cases} 
  dx & x > y \\
  dy & x < y \\
  \text{hull}(dx, dy) & x = y
\end{cases}
\]

\[
\|\max\|^{(k+2)}_{\text{AD}}((x, y); \bar{\nu}) \triangleq \begin{cases} 
  0 & x \neq y \\
  \bot & x = y
\end{cases}
\]

### 4.3.3 Differentiation operator.

To give a semantics to the syntax \( \frac{\partial e_x}{\partial x} |_{x = e_x} \cdot e_{dx} \) for differentiation, we first define a differentiation operator, \text{postfix ‘}’, on smoothish maps, where \( f : A \sim B \) maps to \( f' : A \times A \sim B \). Defining this operator is nontrivial, because all the derivatives of \( f' \) must consider not only perturbations to the function value but also perturbations to the derivative argument, which are not accounted for in the original derivative tower: note that the \( k \)-th derivative of \( f \) is a multilinear map from \( A^k \), whereas the \( k \)-th derivative of \( f' \) is a multilinear map from \( A^{2k} \). We show the value and first few derivatives; because \( x \) will always be applied as the value argument to derivatives of \( f \), we elide those arguments:

\[
f'^{(0)}(x, v) = f^{(1)}(v)
\]

\[
f'^{(1)}((x, v); (dx_a, dv_a)) = f^{(2)}(v, dx_a) + f^{(1)}(dv_a)
\]

\[
f'^{(2)}((x, v); (dx_a, dv_a), (dx_b, dv_b)) = f^{(3)}(v, dx_a, dx_b) + f^{(2)}(dv_a, dx_b) + f^{(2)}(dx_a, dv_b)
\]

The general formula is:

\[
f'^{(k)}((x, v); (dx_1, dv_1), \ldots, (dx_k, dv_k)) \triangleq f^{(k+1)}(x; v, dx_1, \ldots, dx_k) + \sum_{j=1}^{k} f^{(j)}(x; dx_1, \ldots, dx_{j-1}, dv_j, dx_{j+1}, \ldots dx_k).
\]

### 4.3.4 Revisting derivative tower construction.

The ‘ operator is analogous to the tail operator of a stream, in that derivative towers have the section-retraction pair

\[
A \sim B \xrightarrow{\lambda f. (f'^{(0)}, f')} \ (A \rightarrow B) \times (A \times A \sim B)
\]
that characterizes a derivative tower \( f : A \rightarrow B \) as a function \( f^{(0)} : A \rightarrow B \) for the evaluation map of \( f \) together with a derivative tower \( f' : A \times A \rightarrow B \) representing the forward-mode derivative.

Given this observation, we may for convenience in the rest of the paper define a smooth map \( f \) by its value-level function \( f^{(0)} \) and its smoothish derivative \( f' \), denoting an implicit use of \( \text{foldDer} \). For example, we can equivalently define the smooth multiplication operator (§4.3.1) by

\[
\begin{align*}
\left[\star\right]^{(0)}_{\text{AD}} & \triangleq \lambda (x, y). \ x \times y \\
\left[\star\right]^{(1)}_{\text{AD}} & \triangleq \left[\left((x, y), (dx, dy) \mapsto x \star dy + y \star dx\right)\right]_{\text{AD}}.
\end{align*}
\]

### 4.4 Categorical operations

\text{AD} forms a Cartesian monoidal category. We describe the categorical operations here, and prove that they satisfy the expected properties in Appendix F.1. The maps \( \text{id} : A \rightarrow A \) (for all \( A \)), \( ! : \Gamma \rightarrow * \) (for all \( \Gamma \)), \( \text{fst} : A \times B \rightarrow A \) and \( \text{snd} : A \times B \rightarrow B \) (for all \( A, B \)) are all in fact linear maps and so can be made into smooth maps with the linear operator described above. Given \( f : \Gamma \rightarrow A \) and \( g : \Gamma \rightarrow B \), we define their product \( \langle f, g \rangle : \Gamma \rightarrow A \times B \) by

\[
\langle f, g \rangle^{(k)}(x, \overline{\nu}) \triangleq (f^{(k)}(x, \overline{\nu}), g^{(k)}(x, \overline{\nu})),
\]

It only remains to define composition. Composition of smooth maps is given by Faà di Bruno’s formula. The definition is perhaps easier to understand by example for small \( k \). The following shows derivatives of \( g \circ f \) at \( x \); since \( g \) is always differentiated at \( f(x) \) and \( f \) is always differentiated at \( x \), we elide those arguments:

\[
\begin{align*}
(g \circ f)^{(0)}() &= g^{(0)}() \\
(g \circ f)^{(1)}(v_a) &= g^{(1)}(f^{(1)}(v_a)) \\
(g \circ f)^{(2)}(v_a, v_b) &= g^{(2)}(f^{(1)}(v_a), f^{(1)}(v_b)) + g^{(1)}(f^{(2)}(v_a, v_b)) \\
(g \circ f)^{(3)}(v_a, v_b, v_c) &= g^{(3)}(f^{(1)}(v_a), f^{(1)}(v_b), f^{(1)}(v_c)) + g^{(2)}(f^{(2)}(v_a, v_b), f^{(1)}(v_c)) + g^{(2)}(f^{(2)}(v_a, v_c), f^{(1)}(v_b)) + g^{(2)}(f^{(2)}(v_b, v_c), f^{(1)}(v_a)) + g^{(1)}(f^{(3)}(v_a, v_b, v_c)).
\end{align*}
\]

The general formula is

\[
(g \circ f)^{(k)}(x; \overline{\nu}) \triangleq \sum_{\pi \in \mathcal{H}(\{1, \ldots, k\})} \text{let } n \triangleq |\pi| \text{ in } g^{(n)}(f(\pi_1(x); v_{\pi_1}, \ldots, v_{\pi_1|\pi_1|}), \ldots, f(\pi_n(x); v_{\pi_n}, \ldots, v_{\pi_n|\pi_n|})),
\]

where \( \mathcal{H}(S) \) is the set of partitions of a set \( S \), and \( |S| \) is the cardinality of a set. Note that in the general case, the inputs to \( g^{(n)} \) may be elements of \( \mathbb{R}^b \) rather than \( \mathbb{R}^b \) for some \( b \in \mathbb{N} \). Given any nth derivative \( g^{(n)} : \mathbb{R}^b \times (\mathbb{R}^b)^k \rightarrow \mathbb{R}^m \), we extend it to apply to inputs \( x \in \mathbb{R}^b \) and \( dx_1, \ldots, dx_k \in \mathbb{R}^b \) by

\[
g^{(n)}(x; dx_1, \ldots, dx_k) \triangleq \text{hull}\left\{ g^{(n)}(y; dy_1, \ldots, dy_k) \mid y \in x, dy_1 \in dx_1, \ldots, dy_k \in dx_k \right\}.
\]

Faà di Bruno’s formula simplifies drastically in the case that either function is linear:

\[
\begin{align*}
(\text{linear}(g) \circ f)^{(k)}(v_1, \ldots, v_k) &= g(f^{(k)}(v_1, \ldots, v_k)) \\
(g \circ \text{linear}(f))^{(k)}(v_1, \ldots, v_k) &= g^{(k)}(f(v_1), \ldots, f(v_k)),
\end{align*}
\]

and from these formulæ it is apparent that \( \text{id} \circ f = f \circ \text{id} = f \).

\(^2\)For proofs, see Proposition F.25 and Proposition F.20.
The derivatives that our semantics defines are **sound**. Therefore, $AD$ (and similarly for higher-order derivatives). For example, at the value level, $\max x 0 + \min 0 = x = x$, but the derivative of the left-hand side at 0 is $[0, 2]$ while the derivative at the right-hand side is 1, noting $[0, 2] \subseteq 1$. This has important ramifications for $\lambda_S$, where we construct functions as compositions of others and need composition to be computable. Because of the specialization relation, we know that any behavior of a function in $\lambda_S$ (e.g., $[0, 2]$) will be compatible with the ideal derivative of its value-level function (e.g., 1), but it may not return the maximal such value.

Appendix F.1 proves that these operations give AD the structure of a Cartesian monoidal category. Therefore, AD admits the internal language described in Fig. 3.

### 4.5 Soundness

The derivatives that our semantics defines are **sound**: the behaviors of $k$th derivative that is computed, $\llbracket e \rrbracket_{AD}^{(k)}$, are compatible with the derivatives that would be abstractly defined by looking at its value-level behavior, $\partial^k_M \text{Mat}_0(\llbracket e \rrbracket_{AD}^{(0)})$. This proposition follows by first demonstrating that derivative towers are **consistent**.

**Proposition 4.2.** Given any term $\Gamma \vdash e : \tau$, the derivative tower $\llbracket e \rrbracket_{AD}$ is consistent.

**Proof Sketch.** By induction on the typing derivation of $e$. We then see that, to know the proposition is true, we must know that the derivative towers for all primitives are consistent (including product projections) and that pairing and composition preserve consistency. We prove these facts in detail in Appendix F.1 and Appendix F.2.

**Proposition 4.3 (Soundness of Differentiation in the First-Order Language).** Given any term $\Gamma \vdash e : \tau$, for all $k \in \mathbb{N}$, $\text{Cons}_{k+1} \left( \llbracket e \rrbracket_{AD}^{(k+1)}, \partial^k_M \text{Mat}_0(\llbracket e \rrbracket_{AD}^{(0)}) \right)$.

**Proof.** By Proposition 4.2, $\llbracket e \rrbracket_{AD}$ is consistent, and thus this statement is a simple corollary of Proposition F.36.

### 5 Higher-Order Semantics (HAD)

The category AD does not admit exponentiation (function spaces), since its objects are limited to $\mathbb{R}^n$. However, higher-order functions yield novel expressive power that is critical for §7. So in order
5.1 Smooth integral.

The integral \( \text{integral01}\) is defined as follows for any \( f : \Gamma \times \mathbb{R} \rightarrow \mathbb{R} \):

\[
\|\text{integral01}\|_{\text{HAD}} (f)(k)(y; dy_1, \ldots, dy_k) = \int_0^1 f^{(k)}(y, x; (dy_1, 0), \ldots, (dy_k, 0)) \, dx.
\]

Since integration is a linear operator, we essentially just integrate the first-order infinitesimal perturbations arising from \( f \) at every order of derivative. Integration is smooth in the sense that if its input is smooth, its output will be smooth as well. Note the similarity between the above AD tower and the result of postcomposing a linear function \( \ell \) after a function \( f \) arising from Faà di Bruno’s formula described previously. The reader may wonder how a semantics invoking integration might be computable; we discuss this in §6.

5.1.2 Smoothish root finding.

The primitive \( \text{cutRoot} : (\mathbb{R} \rightarrow \mathbb{R}) \rightarrow \mathbb{R} \) smoothly finds the root of any function with a single isolated root that is positive to its left and negative to its right.

Equivalently, \( \text{cutRoot} \) is a map \( (\Gamma \times \mathbb{R} \leadsto \mathbb{R}) \rightarrow (\Gamma \leadsto \mathbb{R}) \). We will define \( \text{cutRoot} \) by using the stream characterization of smooth maps, defining it with a function for its evaluation map and a
smooth map for its derivative:

\[
\text{cutRoot}_{\text{HAD}}(f)^{(0)} \triangleq \lambda y. \sup\{x : \mathbb{R} \mid f(y, x) > 0\}, \inf\{x : \mathbb{R} \mid f(y, x) < 0\}
\]

\[
\text{cutRoot}_{\text{HAD}}(f)' \triangleq \left[ y, dy + \text{let } y \triangleq \left[ \text{cutRoot}_{\text{HAD}}(f) \right](y) \in -\frac{f'}{(y, y), (dy, 0))}{f'}((y, y), (0, 1)) \text{ AD} \right]
\]

The formula for the derivative is a simple application of the implicit function theorem. Note that we have a well-founded recursive reference following the same pattern as with multiplication.

\text{cutRoot} enables root-finding only for functions that have only one root. In graphics, for ray tracing of implicit surfaces, it is useful to be able to find for a function \( f : \mathbb{R} \rightarrow \mathbb{R} \) the least root \( x \in [0, 1] \) such that \( f \) switches from positive for values just less than \( x \) to negative for values just greater than \( x \). \text{firstRoot} : (\mathbb{R} \rightarrow \mathbb{R}) \rightarrow \mathbb{R} \) accomplishes this:

\[
\text{firstRoot}_{\text{HAD}}(f)^{(0)} \triangleq \lambda y. \sup\{x \in [0, 1] \mid \forall q \in [0, x], f(y, q) > 0\}, \inf\{x \in [0, 1] \mid \exists q \in [0, x], f(y, x) < 0\}
\]

\[
\text{firstRoot}_{\text{HAD}}(f)' \triangleq \left[ y, dy + \text{let } y \triangleq \left[ \text{firstRoot}_{\text{HAD}}(f) \right](y) \in -\frac{f'}{(y, y), (dy, 0))}{f'}((y, y), (0, 1)) \text{ AD} \right]
\]

Like with \text{cutRoot}, its derivatives are determined by the implicit function theorem; the only difference is in the definition of the value of the root.

5.1.3 Smoothish optimization. \( \lambda_S \) admits primitives \text{argmax01}, \text{max01} : (\mathbb{R} \rightarrow \mathbb{R}) \rightarrow \mathbb{R} \) that find the maximum and the maximizing argument, respectively, of a function \( f : \mathbb{R} \rightarrow \mathbb{R} \) over the unit interval. Equivalently, each of \text{argmax01} and \text{max01} are maps \((\Gamma \times \mathbb{R} \sim \mathbb{R}) \rightarrow (\Gamma \sim \mathbb{R})\).

We first describe \text{argmax01}. We can find argumentes by keeping track of which intervals survive in the computation of the max itself. At any given step of computation, we will have some collection of intervals representing potential argumentes. If we ever observe that \( f'' > 0 \) over an entire given interval, then that interval has a single argument, whose location is the root of the local equation \( f'(y, x)(0, 1) = 0 \), where \( x \) may vary. It is also possible to have maxima at either end of the unit interval, where on the left end we could have \( f' < 0 \) and on the right \( f' > 0 \).

\[
\text{argmax01}_{\text{HAD}}(f)^{(0)} \triangleq \lambda y. \text{hull}\left(\{x \in [0, 1] \mid f(x) = \max_{z \in [0, 1]} f(z)\}\right)
\]

\[
\text{argmax01}_{\text{HAD}}(f)' \triangleq \left[ y, dy + \text{let } y \triangleq \left[ \text{argmax01}_{\text{HAD}}(f) \right](y) \in -\frac{f''}{f'}((y, y), (dy, 0))}{f'}((y, y), (0, 1)) \text{ AD} \right]
\]

Just as the derivative of max depends on which argument results in the max, similarly the derivative of \text{max01} is a function of the maximizing argument. If we can isolate a single argument, then \text{max01} \( f = f \circ \text{argmax01} \) \( f \), and thus all the derivatives of \text{max01} \( f \) follow from the chain rule and the smooth derivatives of \( f \) and \text{argmax01} \( f \).

\[
\text{max01}_{\text{HAD}}(f)^{(0)} \triangleq \lambda y. \max_{x \in [0, 1]} f(y, x)
\]

\[
\text{max01}_{\text{HAD}}(f)' \triangleq (f \circ \text{argmax01}_{\text{HAD}}(f))'
\]
5.2 Internal derivatives of functions at all types

Following Vákár et al. [2018], we can lift the operation of forward-mode differentiation from the first-order language to the higher-order language. Defining

\[
\text{valueWithDer} : (A \to B) \to (A \times A \to B \times B)
\]

\[
\text{valueWithDer}(f) \triangleq \left[ x, dx \vdash (\lfloor f \rfloor(x), [f'](x, dx)) \right]_{\text{AD}}
\]

we find that valueWithDer defines a functor on $\text{AD}$ acting on objects by $X \mapsto X \times X$ from a space to its tangent bundle.

