

A Language for Evaluating Derivatives of Functionals Using Automatic Differentiation

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Abstract. We present a simple functional programming language, called Dual PCF, that implements **forward mode automatic differentiation using dual numbers** in the framework of exact real number computation. The main new feature of this language is the ability to evaluate correctly up to the precision specified by the user – in a simple and direct way – the directional derivative of functionals as well as first order functions. In contrast to other comparable languages, Dual PCF also includes the recursive operator for defining functions and functionals. We provide a wide range of examples of Lipschitz functions and functionals that can be defined in Dual PCF. We use domain theory both to give a denotational semantics to the language and to prove the correctness of the new derivative operator using logical relations. To be able to differentiate functionals—including on function spaces equipped with their compact-open topology that do not admit a norm—we develop a domain-theoretic directional derivative that is Scott continuous and extends Clarke’s sub-gradient of real-valued locally Lipschitz maps on Banach spaces to real-valued continuous maps on Hausdorff topological vector spaces. Finally, we show that we can express arbitrary computable linear functionals in Dual PCF.

1 Introduction

In this paper, we describe a language for performing automatic differentiation on a wide set of functions, including higher-order functions and non-differentiable Lipschitz functions. This language combines the **dual numbers**—i.e., the algebra consisting of numbers of the form $a + b\varepsilon$ where a and b are real and $\varepsilon^2 = 0$ —with a domain-theoretic directional derivative which we introduce in this paper. The domain-theoretic directional derivative can properly and correctly handle higher-order functions and Lipschitz functions like the absolute value function or ReLU used in machine learning. The dual numbers are used to incorporate automatic differentiation into the language in a straightforward manner.

Due to its wide range of applications, automatic differentiation has been an active theoretical and practical area of research in recent years [28]. While there is a large body of work in the subject, automatic differentiation is not always

implemented in a sound and rigorous way. A standard example is the if-then-else constructor, ubiquitous in numerical programs, which gives incorrect results when evaluated in automatic differentiation software.

In this work, we develop a language, based on dual numbers and called Dual PCF, which has a rich set of definable functions. This set includes locally Lipschitz functions such as the absolute value function and ReLU that are not differentiable everywhere but are widely used in applications and have a set-valued generalised derivative called the Clarke subgradient, which generalises the classical gradient [12].

Several formal calculi, containing a primitive for evaluating the derivative of functions, have been proposed in the literature. All together, three main features distinguish our calculus from these other work: having a recursive operator in the language, the possibility to deal with functions that are not infinitely differentiable, and the ability to compute the derivative of functionals on real-valued functions. None of the existing languages accommodate all these three features together.

The recursive operator allows the recursive definition of functions on real numbers. Most of the programming languages in the literature, instead, assume the existence of a sufficiently rich set of basic functions over the real numbers and construct the other functions by composition, λ -abstraction, and test operator [3,4,32,38,53]. Since the recursive operator is missing, these languages are not Turing complete from the point of view of real number computation. In [38], it is claimed that the approach used in [46], together with other techniques, can be used to solve the problem of dealing with the recursive definition. However, the actual solution is left as future work.

To accommodate the recursive operator, the denotational semantics needs to describe partial elements, either in the form of partially defined functions over the real line as in [1,46] or as partial real numbers, as in the present work. The use of partial real numbers unifies our treatment of the derivative operator to the field of exact real number computation. Other approaches assume that real numbers form a basic type where the arithmetic operations can be computed in constant time, giving the exact result. Therefore, the computation on reals is idealised, and the problem of the infinitary nature of real numbers is wholly avoided.

A second aspect by which our work differs from existing work is that we also consider functions that are Lipschitz but not differentiable, such as the absolute value function, which plays a key role in all applications. The presence of non-differentiable functions makes the repeated application of derivative operator more complex. The calculi in [3,22] assume that all functions are infinitely differentiable; as a consequence, they cannot accommodate, in a coherent way, functions like absolute value or min (evaluating the minimum of two real numbers) that are Lipschitz but not everywhere differentiable. The formal languages developed in [1,46] accommodate a larger set of functions including the if-then-else constructor, but define a restricted domain for the input-values and only ensure the correct evaluation of the derivative in the restricted domain.

However, the main feature of our calculus is the ability to compute the derivative of functionals on real-valued functions. We therefore extend the mechanism of automatic differentiation to provide the directional derivative of functionals. To this end, we have developed a domain-theoretic Scott continuous directional derivative for real-valued functions on Hausdorff topological vector spaces that extends the Clarke subgradient to functionals defined on function spaces where the Scott topology does not admit a norm. In addition, we are able to reduce the problem of definability of linear functionals in the language to the definability of first-order functions.

Automatic differentiation on functionals has also been considered in [10,31,38,53]. In [10], an approach quite different from ours is used: functions on reals are represented through a base of Chebyshev polynomials, and thereby the directional derivative of a functional is evaluated. In [31,53] no recursive definition of functions on reals is possible and we have already commented on [38].

Because both recursion on real numbers and non-differentiable Lipschitz maps are included in our language, we cannot use the approach adopted by [32,53] in the denotational semantics, which creates a serious challenge for defining a denotational semantics as we undertake in this work. Here, we establish the correctness of the results given by automatic differentiation of higher-order functions and relate them to mathematical notions of derivatives.

The new domain-theoretic notion of directional derivative developed in the paper computes the support function of the well-established mathematical concept of the generalized Lebourg's subgradient which reduces, when this subgradient is a singleton, to the Gateaux derivative of real-valued maps on topological vector spaces. In contrast, in [53,32] the directional derivatives developed using category theory are not related to any established mathematical notions of differentiation on topological vector spaces. In this respect, in [32], Section 7.2., which has the title "Canonical derivatives of higher order functions?", concludes with the following remark: "We hope that an exploration of such techniques might lead to an appropriate notion of computable derivative, even for higher order functions." Thus, the authors leave the problem of defining a canonical notion of derivative for higher order functions as an open problem.

Dual PCF is simply a functional programming language with an extra basic type of dual numbers. In fact, dual numbers are at the basis of a standard approach to automatic differentiation, in which one evaluates the derivative of a function at a given point and along one variable. In our language, however, we show also that dual numbers can be used to obtain the directional derivative of a function in several variables, and the directional derivative of a functional. An important contribution is a formal proof of correctness for the computation of the directional derivative inside the language.

We also note that there exists a trick, well-known in functional analysis, to reduce the problem of evaluating the derivative of a functional along a given direction to the problem of evaluating the derivative of a first order function. Given a functional $F : (\mathbb{R} \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$, the derivative of F at $f : \mathbb{R} \rightarrow \mathbb{R}$ in the direction $g : \mathbb{R} \rightarrow \mathbb{R}$ can be reduced to evaluating the derivative of

$\lambda x.F(\lambda y.f(y) + x \cdot g(y))$. However, this technique has its own problems. Without an analysis of how functionals are described in automatic differentiation, there is no guarantee that the above technique will evaluate the derivative correctly. More specifically, our language contains higher-order primitives such as integration or supremum, and it is necessary to check that automatic differentiation is correctly implemented on these primitives. Furthermore, it is useful to be able to evaluate the derivative of a functional directly from the functional itself, without having to plunge the functional into another expression just to extract the derivative.

The wide range of applications of differentiation of functionals, some of which we elaborate in the paper, include: calculus of variations [42], numerical solution of differential equations using Newton's method over function spaces [10], optimal control theory which features some non-differentiable functions such as the absolute value function [13], physical applications in analytical mechanics, Lagrangian and Hamiltonian mechanics [54,29] and in quantum chemistry [50].

1.1 Related works

Several simple calculi with a derivative operator as a primitive have been presented in the literature. A few of these do not aim to implement automatic differentiation [22,16]. Forward-mode automatic differentiation is realized in [44,45,53].

In recent years, driven by application of reverse-mode automatic differentiation in deep learning, a series of formal calculi have been proposed, some of them based on reverse-mode automatic differentiation [11,23,43], others implementing both forward-mode and reverse-mode automatic differentiation [46]. In these works, correctness of automatic differentiation is proved in the context of first order languages [1], or higher order functional languages [3,11,23,38,43,46]. Calculi that use logical relations to prove the correctness of derivative evaluation, a key aspect of our work, are provided in [7,16]. In several of these works, the semantics of differentiation is given using a categorical setting, [3,31,43], in contrast to using the more concrete space of real numbers or its extension in domain theory. With the exception of [16,53], none of these formalisms use the notion of Clarke subgradient.

In the rest of this section, we recall the elementary facts about dual numbers followed by the basic domain-theoretic notions and results required in this paper. In Section 2, we develop the domain-theoretic generalization of Clarke's subgradient for topological vector spaces. In Section 3, we introduce the domain of dual numbers. In Section 4, we present the syntax of Dual PCF, with its denotational and operational semantics, and prove adequacy. In Section 5, a wide range of examples of functions and functionals definable in Dual PCF are presented. In section 6, we define the notion of local consistency between the real and dual part of a function on the dual domain. In Section 7, we show that the semantic interpretations of the functions definable in Dual PCF are locally consistent. Finally, in Section 8, we prove that all linear functionals on real functions that tend to zero at infinity are definable in Dual PCF.

1.2 Dual-number preliminaries

The dual numbers are one of only three 2-dimensional “number systems” that extend the real numbers ([34]). A dual number is an expression of the form $a + \varepsilon b$, where a and b are reals, and ε is a new type of imaginary number with $\varepsilon^2 = 0$.

The ε can also be thought of as representing some very small number ([9]). The number is not *so small* as to be zero, but it is small enough that its product with itself is zero. This leads to an intuitive picture where the dual numbers represent a one-dimensional number line where each number on that line is surrounded by a set of numbers which are infinitely close to it. We call the term a in $a + b\varepsilon$ the *standard part*, and the term b the *infinitesimal part*. This terminology is consistent with that of nonstandard analysis.

To appreciate the properties of dual numbers, let $f(x)$ be some polynomial. It is easy to check that

$$f(x + \varepsilon x') = f(x) + \varepsilon x' \cdot f'(x), \quad (1)$$

where f' is the derivative of f .

As a geometric interpretation, Equation (1) suggests that every function is “infinitesimally straight” ([9,36,49]). In other words, as you zoom into a point on a function’s graph, the function appears to straighten out. When one zooms into the “ ε level”, the function becomes *exactly* straight. This infinitesimal straight line is exactly equal to the tangent line.

On a purely algebraic level, the above equation shows that **the dual numbers are able to “accidentally” differentiate an arbitrary function**. This feature of the dual numbers can be used to “induce” a computer language into computing the derivative of a subroutine, essentially by exploiting operator overloading ([14]). This method is remarkable for not introducing any numerical approximations, and also for avoiding the exponential overhead of naive symbolic differentiation. The term for this method is “forward-mode automatic differentiation” ([30]).

All proofs of this paper are given in the Appendix.

2 Domain-theoretic directional derivative

We first present the elements of domain theory required in the paper; see [2] and [26] for basic references to domain theory. We denote the closure and interior of a subset S of a topological space by \overline{S} and S° respectively. For a map $f : A \rightarrow B$, we denote the image of any subset $S \subset A$ by $f[S]$. If $I \subset \mathbb{R}$ is a compact real interval, we write $I = [I^-, I^+]$.

A directed complete partial order D is a partial order in which every directed set $A \subset D$ has a lub (least upper bound) or supremum $\bigsqcup A$. The way-below relation \ll in a dcpo (D, \sqsubseteq) is defined by $x \ll y$ if whenever there is a directed subset $A \subset D$ with $y \sqsubseteq \bigsqcup A$, then there exists $a \in A$ with $x \sqsubseteq a$. A subset $B \subset D$ is a basis if for all $y \in D$ the set $\{x \in B : x \ll y\}$ is directed with lub y . By a *domain* we mean a dcpo with a basis. Domains are also called continuous dcpo’s. If D has a countable base then it is called a countably based domain.

In a domain D with basis B , we have the interpolation property: The relation $x \ll y$, for $x, y \in D$, implies there exists $z \in B$ with $x \ll z \ll y$. A subset $A \subset D$ is *bounded* if there exists $d \in D$ such that for all $x \in A$ we have $x \sqsubseteq d$. If a pair of elements $d_1, d_2 \in D$ are bounded above (consistent), we write $d_1 \uparrow d_2$ and refer to the predicate \uparrow as the *consistency relation*. If any bounded subset of D has a lub then D is called bounded complete. In particular a bounded complete domain has a bottom element \perp that is the lub of the empty subset. A bounded complete domain D has the property that any non-empty subset $S \subset D$ has an infimum or greatest lower bound $\bigwedge S$. All domains in this paper are bounded complete and countably based.

The set of non-empty compact intervals of the real line ordered by reverse inclusion and augmented with the whole real line as bottom is the prototype bounded complete domain for real numbers denoted by \mathbb{IR} , in which $I \ll J$ iff $J \subset I^\circ$. It has a basis consisting of all intervals with rational endpoints. For two compact intervals I and J , their infimum $I \sqcap J$ is simply the convex closure of $I \cup J$. The Scott topology on a domain D with basis B has sub-basic open sets of the form $\uparrow b := \{x \in D : b \ll x\}$ for any $b \in B$. The upper set of an element $x \in D$ is given by $\uparrow x = \{y \in D : x \sqsubseteq y\}$. The lattice of Scott open sets of a bounded complete domain is continuous. The basic Scott open sets for \mathbb{IR} are of the form $\{J \in \mathbb{IR} : J \subset I^\circ\}$ for any $I \in \mathbb{IR}$. The maximal elements of \mathbb{IR} are the singletons $\{x\}$ for $x \in \mathbb{R}$ which we identify with real numbers as the mapping $x \mapsto \{x\}$ is a topological embedding when \mathbb{R} is equipped with its Euclidean topology and \mathbb{IR} with its Scott topology. Similarly, $\mathbb{I}[a, b]$ is the domain of non-empty compact intervals of $[a, b]$ ordered with reverse inclusion.

If X is any topological space with some open set $O \subset X$ and $d \in D$ lies in the domain D , then the single-step function $d\chi_O : X \rightarrow D$, defined by $d\chi_O(x) = d$ if $x \in O$ and \perp otherwise, is a Scott continuous function. The partial order on D induces by point-wise extension a partial order on continuous functions of type $X \rightarrow D$ with $f \sqsubseteq g$ if $f(x) \sqsubseteq g(x)$ for all $x \in X$. For any two bounded complete domains D and E , the function space $(D \rightarrow E)$ consisting of Scott continuous functions from D to E with the extensional order is a bounded complete domain with a basis consisting of lubs of bounded and finite families of single-step functions. If the lattice ΩX of open sets of X is a domain and if D is a bounded complete domain then for any continuous function $f : X \rightarrow D$ we have $d\chi_O \ll f$ iff $O \ll_{\Omega X} f^{-1}(\uparrow d)$. [26, Proposition II-4.20(iv)].

Proposition 1. [26, Exercise II-3.19] *If $h : A \subset Y \rightarrow D$ is any map from a dense subset A of a topological space Y into a bounded complete domain D , then its envelope*

$$h^* : Y \rightarrow D$$

given by $h^(x) = \bigsqcup \{\bigsqcap h[O] : x \in O \text{ open}\}$ is a continuous map with $h^*(x) \sqsubseteq h(x)$, and in addition $h^*(x) = h(x)$ if h is continuous at $x \in A$. Moreover, h^* is the greatest continuous function $p : Y \rightarrow D$ with $p(x) \sqsubseteq h(x)$ for all $x \in Y$.*

Since $\mathbb{R} \subset \mathbb{IR}$ is dense, any continuous map $f : \mathbb{R} \rightarrow \mathbb{R} \subset \mathbb{IR}$, considered as a continuous map $f : \mathbb{R} \rightarrow \mathbb{IR}$, has a maximal extension $f^* : \mathbb{IR} \rightarrow \mathbb{IR}$ given by $f^*(x) = f[x]$. We also have the following result.

Proposition 2. *The set of functions*

$$\{f^* : \mathbb{IR} \rightarrow \mathbb{IR} : f \in (\mathbb{R} \rightarrow \mathbb{R})\}$$

is dense in $(\mathbb{IR} \rightarrow \mathbb{IR})$ with respect to the Scott topology.

In this paper, we construct a language for differentiation of functions of first-order and functionals of second-order. The input and output of these functions and functionals will be given by bounded complete domains whose set of maximal elements consists of real numbers, in the case of functions, or contains the continuous real-valued functions, in the case of functionals. We will first study the topological properties of the space of first-order real-valued functions in this section.

2.1 Scott topologies on function spaces

The space of maximal elements of a bounded complete domain, equipped with its relative Scott topology, is Hausdorff [33] and is in fact a complete separable metrisable space [39]. Moreover, the domains encountered in this paper are constructed from \mathbb{IR} by using Cartesian product and function space construction, and therefore they inherit the operations for addition and scalar multiplication from interval arithmetic operations on \mathbb{IR} ; e.g., for $f, g : \mathbb{IR} \rightarrow \mathbb{IR}$ we have $f + g : \mathbb{IR} \rightarrow \mathbb{IR}$, with $(f + g)(x) = f(x) + g(x)$, where $f(x) + g(x)$ is the sum of two intervals $f(x)$ and $g(x)$.

As a major example that we work with in this paper, consider the function space $(\mathbb{R} \rightarrow \mathbb{R})$ of all continuous real-valued functions on the real line. This function space is a real vector space with the usual operations of addition of functions and multiplication by real numbers. It is in one to one correspondence with the subset of functions in the maximal elements of the bounded complete domain $(\mathbb{IR} \rightarrow \mathbb{IR})$ consisting of the maximal extensions of continuous real-valued functions. This subset of maximal elements inherits the relative Scott topology from the domain, but does not admit a norm (Proposition 4).

The compact-open topology on the function space $(Y \rightarrow Z)$, the collection of all continuous functions between topological spaces Y and Z , has sub-basic open sets of the form

$$U(C, O) := \{f : Y \rightarrow Z : f[C] \subset O\},$$

for any compact subset $C \subset Y$ and open $O \subset Z$ [19]. There is a simple characterisation of the compact-open topology for the function space $(\mathbb{R} \rightarrow \mathbb{R})$ or $([0, 1] \rightarrow \mathbb{R})$.

Lemma 1. *The compact-open topology on $(\mathbb{R} \rightarrow \mathbb{R})$ is generated by the sub-basis consisting of subsets of the form $U(\overline{O_1}, O_2)$ where O_1 and O_2 are open intervals with compact closures.*

Let $\text{Max}(D)$ denote the set of maximal points of a bounded complete domain D and let $(_)^* : (\mathbb{R} \rightarrow \mathbb{R}) \rightarrow (\mathbb{IR} \rightarrow \mathbb{IR})$ be the maximal extension (envelope) operator given in Proposition 1, where $(\mathbb{R} \rightarrow \mathbb{R})$ is equipped with the compact-open topology.

Proposition 3. *The map $(\cdot)^*$ is a topological embedding, i.e. it is injective, continuous and is an open map onto its image in $\text{Max}(\mathbb{R} \rightarrow \mathbb{R})$ with respect to the relative Scott topology on $\text{Max}(\mathbb{R} \rightarrow \mathbb{R})$.*

The function space $(\mathbb{R} \rightarrow \mathbb{R})$, equipped with the compact-open topology, is an example of a Hausdorff topological vector space. Recall that a Hausdorff topological vector space is a vector space with a Hausdorff topology with respect to which addition of vectors and scalar multiplication are continuous operations.

Proposition 4. *The function space $(\mathbb{R} \rightarrow \mathbb{R})$ equipped with the compact-open topology does not admit a norm.*

We make two additional remarks here. The sup norm topology on the function space $([0, 1] \rightarrow \mathbb{R})$ coincides with the compact-open topology as is easy to check. However, the compact-open topology on the function space $(\mathbb{R} \rightarrow_b \mathbb{R})$, the set of bounded continuous maps, is strictly weaker than the sup norm topology [19, p. 284]. The same is true for the space $C_0(\mathbb{R}) := (\mathbb{R} \rightarrow_0 \mathbb{R})$, the set of continuous maps of type $\mathbb{R} \rightarrow \mathbb{R}$ that vanish at infinity.

Therefore, for computational reasons, we will work with Hausdorff topological vector spaces which are more general than normed vector spaces and give a unifying framework for function spaces as well as the more basic finite dimensional Euclidean spaces we consider in this paper.

Finally, we have the following result which follows from Proposition 2. Consider the function space $(\mathbb{R} \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ with its compact-open topology.

Corollary 1. *Any continuous functional $F : (\mathbb{R} \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ has a continuous extension $F^* : (\mathbb{R} \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ obtained by first extending F by $F(f^*) = F(f)$ for any $f \in (\mathbb{R} \rightarrow \mathbb{R})$, which defines F on a dense subset of $(\mathbb{R} \rightarrow \mathbb{R})$.*

2.2 Directional derivative: topological vector spaces

Let $f : X \rightarrow \mathbb{R}$ be a continuous map on a Banach space X , a complete normed vector space. The *generalised directional derivative* of f at x in the direction of $v \in X$ is defined as the extended real number: [12, p. 25]³

$$f^\circ(x; v) := \limsup_{y \rightarrow x, t \rightarrow 0^+} \frac{f(y + tv) - f(y)}{t}. \quad (2)$$

There is a rich theory of generalised subgradient for a real-valued locally Lipschitz function $f : X \rightarrow \mathbb{R}$. For f to be locally Lipschitz, it means that for any $x \in X$, there exists an open neighbourhood $O \subset X$ of x and a constant $k > 0$ such that $|f(x_1) - f(x_2)| \leq k\|x_1 - x_2\|$ for all $x_1, x_2 \in O$. In particular, for such functions the generalised directional derivative is always a real number.

³ For a topological space Y and function $g : Y \rightarrow \mathbb{R}$, recall that the limit superior $\limsup_{u \rightarrow v} g(u)$ is defined as the unique $a \in [-\infty, \infty]$ with the following two properties: (i) for all $\epsilon > 0$, there exists an open neighbourhood O of v such that $g(x) \leq a + \epsilon$ for all $x \in O$, (ii) for all $\epsilon > 0$ and all neighborhood O of v there exists $x \in O$ with $a - \epsilon < g(x)$. Dually we have the definition of limit inferior \liminf .

Let X^* be the dual of X : the space of all continuous linear functionals $A : X \rightarrow \mathbb{R}$ equipped with the weak* topology, i.e., the weakest topology on X^* that makes all the linear functionals $\hat{x} : X^* \rightarrow \mathbb{R}$ with $\hat{x}(A) = A(x)$ continuous for any $x \in X$. The *Clarke subgradient* $\partial_c f(x) \subset X^*$ of f at $x \in X$ is defined as

$$\partial_c f(x) = \{A \in X^* : f^\circ(x; v) \geq A(v), \text{ for all } v \in X\}, \quad (3)$$

which is a non-empty convex and weak* compact subset of X^* [12, 2.1.2]. E.g., when $X = \mathbb{R}$ and $f(x) = |x|$,

$$f^\circ(x; v) = \begin{cases} v & x > 0 \\ -v & x < 0 \\ |v| & x = 0 \end{cases} \quad \partial_c f(x) = \begin{cases} \{1\} & x > 0 \\ \{-1\} & x < 0 \\ [-1, 1] & x = 0 \end{cases}$$

The generalised directional derivative $f^\circ(x, \cdot) : X \rightarrow \mathbb{R}$ is the *support function* of the convex set $\partial_c f(x)$, i.e., $f^\circ(x; v) = \sup\{A(v) : A \in \partial_c f(x)\}$ [12, p. 28]. The Clarke subgradient satisfies a weaker calculus compared with the classical gradient; e.g., we have the following subadditivity property: $\partial_c(f + g)(x) \subset \partial_c f(x) + \partial_c g(x)$ [12, p. 39]. For example if $X = \mathbb{R}$ and $f(x) = |x|$ and $g(x) = -|x|$, then $\partial_c(f + g)(0) = 0$, whereas $\partial_c f(0) + \partial_c g(0) = 2[-1, 1]$.

Since the function spaces we deal with—such as the space $(\mathbb{R} \rightarrow \mathbb{R})$ of all real-valued continuous functions of a real variable with its compact-open topology—may not admit a norm, we will develop and adopt a domain-theoretic directional derivative for real-valued maps on Hausdorff topological spaces and obtain its calculus and properties that generalise those for Banach spaces. In the case of the so-called locally Lipschitzian maps, as we will see, the domain-theoretic directional derivative is equivalent to that given in [41], which itself is a generalisation of the Clarke construction. From now on in this section, we consider a real-valued continuous map $f : X \rightarrow \mathbb{R}$ on a Hausdorff topological vector space X .

Recall the following notions [12, p. 30] of derivatives of functions which also hold on topological vector spaces. A map $f : X \rightarrow \mathbb{R}$ has a (one-sided) *directional derivative* at x in the direction of x' if $\lim_{r \rightarrow 0^+} \frac{f(x + rx') - f(x)}{r}$ exists, in which case we write $f'(x; x') = \lim_{r \rightarrow 0^+} \frac{f(x + rx') - f(x)}{r}$. We say f has *Gateaux derivative* at $x \in X$ if there exists a continuous linear functional $Df(x, -) \in X^*$ such that for all $x' \in X$, the directional derivative of f at x in the direction x' exists and is given by $Df(x, x')$, i.e., $Df(x, x') = f'(x; x')$.

Given $x' \in X$ we aim to define a domain-theoretic directional derivative of f in the direction of x' at a point $x \in X$, which gives the organising tool for deriving the classical directional derivative of f .

Definition 1. The domain-theoretic directional derivative $Lf : X \times X \rightarrow \mathbb{IR}$ of $f : X \rightarrow \mathbb{R}$ at $x \in X$ in the direction $x' \in X$ is defined as, $Lf(x, x') :=$

$$\left[\liminf_{\substack{y \rightarrow x, z \rightarrow x' \\ r \rightarrow 0^+}} \frac{f(y + rz) - f(y)}{r}, \limsup_{\substack{y \rightarrow x, z \rightarrow x' \\ r \rightarrow 0^+}} \frac{f(y + rz) - f(y)}{r} \right],$$

if both endpoints above are real numbers; otherwise define $Lf(x, x') = (-\infty, \infty)$. We say $Lf(x, x')$ is bounded if it is a compact (i.e., non-bottom) interval.