This functor can be extended to $\text{HAD}$ via a left Kan extension to produce a functor $\text{Tan}$ and its functorial map $\text{tangent A} B : (A \to B) \to \text{Tan A} \to \text{Tan B}$, which runs generalized forward-mode derivatives, interpreted geometrically as a pushforward of the tangent bundles.

**Tangent bundles.** Any space $X$ defines a corresponding space of tangent bundles $\text{Tan} X$, where a point in the tangent bundle $\text{Tan} X$ represents a point of $X$ together with an infinitesimal perturbation to that point. A polymorphic function $\text{tangentValue A} : \text{Tan A} \to A$ projects out the base point. There is an isomorphism $\text{tangent_R} : \text{Tan} \mathbb{R} \cong \mathbb{R} \times \mathbb{R}$, such that $\text{tangentValue} \circ \text{tangent_R} = \text{fst}$, i.e., the first component is the base point and the second is the infinitesimal perturbation. Tangent bundles commute with products, i.e., $\text{Tan} (U \times V) \cong \text{Tan U} \times \text{Tan V}$. Additionally, tangent bundles distribute over functions into $\mathbb{R}$: $\text{Tan} (V \to \mathbb{R}) \cong V \to \text{Tan} \mathbb{R}$. Appendix C details the various operations on and isomorphisms of tangent bundles.

5.3 Soundness

**Proposition 5.1 (Soundness of differentiation in the higher-order language).** Given any term $\Gamma \vdash e : \tau$ in $\lambda_S$ where $\Gamma$ is a context of all ground types and $\tau$ is a ground type, then $\llbracket e \rrbracket_{\text{HAD}}$ is equivalent to some first-order smoothish map $f$, i.e., consistent derivative tower.

**Proof.** Since the Yoneda embedding is full, first-order terms in $\text{HAD}$ correspond to morphisms in $\text{AD}$, so this statement reduces to Proposition 4.3. □

6 COMPUTABILITY AND NUMERICALLY-SOUND IMPLEMENTATION

It is not obvious that the categorical semantics of $\lambda_S$ we present in §4-5 is actually implementable (in a sound manner). The semantics critically uses reals and real arithmetic, rather than some approximation like floating point (which would fail to give even the most basic equalities such as $1/5 + 2/5 = 3/5$). And value-level definitions of higher-order primitives in $\lambda_S$ are expressed in terms of mathematical operations for integration, optimization, and root finding applied to arbitrary continuous maps. In fact, our semantic development is computable, and we have implemented it in a numerically sound manner as an embedded DSL in Haskell.

Our semantics can be developed constructively and interpreted within the internal language of another topos, which we call $\lambda_C$, in order to provide a computable interpretation. We base $\lambda_C$ on MarshallB [Sherman et al. 2019]. Our implementation of $\lambda_S$ more-or-less directly follows interpreting the semantics of $\lambda_S$ within $\lambda_C$ and in turn implementing $\lambda_C$ in Haskell.

Like $\lambda_S$, $\lambda_C$ is a topos of sheaves over a Cartesian monoidal category that we call $\text{CTop}$. $\text{CTop}$ is a category of computably presented topological spaces and computable continuous maps.

Our semantics can be developed constructively and interpreted within the internal language of another topos, which we call $\lambda_C$, in order to provide a computable interpretation. We base $\lambda_C$ on MarshallB [Sherman et al. 2019]. Our implementation of $\lambda_S$ more-or-less directly follows interpreting the semantics of $\lambda_S$ within $\lambda_C$ and in turn implementing $\lambda_C$ in Haskell.

Like $\lambda_S$, $\lambda_C$ is a topos of sheaves over a Cartesian monoidal category that we call $\text{CTop}$. $\text{CTop}$ is a category of computably presented topological spaces and computable continuous maps.

What results is a stack of languages: $\lambda_S$ reducing to $\text{AD}$, implemented in $\lambda_C$, which reduces to $\text{CTop}$, which carries the final executable content of ground terms. We can view it like a stack of metaprogramming languages on top of $\text{CTop}$: ultimately, when a closed term of $\lambda_S$ (or any other language in the stack) of ground type is evaluated and displayed as a sequence of improving approximations, it is in fact a closed term of $\text{CTop}$, i.e., a computable point of a topological space.
Semantics of $\lambda_C$ and implications for $\lambda_S$. $\lambda_C$ is a language whose types are (generalized) topological spaces with computable structure and whose functions are (generalized) computable continuous maps. $\lambda_C$ permits all the higher-order functions and higher-order types that we will seek to define in $\lambda_S$ and enables their computation to arbitrary precision. This section describes $\lambda_C$ by example. In $\lambda_C$, the type $\mathbb{R}$ in $\lambda_C$ represents the interval reals $\mathbb{R}$. One closed term, or value, of type $\mathbb{R}$ is $\sqrt{2}$. A value of $\mathbb{R}$ represents a point of the space $\mathbb{R}$ and is computationally represented by streams of increasingly precise approximations (i.e., monotone with respect to $\sqsubseteq$):

$$\texttt{> sqrt 2 : } \mathbb{R}$$

```
[1.4142135619, 1.4142135624]
[1.414213562370, 1.414213562384]
[1.4142135623729, 1.4142135623733]
...```

Note that these streams of increasingly precise approximations can be used to provide the arbitrary-precision interface where one asks for a precision tolerance and gets a result. Each interval $[x, x']$, where $x \in (-\infty) \cup \mathbb{D}, x' \in \mathbb{D} \cup \{\infty\}$, has either infinite or dyadic-rational ($\mathbb{D} = \{k/2^n \mid k \in \mathbb{Z}, n \in \mathbb{N}\}$) endpoints and represents partial information about $\sqrt{2}$: the first component represents a rational lower bound (with $-\infty$ being a vacuous bound) and the second an upper bound (with $\infty$ vacuous). $\lambda_C$ is sound in the sense that these bounds are guaranteed to hold of the true value. Two closed terms of $\mathbb{R}$ in $\lambda_C$ are considered equivalent if their streams always overlap, even if the streams are not identical. For instance, $(\sqrt{2})^2 = 2$:

$$\texttt{> (sqrt 2)^2 : } \mathbb{R}$$

```
[1.9999999986, 2.0000000009]
[1.9999999995, 2.0000000008]
[1.9999999999991, 2.0000000000009]
...```

The equivalence means that one can substitute $(\sqrt{2})^2$ for 2 within any program without affecting its meaning. Note that this is in contrast to the unsoundness of floating-point computation that for many languages and CPUs returns 2.0000000000000004, which is not 2 and does not itself indicate a larger range of possible values that includes 2, and would not validate the equation $(\sqrt{2})^2 = 2$.

First-order functions in $\lambda_C$ are stream transformers of their approximations. For instance, applying the squaring function $(-)^2 : \mathbb{R} \to \mathbb{R}$ to $\sqrt{2}$ yields the following result:

$$\texttt{> sqrt 2 : } \mathbb{R}$$

```
[1.4142135619, 1.4142135624]
[1.414213562370, 1.414213562384]
[1.4142135623729, 1.4142135623733]
...```

$$\texttt{> (sqrt 2)^2 : } \mathbb{R}$$

```
[1.9999999986, 2.0000000009]
[1.9999999995, 2.0000000008]
[1.9999999999991, 2.0000000000009]
...```

In this case, the squaring function squares each input interval to produce output intervals. The computation is continuous in the sense that the computation of each interval result of $(\sqrt{2})^2$ needs only an interval approximation of $\sqrt{2}$. First-order functions such as $(-)^2$ are continuous maps, meaning that in order to approximate the output to any finite level of precision, it suffices to inspect the input to only a finite level of precision.

Implementing higher-order primitives. The value-level definitions of higher-order primitives in $\lambda_S$ are expressed in terms of mathematical operations for integration, optimization, and root finding. It’s
not obvious that these are computable. However, MarshallB [Sherman et al. 2019] demonstrates how to endow a language with computable implementations of Riemannian integration, maximization over compact sets, as well as a Dedekind cut primitive that is essentially equivalent to the root finding of cutRoot and can be used to implement the root finding of firstRoot. We were able to implement these MarshallB primitives in $\lambda_C$ and use them to implement the higher-order primitives in $\lambda_S$.

**Haskell implementation.** We implemented $\lambda_S$ as an embedded language within Haskell. Because $\mathbb{R}^n$ and $\mathbb{R}^n$ are representable within CTop, we actually implement AD directly using CTop within Haskell, rather than working internally to $\lambda_C$. We implement CTop using an interval-arithmetic library that in turn uses MPFR [Fousse et al. 2007], a library for multi-precision floating-point arithmetic. Our implementation and all code examples are available at https://github.com/psg-mit/smooth. See the readme file for more information about the code.

**Computability and numerical soundness.** The semantics for $\lambda_S$ supports a realistic machine model for computing real-valued results to arbitrary precision. This is in contrast to semantics that permit Boolean-valued comparison of real numbers, and computational models like Real RAM, in which a machine can compare real numbers in constant time. When algorithms are designed based on such models but implemented with floating-point arithmetic, those implementations may fail to be robust to floating-point error (e.g., [Kettner et al. 2008]). In contrast, the continuity inherent in $\lambda_S$'s semantics provides a robustness guarantee: arbitrary-precision approximations of the output can be produced by inspecting only finite-precision approximations of the input.

### 7 Higher-Order Datatypes and Libraries

This section demonstrates the unique expressivity and computability of $\lambda_S$. We use the novel higher-order primitives available in $\lambda_S$ – including integration, optimization, and root-finding – to build libraries for constructing and computing with three different higher-order datatypes: probability distributions (and measures), implicit surfaces, and generalized parametric surfaces. Since these libraries are expressed in $\lambda_S$, we can differentiate through code that uses them (arbitrarily many times). For each library, we compute an example differentiation task. Fig. 7 shows a high-level overview of each example.
7.1 Probability distributions (and measures)
Probability is central to many machine-learning applications. Loss functions for Bayesian neural networks, GANs, etc. involve expectations over probability distributions. However, no previous work on the semantics of AD supports probability distributions. The interaction between probabilistic choice and differentiation is nontrivial, and the lack of a semantic treatment of their interaction has real consequences for machine-learning practitioners using AD libraries who seek to combine them. Practitioners often use Monte Carlo sampling to approximate expectations, but because derivatives cannot be propagated through the samplers in common frameworks such as PyTorch and TensorFlow, code that looks correct and produces appropriate approximations of its value-level output can end up producing incorrect derivatives when AD is applied (as mentioned in the introduction). This common pitfall, which can be difficult to detect, necessitates the reparameterization trick, where code is rewritten such that samplers do not depend on any parameters that are to be differentiated.

\( \lambda_S \) can represent a monad of probability distributions \( P \), making it the first language semantics to support differentiation through probabilistic choice. Supporting probability distributions is hard because they must involve higher-order functions: expectations are higher-order functions \( P(A) \times (A \to \mathbb{R}) \to \mathbb{R} \), as is the monadic bind operator \( P(A) \times (A \to P(B)) \to P(B) \) that supports compositional construction of complex probability distributions from simple ones.

A \( \lambda_S \) library for probability distributions and measures. Probability distributions, measures, and distributions (in the sense of generalized functions) can all be described as integrals,

\[
\text{type } \text{Integral } A = (A \to \mathbb{R}) \to \mathbb{R},
\]
detailed in Fig. 8. Integrals are functions \( i : (A \to \mathbb{R}) \to \mathbb{R} \) which are linear in their arguments. Measures are those integrals \( i \) satisfying \( i(f) \geq 0 \) whenever \( f(x) \geq 0 \) for all \( x \in \mathbb{R} \). Probability distributions are those measures \( i \) satisfying \( i(\lambda x. 1) = 1 \); the integral for a probability distribution computes the expectation of a real-valued function under that distribution.

\[
\begin{align*}
&\text{let } \text{dirac } A \ (x : A) : \text{Integral } A = \lambda f : A \to \mathbb{R} \Rightarrow f x \\
&\text{let } \text{bind } B \ (x : \text{Integral } A) \ (f : A \to \text{Integral } B) : \text{Integral } B \\
&\quad = \lambda k : B \to \mathbb{R} \Rightarrow x \ (\lambda a : A \Rightarrow f a k) \\
&\text{let } \text{zero } A : \text{Integral } A = \lambda f : A \to \mathbb{R} \Rightarrow 0 \\
&\text{let } \text{add } A \ (x y : \text{Integral } A) : \text{Integral } A = \lambda f : A \to \mathbb{R} \Rightarrow x f + y f \\
&\text{let } \text{map } A B \ (f : A \to B) \ (e : \text{Integral } A) : \text{Integral } B = \\
&\quad \lambda k : B \to \mathbb{R} \Rightarrow e \ (\lambda a : A \Rightarrow k (f a)) \\
&\text{let } \text{factor } (x : \mathbb{R}) : \text{Integral } \text{unit} = \lambda f : \text{unit} \to \mathbb{R} \Rightarrow f (\, \) \( \ast x) \\
&\text{let } \text{measToProb } A \ (e : \text{Integral } A) : \text{Integral } A = \lambda f : A \to \mathbb{R} \Rightarrow e f / e \ (\lambda x : A \Rightarrow 1) \\
&\text{let } \text{bernoulli } (p : \mathbb{R}) : \text{Integral } \text{unit} = \lambda f : \text{unit} \to \mathbb{R} \Rightarrow p * f \ tt + (1 - p) * f \ ff \\
&\text{let } \text{uniform } : \text{Integral } \mathbb{R} = \text{integral01} \\
&\text{let } \text{total_mass } A \ (mu : \text{Integral } A) = mu \ (\lambda x : A \Rightarrow 1) \\
&\text{let } \text{mean } (mu : \text{Integral } \mathbb{R}) = mu \ (\lambda x : \mathbb{R} \Rightarrow x) \\
&\text{let } \text{variance } (mu : \text{Integral } \mathbb{R}) = mu \ (\lambda x : \mathbb{R} \Rightarrow (x - \text{mean } mu)^2) \\
\end{align*}
\]

Fig. 8. Integrals and \( \lambda_S \) programs that manipulate them.