If X admits a norm (e.g. $X = \mathbb{R}$) with respect to which f is Lipschitz, then $Lf(x, x')$ is a non-empty compact interval. In fact, for $r > 0$, we then have:

$$\frac{|f(y + rz) - f(y)|}{r} \leq k\|z\|$$

where $k \geq 0$ is a Lipschitz constant for f , and thus $Lf(x, x') \subseteq [-k\|x'\|, k\|x'\|]$.

Lemma 2. $Lf : X \times X \rightarrow \mathbb{IR}$ is Scott continuous.

Proposition 5. If $Lf(x, x')$ is a point for some $x \in X$ and some $x' \in X$, then f has a directional derivative at x and x' given by $f'(x; x') = Lf(x, x')$.

Using the basic rules for limit superiors and limit inferiors of sequences, one can easily deduce the following homogenous, sublinear, subadditive and submultiplicative calculus rules for all continuous $f, g : X \rightarrow \mathbb{R}$ and $x, x', y, z \in X$ with $t \in \mathbb{R}$:

$$\begin{aligned} Lf(x, tx') &= tLf(x, x') \\ Lf(x, y) + Lf(x, z) &\subseteq Lf(x, y + z) \\ Lf(x, x') + Lg(x, x') &\subseteq L(f + g)(x, x') \\ g(x)Lf(x, x') + f(x)Lg(x, x') &\subseteq L(f \cdot g)(x, x') \end{aligned}$$

Finally, we have the following chain rule which is weaker than the classical chain rule and generalises the corresponding rule when X is a Banach space [12, 2.3.9].

Proposition 6. (The Chain rule.) For continuous functions $h : X \rightarrow \mathbb{R}^n$ and $g : \mathbb{R}^n \rightarrow \mathbb{R}$, with $f = g \circ h : X \rightarrow \mathbb{R}$, we have:

$$(Lg)^*(h(x), Lh(x, x')) \subseteq Lf(x, x'), \quad (4)$$

where $(x, x') \in X \times X$ and $(Lg)^* : \mathbb{R}^n \times \mathbb{IR}^n \rightarrow \mathbb{IR}$ is the maximal extension (envelope) of Lg in its second component, while $Lh(x, x') = \times_{i=1}^n Lh_i(x, x')$.

To have a counterpart for Clarke's subgradient, we would require more conditions. As in [41], we define a notion of local Lipschitzian function that coincides with the usual notion of a locally Lipschitz map when X admits a norm. We say $Lf : X \times X \rightarrow \mathbb{IR}$ is bounded in the open set $O \times O' \subset X \times X$ if there exists a compact interval $C \in \mathbb{IR}$ such that $C \subseteq Lf(x, x')$ for all $(x, x') \in O \times O'$.

Definition 2. We say $f : X \rightarrow \mathbb{R}$ is locally Lipschitzian at $x \in X$ if there exists an open neighbourhood $O \subset X$ of x and an open neighbourhood O' of the origin such that the generalised directional derivative $Lf(-, -) : X \times X \rightarrow \mathbb{IR}$ is bounded for $(x, x') \in O \times O'$.

The simplest case is when $X = \mathbb{R}$ and we have:

Proposition 7. *If $f : \mathbb{R} \rightarrow \mathbb{R}$ and $Lf(x, x')$ is bounded at a point $(x, x') \in \mathbb{R}^2$, then f is locally Lipschitzian and locally Lipschitz at x .*

More generally, as we will see in Corollary 2, if X is normed any locally Lipschitzian map is locally Lipschitz.

We use the notation in Equation (2), defined for a continuous real-valued function on a Banach space, for continuous maps on a topological vector space. From now, assume $f : X \rightarrow \mathbb{R}$ is locally Lipschitzian.

Proposition 8. [41, 1.5] *If $f : X \rightarrow \mathbb{R}$ is locally Lipschitzian, then for each $x \in X$ the set*

$$\partial f(x) := \{A \in X^* : \forall x' \in X. A(x') \leq f^\circ(x; x')\}$$

is a non-empty, convex and weak compact subset of X^* . The map $\partial f : X \rightarrow \mathbf{C}(X^*)$, where $\mathbf{C}(X^*)$ is the set of non-empty weak* compact, convex subsets of X^* ordered by reverse inclusion, is upper semi-continuous; any $x \in X$ has a neighbourhood sent by ∂f to a weak* compact set.*

The non-empty, convex and weak* compact set $\partial f(x)$ is called the *generalised subgradient* of f at x . By its weak* compactness, for any $x' \in X$ the set $\{A(x') : A \in \partial f(x)\} \subset \mathbb{R}$ will be a compact interval, a key requirement for our denotational semantics later on. It generalises Clarke's subgradient of a real-valued locally Lipschitz map on a Banach space as defined in Equation (3) to real-valued locally Lipschitzian functions on topological vector spaces. Note that if $X = \mathbb{R}$ and $f : \mathbb{R} \rightarrow \mathbb{R}$, then $Lf(x, -) = \partial f(x)$.

Theorem 1. *Suppose $f : X \rightarrow \mathbb{R}$ is locally Lipschitzian.*

- (i) $Lf(x, x') = \{A(x') : A \in \partial f(x)\}$.
- (ii) *If $Lf(x, x')$ is a point for some $x \in X$ and all $x' \in X$, then f has a Gateaux derivative at x given by $Df(x, -) = Lf(x, -) : X \rightarrow \mathbb{R}$.*
- (iii) *If $Lf(x, x')$ is a point for x in an open set $O \subseteq X$ and all $x' \in X$, then the map $Df(-, -) : O \rightarrow X^*$ with $x \mapsto Df(x, -)$ is continuous with respect to the weak* topology on X^* .*
- (iv) *If X is a finite dimensional Euclidean space and $Lf(x, x')$ is a point for x in an open set $O \subseteq X$ and all $x' \in X$, then f is differentiable in O with $f'(x) = Df(x, -)$ for $x \in O$.*

Item (i), says that for a locally Lipschitzian map f , the domain-theoretic directional derivative Lf factors out with respect to its two components as for a classical differentiable map, and that $f^\circ(x; -) : X \rightarrow \mathbb{R}$ is the support function of $\partial f(x)$ as in the case when X is a Banach space.

We finally state the mean-value theorem below from [41]. For $a, b \in X$, the closed and open line segments are defined respectively as $[a, b] := \{(1-t)a + tb : 0 \leq t \leq 1\}$ and $(a, b) := \{(1-t)a + tb : 0 < t < 1\}$.

Theorem 2. (Mean value theorem) [41, Theorem 1.7] *Suppose $f : X \rightarrow \mathbb{R}$ is a locally Lipschitzian function defined on an open set $O \subset X$ which contains the line segment $[a, b]$. Then, there exist $t \in (a, b)$ and $M \in \partial f(t)$ such that $f(a) - f(b) = M(a - b)$.*

Corollary 2. *If X admits a norm then a locally Lipschitzian map is locally Lipschitz and its generalised subgradient coincides with the Clarke subgradient.*

3 Domain of dual number intervals

This section introduces a hierarchy of continuous domains for dual numbers, \mathbb{D}_τ , and defines a family of mapping, $(-)_\tau^{\mathbf{d}}$, that embeds the spaces of functions on real numbers and those of functionals on functions into these domains. The domain-theoretic directional derivative of a function f on reals defines the *infinitesimal* part of $(f)_\tau^{\mathbf{d}}$. On the other hand, we define two families of maps, $(-)_\tau^{\mathbf{s}}$ and $(-)_\tau^{\mathbf{i}}$, that *extract*, from a *total* function g on \mathbb{D}_τ , the function f on real numbers that g represents as well an infinitesimal perturbation of f that is used in the computation of directional derivatives.

The maps $(-)_\tau^{\mathbf{d}}$, $(-)_\tau^{\mathbf{s}}$, and $(-)_\tau^{\mathbf{i}}$ are given on a limited hierarchy of types τ formally defined by the following. We define *first-order function types* to be the types having the form $\delta \rightarrow (\dots \rightarrow (\delta \rightarrow \delta))$, and *second-order function types* to be the types having the form $\tau_1 \rightarrow (\dots \rightarrow (\tau_n \rightarrow \delta) \dots)$ with τ_1, \dots, τ_n either a first-order function type or equal to δ . Notice that, by the above definition, a first-order function type is always a second-order function type. We define a *first-order function* to be a function f having first-order function type. We define a *second-order function*, or a *functional*, to be a function F having a strictly second-order function type. By uncurrying, a first-order function f can be seen to take n dual values and return a dual value.

The domain for dual number, \mathbb{DR} , is the domain $\mathbb{IR} \times \mathbb{IR}$. The first component is the standard part of a dual number (albeit interval valued instead of single-valued) and the second component is the infinitesimal part. The domains and codomains of the maps, $(-)_\tau^{\mathbf{d}}$, $(-)_\tau^{\mathbf{s}}$, and $(-)_\tau^{\mathbf{i}}$ are defined by the following.

Definition 3. *By induction on the structure of a second-order function type τ , we define the following families of topological spaces:*

- $\mathbb{R}_\delta = \mathbb{R}$ and $\mathbb{R}_{\tau_1 \rightarrow \tau_2}$ is the topological vector space of continuous functions from \mathbb{R}_{τ_1} to \mathbb{R}_{τ_2} with the compact-open topology;
- $\mathbb{R}_\delta^p = \mathbb{IR}$ and $\mathbb{R}_{\tau_1 \rightarrow \tau_2}^p$ is the topological space of continuous functions from \mathbb{R}_{τ_1} to $\mathbb{R}_{\tau_2}^p$ with the Scott topology;
- $\mathbb{D}_\delta = \mathbb{DR}$ and $\mathbb{D}_{\tau_1 \rightarrow \tau_2}$ is the bounded complete domain $(\mathbb{D}_{\tau_1} \rightarrow \mathbb{D}_{\tau_2})$;
- \mathbb{D}_δ^t is the subset of \mathbb{DR} containing elements whose standard part is total, i.e., maximal; $\mathbb{D}_{\tau_1 \rightarrow \tau_2}^t$ is the subset of $\mathbb{D}_{\tau_1 \rightarrow \tau_2}$ containing functions mapping all elements in $\mathbb{D}_{\tau_1 \rightarrow \tau_2}^t$ to elements in $\mathbb{D}_{\tau_2}^t$. Functions in \mathbb{D}_τ^t are called standard maximal preserving.

Notice that, equipped with the compact-open topology, the topological vector space $\mathbb{R}_{\tau_1 \rightarrow \dots \rightarrow \tau_n \rightarrow \delta}$ is homeomorphic to the space $(\mathbb{R}_{\tau_1} \times \dots \times \mathbb{R}_{\tau_n}) \rightarrow \mathbb{R}_\delta$ [19, p. 261]. Moreover, the space of maximal elements of the listed bounded complete domains, in Definition 3, equipped with their relative Scott topology will be Polish, and hence Hausdorff topological vector spaces ([39]) and thus the results at the end of Section 2, and proved in [17, sections 2.1, 2.2], can be used.

Definition 4. The functions: $(_)_{\tau}^{\mathbf{d}} : \mathbb{R}_{\tau} \rightarrow \mathbb{D}_{\tau}^t$, $(_)_{\tau}^{\mathbf{s}} : \mathbb{D}_{\tau}^t \rightarrow \mathbb{R}_{\tau}$, $(_)_{\tau}^{\mathbf{i}} : \mathbb{D}_{\tau}^t \rightarrow \mathbb{R}_{\tau}^p$ are inductively defined on the type τ by:

$$(x)_{\delta}^{\mathbf{d}} := x + \varepsilon 0 \quad (x + \varepsilon x')_{\delta}^{\mathbf{s}} := x \quad (x + \varepsilon x')_{\delta}^{\mathbf{i}} = x' \text{ and}$$

and by:

$$\begin{aligned} (f)_{\vec{\tau} \rightarrow \delta}^{\mathbf{d}} &= h^* \text{ with } h : \mathbb{D}_{\tau_1}^t \rightarrow \dots \rightarrow \mathbb{D}_{\tau_n}^t \rightarrow \mathbb{D}\mathbb{R} \text{ defined by:} \\ h(\vec{d}) &= f(\overrightarrow{(d)^{\mathbf{s}}}) + \varepsilon((Lf)^*(\overrightarrow{(d)^{\mathbf{s}}}, \overrightarrow{(d)^{\mathbf{i}}})) \\ (g)_{\vec{\tau} \rightarrow \delta}^{\mathbf{s}}(\vec{x}) &= (g(\overrightarrow{(x)^{\mathbf{d}}}))_{\delta}^{\mathbf{s}} \quad (g)_{\vec{\tau} \rightarrow \delta}^{\mathbf{i}}(\vec{x}) = (g(\overrightarrow{(x)^{\mathbf{d}}}))_{\delta}^{\mathbf{i}}, \end{aligned}$$

where $(_)^*$ is the envelope operator of Proposition 1. In defining h , we need to use the envelope $(Lf)^*$ because $(d_i)^{\mathbf{i}}$ can be a partial real number, or a function returning partial real numbers. Since the topological space \mathbb{D}_{δ}^t is dense in \mathbb{D}_{δ} , by an obvious generalization of Proposition 2, for any first order type τ , \mathbb{D}_{τ}^t is dense in \mathbb{D}_{τ} ; it follows by Proposition 1 that the envelope h^* exists for both first order and second order functions. The definition of $(_)_{\tau}^{\mathbf{d}}$ can be seen as extension of the construction in [17, Corollary 1] for extending a functional of type $(\mathbb{R} \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ to $(\mathbb{I}\mathbb{R} \rightarrow \mathbb{I}\mathbb{R}) \rightarrow \mathbb{I}\mathbb{R}$.