\( ^3 \) While other works can represent expectations over distributions with finite support as sums, this would not work for distributions with infinite support. Loss functions frequently involve expectations over distributions with infinite support.
Example. What happens if we make an infinitesimal perturbation to the uniform distribution? How will its mean and variance change? Differentiation answers these questions.

The uniform distribution over the interval \([0, 1]\) is equivalent to the integral of \([0, 1]\), namely \(\text{uniform} : \text{Integral } \mathbb{R} = \int_0^1 dx = 1\) (as any probability distribution must), and has mean \(\int_0^1 x dx = 1/2\) and variance \(\int_0^1 (x - 1/2)^2 dx = 1/4\).

Next, we must craft a perturbation to consider. There is an isomorphism \(\text{Tan } (\text{Integral } A) \cong \text{Integral } A \times \text{Integral } A\), which says that a perturbation to an integral itself has the form of an integral as well. Hence, our perturbation must also be an integral. In addition, because we are perturbing a probability distribution, whose total mass must sum to 1, the total mass of our perturbation must be 0: if we are to increase mass somewhere, we must decrease it elsewhere. Given these design considerations, consider the following perturbation to the uniform distribution that makes 1 more likely, 0 less likely, 1/2 equally likely as before, and interpolates between these:

\[
\text{let change} : \text{Integral } \mathbb{R} = \lambda f : \mathbb{R} \rightarrow \mathbb{R} \Rightarrow \int_0^1 (\lambda x : \mathbb{R} \Rightarrow (x - 1/2) * f x)
\]

The perturbation is an integral with total mass 0: \(\int_0^1 (x - 1/2)dx = 0\).

Returning to our question of how this perturbation changes the mean and variance of \(\text{uniform}\), for convenience let \(\text{der} : (\text{Integral } A \rightarrow \mathbb{R}) \rightarrow \text{Integral } A \rightarrow \text{Integral } A \rightarrow \mathbb{R}\) compute the derivative of its argument at a point and infinitesimal perturbation, using the appropriate coercions and projections to and from tangent spaces. Since \(\text{mean}\) is linear, its derivative is independent of the current value and is just the original \(\text{mean}\) function applied to the infinitesimal perturbation:

\[
\text{der mean uniform change} = \text{mean change} = \int_0^1 (\lambda x : \mathbb{R} \Rightarrow (x - 1/2) * x)
\]

And indeed, that’s what we compute:

\[
\text{eps}=1e-3> \text{der mean uniform change} \\
[0.0829, 0.0837]
\]

However, \(\text{variance}\) is nonlinear, so its derivative does depend on the current point. Let’s compute it and then reason about the answer:

\[
\text{eps}=1e-2> \text{der variance uniform change} \\
[-0.005, 0.004]
\]

We can reason about the change in the variance by laws about derivatives, just as we would in first-order cases:

\[
\text{der variance uniform change} = \text{der} (\lambda \mu : \text{Integral } \mathbb{R} \Rightarrow \mu (\lambda x : \mathbb{R} \Rightarrow x^2) - (\text{mean } \mu)^2) \text{ uniform change} \\
= \text{change} (\lambda x : \mathbb{R} \Rightarrow x^2) - 2 * \text{mean uniform} * \text{mean change} \\
= \int_0^1 (\lambda x : \mathbb{R} \Rightarrow (x - 1/2) * x^2) - 2 * 1/2 * 1/12
\]

\(^4\)Fig. 7a shows a schematic of this perturbation.

\(^5\)let \(\text{der} f x dx = \text{snd } (\text{tangetTo_R.to } (\text{tangent } f (\text{tangetTo_R.from } (x, dx))))\)
type Surface A = A → ℜ

let circle (c : ℜ^2) (r : ℜ) : Surface (ℜ^2) =
  λ x : ℜ^2 ⇒ r^2 - (x[0] - c[0])^2 - (x[1] - c[1])^2

let halfplane A (normal : ℜ^2) : Surface (ℜ^2) =
  λ x : ℜ^2 ⇒ dot normal x

let union A (s s' : Surface A) : Surface A =
  λ x : A ⇒ max (s x) (s' x)

let intersection A (s s' : Surface A) : Surface A =
  λ x : A ⇒ min (s x) (s' x)

let complement A (s : Surface A) : Surface A =
  λ x : A ⇒ - (s x)

Fig. 9. A λS library for implicit surfaces.

So it turns out that this infinitesimal perturbation will actually not change the variance.

7.2 Implicit surfaces and root-finding

§2 and Fig. 1 presented a library for implicit surfaces and a function for performing ray tracing on scenes represented by implicit surfaces.

Fig. 9 presents a library for constructing implicit surfaces. An implicit surface is a representation of a surface (such as a sphere or plane) with the zero-set of a differentiable function f : ℜ^n → ℜ (where usually we consider n = 3 for 3-dimensional space). Whether f(x, y) is positive, negative, or zero indicates whether (x, y) is inside, outside, or on the border of the surface, respectively. The angle at which a ray deflects is determined by the surface normal at the location where the ray hits the surface, which is the vector that is orthogonal to the plane that is tangent to the surface.

In λS, we can represent implicit surfaces as type Surface A = A → ℜ. Fig. 9 presents a small library for constructing implicit surfaces. The Boolean operations of Constructive Solid Geometry (CSG) – union, intersection, and complement – are available for these implicit surfaces. Because λS permits nonsmooth functions, it is able to represent implicit surfaces that don’t necessarily correspond to manifolds, such as the union of two spheres that are offset and equally sized. Where they touch, there is a corner, and thus there is no (unique) surface normal.

Our smooth ray tracer, shown in Fig. 1c, renders the image of an implicit surface with a single light source and a Lambertian reflectance model, computing the angle at which light reflects off of the surface using automatic differentiation. The code in Fig. 1c reflects the contributions of Niemeyer et al. [2020], who use a differentiable ray-tracing renderer to learn implicit 3D representations of surfaces, noting their ”key insight is that depth gradients can be derived analytically using the concept of implicit differentiation.”

We can implement a smooth (and thus differentiable) ray tracer for implicit surfaces in λS in just a few lines of code, and the use of implicit differentiation automatically falls out.

7.3 Generalized parametric surfaces and optimization

We now build a library within λS for constructing shapes and computing operations on them. For instance, we can represent the quarter disk and unit square in Fig. 7c as shapes and compute the Hausdorff distance between them, which equals \(\sqrt{2} - 1\), as:

```
eps=1e-3> hausdorffDist d_R2 l_shape (quarterCircle 0)
[0.4138, 0.4145]
```
We can also compute derivatives, such as the infinitesimal perturbation in the Hausdorff distance that would result if the quarter circle were to infinitesimally move up by a unit magnitude:

```plaintext
eps=1e-1> deriv (\ y : \ \mathbb{R} \Rightarrow \text{hausdorffDist d_R2 l_shape (quarterCircle y)}) 0
[-0.752, -0.664]
```

This application is admittedly more speculative in its practical applications, but it demonstrates a novel domain in which we can define and compute derivatives. We will now explain how this library for shapes works.

We represent these generalized parametric surfaces as *maximizers*:

```plaintext
type Maximizer A = (A 
\rightarrow \mathbb{R}) \rightarrow \mathbb{R}.
```

A generalized parametric surface \( k : \text{Maximizer} \ A \), when applied to a function \( f : A \rightarrow \mathbb{R} \), returns the maximum value that \( f \) attains on the region represented by \( k \).

```plaintext
type Maximizer A = (A \rightarrow \mathbb{R}) \rightarrow \mathbb{R}
let point A (x : A) : Maximizer A = \( \lambda \ f : A \rightarrow \mathbb{R} \Rightarrow f \ x \)
let indexedUnion A B (ka : Maximizer A) (kb : A \rightarrow \text{Maximizer} B) : Maximizer B =
\( \lambda \ f : B \rightarrow \mathbb{R} \Rightarrow \text{ka} (\lambda \ A : \mathbb{R} \Rightarrow \text{kb} \ a \ f) \)
let union A (k1 k2 : Maximizer A) : Maximizer A =
\( \lambda \ f : A \rightarrow \mathbb{R} \Rightarrow \text{max} (k1 \ f) (k2 \ f) \)
let map A B (g : A \rightarrow B) (k : Maximizer A) : Maximizer B =
\( \lambda \ f : B \rightarrow \mathbb{R} \Rightarrow \text{k} (\lambda \ a : \mathbb{R} \Rightarrow f \ (g \ a)) \)
let sup A (k : Maximizer A) : \mathbb{R} = sup (\lambda \ x1 : A \Rightarrow \text{inf} k2 (\lambda \ x2 : A \Rightarrow \text{d_R2} x1 x2))
let inf A (k : Maximizer A) : \mathbb{R} = \text{sup} k1 (\lambda \ x1 : A \Rightarrow \text{inf} k2 (\lambda \ x2 : A \Rightarrow \text{d_R2} x1 x2))
```

```plaintext
let unitInterval : Maximizer \( \mathbb{R} \) = \text{max01}
let quarterCircle (y : \mathbb{R}) : Maximizer (\mathbb{R}^2) = \text{map}
(\lambda \ \text{theta} : \mathbb{R} \Rightarrow (\text{cos} (\pi \ / \ 2 \ * \ \text{theta}), \ \text{sin} (\pi \ / \ 2 \ * \ \text{theta}) + y))
unitInterval
let l_shape : Maximizer (\mathbb{R}^2) =
union (\lambda \ x : \mathbb{R} \rightarrow (x, 1)) \text{unitInterval})
(\lambda \ y : \mathbb{R} \Rightarrow (1, y)) \text{unitInterval})
let d_R2 (a b : \mathbb{R}^2) : \mathbb{R} = \text{sqrt} ((a[0] - b[0])^2 + (a[1] - b[1])^2)
```

Fig. 10 shows an excerpt of the library for generalized parametric surfaces. Note that generalized parametric surfaces shapes form a monad (representing nondeterminism), with \text{point} and \text{indexedUnion} as \text{return} and \text{bind}, yielding a programming model for constructing shapes.

Returning to the earlier Hausdorff-distance example, note that the maximal distance on the “L” shape occurs at the corner point, which is represented twice, as the endpoint of each line; thus, a maximum is taken over two equal distances. In [Abadi and Plotkin 2020], because the maximum operator is defined with a partial conditional statement, the result — not to mention the derivative — would be undefined. Because both the values and the derivatives are the same for the two representations of this corner point, we in fact get a maximal element as the derivative. Also note that we need second derivatives in order to compute the derivative of the Hausdorff distance, due to the use of \text{max01}.
8 DISCUSSION

In this section, we discuss the capability of $\lambda_S$ to represent control flow as well as the opportunity to soundly speed up execution of higher-order primitives using derivative information. Appendix E describes representation of reverse-mode differentiation, a modal type operator for (completely) nondifferentiable code, as well as support for manifolds via quotients.

8.1 Control flow: conditionals and recursion

$\lambda_S$ supports discrete spaces, including in particular the Booleans $\mathbb{B}$ and any well-founded set (such as the natural numbers). The recursion principles for these yield, respectively, if-then-else expressions and well-founded recursion. These control-flow expressions must be independent of "continuous data": all maps from connected spaces to discrete spaces are constant. This property defines connected spaces. Connected spaces include all vector spaces, such as $\mathbb{R}^n$. Di Gianantonio and Edalat [2013] explain some particular issues that demonstrate why implementing piecewise-differentiable functions with branching is problematic.

8.2 Optimizing higher-order primitives with derivative information

We can also use the fact that functions in $\lambda_S$ come equipped with all their derivatives to opportunistically speed up some operations. For instance, consider applying $\text{cut\_root}$ to some function $f$. Its value-level definition naturally maps to a bisection-like algorithm on the values of $f$. However, since we have access to $f^{(1)}$, we can use a variation of Newton’s method generalized to interval arithmetic to speed up the convergence drastically, and indeed we do this in our implementation. Note that we are guaranteed that this optimization is sound, because soundness of differentiation ensures that $f^{(1)}$ appropriately reflects $f^{(0)}$. It may be the case that $f^{(1)}$ returns $\perp$ at some points, or even everywhere, in which case the algorithm falls back on bisection to ensure progress.

Similarly, the literal interpretation of the value-level definition of Riemannian integration in §5 maps to a quadrature method that uses only the values $f^{(0)}$ of $f$. However, the availability of higher derivatives of $f$ makes it possible to use interval-based versions of higher-order integration methods, which can also drastically speed up the convergence. We do not use these higher-order methods by default in our actual implementation.

9 RELATED WORK

Our work is unique in supporting higher-order functions, higher-order derivatives, and nondifferentiable functions. Table 1 summarizes related work on differentiable-programming semantics and their support for these features. In addition to the following discussion, Appendix D covers additional related work.

We combine the use of Clarke derivatives in Di Gianantonio and Edalat [2013] to support nondifferentiable functions, the diffeological approach of Vákár et al. [2018] to support higher-order functions, and the derivative towers of Elliott [2008] to support higher-order derivatives. Merging these techniques gives us a platform to accomplish the other contributions.

Di Gianantonio and Edalat [2013] describe a programming language for nonexpansive (i.e., Lipschitz constant 1) functions on the interval $[-1, 1]$ with a differentiation operator that applies to functions from $[-1, 1]$ to $[-1, 1]$. The semantics of this differentiation operator are that of the L-derivative [Edalat 2008; Edalat and Lieutier 2004], a domain-theoretic analogue of Clarke’s generalized derivatives, which is well-defined for all locally Lipschitz functions. Their domain-theoretic account ensures computability: in theory, results can be computed to arbitrary precision. Their semantics is fundamentally limited to first-order derivatives: their interval type denotes $[-1, 1] \times [-1, 1]$, corresponding to a dual-number representation, baking in that limited capability. It is
Higher-order derivatives: The differentiation operator can be iterated arbitrarily many times (when applied to smooth functions). Higher-order functions: A concrete test: is twice \( f : \mathbb{R} \rightarrow \mathbb{R} \) (\( x : \mathbb{R} \)) \( \Rightarrow f(f(x)) \) admitted? Non-differentiable functions: Some nondifferentiable functions are admitted. A concrete test: is \( \text{max} : \mathbb{R}^2 \rightarrow \mathbb{R} \) admitted? “Clarke derivative” indicates that locally Lipschitz functions support derivatives in the sense of Clarke derivatives or L-derivatives [Edalat and Lieutier 2004], whereas “partiality” indicates that nondifferentiable maps are supported by considering them to be partial at their discontinuities.

Unclear how that representation could be generalized directly to permit higher-order differentiation and appropriately handle nested differentiation (without the perturbation confusion [Siskind and Pearlmutter 2005] that is possible when multiple derivatives are involved).

Elliott [2008] (blog post) presents a data type for representing smooth maps, where a smooth map \( f \) is represented by the collection of its \( k \)th derivatives for all \( k \). Elliott [2008] defines the derivatives of some arithmetic functions as well as some categorical operations, though the definition of composition of smooth maps is incorrect. We support higher-order derivatives by adapting this representation for the Clarke derivative.

Vákár et al. [2018] (slide deck) presents the semantics of a differentiable programming language that supports higher-order functions and higher-order derivatives using the quasitopos of diffeological spaces. As a quasitopos, the semantics supports higher-order functions and quotient types. Vákár et al. [2018] show an internal derivative operator that can be applied to any function of any type, and thus can be applied repeatedly for higher-order derivatives. This derivative operator is based on a left Kan extension of a functor characterizing derivatives on Cartesian spaces \( \mathbb{R}^n \). Functions such as \( \text{max} \) that are not smooth are not admissible. It is not made clear how one could implement a differentiable programming language supporting the expressive possibilities suggested by the semantics.

None of the works in Table 1 describe higher-order functions for root-finding, optimization, or integration, nor do they describe datatypes for implicit surfaces, compact shapes, or probability distributions. Edalat and Lieutier [2004] describe an integration operator in a domain-theoretic framework for differential calculus, but it does not handle higher-order derivatives. Sherman et al. [2019] describe computable higher-order functions and libraries for root-finding, optimization, and integration, but does not admit differentiation of any sort.

We follow Sherman et al. [2019] in our approach to computability. We are unaware of any system that computes arbitrary-precision derivatives (given the definition of the function) in any capacity.

### 10 Conclusion

This paper demonstrates how to compute and make sense of derivatives of higher-order functions, such as integration, optimization, and root-finding and at higher-order types, such as probability...
distributions, implicit surfaces, and generalized parametric surfaces. Our libraries and case studies model existing differentiable algorithms, for instance, a differentiable ray tracer for implicit surfaces, without requiring any user-level differentiation code, in addition to demonstrating new differentiable algorithms, such as computing derivatives of the Hausdorff distance of generalized parametric surfaces. Ideally, the ideas λS demonstrates may enable differentiable programming frameworks to support the new abstractions and expressivity suggested by this paper.

REFERENCES

Martín Abadi and Gordon D. Plotkin. A simple differentiable programming language. In Principles of Programming Languages, 2020.

Matan Atzmon, Niv Haim, Lior Yariv, Ofer Israelov, Haggai Maron, and Yaron Lipman. Controlling neural level sets. In Advances in Neural Information Processing Systems, 2019.

Shaojie Bai, J Zico Kolter, and Vladlen Koltun. Deep equilibrium models. In Advances in Neural Information Processing Systems, 2019.

Michael Betancourt. A geometric theory of higher-order automatic differentiation. arXiv preprint arXiv:1812.11592, 2018.

J Daniel Christensen and Enxin Wu. Tangent spaces and tangent bundles for diffeological spaces. American Mathematical Society, 2017.

Frank H Clarke. Optimization and nonsmooth analysis. 1990.

Pietro Di Gianantonio and Abbas Edalat. A language for differentiable functions. In Foundations of Software Science and Computational Structures, 2013.

Abbas Edalat. A continuous derivative for real-valued functions. In New Computational Paradigms, 2008.

Abbas Edalat and André Lieutier. Domain theory and differential calculus (functions of one variable). Mathematical Structures in Computer Science, 14(6), 2004.

Thomas Ehrhard and Laurent Regnier. The differential lambda-calculus. Theoretical Computer Science, 309(1-3), 2003.

Conal Elliott. Higher-dimensional, higher-order derivatives, functionally. 2008. URL http://conal.net/blog/posts/higher-dimensional-higher-order-derivatives-functionally.

Conal Elliott. The simple essence of automatic differentiation. In International Conference on Functional Programming, 2018.

Mikhail Figurnov, Shakir Mohamed, and Andriy Mnih. Implicit reparameterization gradients. In Advances in Neural Information Processing Systems, 2018.

Laurent Fousse, Guillaume Hanrot, Vincent Lefèvre, Patrick Pélissier, and Paul Zimmermann. MPFR: A multiple-precision binary floating-point library with correct rounding. ACM Transactions on Mathematical Software, 33(2), 2007.

Mathieu Huot, Sam Staton, and Matthijs Vákár. Correctness of automatic differentiation via diffeologies and categorical gluing. In Foundations of Software Science and Computation Structures, 2020.

Eric Jang, Shixiang Gu, and Ben Poole. Categorical reparameterization with gumbel-softmax. International Conference on Learning Representations, 2017.

Martin Jankowiak and Fritz Obermeyer. Pathwise derivatives beyond the reparameterization trick. In International Conference on Machine Learning, 2018.

Sham M Kakade and Jason D Lee. Provably correct automatic sub-differentiation for qualified programs. In Advances in Neural Information Processing Systems, 2018.

Lutz Kettner, Kurt Mehlhorn, Sylvain Pion, Stefan Schirra, and Chee Yap. Classroom examples of robustness problems in geometric computations. Computational Geometry, 40(1), 2008.

Anders Kock. Synthetic differential geometry, volume 333. 2006.

Tzu-Mao Li, Miika Aittala, Frédéric Durand, and Jaakko Lehtinen. Differentiable Monte Carlo ray tracing through edge sampling. In Special Interest Group on Computer Graphics and Interactive Techniques, 2018.

Jonathan Lorraine, Paul Vicol, and David Duvenaud. Optimizing millions of hyperparameters by implicit differentiation. arXiv preprint arXiv:1911.02590, 2019.

Christian A. Naesseth, Francisco J. R. Ruiz, Scott W. Linderman, and David M. Blei. Reparameterization gradients through acceptance-rejection sampling algorithms. In Artificial Intelligence and Statistics, 2017.

Michael Niemeyer, Lars Mescheder, Michael Oechsle, and Andreas Geiger. Differentiable volumetric rendering: Learning implicit 3D representations without 3D supervision. In Computer Vision and Pattern Recognition, 2020.

Zsolt Páles and Vera Zeidan. Infinite dimensional clarke generalized jacobian. Journal of Convex Analysis, 14(2), 2007.

Benjamin Sherman, Jesse Michel, and Michael Carbin. Sound and robust solid modeling via exact real arithmetic and continuity. In International Conference on Functional Programming, 2019.

Jesse Sigal. Denotational semantics for differentiable programming with manifolds. In Student Research Competition at the Internation Conference on Functional Programming, 2018.
Jeffrey Mark Siskind and Barak A Pearlmutter. Perturbation confusion and referential transparency: Correct functional implementation of forward-mode ad. Workshop on Implementation and Application of Functional Languages, 2005.

Dimitrios Vytiniotis, Dan Belov, Richard Wei, Gordon Plotkin, and Martin Abadi. The differentiable curry. In Neural Information Processing Systems Workshop Program Transformations, 2019.

Matthijs Vákár, Ohad Kammar, and Sam Staton. Diffeological spaces and semantics for differential programming. In Domains, 2018. URL https://andrejbauer.github.io/domains-floc-2018/slides/Matthijs-Kammar-Staton.pdf.

Yuanhao Wang, Guodong Zhang, and Jimmy Ba. On solving minimax optimization locally: A follow-the-ridge approach. In International Conference on Learning Representations, 2020.
A SEMANTICS OF VARIABLE REFERENCES AND CONTEXT MEMBERSHIP

The semantics of a variable reference is the projection out of the product that defines it to find the appropriate variable in the context:

\[(x : \tau) \in (\Gamma, x : \tau) \quad \text{and} \quad (x : \tau) \in (\Gamma, x' : \tau')\]

\[
\begin{align*}
\llbracket (x : \tau) \in \Gamma \rrbracket & \in \llbracket \Gamma \rrbracket \rightarrow C \llbracket \tau \rrbracket \\
\llbracket (x : \tau) \in (\Gamma, x : \tau) \rrbracket & \triangleq \pi_2 \\
\llbracket (x : \tau) \in (\Gamma, x' : \tau') \rrbracket & \triangleq \llbracket (x : \tau) \in \Gamma \rrbracket \circ \pi_1
\end{align*}
\]

B SEMANTICS OF SECOND-ORDER FUNCTIONS

In the category of presheaves \([C^{op}, \text{Set}]\), let \(\tau\) denote the Yoneda embedding, and let \(\Rightarrow\) denote the internal hom. Then there is an equivalence between constants with the second-order type \((\overline{A} \Rightarrow \overline{B}) \Rightarrow \overline{C}\) and the end \(\int_{\Gamma}(\Gamma \times A \rightarrow C B) \rightarrow (\Gamma \rightarrow C C)\):

\[1 \rightarrow\llbracket\text{C}^{op}, \text{Set}\rrbracket(\overline{A} \Rightarrow \overline{B}) \Rightarrow \overline{C}\](\overline{A} \Rightarrow \overline{B}) \Rightarrow \overline{C} \cong (\overline{A} \Rightarrow \overline{B}) \Rightarrow\llbracket\text{C}^{op}, \text{Set}\rrbracket \overline{C}
\]

\[= \int_{\Gamma}(\overline{A} \Rightarrow \overline{B})(\Gamma) \rightarrow \overline{C}(\Gamma)
\]

\[\cong \int_{\Gamma}(\Gamma \times A \rightarrow C B) \rightarrow (\Gamma \rightarrow C C)
\]

C SEMANTICS OF TANGENT BUNDLES IN \(\lambda_S\)

To define tangent bundles and forward-mode differentiation on smooth spaces, we begin by defining them on the underlying category of vector spaces and smooth maps.

For vector spaces, we have for any smooth map \(f : A \rightarrow B\) a smooth map \(\text{fwd}(f) : A \times A \rightarrow B \times B\) for its forward-mode derivative. The forward-mode derivative defines a functor, and it is this that can be extended to the smooth spaces via a left Kan extension.

Our notion of tangent spaces, \(\text{Tan}\), should correspond to the dvs diffeology on internal tangent bundles as described by Christensen and Wu [2017]. We get the equivalence \(\text{Tan} (A \ast B) \cong \text{Tan} A \ast \text{Tan} B\) by [Christensen and Wu 2017, Proposition 4.13.2], and \(\text{Tan} (A \rightarrow \mathcal{R}) \cong A \rightarrow \text{Tan} \mathcal{R}\) by [Christensen and Wu 2017, Proposition 4.27].

More concretely, left Kan extensions correspond to coends:

\[\text{Tan}(F)(\Gamma) \cong \int_{\Delta} (\Delta \rightarrow \Delta^2) \times F(\Delta).
\]

We first show \(\text{Tan}(yA) \cong y(A^2)\), where \(y\) is the Yoneda embedding:

\[\text{Tan}(yA)(\Gamma) \cong \int_{\Delta} (\Delta \rightarrow \Delta^2) \times (\Delta \rightarrow A)
\]

Given \(f : A^2(\Gamma) \rightarrow \Gamma \rightarrow A^2\), we can take \(\Delta = A\) and use \((f, \text{id})\). Given an element of \(\text{Tan}(A)(\Gamma)\), i.e., some \(\Delta\) and \(f : \Gamma \rightarrow \Delta^2\) and \(g : \Delta \rightarrow A\), then \(\text{fwd}(g) \circ f : A^2(\Gamma)\).

We will now show \(\text{Tan}(F \times G) \cong \text{Tan}(F) \times \text{Tan}(G)\). We easily have the product projections \(\text{Tan}(F \times G) \rightarrow \text{Tan}(F)\) and \(\text{Tan}(F \times G) \rightarrow \text{Tan}(G)\). Conversely, given \((\text{Tan}(F) \times \text{Tan}(G))(\Gamma)\), we get
The differential \( \pi \) fundamentally depends on this geometric inner-product structure in a way that the unique linear map satisfying \( D f \mapsto \gamma \) in reverse-mode differentiation, a smooth map \( f : \mathbb{R}^n \to \mathbb{R}^k \) determines at a point \( x \in \mathbb{R}^n \) a linear map \( D f_x^* : \mathbb{R}^k \to \mathbb{R}^n \), which is the adjoint of the forward-mode derivative. When vector spaces \( U \) and \( V \) have inner-product structures, the adjoint \( f^* : V \to U \) of a linear map \( f : U \to V \) is the unique linear map satisfying \( \langle u, f^*(v) \rangle_U = \langle f(u), v \rangle_V \) for all \( u \in U \) and \( v \in V \). Reverse-mode differentiation fundamentally depends on this geometric inner-product structure in a way that

\[ f(y) = ((x, y), (dx, dy)) \]

where \( (x, dx) = f(y) \) and \( (y, dy) = g(y) \). Using the pullbacks \( \pi_1 : F(\Delta_1) \to F(\Delta_1 \times \Delta_2) \) and \( \pi_2 : G(\Delta_2) \to G(\Delta_1 \times \Delta_2) \), we can produce \( \text{Tan}(F \times G)(\Gamma) \).

Next, we can show that \( \text{Tan}(A \Rightarrow \mathbb{R}) \equiv A \Rightarrow \text{Tan}(\mathbb{R}) \equiv A \Rightarrow y(\mathbb{R}^2) \), noting these are:

\[
\text{Tan}(A \Rightarrow \mathbb{R})(\Gamma) \equiv \int_\Delta (\Gamma \Rightarrow \Delta^2) \times \int_X (X \Rightarrow \Delta) \to A(X) \to (X \Rightarrow \mathbb{R})
\]

\[
(A \Rightarrow \mathbb{R}^2)(\Gamma) \equiv \int_X (X \Rightarrow \Gamma) \to A(X) \to (X \Rightarrow \mathbb{R}^2)
\]

Given \( f : (A \Rightarrow \mathbb{R}^2) \), we take \( \Delta = \Gamma \times \mathbb{R} \), and use

\[
\exists \Gamma \times \mathbb{R}. (\lambda y. ((y, 0), (0, 1)), \Lambda X. \lambda(e : X \Rightarrow \Gamma \times \mathbb{R}). \lambda(a : A(X)).
\]

\[
\lambda(y, 0, (0, 1), \Lambda X. \lambda(e : X \to \Gamma \times \mathbb{R}). \lambda(a : A(X)).
\]

Conversely, given a member of \( \text{Tan}(A \Rightarrow \mathbb{R})(\Gamma) \), i.e., a \( \Delta \) with \( d : \Gamma \Rightarrow \Delta^2 \) and \( f : \int_X (X \Rightarrow \Delta) \to A(X) \to (X \Rightarrow \mathbb{R}) \), we can provide

\[ \Lambda X. \lambda(e : X \Rightarrow \Gamma). \lambda(a : A(X)). \text{fwd}(f(X, \pi_1(f(X, \pi_1 \circ d \circ e, a), f(X, \pi_2 \circ d \circ e, a)))). \]

## D ADDITIONAL RELATED WORK

The differential \( \lambda \)-calculus [Ehrhard and Regnier 2003] supports higher-order functions but requires every type to have a zero element and addition, which rules out features we support such as discrete types (§8.1).