Proposition 9. For any second order type $\tau = \vec{\tau}^i \rightarrow \delta$, functionals $f_1, f_2 \in \mathbb{R}_{\tau}$ and list of values $\vec{x}_1, \vec{x}_2 \in \mathbb{R}_{\vec{\tau}}$, by the infinitesimal property of ε , we have:

- (i) $f_1 = ((f_1)_{\tau}^{\mathbf{d}} + \varepsilon(f_2)_{\tau}^{\mathbf{d}})_{\tau}^{\mathbf{s}}$
- (ii) $f_2 = ((f_1)_{\tau}^{\mathbf{d}} + \varepsilon(f_2)_{\tau}^{\mathbf{d}})_{\tau}^{\mathbf{i}}$
- (iii) $Lf_1 \vec{x}_1 \vec{x}_2 = ((f_1)_{\tau}^{\mathbf{d}}(\overrightarrow{(x_1)^{\mathbf{d}}}) + \varepsilon \overrightarrow{(x_2)^{\mathbf{d}}})_{\delta}^{\mathbf{i}}$

Note that for first-order types τ , the functions $(_)_{\tau}^{\mathbf{d}}$ are just set-theoretic functions since they are not continuous functions on the infinitesimal component. In the above and in the following, we use the point-wise extension of the multiplication by the dual number ε , and the addition operation $+$. That is, if $*$ is an operation defined on the domain D , the operation $*$ on the domain $C \rightarrow D$, is defined by:

$$(f_1 * f_2)(c) = f_1(c) * f_2(c)$$

and similarly for other operations and functions.

In the following, we will sometimes omit the type τ from $(_)_{\tau}^{\mathbf{d}}$, $(_)_{\tau}^{\mathbf{s}}$, $(_)_{\tau}^{\mathbf{i}}$ when the type of τ is clear from the context. We will also implicitly assume, where necessary, that any real number is automatically “cast” to a dual number.

Denote by St and In the envelopes of the functions $(_)_{\delta}^{\mathbf{s}}$ and $(_)_{\delta}^{\mathbf{i}}$ respectively. They are functions in $\mathbb{D}\mathbb{R} \rightarrow \mathbb{I}\mathbb{R}$ defined by: $\text{St}(x + \varepsilon x') = x$, $\text{In}(x + \varepsilon x') = x'$.

4 A language for differentiable functionals

Next we present Dual PCF, a language with a primitive operator for the evaluation of directional derivatives of functionals. The language is a simply typed λ -calculus extended with a suitable set of constants.

The types of the Dual PCF are defined by the grammar:

$\tau ::= o \mid \nu \mid \pi \mid \delta \mid \tau \rightarrow \tau$, where o is the type of booleans, ν is the type of natural numbers, π is the type of real numbers, and δ is the type of dual numbers. The derivative operator is defined only on the type of dual numbers δ . We assign to variable x the type π if we are not interested in evaluating the derivative with respect to x ; values of type π have implicitly an infinitesimal part equal to 0.

The set of expressions in the language is defined by the grammar:

$$e ::= c \mid x^\tau \mid e_1 e_2 \mid \lambda x^\tau. e \quad (5)$$

where x^τ ranges over a set of typed variables and c over a set of constants. For simplicity, here we present only a minimal set of basic constants, sufficient to express any other computable function. In a real programming language this minimal set will be extended with other functions. All constants defining functions on dual numbers, for example $\max : \delta \rightarrow \delta \rightarrow \delta$ have a corresponding version on real numbers $\max : \pi \rightarrow \pi \rightarrow \pi$, acting in the obvious way. To avoid repetition, we present just the dual number versions, implicitly assuming the definition for the real number version.

The basic constants in the language are:

- the three total arithmetic operations, $+, -, * : \delta \rightarrow \delta \rightarrow \delta$;
- division by a positive natural number, $/ : \delta \rightarrow \nu \rightarrow \delta$;
- minimum and maximum $\min, \max : \delta \rightarrow \delta \rightarrow \delta$, evaluating the minimum and maximum of two dual numbers;
- two casting functions (explicit conversion), from naturals to reals $\text{in}_\pi : \nu \rightarrow \pi$, and from reals to duals $\text{in}_\delta : \pi \rightarrow \delta$;
- a zero-test on reals $(0 <) : \pi \rightarrow o$, that cannot be applied to dual values. This restriction assures that functions on dual numbers do not have points of discontinuity on maximal elements. For example, a function, from dual values to dual values, returning 0 on strictly negative values and 1 on strictly positive values, will not be definable. This fact, in turn, is necessary to guarantee the correctness of the derivative operator.
- A projection function $\text{pr} : \delta \rightarrow \delta$, projecting a value on the unit interval $[-1, 1]$. On real values, the behaviour of pr is defined by $\text{pr}(x) = \max(-1, \min(x, 1))$.
- An integration functional $\text{int}_\delta : (\pi \rightarrow \delta) \rightarrow \delta$, giving the Riemann integral of a function on the interval $[0, 1]$,
- A supremum functional, $\text{sup} : (\pi \rightarrow \delta) \rightarrow \delta$, evaluating the supremum of functions in the interval $[0, 1]$,
- For second-order function types, $\tau = \vec{\tau} \rightarrow \delta$, a directional derivative operator $L_{\vec{\tau}} : ((\tau \rightarrow \vec{\tau}_\pi \rightarrow \vec{\tau}_\pi \rightarrow \pi))$. Each type τ_i in the list $\vec{\tau}$ must be equal to δ , or be a first order type, in the form $\sigma_1 \rightarrow \dots \sigma_n \rightarrow \delta$, with σ_1 a ground type, while the type τ_π is recursively defined by $\delta_\pi = \pi$ and $(\sigma_1 \rightarrow \dots \sigma_n \rightarrow \delta)_\pi = \sigma_1 \rightarrow \dots \sigma_n \rightarrow \pi$. Given a function f in several arguments and returning a dual number, $L_{\vec{\tau}} f \vec{x} \vec{y}$ evaluates the derivative of f at \vec{x} along the direction \vec{y} . In the expression $L_{\vec{\tau}} f \vec{x} \vec{y}$, we need to add the syntactic condition that the derivative operator L does not appear inside $f \vec{x} \vec{y}$.

– The standard PCF constants on natural numbers, a sequential if-then-else test function and a fixed-point operator on arbitrary types $Y_\tau : (\tau \rightarrow \tau) \rightarrow \tau$.

4.1 Operational semantics

We define a small-step operational semantics. We note that we cannot use a standard PCF operational semantics as in [46] because in our work, unlike [46], we implement exact computation on real numbers, so a real number cannot be defined by a single finite value. In [15,16], an operational semantics to exact computation on real numbers is given using lazy evaluation, but this has its drawbacks. It relies on parallel computation and is difficult to simulate in a programming language. In this paper, we propose an alternative approach, reminiscent of some work in [8,53], with the advantage of a fairly direct translation into Haskell.

In the operational semantics, we use a set of basic constants for the rational intervals $[a, b]$, together with a set of basic constants on dual numbers, made up of pairs of rational intervals, $[a, b] + \varepsilon[a', b']$. We consider the infinite interval $(-\infty, +\infty)$ to be a special case of a rational interval. We avoid introducing these values directly in the main syntax of the language because they are partial values, and we prefer to have constants only for totally defined values, as it is common in most programming languages. Using the functions $\text{in}_\pi : \nu \rightarrow \pi$ and $\text{in}_\delta : \pi \rightarrow \delta$ and the arithmetic operations, all rational values are readily available in the language.

In the operational semantics, we need to address the problem that by unfolding the fixed-point operator Y_τ , on the one hand, one can obtain better and better approximations for a real value, but, on the other hand, the unfolding needs to be stopped at some point; otherwise, the computation diverges. In exact real number computation, which deals with infinitary objects, one rarely has base cases in recursive definitions. For example, one can define a real number by the recursive equation $x = 1/4 + x/4$, and the infinite unfolding of this definition is an infinitary expression representing the value $1/3$. The partial approximations of $1/3$ actually used in the computation are obtained by forcing a stop in the infinite unfolding. Similar considerations hold for the Riemann integral, by increasing the number of sub-intervals with which the unit interval is partitioned, one obtains better approximations of the integral, but the partition of the unit interval cannot be refined indefinitely.

Similar considerations hold for the Riemann integral: by increasing the number of sub-intervals with which the unit interval is partitioned, one obtains better approximations of the integral, but the partition of the unit interval cannot be refined indefinitely.

To solve this problem, we extend the syntax, used in the operational semantics, by building expressions in the form $\langle e, n \rangle$ (or $\langle e, (m, n) \rangle$). The parameter n (or (m, n)) represents a measure of the complexity of the computation along which the expression e is going to be evaluated. The operational semantics allows to derive judgements in the form $\langle e, n \rangle \rightarrow_* [a, b] + \varepsilon[a', b']$, whose

intended meaning is that with a computation bounded by a cost n , the expression e reduces to the rational dual $[a, b] + \varepsilon[a', b']$. In more detail, Dual PCF has two forms of the recursive operator Y_τ : a bounded one, when τ is a *continuous type*, a function type having a continuous range space, that is $\tau = \vec{\tau}' \rightarrow \pi$ or $\tau = \vec{\tau}' \rightarrow \delta$, and a standard one for any other value of type τ . Higher values of the parameter n imply more effort in the computation so it will be always the case that if $m \leq n$, $(e, m) \rightarrow [a, b] + \varepsilon[a', b']$ and $(e, n) \rightarrow [c, d] + \varepsilon[c', d']$ then $[a, b] + \varepsilon[a', b'] \sqsubseteq [c, d] + \varepsilon[c', d']$. In other words, the evaluation of $\langle e, 0 \rangle, \langle e, 1 \rangle, \langle e, 2 \rangle, \dots$, produces a sequence of intervals each one contained in the previous one and converging to the denotational semantics of e . This approach to the operational semantics is somewhat similar to and inspired by [53,8]. Moreover we have used the above ideas in a proof-of-concept implementation in Haskell of exact dual numbers and derivative operators that can be found in [5].

Formally for the operational semantics, we consider an extended language obtained by adding extra constants and three extra production rules to the expression grammar of Dual PCF, as in Equation (5):

$$e ::= \langle e, n \rangle \mid \langle \text{int}, (m, n) \rangle \mid \langle \text{sup}, (m, n) \rangle$$

with $n, m \in \mathbb{N}$.

The set of constants is extended by:

- a set of constants $[a, b] : \pi$, and $[a, b] + \varepsilon[a', b'] : \delta$, with $[a, b]$ and $[a', b']$ rational intervals, or the value $(-\infty, +\infty)$;
- a constant In for a function $\delta \rightarrow \pi$ returning the infinitesimal part of a dual number.

The evaluation contexts are the standard ones for a call-by-value reduction:

$$\begin{aligned} E[_] ::= [_] \mid E[_] e \mid E[_] \text{op} e \mid c \text{op} E[_] \\ \mid \text{if } E[_] \text{if } e_1 \text{ else } e_2 \mid \text{In } E[_] \end{aligned}$$

The reduction rules for generic terms are:

$$\langle e_1 e_2, n \rangle \rightarrow \langle e_1, n \rangle e_2 \quad \langle \lambda x. e_1, m \rangle e_2 \rightarrow \langle e_1[e_2/x], m \rangle$$

The reduction rules for a generic binary operation on dual numbers op are:

$$\langle e_1 \text{ op } e_2, n \rangle \rightarrow \langle e_1, n \rangle \text{ op } \langle e_2, n \rangle$$

together with the rules defining operations on rational intervals; e.g.:

$$\begin{aligned} \langle x + \varepsilon x', n \rangle &\rightarrow x + \varepsilon x' \\ (x + \varepsilon x') + (y + \varepsilon y') &\rightarrow (x + y) + \varepsilon(x' + y') \\ (x + \varepsilon x') * (y + \varepsilon y') &\rightarrow (x * y) + \varepsilon(x * y' + y * x') \end{aligned}$$

The remaining rules can be found in the Appendix. The reduction rules for the functionals on dual numbers make use of the parameter n and are the following:

$$\begin{aligned}
\langle \text{int}, n \rangle f &\rightarrow \langle \text{int}, (n, n) \rangle f \\
\langle \text{int}, (0, n) \rangle f &\rightarrow \langle f, n \rangle ([0, 1]) \\
\langle \text{int}, (m, n) \rangle f &\rightarrow (\langle \text{int}, (m-1, n) \rangle \lambda x. f(x/2)) / 2 \\
&\quad + (\langle \text{int}, (m-1, n) \rangle \lambda x. f((x+1)/2)) / 2 \\
\langle \text{sup}, n \rangle f &\rightarrow \langle \text{sup}, (n, n) \rangle f \\
\langle \text{sup}, (0, n) \rangle f &\rightarrow \langle f, n \rangle ([0, 1]) \\
\langle \text{sup}, (m, n) \rangle f &\rightarrow \max (\langle \text{sup}, (m-1, n) \rangle \lambda x. f(x/2)) \\
&\quad (\langle \text{sup}, (m-1, n) \rangle \lambda x. f((x+1)/2))
\end{aligned}$$

The operational semantics for the derivative operator is defined by:

$$\begin{aligned}
\langle L_{\vec{\tau}}, n \rangle f \vec{e} \vec{e}' &\rightarrow \text{In} \langle f(\vec{e} +_{\tau_i} (\epsilon_{\tau} \vec{e}')), n \rangle \\
\text{In}([a, b] + \varepsilon[a', b']) &\rightarrow [a', b']
\end{aligned}$$

where $+_{\tau}$ and ϵ_{τ} denote the expressions: $+_{\sigma \rightarrow \tau} = \lambda f. \lambda g. \lambda x. (fx) +_{\tau} (gx)$ and $\epsilon_{\sigma \rightarrow \tau} = \lambda f. \lambda x. \epsilon_{\tau}(fx)$, while $\epsilon(x + \varepsilon x')$ is a shorthand for $(0 + \varepsilon) * (x + \varepsilon x')$.