Abadi and Plotkin [2020] and Sigal [2018] admit nondifferentiable functions like ReLU by allowing branching on real-valued comparisons, where the branch is partial when the quantities are equal.

Thus, at nondifferentiable points of a function, both the value and its derivative are undefined. Neither support higher-order functions.

Betancourt [2018] defines various algorithms for higher-order derivatives of smooth functions on manifolds. It does not define a programming language that supports these operations.

Synthetic differential geometry (SDG) [Kock 2006] is the study of toposes (which, in particular, are CCCs) that have notions of arbitrary derivatives, along the lines of forward-mode AD with arbitrary-order derivatives, as well as notions of infinitesimal objects which contain only elements that are infinitely small, but behave in nontrivial ways. In smooth differential geometry, the objects are generalized manifolds. Diffeological spaces are not a model of SDG.

Kakade and Lee [2018] define a method of computing subgradients that is “provably correct.” However, their method does not permit arbitrary composition of locally Lipschitz functions; there is a nonsyntactic restriction on which functions are admitted. For instance, \( f(x) = \text{ReLU}(x^2) \) is not admitted, where \( \text{ReLU}(x) = \max(x, 0) \).

## E ADDITIONAL DISCUSSION

### E.1 Reverse-mode differentiation

In reverse-mode differentiation, a smooth map \( f : \mathbb{R}^n \to \mathbb{R}^k \) determines at a point \( x \in \mathbb{R}^n \) a linear map \( D f_x^* : \mathbb{R}^k \to \mathbb{R}^n \), which is the adjoint of the forward-mode derivative. When vector spaces \( U \) and \( V \) have inner-product structures, the adjoint \( f^* : V \to U \) of a linear map \( f : U \to V \) is the unique linear map satisfying \( \langle u, f^*(v) \rangle_U = \langle f(u), v \rangle_V \) for all \( u \in U \) and \( v \in V \). Reverse-mode differentiation fundamentally depends on this geometric inner-product structure in a way that
forward-mode differentiation does not: the Gateaux formulation of forward-mode differentiation can be formulated for any locally convex topological vector spaces, without requiring any geometric structure.

Higher-order types such as \texttt{Integral} do not admit any such inner-product structure, so reverse-mode differentiation cannot be extended to \( \lambda_S \) in general unless it is generalized. Rather than considering the adjoints of a linear map \( f : U \rightarrow V \), we can instead consider the transpose, which is a linear map \( f^T : B^* \rightarrow A^* \), where \( B^* \triangleq B \rightarrow \mathbb{R} \) is the dual space of \( B \). For Cartesian spaces \( \mathbb{R}^n \), the transpose is related to the adjoint via the isometry \( \mathbb{R}^n^* \cong \mathbb{R}^n \) that associates elements of its dual space with vectors in the original spaces.

We now describe how we can represent this generalized reverse-mode differentiation in \( \lambda_S \). Using the projection \( \text{tangentValue} \ A : \text{Tan} \ A \rightarrow A \), we can get a dependent type \( T : \text{Type} \), such that \( \text{Tan}(\ A) \triangleq \sum_{a : A} T(a) \). For a point \( a : A \), we call \( T(a) \) the tangent space on \( a \). We can then characterize how forward-mode differentiation maps tangent spaces by

\[
\text{der}_L : \bigotimes_{f : A \rightarrow B} \bigotimes_{a : A} T(a) \rightarrow T(f(a)).
\]

We define the cotangent space on \( a \) as its dual \( T(a)^* \). We can then define a pullback of cotangent spaces,

\[
\text{rev} : \bigotimes_{f : A \rightarrow B} \bigotimes_{a : A} T(f(a))^* \rightarrow T(a)^*
\]

\[
\text{rev}(f)(a)(k) \triangleq k \circ \text{der}_L(f)(a).
\]

Note that this does not address the efficiency concerns that motivate reverse-mode differentiation, in part because converting from \( \mathbb{R}^n^* \) to \( \mathbb{R}^n \) could be expensive, depending on the underlying implementation.

E.2 Nondifferentiable code, discrete objects and the reparameterization trick

Not all parts of a computation may be differentiable. For instance, many machine-learning techniques use Monte Carlo sampling to sample from distributions, and they cannot compute how infinitesimal perturbations to those distributions result in infinitesimal perturbations to the sampled results. Failure to account for this lack of propagation of derivatives is a common error in engineering machine learning systems. The reparameterization trick enables the use of Monte Carlo sampling despite its nondifferentiability by sampling from constant distributions and then differentiably transforming its results.

We can model nondifferentiable code like a black-box Monte Carlo sampler in \( \lambda_S \). For each space \( A \) in \( \lambda_S \), there is a corresponding space \( \Box A \) that has the same global points as \( A \) but lacks its differentiable structure. For instance, we have \( \text{Tan}(\Box A) \cong \Box A \): the tangent bundle is identical to the original space, meaning the tangent spaces are all trivial. We call types discrete when they are isomorphic to \( \Box A \) for some \( A \). The \( \Box \) operator is a comonadic modal operator that can be viewed as a kind of staging: values of \( \Box A \) can only be formed by operating on other discrete types, and they cannot depend on any nondiscrete types in the context.

We can model a Monte Carlo sampler with the \( \Box \) modality. For instance, we may have a function

\[
\text{sampleNormal} : \Box \mathbb{R} \rightarrow \Box \mathbb{R} \rightarrow \Box \text{(Integral} \ \mathbb{R})
\]
that samples from a normal distribution with fixed constant mean and variance. The reparameterization trick can use this sampler to implement a fully differentiable normal distribution:

```haskell
normal (mu : ℜ) (stdDev : ℜ) : Integral ℜ =
  let Box stdNormal = sampleNormal (Box 0) (Box 1) in
  map (λ x : ℜ ⇒ mu + stdDev * x) stdNormal
```

Our modal types yield a semantic understanding of treating nondifferentiable functions within differentiable programming languages and provide a type discipline that prevents the error of forgetting to perform the reparameterization trick and getting silently incorrect derivatives, which is the norm in modern deep-learning frameworks.

### E.3 Manifolds

Because manifolds form a subcategory of HAD, all manifolds are admissible as types in λS. Since HAD is a topos, admitting images and quotients, we can easily define certain manifolds. For instance, the circle is the image of the map \( f : \mathbb{R} \to \mathbb{R}^2 = (\sin x, \cos x) \). Accordingly, it can be defined as the quotient of \( \mathbb{R} \) by the smooth equivalence relation \( x \sim y \iff (\sin(x), \cos(x)) = (\sin(y), \cos(y)) \). We can further characterize the tangent space of the circle as \( \text{Tan Circle} \cong \mathbb{R} \) as well as define its exponential map \( \exp \circ \text{Circle} : \text{Tan Circle} \to \text{Circle} \) that rotates a point on the circle by the amount indicated by its tangent vector. Implementations may represent values on the circle with \( \mathbb{R} \), the space prior to quotienting, and use abstract datatypes (like newtype in Haskell).

### F DETAILED TECHNICAL RESULTS

We now proceed to prove a collection of technical results. These results principally work towards two major propositions: Propositions F.14 and F.15, which claim that the definition of smooth composition preserves consistency of derivative towers and soundly gives derivatives of value-level composition, and Proposition F.32, which shows that the derivative tower for \( \max \) is consistent with our definitions.

#### F.1 AD is a Cartesian monoidal category

To prove that the category AD of smoothish maps is indeed a Cartesian monoidal category, we must first prove that all of the categorical operations preserve consistency: the categorical operations are defined on derivative towers, but smoothish maps are consistent derivative towers, so we must know that the categorical operations preserve consistency. Then, we must prove that all of the equational laws expected of Cartesian monoidal categories are satisfied.

**F.1.1 Categorical operations preserve consistency.**

*Identity maps are consistent.* Identity maps are consistent; their consistency follows from the consistency of linear maps in general, Proposition F.31.

*Composition (Faà di Bruno) preserves consistency.* We begin with many lemmas that lead to the ultimate

**Proposition F.1 (Chain rule for \( \partial \)).** Given \( f : \mathbb{R}^n \to \mathbb{R}^m \) locally Lipschitz on \( X \subseteq \mathbb{R}^n \), and \( g : \mathbb{R}^m \to \mathbb{R}^k \) locally Lipschitz on \( Y \subseteq \mathbb{R}^m \), then on \( f(X) \cap Y \) we have the relation for all \( dx \in \mathbb{R}^n \)

\[
\text{hull} \left( \{ G \cdot F \cdot dx \mid G \in (\partial g)(f(x)), F \in \partial f(x) \} \right) \subseteq \partial(g \circ f)(x) \cdot dx.
\]

**Proof.** [Clarke 1990, Corollary on page 75]
Proposition F.2 (Chain rule for $\partial_\perp$). Given $f : \mathbb{R}^n \to \mathbb{R}^m_\perp$ and $g : \mathbb{R}^m \to \mathbb{R}^k_\perp$ we have the relation for all $x \in \mathbb{R}^n$ and all $dx \in \mathbb{R}^n$

$$\text{hull}\{ G \cdot F \cdot dx \mid G \in (\partial_\perp g)(f(x)), F \in \partial_\perp f(x)\} \subseteq \partial_\perp (g \circ f)(x) \cdot dx.$$ 

**Proof.** The left-hand side will be not $\perp$ only when $x$ lies in the set under which Proposition F.1 is applicable, and in this case, Proposition F.1 directly applies and proves the result. $\square$

Given two convex sets of tensors $X \in C(\mathbb{R}^{mxn})$ and $Y \in C(\mathbb{R}^{nxk})$, write

$$X : Y \doteq \text{hull}\{ x \cdot y \mid x \in X, y \in Y \}.$$ 

Note that $X : Y \in C(\mathbb{R}^{nxk})$. Note that if either $X$ or $Y$ is just a singleton set, the convex hull is unnecessary, and we may just use the symbol $\cdot$ rather than $:$ accordingly, as we do in the following definition. The $:$ operator is associative:

**Proposition F.3.** For convex sets $X \in C(\mathbb{R}^{mxn})$, $Y \in C(\mathbb{R}^{nxk})$, and $Z \in C(\mathbb{R}^{nxl})$, we have the equality

$$\text{hull}\{ xyz \mid x \in X, y \in Y, z \in Z \} = X : (Y : Z) = (X : Y) : Z.$$ 

**Proof.** Without loss of generality, we only prove the first equality

$$\text{hull}\{ xyz \mid x \in X, y \in Y, z \in Z \} = X : (Y : Z).$$ 

Obviously the left-hand side is included in the right hand side, so we only prove the inclusion in the other direction. Suppose we have $a \in X : (Y : Z)$. Carathéodory’s theorem states that every point in the convex hull of a set is a finite combination of elements from that set. Thus, we have $N \in \mathbb{N}$,$p_i \in [0, 1]$ and $x_i \in X$ for each $i \in \{1, \ldots, N\}$ such that $\sum_{i=1}^N p_i = 1$, and for each $i \in \{1, \ldots, N\}$, we have some $M_i \in \mathbb{N}$ and $q_{ij} \in [0, 1]$, $y_{ij} \in Y$, and $z_{ij} \in Z$ for each $j \in \{1, \ldots, M_j\}$, such that $\sum_{j=1}^{M_j} q_{ij} = 1$, such that

$$a = \sum_{i=1}^N p_ix_i \left( \sum_{j=1}^{M_i} q_{ij}y_{ij}z_{ij} \right),$$ 

and by multilinearity of tensor contractions, we can reassociate the sum to find

$$a = \sum_{i=1}^N \sum_{j=1}^{M_i} (p_iq_{ij}) x_iy_{ij}z_{ij},$$

noting that

$$\sum_{i=1}^N p_iq_{ij} = \sum_{i=1}^N p_i \sum_{j=1}^{M_i} q_{ij} = \sum_{i=1}^N p_i = 1,$$

which shows that $a$ is a finite convex combination of points from the set

$$\{ xyz \mid x \in X, y \in Y, z \in Z \},$$

and thus $a$ is in the convex hull of that set. $\square$

Note that an $n$-ary generalization of this statement holds. We see that $:$ is associative, so we may let the association be ambiguous:

**Corollary F.4.** Given $f : \mathbb{R}^n \to \mathbb{R}^m_\perp$ and $g : \mathbb{R}^m \to \mathbb{R}^k_\perp$, we have the relation for all $x \in \mathbb{R}^n$ and all $dx \in \mathbb{R}^n$

$$(\partial_\perp g)(f(x)) : (\partial_\perp f(x) \cdot dx) \subseteq \partial_\perp (g \circ f)(x) \cdot dx.$$
Given a function \( f : A \to C(B) \), let \( \hat{f} : C(A) \to C(B) \) denote its extension to convex sets of inputs taken by applying \( f \) set-wise and then taking a convex hull, for \( X \in C(A) \).

\[
\hat{f}(X) \triangleq \text{hull} \{ f(x) \mid x \in X \}.
\]

**Corollary F.5.** Given \( f : \mathbb{R}^n \to \mathbb{R}^m \) and \( g : \mathbb{R}^m \to \mathbb{R}^k \), we have the relation for all \( x \in \mathbb{R}^n \) and all \( dx \in \mathbb{R}^n \)

\[
(\partial_1 g)(\hat{f}(x)) \cdot \partial_1 f(x) \cdot dx \subseteq \partial_1(g \circ f)(x) \cdot dx.
\]

**Proof.** Directly from Corollary F.4, we can get that for all \( x \in \mathbb{R}^n \) and all \( dx \in \mathbb{R}^n \),

\[
(\partial_1 g)(f(x)) \cdot \partial_1 f(x) \cdot dx \subseteq \partial_1(g \circ f)(x) \cdot dx.
\]

This implies that for all \( x \in \mathbb{R}^n \) and all \( dx \in \mathbb{R}^n \), we have

\[
\text{hull} \{ (\partial_1 g)(f(z)) \cdot \partial_1 f(z) \cdot dx \mid z \in x \} \subseteq \text{hull} \{ \partial_1(g \circ f)(z) \cdot dx \mid z \in x \}.
\]

By bilinearity of \( \cdot \), we can rewrite each side as follows:

\[
\text{hull} \{ (\partial_1 g)(f(z)) \cdot \partial_1 f(z) \mid z \in x \} \cdot dx \subseteq \text{hull} \{ \partial_1(g \circ f)(z) \mid z \in x \} \cdot dx.
\]

The right-hand side is equivalent to the right-hand side in the theorem, whereas the left-hand side is clearly an upper bound for the left-hand side in the theorem. \( \square \)