The operational semantics for the fixed-point Y_{σ} operator on a continuous type σ is defined by:

$$\begin{aligned}
\langle Y_{\sigma}, 0 \rangle f &\rightarrow \perp_{\sigma} \\
\langle Y_{\sigma}, (n+1) \rangle f &\rightarrow \langle f(Y_{\sigma} f), n \rangle
\end{aligned}$$

where \perp_{σ} is defined as follows $\perp_{\delta} = (-\infty, +\infty) + \varepsilon(-\infty, +\infty)$, $\perp_{\pi} = (-\infty, +\infty)$, $\perp_{\sigma \rightarrow \tau} = \lambda x_{\sigma}. \perp_{\tau}$.

The rules for the constants $+$, $-$, $*$, $/$, \min , \max , pr , int , and sup acting on real values, are the obvious restriction of the corresponding rules for dual numbers.

The reduction rules for the PCF constructors and constants are the standard ones, together with the rules:

$$\begin{aligned}
\langle \text{if } e \text{ then } e_1 \text{ else } e_2, n \rangle &\rightarrow \text{if} \langle e, n \rangle \text{ then } \langle e_1, n \rangle \text{ else } \langle e_2, n \rangle \\
\langle c, n \rangle &\rightarrow c
\end{aligned}$$

with c any PCF constant, different from Y_{σ} , and with σ a continuous type.

Note that, since we do not consider intervals in the form $(-\infty, a]$ or $[a, +\infty)$ as values, pr is not definable in terms of \min , \max . Moreover, pr is the only language constant that defines a function on partial real values mapping the bottom $(-\infty, +\infty)$ to a value different from $(-\infty, +\infty)$; therefore, it is necessary to recursively define real (dual) values and functions on real (dual) values.

4.2 Denotational semantics

The continuous Scott domain \mathbb{D}_{τ} , used to give a semantic interpretation to expressions having arbitrary type τ , is recursively defined by: $\mathbb{D}_o = \{\text{ff}, \text{tt}\}_{\perp}$, $\mathbb{D}_{\nu} = \mathbb{N}_{\perp}$, $\mathbb{D}_{\pi} = \mathbb{IR}$, $\mathbb{D}_{\delta} = \mathbb{DR}$, $\mathbb{D}_{\sigma \rightarrow \tau} = (\mathbb{D}_{\sigma} \rightarrow \mathbb{D}_{\tau})$.

The semantic interpretation of any PCF constant is the usual one. The general schema to give semantics to constants representing functions on dual numbers is the following: given a constant c of type τ that denotes a function f_c on the real line (\mathbb{R}), the semantic interpretation of c is given by $B\llbracket c \rrbracket$ defined by:

$$B\llbracket c \rrbracket = (f_c)_{\tau}^{\mathbf{d}}$$

To help the reader, we explicitly define the semantic interpretation of some of these constants:

$$B\llbracket \min \rrbracket (x + \varepsilon x')(y + \varepsilon y') = (\min x y) + \varepsilon \begin{cases} x' & x < y \\ y' & y < x \\ x' \sqcap y' & \text{o/w} \end{cases}$$

$$B\llbracket \text{int} \rrbracket f = \int_{[0,1]}^d f(x) dx$$

Integration on the dual domain is reduced as

$$\int_{[0,1]}^d f(x) dx = \int_{[0,1]}^{\star} \text{St}(f(x)) dx + \varepsilon \int_{[0,1]}^{\star} \text{In}(f(x)) dx,$$

where $\int_{[0,1]}^{\star} : (\mathbb{I}[0,1] \rightarrow \mathbb{IR}) \rightarrow \mathbb{IR}$ is the envelope of the Riemann integral functional $\int_{[0,1]} : ([0,1] \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ as in Proposition 1; it coincides with integration constructor developed in Real PCF and in interval analysis [20], [48]. It sends a continuous function of type $\mathbb{I}[0,1] \rightarrow \mathbb{IR}$ to an interval in the domain of reals \mathbb{IR} and extends the Riemann integral in the sense that if $f : [0,1] \rightarrow \mathbb{R}$ is continuous then $\int_{[0,1]}^{\star} f(x) dx = \int_0^1 f(x) dx$, where as usual we identify a real number with its singleton. Note that the integration constructor, using the above method, can compute the value of $\int_{[a,b]} f(x) dx$ by a simple change of variable invoked by the linear re-scaling $x = h(y) = (b-a)y + a$ so that

$$\int_{[a,b]} f(x) dx = (b-a) \int_{[0,1]} f \circ h^{\star}(y) dy. \quad (6)$$

For clarity, to distinguish the classical Riemann integral from the domain-theoretic integral, we always denote the classical Riemann integral of $f : [0,1] \rightarrow \mathbb{R}$ over any interval $[a,b]$ by $\int_a^b f(x) dx$ while $\int_{[u,v]} g(x) dx$, i.e., with the range of integration as a subscript to the integral sign, always denotes the extended interval-valued Riemann integral for a continuous function $g : \mathbb{IR} \rightarrow \mathbb{IR}$.

The semantic interpretation of the derivative operator $L_{\vec{\tau}}$ is defined by:

$$B\llbracket L_{\vec{\tau}} \rrbracket f \vec{d} \vec{e} = \text{In}(f(\vec{d} + \varepsilon \vec{e}))$$

The interpretation of the other constants that cannot be obtained by the general scheme is the following:

$$\begin{aligned} B[\text{in}_\delta]x &= x + \varepsilon 0 \\ B[(0 <)]x &= \begin{cases} \text{tt}, & x > 0 \\ \text{ff}, & x < 0 \\ \perp, & \text{otherwise} \end{cases} \\ B[Y_\sigma]f &= \bigsqcup_{i \in \mathbb{N}} f^i(\perp_\sigma) \end{aligned}$$

We point out that quite often dual numbers or functions on dual numbers obtained by using the recursion operator Y have an unbounded infinitesimal part, meaning that, depending on the type, the infinitesimal part is $\perp = (-\infty, +\infty)$, or is the function that maps every element to \perp . A simple example is the following recursive definition of the the value 1: $Y(\lambda x^\delta. (\text{pr } x^\delta + 1)/2)$. This fact can be explained as follows: the semantic interpretation functions are linear on the infinitesimal parts, and a linear function when applied to the bottom value $(-\infty, +\infty)$ returns either 0 (if the linear map is identically 0) or the bottom value itself. It follows that each element in the chain $(f^i(\perp_\sigma))_{i \in \mathbb{N}}$, whose least upper bound gives the semantics interpretation of Yf , has an unbounded infinitesimal part.

A solution for this problem, as in [16], consists of introducing a second type of dual values, δ^l , having the infinitesimal part bounded by the interval $[-1, 1]$. The basis functions on the type δ^l need to be non-expansive. Therefore most of the basic functions defined on δ must be replaced by non-expansive versions of them. For example, addition $+$ is replaced by a function evaluating the average of two values. To motivate this restriction, notice that using addition it is possible to build a function that doubles its argument: $\lambda x.x + x$; this function maps $0 + \varepsilon 1$ to $0 + \varepsilon 2$, and therefore cannot have type $\delta^l \rightarrow \delta^l$. Inside the type δ^l , it is possible to use the fixed point operator to obtain functions with informative infinitesimal part. The functions obtained in this way can later be embedded in the larger type δ . For lack of space and to focus on the main subject of this paper, which is evaluating derivatives of second-order functionals, we do not fully present this solution and refer the interested reader to [16].

The semantic interpretation function E is defined, by structural induction, in the standard way:

$$\begin{aligned} E[c]_\rho &= B[c] & E[x]_\rho &= \rho(x) \\ E[e_1 e_2]_\rho &= E[e_1]_\rho(E[e_2]_\rho) \\ E[\lambda x^\sigma. e]_\rho &= \lambda d \in D_\sigma. E[e]_{(\rho[d/x])} \end{aligned}$$

4.3 Adequacy

The correspondence between the denotational and the operational semantics is shown by the following result.

For a closed expression e of type δ , let us denote by $[a, b] + \varepsilon[a', b'] \ll \text{Eval}(e)$ the property that there exists a natural number n and a dual rational interval $[c, d,] + \varepsilon[c', d']$ such that $\langle e, n \rangle \rightarrow^* [c, d] + \varepsilon[c', d']$ and $[a, b] + \varepsilon[a', b'] \ll [c, d] + \varepsilon[c', d']$.

Theorem 3. *On type δ the operational semantics is sound and complete with respect to the denotational semantics, that is for any closed expression $e : \delta$, for any partial rational dual number $[a, b] + \varepsilon[a', b']$, we have: $[a, b] + \varepsilon[a', b'] \ll E[e]$ iff $[a, b] + \varepsilon[a', b'] \ll \text{Eval}(e)$.*

5 Some functions/functionals in Dual PCF

In this section, we will give various examples of functions and functionals expressible in our language. In some cases, we will also show how to use the operational semantics to compute the derivatives of these functionals. Some of these examples are motivated by actual areas of application. In many cases (for instance, [18]), the problem of solving an integral or differential equation can be reduced to finding the roots of an integral or differential operator; being able to evaluate the derivative of a functional is required for such problems:

1- Absolute value function. $f(x) = |x|$ can be written in the language as $\lambda x. \max(x, -x)$. The domain-theoretic directional derivative of this function at 0 is then correctly evaluated by the following reduction:

$$\begin{aligned} L_\delta f \ 0 \ 1 &\rightarrow \text{In}(f(0 + \varepsilon 1)) \rightarrow \text{In}(\max(0 + \varepsilon 1, 0 - \varepsilon 1)) \\ &\rightarrow \text{In}(0 + [-1, 1]\varepsilon) \rightarrow [-1, 1] \end{aligned}$$

2- Comparison with Chebyshev software. From [10, section 3.2], consider taking the directional derivative of the operator $G = \lambda g. \lambda x. x + g(x)^2$ at the point $f = \lambda u. u^2$ in the direction k . We refer to the operational semantics:

$$\begin{aligned} L_{\delta \rightarrow \delta, \delta} G(\lambda u. u^2) y \ k \ 0 &\rightarrow \text{In}(G(\lambda u. u^2 + \varepsilon k(u))(y + \varepsilon 0)) \\ &\rightarrow \text{In}(\lambda x. x + (x^2 + \varepsilon k(x)) * (x^2 + \varepsilon k(x)))(y + \varepsilon 0)) \\ &\rightarrow \text{In}(y + (y^4 + \varepsilon 2y^2 k(y))) \rightarrow 2y^2 k(y) \end{aligned}$$

So in other words, we have that $LG(f, k) = \lambda y. 2y^2 k(y)$. This is the same result as was obtained by the software system in the above paper, except that their autodiff procedure is far more involved than ours.

3- Laplace and Fourier series. We can express in the language all continuous linear functionals like the Fourier-series finding operator and the Laplace transform of functions with compact support; see Section 8. The dual-number formalism implies that given a continuous linear functional F and function f , we have: $F(f + \varepsilon g) = F(f) + \varepsilon F(g)$ for any function g . So we can deduce: $LF(f, g) = F(g)$.

4- Lagrangian. Consider a functional of the form $F(f) = \int_0^1 \mathfrak{L}(t, f(t), f'(t)) dt$ where $\mathfrak{L} : \mathbb{R}^3 \rightarrow \mathbb{R}$, called the Lagrangian, and $f : \mathbb{R} \rightarrow \mathbb{R}$ are differentiable. This is what is called an action functional that is used for finding the

time evolution of a system in analytical mechanics and quantum mechanics ([35,54,55]). Assuming a term $\mathfrak{L} : \delta \rightarrow \delta \rightarrow \delta \rightarrow \delta$, in our language F is expressed as $\lambda f . \text{int} (\lambda t . \mathfrak{L}(\text{in}_\delta t)(f(\text{in}_\delta t))(\text{L}_\delta f t 1))$. Our language can not be used to differentiate such a functional directly (because we cannot differentiate expressions that themselves contain the derivative operator). Instead, consider $G(g) = F(\int g) = \int_0^1 \mathfrak{L}(t, \int_0^t g(u) du, g(t)) dt$. The functional G can be expressed in our language as

$\lambda g . \text{int} (\lambda t . \mathfrak{L}(\text{in}_\delta t)(\text{int} (\lambda u . (\text{in}_\delta t) * (g(\text{in}_\delta(u * t))))) (g(\text{in}_\delta t)))$, and can be differentiated (along g and along the variables appearing in \mathfrak{L}). Whenever the functional G is locally stationary at g , the functional F is locally stationary at the function $x \mapsto \int_0^x g(t) dt$. We can also fix the value of $\int_0^1 g(t) dt$ using Lagrange multipliers, to ensure that the starting and ending points of a particle are fixed, as is usually required when applying the principle of stationary action.

5- Solving initial value problems (IVP). Consider the one dimensional initial value problem,

$$\dot{y}'(x) = v(y(x)), \quad y(0) = 0 \quad (7)$$

where $v : O \rightarrow \mathbb{R}$ is a continuous one dimensional vector field in an open neighbourhood $O \subset \mathbb{R}$ of the origin.

In our language the solution of the initial value problem can be expressed in the following way. Let $e_v : \pi \rightarrow \pi$, be an expression defining the function v in its domain of definition. The solution of IVP is given by the expression:

$$Y(\lambda f . \lambda x . \text{int} \lambda t . x * \text{pr}_M(e_v(f(t * x))))$$

where pr_M is a function projecting the real line onto the interval $[-M, M]$ and defined as $\lambda x . (\text{in}_\pi M) * \text{pr} x / M$, with M a rational constant. The proof of correctness is in the Appendix. By using currying, the above construction can be easily extended to solve the IVP in \mathbb{R}^n .

6- Legendre-Fenchel transform. Consider a function $f : [0, 1] \rightarrow \mathbb{R}$. Extend it to real values outside $[0, 1]$ by setting $f(x) = +\infty$ whenever $x \in \mathbb{R} \setminus [0, 1]$. We may define the *Legendre-Fenchel transform* ([51]) of such functions as $F(f)(p) = \sup_{x \in [0, 1]} (px - f(x))$. The resulting functional is definable in our language and is differentiable in the generalised sense we consider.

7- Thomas-Fermi kinetic energy functional. ([50]) is a classic example of a non-linear functional in quantum theory. It expresses in an approximate way the total kinetic energy of the electrons in a region of space purely in terms of their density distribution n . It is given by

$$T(n) = C_{\text{kin}} \int [n(\mathbf{r})]^{5/3} d^3r,$$

where C_{kin} is a constant involving the mass of an electron. If we suppose that $n : \mathbb{R}^3 \rightarrow \mathbb{R}$ is zero outside $[0, 1]^3$, we can express the above functional in our language as:

$$T(n) = C_{\text{kin}} \int_0^1 \int_0^1 \int_0^1 (n(x, y, z))^{5/3} dx dy dz.$$

6 Local consistency in the dual domain

To use dual numbers in a useful way, one needs to ensure that the infinitesimal value can actually be used to evaluate the derivative of a function. In other words, one needs to prove that automatic differentiation provides correct results. The problem of correctness of automatic differentiation is often considered in the literature; see for example [1] and [46]. In our setting, where we admit also partial values, we require that the information about a function contained in the value part is not in contradiction with that of the derivative contained in the infinitesimal part. We call this notion *local consistency*.

Definition 5. *An element $x + \varepsilon x' : \mathbb{D}\mathbb{R}$ is locally consistent if x' is an interval containing 0. Given a function type $\vec{\tau} \rightarrow \delta$ with dual numbers δ as its codomain, a continuous functional $F : \mathbb{D}_{\vec{\tau} \rightarrow \delta}$ is locally consistent if it satisfies:*

- (i) *it is standard-robust, i.e., for any pair of lists of standard robust values \vec{d}, \vec{d}' ,*

$$\text{St}(\vec{d}) = \text{St}(\vec{d}') \Rightarrow \text{St}(F(\vec{d})) = \text{St}(F(\vec{d}')),$$

- (ii) *for any pair of lists of standard maximal preserving, locally consistent values \vec{d}, \vec{d}' , and rational $r > 0$,*

$$\text{In}(F((\vec{d} \sqcap (\vec{d} + r\vec{d}')) + \varepsilon\vec{d}')) \uparrow \frac{\text{St}(F(\vec{d} + r\vec{d}') - F(\vec{d}))}{r}.$$

Lemma 3. *Suppose $F : \mathbb{D}_{\vec{\tau} \rightarrow \delta}$ is a standard-robust and standard maximal preserving continuous functional. If $L(F)^{\mathbf{s}}((\vec{d})^{\mathbf{s}}, (\vec{d}')^{\mathbf{s}})$ is bounded for some pair (\vec{d}, \vec{d}') of lists of locally consistent and standard preserving elements, then the restriction of $(F)^{\mathbf{s}}$ to the space of maximal preserving elements is locally Lipschitzian at $((\vec{d})^{\mathbf{s}}, (\vec{d}')^{\mathbf{s}})$.*

The following result states that local consistency exactly characterizes the set of functions on $\mathbb{D}\mathbb{R}$ for which the infinitesimal part gives a correct approximation of the directional derivative of the function represented by the standard part.

Proposition 10. *A standard-robust and standard maximal preserving continuous functional $F : \mathbb{D}_{\vec{\tau} \rightarrow \delta}$ is locally consistent if and only if for any pair of lists of locally consistent and standard maximal preserving elements \vec{d} and \vec{d}' , we have:*

$$\text{In}(F(\vec{d} + \varepsilon\vec{d}')) \sqsubseteq L(F)^{\mathbf{s}}((\vec{d})^{\mathbf{s}}, (\vec{d}')^{\mathbf{s}}). \quad (8)$$

If the left hand side of Equation (8), evaluates to a non-bottom element then by Lemma 3, f is locally Lipschitzian and thus Theorem 1(i) implies that the left hand side of Equation (8) computes approximations to the support function of the generalised subgradient of the standard part of F .

7 Correctness of the derivative operator

By Proposition 10, on locally consistent functions, one can evaluate the derivative of a function by evaluating the function on dual numbers. We aim now to prove that the semantic interpretations of the functions definable in the language are locally consistent.

To obtain these results we need to extend the notion of consistency to all functions definable in our language, and in particular to functions of higher order than 2, and then prove that local consistency is preserved by the basic constructors of the language: these being function composition, λ -abstraction, lub of chains. In order to obtain these results it is convenient to introduce a second, equivalent definition of consistency that is more suitable for extension to higher types. Note that with the present definition of local consistency, the simple statement that composition of two locally consistent functions is locally consistent does not have a straightforward proof. The second definition of consistency is based on logical relations. Logical relations are a standard proof technique used in the semantics of functional languages; they are used for proving that the semantic interpretation of terms satisfies some desired properties. A general introduction to logical relations can be found in [47], while in [7,16], logical relations are used in a way similar to our work.

We define a set of logical relations which, if they are preserved by a function f , imply that the function f is locally consistent. For any rational number $r > 0$ let R_δ^r be a ternary relation over generalised dual numbers $\mathbb{D}\mathbb{R}$ defined by: $R_\delta^r(x_1, x_2, x_3)$ holds whenever

$$\text{St}(x_3) \sqsubseteq \text{St}(x_1) \sqcap \text{St}(x_2) \text{ and } \text{In}(x_3) \uparrow \frac{\text{St}(x_2 - x_1)}{r}$$

or, equivalently, $R_\delta^r(I_1 + \varepsilon I'_1, I_2 + \varepsilon I'_2, I_3 + \varepsilon I'_3)$ holds whenever $I_3 \sqsubseteq I_1 \sqcap I_2$ and $r I'_3 \uparrow I_2 - I_1$.

For the other ground domains, \mathbb{D}_o and \mathbb{D}_ν , R_o^r and R_ν^r are defined as follows: $R_\nu^r(n_1, n_2, n_3)$ holds whenever $n_3 \sqsubseteq n_1 \sqcap n_2$, and n_1, n_2 are consistent. The rationale behind this definition consists in repeating the definition of R_δ^r by considering Boolean values and natural numbers as having a hidden infinitesimal part equal to zero.

The relations are extended inductively to higher order domains in the usual way for logical relations: $R_{\sigma \rightarrow \tau}^r(f_1, f_2, f_3)$ iff for every $d_1, d_2, d_3 \in \mathbb{D}_\sigma$, the relation $R_\sigma^r(d_1, d_2, d_3)$ implies $R_\tau^r(f_1(d_1), f_2(d_2), f_3(d_3))$.

Definition 6. *An element f in the domain \mathbb{D}_σ is logically consistent if it is self-related by R_σ^r , i.e. $R_\sigma^r(f, f, f)$, for any positive rational number r . We call a constant c in the language logically consistent if its semantic interpretation $B[[c]]$ is logically consistent.*

Proposition 11. *Any first-order function $f : \mathbb{D}_\tau$ is locally consistent if and only if it is logically consistent.*

Next, we have the following implication regarding functionals. We conjecture that the reverse implication also holds, but since the reverse implication is not required in this work, we avoid considering it here.

Proposition 12. *Any second-order function $F : D_{\vec{\tau} \rightarrow \delta}$ is locally consistent if it is logically consistent.*

Note that, with the single exception of $L_{\vec{\tau}}$, all the constants in the language are logically consistent. The proof is routine for almost all constants. To prove that the fixed-point operator preserves the above relations, one shows that the bottom elements are self-related by R_{σ}^r , and that the relation is closed under the lub of chains. Note that (< 0) preserves the relation when applied to the domain \mathbb{D}_{π} , but it has no logically consistent extension to the domain \mathbb{D}_{δ} .

Using the technique of logical relations [47], it is straightforward to show:

Proposition 13. *The semantic interpretation $E[e]$ of any closed expression $e : \tau$ not containing L is logically consistent.*

Corollary 3. *The semantic interpretation $E[e]$ of any closed expression e having second-order function type and not containing L is locally consistent.*

Corollary 4. *The derivative operator L is sound, i.e., for any closed expression $LF(\vec{f})(\vec{g})$, if F is a second-order function, $E[F], E[\vec{f}], E[\vec{g}]$ are standard maximal preserving, and L is not contained in F, \vec{f}, \vec{g} then*

$$E[LF(\vec{f})(\vec{g})] \sqsubseteq L(E[F])^s((E[\vec{f}])^s, (E[\vec{g}])^s)$$

Since our language contains the if-then-else operator, and it is a well-known problem that the if-then else constructor produces an inconsistent result with automatic differentiation, the above result may appear contradictory. Note, however, that there are restrictions on the functions that can be defined on dual numbers. In particular, it is impossible to convert a dual number into a real number, or to test whether a dual value is less or greater than 0. Consequently, all functions from duals to Booleans are constant, so the if-then-else operator cannot be used to define functions on duals that have no generalised derivative. As in [16], we have used the min/max operators as a safe alternative to if-then-else.

8 Definability of Linear functionals

We show that any computable continuous linear functional on $C_0(\mathbb{R})$, the set of continuous real functions that vanish at infinity, can be expressed in our language. We start with continuous linear functionals on $([0, 1] \rightarrow \mathbb{R})$.

Proposition 14. *If $F : ([0, 1] \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ is a continuous linear functional then there exist two right continuous non-decreasing maps $g_i^{\dagger} : [c_i, d_i] \rightarrow [0, 1]$ with $i = 1, 2$ such that for any continuous map $f : [0, 1] \rightarrow \mathbb{R}$ we have*

$$F(f) = \int_{c_1}^{d_1} f \circ g_1^{\dagger}(x) dx - \int_{c_2}^{d_2} f \circ g_2^{\dagger}(x) dx.$$

By employing the envelopes of g_1^\dagger and g_2^\dagger as in Proposition 1, we can then deduce the following result.

Theorem 4. *The continuous linear functional $F : ([0, 1] \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ has a conservative extension $F^* : (\mathbb{I}[0, 1] \rightarrow \mathbb{I}\mathbb{R}) \rightarrow \mathbb{I}\mathbb{R}$ given by*

$$F^*(f) = \int_{[c_1, d_1]} f \circ (g_1^\dagger)^*(x) dx - \int_{[c_2, d_2]} f \circ (g_2^\dagger)^*(x) dx.$$

Similarly, the embedding $(F)^\mathbf{d}$ of F in the dual domain $\mathbb{D}_{(\delta \rightarrow \delta) \rightarrow \delta}$ is given by: $(F)^\mathbf{d}(f) =$

$$\int_{[c_1, d_1]}^\mathbf{d} f((g_1^\dagger)^*(x)^\mathbf{s})^\mathbf{d} dx - \int_{[c_2, d_2]}^\mathbf{d} f((g_2^\dagger)^*(x)^\mathbf{s})^\mathbf{d} dx.$$

Theorem 4 reduces the definability of a computable linear functional F to the definability of computable functions $(g_1^\dagger)^*$ and $(g_2^\dagger)^*$. The latter result is proved in [24], for a calculus whose expressing power, on first order functions, is equivalent to the present calculus. Thus, in our calculus computable linear functionals of type $([0, 1] \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ are definable. Next, note the following.