**Corollary F.6.** Given \( f : \mathbb{R}^n \to \mathbb{R}^m \), and \( g : \mathbb{R}^m \to \mathbb{R}^k \) we have the relation for all \( x \in \mathbb{R}^n \) and all \( dx \in \mathbb{R}^n \)

\[
(\partial_1 g)(f(x)) \cdot \partial_1 f(x) \cdot dx \subseteq \partial_1(g \circ f)(x) \cdot dx.
\]

**Proof.** By Corollary F.5, we know that

\[
(\partial_1 \text{Mat}_0 g)(\text{Mat}_0 f(x)) \cdot \partial_1 \text{Mat}_0 f(x) \cdot dx \subseteq \partial_1(\text{Mat}_0 g \circ \text{Mat}_0 f)(x) \cdot dx,
\]

which is equivalent to (using Propositions F.13 and F.35)

\[
(\partial_1 g)(\text{Mat}_0 f(x)) \cdot \partial_1 f(x) \cdot dx \subseteq \partial_1(g \circ f)(x) \cdot dx.
\]

\( \square \)

Given two convex sets \( X, Y \in C(A) \), we write \( X + Y \) to denote

\[
X + Y \triangleq \{ x + y \mid x \in X, y \in Y \}.
\]

We note that \( X + Y \in C(A) \), since

\[
c(x_1 + y_1) + (1 - c)(x_2 + y_2) = (cx_1 + (1 - c)x_2) + (cy_1 + (1 - c)y_2).
\]

**Proposition F.7** (Product rule for \( \partial \)). Given \( f : D \to \mathbb{R}^{n \times m} \) and \( g : D \to \mathbb{R}^{m \times k} \) both locally Lipschitz on \( D \), for all \( x \in D \),

\[
\partial f(x) \cdot g(x) + f(x) \cdot \partial g(x) \subseteq \partial(f \cdot g)(x).
\]

**Proof.** [Páles and Zeidan 2007, Corollary 3.6]. \( \square \)

**Proposition F.8** (Product rule for \( \partial_1 \)). Given \( f : D \to \mathbb{R}^{n \times m}_1 \) and \( g : D \to \mathbb{R}^{m \times k}_1 \), for all \( x \in D \),

\[
\partial_1 f(x) \cdot g(x) + f(x) \cdot \partial_1 g(x) \subseteq \partial_1(f \cdot g)(x).
\]

**Proof.** The left-hand side is only not \( \perp \) in the case where all four terms in the left-hand side are not \( \perp \). On the region where this holds, we are guaranteed that the right-hand side is not \( \perp \), and in this case, the relation follows from Proposition F.7. \( \square \)
PROPOSITION F.9 (Tensor product rule for $\partial_\perp$). Given $g : D \to \mathbb{R}_{\perp}^{m \times n_j \times \ldots \times n_i}$ and for all $i \in \{1, \ldots, j\}$, $f_i : D \to \mathbb{R}_{\perp}^{n_i}$, for all $x \in D$,

\[
\partial_\perp g(x) \cdot (f_1(x) \otimes \ldots \otimes f_j(x)) + \sum_{i=1}^{j} g(x) \cdot (f_1(x) \otimes \ldots \otimes f_{i-1}(x) \otimes \partial_\perp f_i(x) \otimes f_{i+1}(x) \otimes \ldots \otimes f_j(x)) \subseteq \\
\partial_\perp (g \cdot (f_1 \otimes \ldots \otimes f_j))(x).
\]

**Proof.** By repeated application of the product rule (Proposition F.8), and transitivity of $\subseteq$. $\square$

PROPOSITION F.10 (Sum rule). Given $f, g : D \to \mathbb{R}_{\perp}^{n}$, for all $x \in D$,

\[
\partial_\perp f(x) + \partial_\perp g(x) \subseteq \partial_\perp (f + g)(x)
\]

**Proof.** At a point $x$, if $f + g$ has a Bouligand subdifferential $H$, then there is a sequence $x_j$ such that

\[
H = \lim_{j \to \infty} J(f + g)(x_j) = \lim_{j \to \infty} Jf(x_j) + Jg(x_j) = \left( \lim_{j \to \infty} Jf(x_j) \right) + \left( \lim_{j \to \infty} Jg(x_j) \right),
\]

meaning that $f$ has a Bouligand subdifferential $H_f \triangleq \lim_{j \to \infty} Jf(x_j)$ and $g$ has a Bouligand subdifferential $H_g \triangleq \lim_{j \to \infty} Jg(x_j)$ such that $H = H_f + H_g$. $\square$

PROPOSITION F.11 (Faà di Bruno for $\partial_\perp$). Given $f : \mathbb{R}^n \to \mathbb{R}_{\perp}^m$, and $g : \mathbb{R}^m \to \mathbb{R}_{\perp}^k$, for every $j \in \mathbb{N}$, we have the relation for all $x \in \mathbb{R}^n$ and all $v_1, \ldots, v_j \in \mathbb{R}^n$

\[
\sum_{\pi \in \mathcal{H}(\{1, \ldots, j\})} \text{let } i = |\pi| \text{ in } (\partial_\perp^j g)(f(x)) : \\
\quad \left( (\partial_\perp^{\pi_i} f)(x) \cdot v_{\pi_1} \otimes \ldots \otimes v_{\pi_i \mid \pi_i} \right) \otimes \\
\quad \left( (\partial_\perp^{\pi_j} f)(x) \cdot v_{\pi_1} \otimes \ldots \otimes v_{\pi_i \mid \pi_i} \right) \subseteq \\
\quad \partial_\perp^j (g \circ f)(x) \cdot v_1 \cdot \ldots \cdot v_j
\]

where in the big tensor product of convex-set-valued derivatives of $f$, we mean that we construct the convex set of tensor products that is the convex hull of elements drawn from each of the convex sets in each position, and where $\mathcal{H}(S)$ is the set of partitions of a set $S$, and $|S|$ is the cardinality of a set.

**Proof sketch.** By induction, starting with $j = 1$ ($j = 0$ holds by convention with particular interpretations of set partitions, but this is unimportant). In the case $j = 1$, this just reduces to the chain rule, F.4. In the inductive case, we know the relation holds for some $j$ and must prove that it holds for $j + 1$. Consider both sides as functions from $x \in \mathbb{R}^n$ to $C_{\perp}(\mathbb{R}^m)$. Then, we can see that $\partial_\perp$ is monotone, i.e., if $f \subseteq g$ then $\partial_\perp f \subseteq g$, so apply it to both sides. On the right side we have

\[
\partial_\perp^{j+1} (g \circ f)(x) \cdot v_1 \cdot \ldots \cdot v_j,
\]

which is our goal as the upper bound. We can lower-bound the left-hand side by using the sum rule (Proposition F.10) to lower-bound each term in the sum, and then using the tensor-product rule (Proposition F.9) to lower bound each term by the sum of products. Suppose we are lower-bounding a term in the sum corresponding to a partition $\pi$, letting $i = |\pi|$ be the cardinality of the partition. Then we will have $i + 1$ terms in the sum using the tensor-product rule. Those $i + 1$ correspond to adding a new element to this partition, either by creating a new set in the partition (which
corresponds to differentiating with respect to the “$g$”), or by adding the element to one of the existing partitions (which corresponds to differentiation with respect to one of the $f_i$s).

Let $I_n : \mathbb{R}^n \to \mathbb{R}^n_+$ send maximal elements $\{x\} \in \mathbb{R}^n$ to $x$ and all other elements to $\bot$. Note that there is an embedding of $\mathbb{R}^n_+$ into $\mathbb{R}^n$ that maps $\bot \in \mathbb{R}^n_+$ to $(\bot, \ldots, \bot) \in \mathbb{R}^n$. Then, implicitly using this embedding, we have for all $x \in \mathbb{R}^n$,

$$I_n(x) \subseteq x.$$ 

**Proposition F.12.** For any $f : \mathbb{R}^n \to \mathbb{R}^m$ and any $x \in \mathbb{R}^n$, $\text{Mat}_0 : (\mathbb{R}^n \to \mathbb{R}^m) \to \mathbb{R}^n \to \mathbb{R}^m_+$ acts on $f$ by

$$\text{Mat}_0 f = I_m \circ f$$

**Proof.** Follows from the definition of Mat.

**Proposition F.13.** For any $f : \mathbb{R}^n \to \mathbb{R}^m$ and $g : \mathbb{R}^m \to \mathbb{R}^k$,

$$\text{Mat}_0 g \circ f = \text{Mat}_0 (g \circ f).$$

**Proof.** Note that this equality relation on functions $\mathbb{R}^n \to \mathbb{R}^k_+$ is meant to be interpreted pointwise over all inputs $x \in \mathbb{R}^n$. By Proposition F.12,

$$\text{Mat}_0 (g \circ f) = I_k \circ (g \circ f) = (I_k \circ g) \circ f = \text{Mat}_0 g \circ f$$

**Proposition F.14 (Faà di Bruno for derivative towers is consistent).** Given consistent derivative towers $g : \mathbb{R}^n \to \mathbb{R}^m$ and $f : \mathbb{R}^m \to \mathbb{R}^k$, the Faà di Bruno derivative tower described in the main text as $g \circ f$ is a consistent derivative tower.

**Proof Sketch.** We must prove that for all $j \in \mathbb{N}$, we have $\text{Cons}_{j+1}((g \circ f)^{(j+1)}, \partial_\perp \text{Mat}_j((g \circ f)^{(j)}))$. We do so by induction on $j$.

**Base case: chain rule.** In the base case $j = 0$, this reduces to proving that for all $x \in \mathbb{R}^n$ and for all $dx \in \mathbb{R}^n$, we have

$$g^{(1)}(f^{(0)}(x); f^{(1)}(x; dx)) \subseteq (\partial_\perp \text{Mat}_0((g \circ f)^{(0)}))(x) \cdot dx.$$ 

(Recall that the left-hand side is a product of intervals that we treat as a hyperrectangular convex set.)

By definition of $(g \circ f)^{(0)}$ and by Proposition F.13, we can reduce this to

$$g^{(1)}(f^{(0)}(x); f^{(1)}(x; dx)) \subseteq (\partial_\perp (\text{Mat}_0(g^0) \circ f^{(0)}))(x) \cdot dx.$$ 

By the chain rule (Corollary F.6), we can reduce this to

$$g^{(1)}(f^{(0)}(x); f^{(1)}(x; dx)) \subseteq (\partial_\perp \text{Mat}_0(g^0))(f^{(0)}(x)) \cdot (\partial_\perp \text{Mat}_0(f^{(0)}))(x) \cdot dx.$$ 

By consistency of $g$ we know

$$g^{(1)}(f^{(0)}(x); f^{(1)}(x; dx)) \subseteq \partial_\perp \text{Mat}_0(g^0)(f^{(0)}(x)) \cdot f^{(1)}(x; dx),$$

and by consistency of $f$ we know

$$f^{(1)}(x; dx) \subseteq \partial_\perp \text{Mat}_0(f^{(0)})(x) \cdot dx.$$ 

Putting these together, and using the monotonicity of $\cdot$, we get

$$g^{(1)}(f^{(0)}(x); f^{(1)}(x; dx)) \subseteq \partial_\perp \text{Mat}_0(g^0)(f^{(0)}(x)) \cdot \partial_\perp \text{Mat}_0(f^{(0)})(x) \cdot dx,$$

which is exactly the relation that we need.
Inductive case. Essentially the same as in Proposition F.11, using the consistency of higher-order derivatives of \(g\) and \(f\) to rewrite applications of higher-order derivatives as tensor products, and then using the tensor-product rule (Proposition F.9) to find the derivatives of these programs that approximate the tensor products. \(\square\)

**Corollary F.15 (Faà di Bruno for derivative towers is sound).** Given consistent derivative towers \(g : \mathbb{R}^n \rightsquigarrow \mathbb{R}^m\) and \(f : \mathbb{R}^m \rightsquigarrow \mathbb{R}^k\), the Faà di Bruno derivative tower described in the main text as \(g \circ f\) satisfies the relation for all \(j \in \mathbb{N}\),

\[
\text{Cons}_{j+1} \left( (g \circ f)^{(j+1)}, \frac{\partial (g \circ f)}{\partial x} \bigg|_{x = 0} \right).
\]

**Proof.** We can compute that the Faà di Bruno derivative tower program at the value level gives for all \(x \in \mathbb{R}^n\)

\[
(g \circ f)^{(0)}(x) = g^{(0)}(f^{(0)}(x)),
\]

so our goal is equivalent to

\[
\text{Cons}_{j+1} \left( (g \circ f)^{(j+1)}, \frac{\partial (g \circ f)}{\partial x} \bigg|_{x = 0} \right).
\]

which follows from consistency of \(g \circ f\) (Proposition F.14) and Proposition F.36. \(\square\)

In general, we see that proving soundness of derivative towers can be reduced to proving that the derivative towers are consistent and that their value-level operation is as desired.

Pairing preserves consistency.

**Proposition F.16.** Given two maps \(f : \mathbb{R}^n \rightarrow \mathbb{R}_1^m\) and \(g : \mathbb{R}^n \rightarrow \mathbb{R}_1^k\), for any \(x \in \mathbb{R}^n\),

\[
\{ [u, v] \mid u \in \partial_{\perp} f(x), v \in \partial_{\perp} g(x) \} \subseteq \partial_{\perp} (\lambda z. (f(z), g(z)))(x),
\]

where the pairing operation \((\cdot, \cdot) : \mathbb{R}_1^m \times \mathbb{R}_1^k \rightarrow \mathbb{R}_1^{m+k}\) returns \(\perp\) if either of its arguments it \(\perp\), or the pair of values if both inputs are not \(\perp\).

**Proof sketch.** Note that the set defined by the set comprehension on the left-hand side of the relation is convex, since both \(\partial_{\perp} f(x)\) and \(\partial_{\perp} g(x)\) are. Suppose \([H, L]\) is in the Bouligand subdifferential of \(\lambda z. (f(z), g(z))\) at \(x\). Then it must be the case that \(H\) is in the Bouligand subdifferential for \(f\) and that \(L\) is in the Bouligand subdifferential for \(g\). \(\square\)

**Proposition F.17.** For any \(f : \mathbb{R}^n \rightarrow C(\mathbb{R}^{\ell \times k})\) and \(g : \mathbb{R}^n \rightarrow C(\mathbb{R}^{\ell \times m})\), defining \((f, g) : \mathbb{R}^n \rightarrow C(\mathbb{R}^{\ell \times m+k})\) by

\[
(f, g)(x) = \{ [H, L] \mid H \in f(x), L \in g(x)\},
\]

for all \(x \in \mathbb{R}^n\) and for all \(dx_1, \ldots, dx_k \in \mathbb{R}^n\), we have

\[
\{ (u, v) \mid u \in f(x) \cdot (dx_1 \otimes \ldots \otimes dx_k), v \in g(x) \cdot (dx_1 \otimes \ldots \otimes dx_k) \} = (f, g)(x) \cdot (dx_1 \otimes \ldots \otimes dx_k).
\]

**Proof.** Note that the set defined by the set comprehension on the left-hand side of the relation is convex, since both \(f(x) \cdot (dx_1 \otimes \ldots \otimes dx_k)\) and \(g(x) \cdot (dx_1 \otimes \ldots \otimes dx_k)\) are. This equality follows simply from following the definitions and noting that

\[
[H, L] \cdot v = (H \cdot v, L \cdot v),
\]

\(\square\)

**Proposition F.18 (Pairing preserves consistency).** Given two consistent derivative towers \(f : \mathbb{R}^n \rightsquigarrow \mathbb{R}^m\) and \(g : \mathbb{R}^n \rightsquigarrow \mathbb{R}^k\), the derivative tower \((f, g) : \mathbb{R}^n \rightarrow \mathbb{R}^{m+k}\) is consistent.