Theorem 5. [6, Theorem 1.4] *If $F : C_0(\mathbb{R}) \rightarrow \mathbb{R}$ is a continuous linear functional, then there exists a finite signed measure ν , such that $F(f) = \int_{-\infty}^{\infty} f d\nu$.*

We will show in the Appendix, using Theorem 5, known as Riesz-Markov representation theorem, and Hahn decomposition of finite signed measures, that Theorem 4 can be extended to continuous linear functionals on $C_0(\mathbb{R})$. Therefore, any computable continuous linear functional on $C_0(\mathbb{R})$ can be expressed in our language. In particular, this holds for any continuous linear functional on $C_0(\mathbb{R})$ equipped with the compact-open topology, since the compact-open topology is weaker than the sup norm topology on $C_0(\mathbb{R})$.

9 Conclusions and future work

We have for the first time developed a language to compute the derivatives of functionals on real-valued functions. Dual PCF contains, as basic primitives, the operations of integration and sup. Using this language it is possible to numerically evaluate the directional derivative of functionals. We have also reduced the problem of definability of continuous linear functionals to the previously solved problem of definability of real functions.

The present work can be expanded in different directions. As an immediate application, one can properly implement the primitives of Dual PCF in a programming language. This will provide a simple and new method to numerically evaluate the derivative of functionals. In this paper, to ensure correctness of computations, and to avoid dealing with errors induced by floating point arithmetic, we assume that we are computing with exact real numbers. However, there would be no problems in defining our primitive operations over floating

point numbers instead. One just needs to encode the infinitesimal part of a dual number, representing the directional derivative of a function, by an interval.

We conjecture that using supremum and integration all computable functionals, and not just the computable linear functionals, would be definable.

We may extend our language to support nested differentiation. A common approach is to introduce a set of “independent” infinitesimals, each like ε in that they square to zero, but such that their mutual products are not zero [45].

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Appendix

Here we provide the proofs of the results in the paper.

9.1 Proof of Section 2

Proposition 2. The set of functions

$$\{f^* : \mathbb{IR} \rightarrow \mathbb{IR} : f \in (\mathbb{R} \rightarrow \mathbb{R})\}$$

is dense in $(\mathbb{IR} \rightarrow \mathbb{IR})$ with respect to the Scott topology.

Proof. Let $h : \mathbb{IR} \rightarrow \mathbb{IR}$ be a step function with $h = \sup_{i \in I} a_i \chi_{\uparrow A_i}$, where, a_i and A_i are compact intervals with non-empty interior, I is a finite indexing set and $\uparrow h \neq \emptyset$. Consider the induced step function $h_0 : \mathbb{R} \rightarrow \mathbb{IR}$ with $h_0 = \sup_{i \in I} a_i \chi_{A_i^\circ}$. Let (a, b) be a connected component of h_0 where the function is not bottom valued. Then, in (a, b) , we have $h_0 = [h_0^-, h_0^+]$ where h_0^- and h_0^+ are, respectively, lower and upper semicontinuous, piecewise constant map with $h^-(x) < h^+(x)$ for $x \in (a, b)$. In fact, (a, b) induces a partition $P : a = q_0 < q_1 < \dots, q_{t-1} < q_t = b$ of (a, b) into a finite number of (open, closed or half-open/half-closed) intervals on each of which h^- and h^+ are constant. The Scott continuity of h_0 at q_i for $0 < i < t$ implies that $h_0(x) \subseteq h_0(y)$ or $h_0(y) \subseteq h_0(x)$ for $x \in (q_{i-1}, q_i)$ and $y \in (q_i, q_{i+1})$. Let $u_i, v_i \in \mathbb{IR}$ with $u_i \subset v_i$ be the value of $h(x)$ in the interiors of the two intervals in P with common boundary q_i . Then u_i is compact. Put $c_i = (u_i^- + u_i^+)/2$ for $0 \leq i \leq t$. Now consider the piecewise linear map $g : (a, b) \rightarrow \mathbb{R}$ with $g(q_i) = c_i$, linear in each interval $[q_i, q_{i+1}]$ for $0 \leq i \leq t-1$. We can then continuously glue the piecewise linear functions g so constructed for all components of the domain of h_0 by defining it to be affine in between any two closest components and extending the resulting map from the rightmost, respectively leftmost, component to $+\infty$, respectively to $-\infty$, as a constant map to obtain a continuous map $G : \mathbb{R} \rightarrow \mathbb{R}$. Now we have a continuous map $G^* : \mathbb{IR} \rightarrow \mathbb{IR}$ that satisfies $h \ll G^*$.

Lemma 1. The compact-open topology on $(\mathbb{R} \rightarrow \mathbb{R})$ is generated by the sub-basis consisting of subset of the form $U(\overline{O_1}, O_2)$ where O_1 and O_2 are open intervals with compact closures.

Proof. Note that the open intervals with compact closure form a basis of the Euclidean topology. If $C \subset \mathbb{R}$ is compact and $O \subset \mathbb{R}$ is open with $C \subset O$, then there exists, by compactness of C , a finite set of open intervals O_i , $i \in I$, with compact closures such that $C \subset \bigcup_{i \in I} O_i \subset O$. The result now follows from [19, p. 264].

Proposition 3. The map E is a topological embedding, i.e. it is injective, continuous and is an open map onto its image $\text{Image}(E) \subset \text{Max}(\mathbb{IR} \rightarrow \mathbb{IR})$ with respect to the relative Scott topology on $\text{Max}(\mathbb{IR} \rightarrow \mathbb{IR})$.

Proof. By Lemma 1, a sub-basic compact-open set of $\mathbb{R} \rightarrow \mathbb{R}$ is of the form $U(\overline{O_1}, O_2)$ where O_1 and O_2 are open intervals with compact closures. A sub-basic Scott open subset of a bounded complete domain $(\mathbb{IR} \rightarrow \mathbb{IR})$ is the way-above set of a single-step function of the form $\uparrow(\overline{O_2}\chi_{\uparrow\overline{O_1}})$, where O_1 and O_2 are open intervals with compact closures. Let $E(-) := (-)^*$. It is sufficient to show that

$$E[U(\overline{O_1}, O_2)] = \text{Image}(E) \cap (\uparrow(\overline{O_2}\chi_{\uparrow\overline{O_1}})),$$

i.e., $f \in U(\overline{O_1}, O_2)$ iff $f^* \in \uparrow(\overline{O_2}\chi_{\uparrow\overline{O_1}})$. Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be continuous. Since the lattice of open sets of the bounded complete domain $(\mathbb{IR} \rightarrow \mathbb{IR})$ is continuous, by [26, Proposition II-4.20(iv)], we have: $\overline{O_2}\chi_{\uparrow\overline{O_1}} \ll f^*$ iff $\uparrow\overline{O_1} \ll (f^*)^{-1}(\uparrow\overline{O_2})$ iff $\uparrow\overline{O_1} \subset (f^*)^{-1}(\uparrow\overline{O_2})$ iff $f^*(\overline{O_1}) \subset O_2$ iff $f[\overline{O_1}] \subset O_2$, and the result follows.

Proposition 4.

The function space $(\mathbb{R} \rightarrow \mathbb{R})$ equipped with the compact-open topology does not admit a norm.

Proof. Recall that a topological vector space is locally convex if it has a local basis at 0 whose members are convex. It is locally bounded if 0 has a bounded neighborhood W , i.e., for all neighbourhood V of 0 there exists $s > 0$ such that $W \subset tV$ for any $t > s$; see [52]. For any topological space Y , the function space $(Y \rightarrow \mathbb{R})$, equipped with the compact-open topology, is a locally convex topological vector space [19, p. 279]. Next, recall that a topological vector space admits a norm iff it is locally convex and locally bounded [52, 1.39]. Therefore, it suffices to show that $(\mathbb{R} \rightarrow \mathbb{R})$, equipped with the compact-open topology, is not locally bounded. Let $f_0 : \mathbb{R} \rightarrow \mathbb{R}$ be the constant function with value 0 $\in \mathbb{R}$, i.e., f_0 is the origin of the vector space $\mathbb{R} \rightarrow \mathbb{R}$. Let $W = \bigcap_{i \in I} U(C_i, A_i)$ —for a finite set I , compact subsets C_i and open subsets A_i with $0 \in A_i$ for all $i \in I$ —be any basic compact-open neighbourhood of f_0 . Consider any sub-basic compact-open set $V = U(C, A)$ with $0 \in A$ and

$$C \cap \left(\bigcup_{i \in I} C_i \right) = \emptyset. \quad (9)$$

Then, $f_0 \in V$, and thus V is an open neighbourhood of f_0 . Note that for a positive $t > 0$, we have: $tU(C, A) = U(C, tA)$. It follows that $W \not\subset tV$ for any $t > 0$, since, in view of Relation (9), we can always find a continuous function $g \in U(C, A)$ such that $g \notin \bigcap_{i \in I} U(C_i, tA_i)$. Thus the function space is not locally bounded and the result follows.

Lemma 2.

The map $Lf : X \times X \rightarrow \mathbb{IR}$ is Scott continuous.

Proof. Assume that $Lf(x, x')$, for some $(x, x') \in X \times X$, is a compact interval. Given $\epsilon > 0$, by the definition of \limsup and \liminf , there exists open sets $O \times O' \subset X \times X$ and $U \subset \mathbb{R}$ such that for $(y, z) \in O \times O'$ and $r \in U$, $r > 0$,

we have: $Lf(x, x')^- - \epsilon < \frac{f(y+rz) - f(y)}{r} < (Lf(x, x')^+ + \epsilon)$. This shows that Lf is continuous at (x, x') . The continuity of Lf at (x, x') with $Lf(x, x') = \perp$ is trivial.

Proposition 5. If $Lf(x, x')$ is a point for some $x \in X$ and some $x' \in X$, then f has a directional derivative at x and x' given by $f'(x; x') = Lf(x, x')$.

Proof. From $(Lf(x, x'))^+ = (Lf(x, x'))^-$, we obtain $\lim_{r \rightarrow 0^+} \frac{f(x+rx') - f(x)}{r}$ exists and is equal to $(Lf(x, x'))^+ = (Lf(x, x'))^-$ as required.

Note that from the homogeneous property in the calculus, we have:

$$Lf(x, -x') = -Lf(x, x') = [-(Lf(x, x'))^+, -(Lf(x, x'))^-]$$

It follows that in computing the limit superiors in our expressions for the domain-theoretic directional derivative we can always replace $r \rightarrow 0^+$ with $r \rightarrow 0$ since we have:

$$\begin{aligned} & \limsup_{x_i \rightarrow x, x'_i \rightarrow x', r_i \rightarrow 0^-} \frac{f(x_i + r_i x'_i) - f(x_i)}{r_i} \\ &= \limsup_{x_i \rightarrow x, x'_i \rightarrow x', r_i \rightarrow 0^+} \frac{f(x_i - r_i x'_i) - f(x_i)}{r_i} \\ &= - \liminf_{x_i \rightarrow x, x'_i \rightarrow x', r_i \rightarrow 0^+} \frac{f(x_i - r_i x'_i) - f(x_i)}{r_i} \\ &= \limsup_{x_i \rightarrow x, x'_i \rightarrow x', r_i \rightarrow 0^+} \frac{f(x_i + r_i x'_i) - f(x_i)}{r_i}. \end{aligned}$$

Proposition 6. (The Chain rule) For continuous functions $h : X \rightarrow \mathbb{R}^n$ and $g : \mathbb{R}^n \rightarrow \mathbb{R}$, with $f = g \circ h : X \rightarrow \mathbb{R}$, we have:

$$(Lg)^*(h(x), Lh(x, x')) \subseteq Lf(x, x'), \quad (10)$$

where $(x, x') \in X \times X$ and $(Lg)^* : \mathbb{R}^n \times \mathbb{IR}^n \rightarrow \mathbb{IR}$ is the maximal extension of Lg in its second component, while $Lh(x, x') = \times_{i=1}^n Lh_i(x, x')$.

Proof. If the left hand side of Relation (10), evaluates to bottom, there is nothing to prove. Assume therefore that for some $(x, x') \in X \times X$, the values $Lh(x, x')$ and $Lg(h(x), y')$ are compact for all $y' \in Lh(x, x')$, and $C \ll (Lg)^*(h(x), Lh(x, x'))$ for some compact interval $C \subset \mathbb{R}$. For each $y' \in Lh(x, x')$, by the definition of directional derivative for g at $(h(x), y')$, there exists an open set $O \times O' \subset \mathbb{R}^n \times \mathbb{R}^n$ with $(h(x), y') \in O \times O'$ such that

$$(g(z + rz') - g(z))/r \in C,$$

for $z \times z' \in O \times O'$ and sufficiently small $r > 0$. By compactness of $Lh(x, x')$, there exist a finite number of open sets $O_i \times O'_i \subset \mathbb{R}^n \times \mathbb{R}^n$, for $i \in I$, such that $h(x) \in O_i$, $Lh(x, x') \subset \bigcup_{i \in I} O'_i$ and $(g(z + rz') - g(z))/r \in C$ for $z \times z' \in O_i \times O'_i$ for each $i \in I$. Let $O = \bigcap_{i \in I} O_i$ and $O' = \bigcup_{i \in I} O'_i$. Then $h(x) \in O$, $Lh(x, x') \subset O'$ and

$$(g(z + rz') - g(z))/r \in C, \quad (11)$$

for $z \times z' \in O \times O'$ and sufficiently small $r > 0$. By the continuity of h and the Scott continuity of Lh , there exists an open set $U \times U' \subset X \times X$ with $(x, x') \in U \times U'$ such that $h(u) \in O$ and

$$(h(u + tu') - h(u))/t \in O', \quad (12)$$

for $(u, u') \in U \times U'$ and small enough $t > 0$. Therefore, using Relations (11) and (12), for small $r, t > 0$ we have

$$\frac{g(h(u) + r(h(u + tu') - h(u))/t) - g(h(u))}{r} \in C.$$

Hence, for small value of $r = t > 0$, with $s = r = t$, we obtain

$$\frac{g(h(u + su') - g(h(u))}{s} \in C.$$

Since $C \ll (Lg)^*(h(x), Lh(x, x'))$ is arbitrary, the result follows.