**Proof sketch.** Follows in a straightforward manner from Proposition F.16 and Proposition F.17. \(\square\)
F.1.2 Equational laws hold for categorical operations. To know that these categorical operations indeed form a Cartesian monoidal category, we need to know that several equational laws hold, like $f \circ \text{id} = \text{id} \circ f = f$. We will prove these laws in this section.

**Proposition F.19.** The composition operator $\circ$ given by the Faà di Bruno formula is associative, i.e.,

\[ h \circ (g \circ f) = (h \circ g) \circ f. \]

**Proof sketch.** The proof of this fact relies on two important facts. Firstly, the $+$ operator is associative and commutative. Second, taking partitions of partitions is associative in the appropriate sense.

Next, we will prove that composition with linear maps works as expected. These facts will be critical for demonstrating that various equational laws hold.

**Proposition F.20.** For any $g : B \to C$ and any derivative tower $f : A \leadsto B$, for any $k \in \mathbb{N}$ and any $x \in A$ and $v_1, \ldots, v_k \in A$,

\[ (\text{linear}(g) \circ f)^{(k)}(x; v_1, \ldots, v_k) = g(f^{(k)}(v_1, \ldots, v_k)) \]

**Proof.** Because $\text{linear}(g)^{(j)}(v_1, \ldots, v_j) = 0$ whenever $j > 1$ by definition of linear, all terms in the sum given by the Faà di Bruno formula where $|\pi| > 1$ will be 0. By Proposition F.34, we can remove those terms, and the only term in the sum that will remain is the one where $|\pi| = 1$ (i.e., the partition puts all elements into the same set), and yields

\[ (\text{linear}(g) \circ f)^{(k)}(x; v_1, \ldots, v_k) = \text{linear}(g)^{(1)}(x; f^{(k)}(v_1, \ldots, v_k)), \]

which by the definition $\text{linear}(g)^{(1)}(x; \nu) = g(\nu)$ gives the stated equation.

It turns out that proving that precomposing with a linear map works as expected is significantly more difficult, so we need several lemmas before getting to the principal theorem, Proposition F.25.

**Lemma F.21.** Given $L \in C(\mathbb{R}^{n \times k})$ and $X \in C(\mathbb{R}^k)$, then if $L = \perp$ and $X \neq \{0\}$, then $L \circ X = \perp$.

**Proof.** It suffices to know that for every $y \in \mathbb{R}^n$, there exists some $\ell \in L$ and some $x \in X$ such that $y = \ell \cdot x$. Given the correspondence between matrix-vector multiplication and linear maps, equivalently, we can find some linear map $\ell : \mathbb{R}^n \to \mathbb{R}^k$ and some $x \in X$ such that $y = \ell(x)$. Since $X$ is nonempty and $X \neq \{0\}$, there exists some $x \in X$ such that $x \neq 0$. Then let $x \in X$ be such a nonzero value. Then define $\ell$ to be the projection operator

\[ \ell(v) \triangleq \frac{\langle v, x \rangle}{\langle x, x \rangle} y. \]

We can compute that $\ell(x) = y$ and confirm that $\ell$ is linear (since inner products are bilinear). Hence, $L \circ X = \perp$.

**Lemma F.22.** Given $X \in C(\mathbb{R}^n)$ and $Y \in C(\mathbb{R}^k)$, if $X \hat{\otimes} Y = \{0\}$, then either $X = \{0\}$ or $Y = \{0\}$.

**Proof.** Since $X \hat{\otimes} Y = \{0\}$, we know that for all $x \in X$ and for all $y \in Y$, and for all $i \in \{1, \ldots, n\}$ and all $j \in \{1, \ldots, k\}$, $x_i y_j = 0$. We will prove that if $X \neq \{0\}$ then $Y = \{0\}$. If $X \neq \{0\}$, then there is some $x^* \in X$ such that $x^* \neq 0$, meaning that there is some $i \in \{1, \ldots, n\}$ such that $x_i^* \neq 0$. Since for all $y \in Y$ and $j \in \{1, \ldots, k\}$, $x^*_j y_j = 0$, it must be that $y_j = 0$, and thus $y = 0$, and thus $Y = \{0\}$.

**Lemma F.23.** Given a function $g : \mathbb{R}^n \times (\mathbb{R}^k)^k \to \mathbb{R}^m$ and a function $f : \mathbb{R}^n \to C(\mathbb{R}^{n^k \times m})$ such that $\text{Cons}_k(g, f)$, then for all $x \in \mathbb{R}^n$ and $v_1, \ldots, v_k \in \mathbb{R}^n$, if $g(x; v_1, \ldots, v_k) \neq \perp$, then either

\[ (1) \hat{f}(x) \neq \perp, \text{ or} \]

\[ (2) \hat{g}(x; v_1, \ldots, v_k) \neq \perp. \]

We can compute that $\hat{f}(x) = y$ and confirm that $\hat{f}$ is linear (since inner products are bilinear). Hence, $L \circ X = \perp$. □
(2) \( g(\vec{x}; \vec{v}_1, \ldots, \vec{v}_k) \subseteq \bot \) and there is some \( i \in \{1, \ldots, k\} \) such that \( v_i = 0 \).

Furthermore, if \( g \) is Scott-continuous, then \( \hat{f}(x) \neq \bot \), i.e., the second case is impossible.

**Proof.** We assume \( \hat{f}(x) = \bot \) and prove that the second case must hold. Since

\[
g(\vec{x}; \vec{v}_1, \ldots, \vec{v}_k) \subseteq \hat{f}(x) \hat{\otimes} (\vec{v}_1 \hat{\otimes} \ldots \hat{\otimes} \vec{v}_k)
\]

and the left-hand side is not \( \bot \) (by assumption), neither is the right-hand side. By the contrapositive of Lemma F.21, it must be that \( \vec{v}_1 \hat{\otimes} \ldots \hat{\otimes} \vec{v}_k = \{0\} \). Thus, the entire right-hand side is 0, so \( g(\vec{x}; \vec{v}_1, \ldots, \vec{v}_k) \subseteq \{0\} \). By Lemma F.22, we also know that there is some \( i \in \{1, \ldots, k\} \) such that \( v_i = 0 \).

This establishes that one of those two cases must hold. We now show that if \( g \) is Scott-continuous, the second case is impossible. Note that if there is no \( i \in \{1, \ldots, k\} \) such that \( v_i = 0 \), or equivalently, \( \vec{v}_1 \hat{\otimes} \ldots \hat{\otimes} \vec{v}_k \neq \{0\} \), then \( \hat{f}(x) \neq \bot \), since the second case must be false. But we claim that if we can find \( \vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^n \) such that \( g(\vec{x}; \vec{v}_1, \ldots, \vec{v}_k) \neq \bot \) and there is some \( i \in \{1, \ldots, k\} \) such that \( v_i = 0 \), we can also find \( \vec{v}'_1, \ldots, \vec{v}'_k \in \mathbb{R}^n \) such that for all \( i \in \{1, \ldots, k\} \), \( v'_i \neq 0 \) but still \( g(\vec{x}; \vec{v}'_1, \ldots, \vec{v}'_k) \neq \bot \). This follows from the fact that the set on which \( g(\vec{x}; \cdot) \neq \bot \) is open, so \( g \) must not be \( \bot \) on an open neighborhood, whereas the set of tuples of vectors with all nonzero components is dense, so it must intersect that neighborhood. \( \square \)

**Corollary F.24.** Given any consistent derivative tower \( f : A \rightarrow B \), any \( k \in \mathbb{N} \), any \( x \in A \) and any \( \vec{v}_1, \ldots, \vec{v}_k \in A \), either \( f^{(k-1)} \) has a (compact) Clarke derivative at \( x \) or \( f^{(k)}(\vec{v}_1, \ldots, \vec{v}_k) = \bot \).

**Proof.** Recall that all of the derivative maps in a derivative tower are continuous, and by consistency, we have

\[
\text{Cons}_k(f^{(k)}, \partial_{\bot} \text{Mat}_{k-1}(f^{(k-1)})).
\]

By Lemma F.23, using the stronger statement with continuity, and taking the contrapositive, we find that if \( \partial_{\bot} \text{Mat}_{k-1}(f^{(k-1)}(x)) = \bot \), then \( f^{(k)}(x; \vec{v}_1, \ldots, \vec{v}_k) = \bot \). Note that the condition \( \partial_{\bot} \text{Mat}_{k-1}(f^{(k-1)}(x)) = \bot \) is equivalent to \( f^{(k-1)} \) not having a (compact) Clarke derivative at \( x \). \( \square \)

**Proposition F.25.** For any consistent derivative tower \( g : B \rightarrow C \) and any \( f : A \rightarrow B \) that maps maximal elements to maximal elements, for any \( k \in \mathbb{N} \) and any maximal \( x \in A \) and maximal \( \vec{v}_1, \ldots, \vec{v}_k \in A \),

\[
(g \circ \text{linear}(f))^{(k)}(x; \vec{v}_1, \ldots, \vec{v}_k) = g^{(k)}(f(\vec{v}_1), \ldots, f(\vec{v}_k)).
\]

**Proof.** Note that the term in the sum given by the Faà di Bruno formula where \( |\pi| = k \) gives the right-hand side \( g^{(k)}(f(\vec{v}_1), \ldots, f(\vec{v}_k)) \). For all other terms in the sum, where \( |\pi| < k \), we have that one of the inputs to \( g^{(|\pi|)} \) will be 0, because we have \( \text{linear}(f)^{(j)}(\vec{v}_1, \ldots, \vec{v}_j) = 0 \) whenever \( j > 1 \) by definition of linear.

We need to know that adding all these terms to the term \( |\pi| = k \) makes no difference to the sum, which can happen either if all of the terms are 0, or if already \( g^{(k)}(f(\vec{v}_1), \ldots, f(\vec{v}_k)) = \bot \), in which case the addition of any elements will not change the result. Thus, it suffices to prove that if \( g^{(k)}(f(\vec{v}_1), \ldots, f(\vec{v}_k)) \neq \bot \), then all of those other terms in the sum are 0.

Suppose \( g^{(k)}(f(\vec{v}_1), \ldots, f(\vec{v}_k)) \neq \bot \). Then by Corollary F.24, it must be the case that \( g^{(k-1)} \) has a (compact) Clarke derivative at \( x \). Therefore, for all \( j < k \), \( g^{(j)}(x; \cdot) \) is maximal. Since it is maximal, and is implementing a linear operator, whenever all of its multilinear arguments are not bottom and when one of those arguments is 0, the result will be 0. One of those multilinear arguments will be the result of applying a higher derivative of the linear function \( f \) to (at least) two maximal arguments \( v_a \) and \( v_b \) for some \( a, b \in \{1, \ldots, k\} \). Since \( f \) is linear, its result will be 0, and hence the result of the entire term \( g^{(j)}(x; \cdot) \) will be 0. \( \square \)
Proposition F.26. For any smoothish map \( f \),
\[
f \circ \text{linear}(\text{id}) = \text{linear}(\text{id}) \circ f = f.
\]

Proof. By Proposition F.25, we get that
\[
(f \circ \text{linear}(\text{id}))^{(k)}(x; v_1, \ldots, v_k) = \text{id}(f^{(k)}(x; v_1, \ldots, v_k)) = f^{(k)}(x; v_1, \ldots, v_k),
\]
thus showing that \( f \circ \text{linear}(\text{id}) = f \).

Similarly, by Proposition F.20, we get that
\[
(\text{linear}(\text{id}) \circ f)^{(k)}(x; v_1, \ldots, v_k) = f^{(k)}(x; \text{id}(v_1), \ldots, \text{id}(v_k)) = f^{(k)}(x; v_1, \ldots, v_k),
\]
thus showing that \( \text{linear}(\text{id}) \circ f = f \). \( \square \)

Lemma F.27. \text{linear} is a functor from the category whose arrows are linear maps to the category whose arrows are smoothish maps. In particular, \text{linear}(\text{id}) = \text{id}, and given \( f : \mathbb{R}^n \to \mathbb{R}^m \) and \( g : \mathbb{R}^m \to \mathbb{R}^k \), if both \( f \) and \( g \) are linear, then
\[
\text{linear}(g) \circ \text{linear}(f) = \text{linear}(g \circ f).
\]

Proof. The fact \( \text{linear}(\text{id}) = \text{id} \) is just a restatement of Proposition F.26.

Now we show that \text{linear} commutes with composition. By Proposition F.25, we get that
\[
(\text{linear}(g) \circ \text{linear}(f))^{(k)}(x; v_1, \ldots, v_k) = g(\text{linear}(f)^{(k)}(x; v_1, \ldots, v_k)).
\]

Unfolding the definition of \( \text{linear}(f)^{(k)} \), we get
\[
(\text{linear}(g) \circ \text{linear}(f))^{(0)}(x) = g(f(x))
\]
\[
(\text{linear}(g) \circ \text{linear}(f))^{(1)}(x; v) = g(f(v))
\]
\[
(\text{linear}(g) \circ \text{linear}(f))^{(k+2)}(x; \vec{v}) = 0,
\]
which exactly matches the definition of the right-hand side of the original equation, \( \text{linear}(g \circ f) \). \( \square \)

Lemma F.28. \text{linear} commutes with pairing, i.e.,
\[
\text{linear}(\langle f, g \rangle) = \langle \text{linear}(f), \text{linear}(g) \rangle.
\]

Proof. Note that for both definitions, second and higher derivatives are identically zero maps, since
\[
\langle \text{linear}(f), \text{linear}(g) \rangle^{(k+2)}(x; \vec{v}) = (0, 0).
\]

For the value-level definition, we have
\[
\text{linear}(\langle f, g \rangle)^{(0)}(x) = \langle f, g \rangle(x) = (f(x), g(x))
\]
\[
= (\text{linear}(f)^{(0)}(x), \text{linear}(g)^{(0)}(x))
\]
\[
= \langle \text{linear}(f), \text{linear}(g) \rangle^{(0)}(x).
\]

Likewise for the first derivative:
\[
\text{linear}(\langle f, g \rangle)^{(1)}(x; v) = \langle f, g \rangle(v) = (f(v), g(v))
\]
\[
= (\text{linear}(f)^{(1)}(x; v), \text{linear}(g)^{(1)}(x; v))
\]
\[
= \langle \text{linear}(f), \text{linear}(g) \rangle^{(1)}(x; v).
\]
\( \square \)
**Proposition F.29 (β law for product projections).** For all smoothish maps \( f \) and \( g \),
\[
\text{linear}(\text{fst}) \circ \langle f, g \rangle = f
\]
(and similarly for \( \text{snd} \)).

**Proof.** By Proposition F.20, the derivatives are
\[
(\text{linear}(\text{fst}) \circ \langle f, g \rangle)^{(k)}(x; \overline{v}) = \text{fst}(f^{(k)}(x; \overline{v}), g^{(k)}(x; \overline{v})) = f^{(k)}(x; \overline{v}).
\]
□

**Proposition F.30 (η law for product projections).** For all smoothish maps \( f \),
\[
\langle \text{linear}(\text{fst}) \circ f, \text{linear}(\text{snd}) \circ f \rangle = f;
\]

**Proof.** Again using Proposition F.20 as well as the definition of pairing, we compute
\[
(\text{linear}(\text{fst}) \circ f, \text{linear}(\text{snd}) \circ f)^{(k)}(x; \overline{v}) = (\text{fst}(f^{(k)}(x; \overline{v})), \text{snd}(f^{(k)}(x; \overline{v}))) = f^{(k)}(x; \overline{v}).
\]
□

Together, Proposition F.29 and Proposition F.30 demonstrate that pairing, \( \text{linear}(\text{fst}) \), and \( \text{linear}(\text{snd}) \) indeed define a Cartesian product structure for \( \text{AD} \).

**F.2 Consistency of language primitives**

**Proposition F.31.** Call a map \( f : \mathbb{R}^n \to \mathbb{R}^k \) linear if it always outputs values in \( \mathbb{R}^k \) and if it is linear in the traditional sense, i.e., \( f(u) + f(v) = f(u + v) \) for all \( u, v \in \mathbb{R}^n \) and \( c \cdot f(v) = f(c \cdot v) \) for all \( c \in \mathbb{R} \) and all \( v \in \mathbb{R}^n \). Whenever \( f : \mathbb{R}^n \to \mathbb{R}^k \) is linear, \( \text{linear}(f) \) is consistent.

**Proof.** Since \( f \) is linear in the above-defined sense, it is smooth, and so its derivatives will always be maximal, and will coincide with the traditional derivatives, which is exactly what \( \text{linear}(f) \) computes. □

Note that this in particular implies that product projections, which are defined as linear maps, are consistent. This completes the proof that consistency is preserved by the categorical operations as well as the Cartesian product operations, such that the smoothish maps are indeed closed under these operations.

It also implies that addition and subtraction preserve consistency, since they are defined by linear maps.

**Consistency of \( \text{max} \).** We define \( \max \) by
\[
\begin{align*}
\llbracket \max \rrbracket^{(0)}_{\text{AD}}(x, y) &\triangleq \max(x, y) \\
\llbracket \max \rrbracket^{(1)}_{\text{AD}}((x, y); (dx, dy)) &\triangleq \\
&\begin{cases}
  dx & x > y \\
  dy & y < x \\
  \text{hull}(dx, dy) & \text{otherwise}
\end{cases} \\
\llbracket \max \rrbracket^{(k+2)}_{\text{AD}}((x, y); \overline{v}) &\triangleq \\
&\begin{cases}
  0 & x \neq y \\
  \bot & \text{otherwise}
\end{cases}
\end{align*}
\]

We will now show that this is consistent with our definition.

**Proposition F.32 (\( \text{max is consistent} \)).** The tower \( \llbracket \max \rrbracket_{\text{AD}} : \mathbb{R}^2 \to \mathbb{R} \) is consistent.
Proof. First, we will show that all derivatives of order \( k + 2 \) for \( k \in \mathbb{N} \) are consistent, and finally we will show that the first derivative is consistent. Note that we have

\[
\text{Mat}_k \left[ \text{max} \right]^{(1)}_{\text{AD}} (x) = \begin{cases} 
1 & x > y \\
0 & x < y \\
\perp & \text{otherwise} 
\end{cases}
\]

It is \( \perp \) when \( x = y \) because there is no matrix \( M \in \mathbb{R}^2 \) such that for all \( dx, dy \in \mathbb{R} \),

\[
\text{hull}\{dx, dy\} = M \begin{bmatrix} dx \\ dy \end{bmatrix}.
\]

We observe that \( \text{Mat}_k \left[ \text{max} \right]^{(1)}_{\text{AD}} \) is a constant function where it is defined, which is when \( x \neq y \), and so all of its derivatives will be 0 when \( x \neq y \) and undefined elsewhere.

It now remains to show that the first derivative is consistent with the value-level function. We must show that for all \((x, y) \in \mathbb{R}^2\) and for all \((dx, dy) \in \mathbb{R}^2\),

\[
\left[ \text{max} \right]^{(1)}_{\text{AD}} ((x, y); (dx, dy)) \subseteq \left( \partial_\perp \left[ \text{max} \right]^{(0)}_{\text{AD}} \right)(x, y) : \begin{bmatrix} dx \\ dy \end{bmatrix}.
\]

Here, we see that

\[
\left( \partial_\perp \left[ \text{max} \right]^{(0)}_{\text{AD}} \right) (x, y) = \begin{cases} 
1 & x > y \\
0 & x < y \\
\text{hull}\left\{ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\} & \text{otherwise} 
\end{cases}
\]

If \( x > y \) or \( y > x \) (meaning that the intervals are disjoint), clearly these two sides have the same behavior. Thus the only remaining case is when \( x \) and \( y \) overlap, in which case we must show

\[
\text{hull}\{dx, dy\} \subseteq \text{hull}\left\{ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\} : \begin{bmatrix} dx \\ dy \end{bmatrix}
\]

By inspection, we see that the two sides are in fact equal.

\[\square\]

Smooth maps. For smooth maps like \( \times \), \( \sin \), \( \cos \), and \( \exp \), the derivative towers should simply reflect the known classical derivatives of these maps, and indeed they do.

F.3 Higher-order semantics

§5 defines a category \( \text{HAD} \) to give semantics to \( \lambda_S \), and defines the primitives of \( \lambda_S \) detailed in Fig. 2. The definitions of these primitives in the main text does not justify in detail that the definitions satisfy the necessary requirements in order to in fact belong to \( \text{HAD} \). In this section, we sketch those requirements and why they hold for the various primitives.

F.3.1 Primitive types. The only primitive type in the higher-order language is \( \mathbb{R} \). It is defined via the Yoneda embedding of \( \mathbb{R} \), giving a presheaf. We must know that this is a sheaf with respect to the open cover topology. It suffices to know the far more general property, that the open cover topology is subcanonical. This is true in \( \text{HAD} \) for the same reason that it is true in \( \text{Diff} \), the category of diffeological spaces and smooth maps.
F.3.2 Tangent bundles. In §5.2, we claim that valueWithDer is a functor, which we now prove:

**Proposition F.33.** valueWithDer is a functor.

**Proof.** We observe that
\[
\text{valueWithDer}(\text{id}) = \langle x, dx \vdash (\text{id}(x), [\text{id}]'(x, dx)) \rangle_{\text{AD}} = \langle x, dx \vdash (x, dx) \rangle_{\text{AD}},
\]
which is evidently the identity map. For compositions, we have
\[
\text{valueWithDer}(\text{g} \circ f) = \langle x, dx \vdash ((\text{g} \circ f)(x), (\text{g} \circ f)'(x, dx)) \rangle_{\text{AD}}
\]
\[
= \langle y, dy \vdash ([\text{g}](y), [\text{g}'](y, dy)) \rangle_{\text{AD}} \circ \langle x, dx \vdash ([f](x), [f'](x, dx)) \rangle_{\text{AD}}
\]
\[
= \text{valueWithDer}(\text{g}) \circ \text{valueWithDer}(f)
\]
\[\square\]

Note that the types to represent isomorphisms of tangent bundles are not necessarily isomorphisms: the type \(\text{just} \equiv \text{pairs of maps back and forth. The isomorphism tangent}_R: \text{Tan} \mathcal{R} \cong \mathcal{R} \times \mathcal{R} \) holds only when restricted to \(\mathcal{R}\), i.e., indeed \(\text{Tan}(\mathcal{R}) \cong \mathcal{R} \times \mathcal{R}\). Similarly, the mappings \(\text{tangentTo}_R A : \text{Tan} (A \to \mathcal{R}) \equiv (A \to \mathcal{R}) \times (A \to \mathcal{R})\) only give an isomorphism if we actually restrict to the type \(\mathcal{R}\) rather than \(\mathcal{R}\), because we for the isomorphism to hold, we need to know that \(x + 0 \cdot y = x\) for all \(y\), but if we allow \(y \in \mathcal{R} \setminus \mathcal{R}\), there is the counterexample \(x + 0 \cdot \perp = \perp\). The mapping \(\text{tangentProd} A B : \text{Tan} (A \times B) \equiv \text{Tan} A \times \text{Tan} B\) indeed defines an isomorphism when \(A\) and \(B\) are representable, since it only uses categorical operations that are preserved by the Kan extension.

F.3.3 Second-order primitives. In this section, we outline the properties that are required in order to confirm that each of the second-order primitives are indeed constants in HAD.

All second-order primitives are of type \((\mathcal{R} \to \mathcal{R}) \to \mathcal{R}\). Because sheafification preserves internal homs (i.e., exponentiation), and since the open cover topology is subcanonical, this means that the type \((\mathcal{R} \to \mathcal{R}) \to \mathcal{R}\) is be the same as it would be in the category of presheaves. In the category of presheaves, the set of these constants for this type is equivalent to the end
\[
\int_{\Gamma \in \text{AD}} (\Gamma \times \mathcal{R} \rightsquigarrow \mathcal{R}) \to (\Gamma \rightsquigarrow \mathcal{R}),
\]
which is just a natural transformation from the functor \(- \times \mathcal{R} \rightsquigarrow \mathcal{R}\) in \(\text{AD}^{\text{op}}\) to \(- \rightsquigarrow \mathcal{R}\) in \(\text{AD}^{\text{op}}\). We defined these second-order primitives with parametrically polymorphic mappings of derivative towers. We must confirm that these definitions preserve consistency, i.e., mapping consistent derivative towers to consistent derivative towers. But I think the main thing, really the only important and potentially problematic thing, to show is that each of these second-order primitives take consistent derivative towers to consistent derivative towers, i.e., they preserve consistency. In general, this boils down to confirming that taking the derivative of the value-level definitions of each of these primitives yields the definitions for the derivatives of these primitives. It is possible to confirm for each definition that this is the case.

F.4 Miscellaneous theorems

**Proposition F.34.** For all \(x \in \mathcal{R}^n\), \(0 + x = x\).

**Proposition F.35.** For any \(f : \mathcal{R}^m \to \mathcal{R}^n\),
\[
\partial \perp \text{Mat}_0 f = \partial \perp f,
\]
where on the right side $f$ is implicitly treated as having type $\mathbb{R}^m \to \mathbb{R}^n$, by restricting to $\mathbb{R}^m$ and mapping all nonmaximal elements to $\perp$.

**Proposition F.36 (Consistency for all derivatives).** Given any consistent derivative tower $f$, for all $k \in \mathbb{N}$, $\text{Cons}_{k+1} \left(f^{(k+1)}, \partial_{\perp}^{k+1} f^{(0)}\right)$.

**Proof.** By induction on $k$. Base case follows directly from the fact that $f$ is consistent. In the inductive case, we must prove the following:

- Given any consistent derivative tower $f : \mathbb{R}^n \to \mathbb{R}^m$, for all $k \in \mathbb{N}$, if $\text{Cons}_k \left(f^{(k)}, \partial_{\perp}^k \text{Mat}_0(f^{(0)})\right)$, then $\text{Cons}_{k+1} \left(f^{(k+1)}, \partial_{\perp}^{k+1} \text{Mat}_0(f^{(0)})\right)$.

We must prove that for all $x \in \mathbb{R}^n$ and for all $dx_1, \ldots, dx_{k+1} \in \mathbb{R}^n$,

$$f^{(k+1)}(x; dx_1, \ldots, dx_{k+1}) \subseteq (\partial_{\perp}^{k+1} \text{Mat}_0(f^{(0)}))(x) : (dx_1 \otimes \ldots \otimes dx_{k+1}).$$

We know by consistency of $f$ that $\text{Cons}_{k+1} \left(f^{(k+1)}, \partial_{\perp} \text{Mat}_k(f^{(k)})\right)$, meaning

$$f^{(k+1)}(x; dx_1, \ldots, dx_{k+1}) \subseteq \left(\partial_{\perp} \text{Mat}_k(f^{(k)})\right)(x) : (dx_1 \otimes \ldots \otimes dx_{k+1})$$

so what we must prove reduces to

$$\left(\partial_{\perp} \text{Mat}_k(f^{(k)})\right)(x) : (dx_1 \otimes \ldots \otimes dx_{k+1}) \subseteq (\partial_{\perp}^{k+1} \text{Mat}_0(f^{(0)}))(x) : (dx_1 \otimes \ldots \otimes dx_{k+1}).$$

It would suffice to know that

$$\partial_{\perp} \text{Mat}_k(f^{(k)}) \sqsubseteq \partial_{\perp}^{k+1} \text{Mat}_0(f^{(0)})$$

(where the $\sqsubseteq$ relation is defined on functions by pointwise application).

By Proposition F.37 (just below), it suffices to know precisely the hypothesis stated in the lemma. \hfill \Box

**Proposition F.37.** For all $k \in \mathbb{N}$, for all $g : \mathbb{R}^n \times (\mathbb{R}^n)^k \to \mathbb{R}^m$, for all $f : \mathbb{R}^n \to C(\mathbb{R}^n \times \mathbb{R}^m)$, if $\text{Cons}_k(g, f)$ holds, then

$$\partial_{\perp} \text{Mat}_k(g) \sqsubseteq \partial_{\perp} f$$

(where the $\sqsubseteq$ relation is defined on functions by pointwise application).

**Proof.** It suffices to know that the largest open set on which $\text{Mat}_k(g)$ is both defined (i.e., not $\perp$) and locally Lipschitz is included in the largest open set on which $f$ is singly defined (i.e., maximal) and locally Lipschitz, and that they are equal on this set.

To prove that, it suffices to know that whenever $\text{Mat}_k(g)$ is not $\perp$, $\text{Mat}_k(g)$ is equal to $f$, because then the largest open set where $\text{Mat}_k(g)$ is locally Lipschitz must be included in the largest open set where $f$ is locally Lipschitz.

This follows precisely from the definition of $\text{Mat}_k$, as we observe that if $\text{Mat}_k(g)$ is not $\perp$ at the point $x$, then $f(x)$ must be maximal and also agree exactly with $(\text{Mat}_k(g))(x)$. \hfill \Box