Proposition 7. If $f : \mathbb{R} \rightarrow \mathbb{R}$ and $Lf(x, x')$ is bounded at a point $(x, x') \in \mathbb{R}^2$, then f is locally Lipschitzian and locally Lipschitz at x .

Proof. Suppose $Lf(x, x') = I$ is compact. Then, by homogeneity, $Lf(x, tx') = tLf(x, x') \subset I \cap (-I)$ for $t \in [-1, 1]$. Let $k := 1 + \max(|I^-|, |I^+|)$. Then by Scott continuity of Lf there exist open intervals O with $x \in O$ and an open interval $(-a, a)$ with $x' \in (a, -a)$, for some $a > 0$, such that $Lf(y, y') \subset (-k, k)$. Hence f is locally Lipschitzian, and is locally Lipschitz with Lipschitz constant k .

Proposition 15. If $f : X \rightarrow \mathbb{R}$ is locally Lipschitzian then for all $x \in X$ and $x' \in X$

$$\begin{aligned} & \limsup_{y \rightarrow x, z \rightarrow x', r \rightarrow 0^+} \frac{f(y + rz) - f(y)}{r} \\ &= \limsup_{y \rightarrow x, r \rightarrow 0^+} \frac{f(y + rx') - f(y)}{r} = f^\circ(x; x'), \end{aligned}$$

with a similar relation for \liminf , and thus

$$\begin{aligned} (Lf(x, x'))^+ &= \limsup_{y \rightarrow x, r \rightarrow 0^+} \frac{f(y + rx') - f(y)}{r} \\ (Lf(x, x'))^- &= \liminf_{y \rightarrow x, r \rightarrow 0^+} \frac{f(y + rx') - f(y)}{r}. \end{aligned}$$

Proof. Since f is continuous, we always have:

$$\begin{aligned} & \limsup_{y \rightarrow x, z \rightarrow x', r \rightarrow 0^+} \frac{f(y + rz) - f(y)}{r} \\ & \geq \limsup_{y \rightarrow x, r \rightarrow 0^+} \frac{f(y + rx') - f(y)}{r}. \end{aligned}$$

For the reverse inequality, let $\epsilon > 0$ be given. Since f is locally Lipschitzian, it has the following equi-continuous property [41, 1.2]: for each $x \in X$, there exists a neighbourhood $A \subset X$ of x and a neighbourhood $V \subset X$ of the origin such that for all $y \in A$ and $u, v \in V$, we have,

$$|f^\circ(y; u) - f^\circ(y; v)| < \epsilon.$$

By the general properties of limsup, we have:

$$\begin{aligned}
& \limsup_{\substack{y \rightarrow x, z \rightarrow x' \\ r \rightarrow 0^+}} \frac{f(y+rz) - f(y)}{r} \\
& \leq \limsup_{\substack{y \rightarrow x, z \rightarrow x' \\ r \rightarrow 0^+}} \frac{f(y+r(z-x') + rx') - f(y+r(z-x'))}{r} \\
& \quad + \limsup_{\substack{y \rightarrow x, z \rightarrow x' \\ r \rightarrow 0^+}} \frac{f(y+r(z-x')) - f(y)}{r} \\
& \leq \liminf_{y \rightarrow x, r \rightarrow 0^+} \frac{f(y+rx') - f(y)}{r} + \epsilon
\end{aligned}$$

since for $z - x' \in V$ and $y \in A$ we have

$$\limsup_{\substack{y \rightarrow x, z \rightarrow x' \\ r \rightarrow 0^+}} \frac{f(y+r(z-x')) - f(y)}{r} \leq \epsilon$$

as $f^\circ(y; 0) = 0$.

Proposition 15 says that for a locally Lipschitzian map the triple limit superior in the definition of the domain-theoretic directional derivative $Lf(x, x')$ can be replaced with the double limit superior by taking the input direction x' as fixed as is the case for the generalised directional derivative in Equation (2).

Recall that the weak* topology on X^* is the weakest topology on X^* such that for each $x \in X$ the evaluation map $X^* \rightarrow \mathbb{R}$ with $A \mapsto A(x)$ is continuous. From now on, in this section, we assume $f : X \rightarrow \mathbb{R}$ is locally Lipschitzian.

Theorem 1. Suppose $f : X \rightarrow \mathbb{R}$ is locally Lipschitzian.

- (i) $Lf(x, x') = \{A(x') : A \in \partial f(x)\}$.
- (ii) If $Lf(x, x')$ is a point for some $x \in X$ and all $x' \in X$, then f has a Gateaux derivative at x given by $Df(x, -) = Lf(x, -) : X \rightarrow \mathbb{R}$.
- (iii) If $Lf(x, x')$ is a point for x in an open set $O \subseteq X$ and all $x' \in X$, then the map $Df(-, -) : O \rightarrow X^*$ with $x \mapsto Df(x, -)$ is continuous with respect to the weak* topology on X^* .
- (iv) If X is a finite dimensional Euclidean space and $Lf(x, x')$ is a point for x in an open set $O \subseteq X$ and all $x' \in X$, then f is differentiable in O with $f'(x) = Df(x, -)$ for $x \in O$.

Proof. (i) This follows immediately from Proposition 8.

(ii) Let $A \in \partial f(x)$. Note that $(Lf(x, x'))^- = -f^\circ(x; -x')$ and $-A(x') = A(-x') \leq f^\circ(x; -x')$. Then, $(Lf(x, x'))^+ = f^\circ(x; x') \geq A(x') \geq -f^\circ(x; -x') = (Lf(x, x'))^-$. If $Lf(x, x')$ is a point for all $x' \in X$, it follows that $(Lf(x, x'))^+ = (Lf(x, x'))^-$ and thus $f^\circ(x; x') = A(x')$ for all $x' \in X$. Hence, $\partial f(x) = \{A\}$. From Proposition 8, it follows that the directional derivative $\lim_{r_i \rightarrow 0^+} \frac{f(x+rx_i) - f(x)}{r_i}$ exists and is equal to $A(x') = Lf(x, x')$, i.e., $Df(x, -) = Lf(x, -)$.

(iii) Given $x' \in X$ and an open set $U \subseteq \mathbb{R}$, a sub-basic open set of X^* is given by $\{A \in X^* : A(x') \in U\}$. Since $Df(-, -) = Lf(-, -) : O \times X \rightarrow \mathbb{R}$ is continuous in both inputs, it follows that $\{x \in O : Df(x, x') \in U\}$ is open.

(iv) This follows from [12, Corollary, p.33].

Corollary 2. If X admits a norm then a locally Lipschitzian map is locally Lipschitz and its generalised subgradient coincides with the Clarke subgradient.

Proof. Given $x \in X$, there exists, by Proposition 8, an open neighbourhood O of x that is mapped to a weak* compact subset C of X^* . For distinct $a, b \in O$, we have, by the mean value theorem (Theorem 2), $f(a) - f(b) \in M(a - b)$ with $M \in \partial f(t) \subset C$ for some $t \in (a, b)$. Since any weak* compact set is norm bounded, there exists $k \geq 0$ such that have $\|M\| \leq k$ for all $M \in C$. It follows that $|f(a) - f(b)| \leq k\|a - b\|$, i.e., f is locally Lipschitz at x .

9.2 Proofs of Section 3

Proposition 9 For any second order type $\tau = \vec{\tau}' \rightarrow \delta$, functionals $f_1, f_2 \in \mathbb{R}_\tau$ and list of values $\vec{x}_1, \vec{x}_2 \in \mathbb{R}_{\vec{\tau}'}$, by the infinitesimal property of ε , we have:

- (i) $f_1 = ((f_1)_\tau^{\mathbf{d}} + \varepsilon(f_2)_\tau^{\mathbf{d}})_\tau^{\mathbf{s}}$
- (ii) $f_2 = ((f_1)_\tau^{\mathbf{d}} + \varepsilon(f_2)_\tau^{\mathbf{d}})_\tau^{\mathbf{i}}$
- (iii) $Lf_1 \vec{x}_1 \vec{x}_2 = ((f_1)_\tau^{\mathbf{d}} ((x_1)^{\mathbf{d}} + \varepsilon(x_2)^{\mathbf{d}}))_\delta^{\mathbf{i}}$

Proof. Items (i) and (ii) follow by induction on the type τ and a simple calculation. Item (iii) can then be derived by induction on the type τ and a simple calculation using items (i) and (ii).

9.3 Proofs of Section 4

We complete the definition of the operational semantics by adding the following rules:

$$\begin{aligned} (x + \varepsilon x') - (y + \varepsilon y') &\rightarrow (x - y) + \varepsilon(x' - y') \\ (x + \varepsilon x') / 0 &\rightarrow (-\infty, +\infty) + \varepsilon(-\infty, +\infty) \\ (x + \varepsilon x') / n &\rightarrow (x/n + \varepsilon x'/n) \end{aligned}$$

$$\begin{aligned} \max(x + \varepsilon x')(y + \varepsilon y') &\rightarrow x + \varepsilon x' \text{ if } x > y \\ \max(x + \varepsilon x')(y + \varepsilon y') &\rightarrow y + \varepsilon y' \text{ if } y > x \\ \max((-\infty, +\infty) + \varepsilon x')(y + \varepsilon y') &\rightarrow (-\infty, +\infty) + \varepsilon(x' \sqcap y') \\ \max(x + \varepsilon x')((-\infty, +\infty) + \varepsilon y') &\rightarrow (-\infty, +\infty) + \varepsilon(x' \sqcap y') \\ \max(x + \varepsilon x')(y + \varepsilon y') &\rightarrow I + \varepsilon(x' \sqcap y') \text{ o/w} \\ \text{with } I &= [\max(x^-, y^-), \max(x^+, y^+)] \end{aligned}$$

$$\begin{aligned} \text{pr}(x + \varepsilon x') &\rightarrow (-1 + \varepsilon 0) \text{ if } x < -1 \\ \text{pr}(x + \varepsilon x') &\rightarrow (1 + \varepsilon 0) \text{ if } x > 1 \\ \text{pr}(x + \varepsilon x') &\rightarrow (x + \varepsilon x') \text{ if } -1 < x < 1 \\ \text{pr}(x + \varepsilon x') &\rightarrow (x \sqcup [-1, 1]) + \varepsilon(x' \sqcap 0) \text{ o/w} \end{aligned}$$

Theorem 3. On type δ the operational semantics is sound and complete with respect to the denotational semantics, that is for any closed expression $e : \delta$, for any partial rational dual number $[a, b] + \varepsilon[a', b']$, we have: $[a, b] + \varepsilon[a', b'] \ll E[e]$ iff $[a, b] + \varepsilon[a', b'] \ll Eval(e)$.

Proof. We use the standard proof technique of computability predicates.

We define a computability predicate $Comp$, first on closed terms of type o, ν , by requiring that the denotational and operational semantics coincide. That is, $Comp(e)$ when $E[e] = v \iff \exists n. \langle e, n \rangle \rightarrow^* v$.

A closed term e having type δ satisfies the predicate $Comp_\delta$ if for every closed rational dual number $[a, b] + \varepsilon[a', b']$ we have: $[a, b] + \varepsilon[a', b'] \ll Eval(e)$ iff $[a, b] + \varepsilon[a', b'] \ll E[e]_\rho$.

The predicate $Comp$ is defined on closed expressions of type π analogously.

The computability predicate is then extended to closed expressions of arrow type by requiring the preservation, to closed elements of any type, and by closure, to arbitrary elements.

Using the standard technique of computability predicates, it is possible to prove that all constants are computable, and that λ -abstraction preserves the computability of expressions. Therefore all expressions are computable.

As an example, we will prove by induction the computability of the constant $Y_{\tau_1 \rightarrow \dots \tau_n \rightarrow \delta}$. Assume that f, x_1, \dots, x_n are computable closed expressions. We will first show that $[a, b] + [a', b']\varepsilon \ll E[Yf x_1 \dots x_n]$ implies $[a, b] + [a', b']\varepsilon \ll Eval(Yf x_1 \dots x_n)$. We have:

$$[a, b] + [a', b']\varepsilon \ll E[Yf x_1 \dots x_n].$$

This implies that there is some m such that:

$$[a, b] + [a', b']\varepsilon \ll E[f^m \perp x_1 \dots x_n].$$

By the computability of f, x_1, \dots, x_n we have

$$[a, b] + [a', b']\varepsilon \ll Eval(f^m \perp x_1 \dots x_n).$$

Therefore there exists l such that $\langle f^m \perp x_1 \dots x_n, l \rangle \rightarrow_* [c, d] + [c', d']\varepsilon$ with $[a, b] + [a', b']\varepsilon \ll [c, d] + [c', d']\varepsilon$. It's possible to check that by the operational rules for Y , $\langle Yf x_1 \dots x_n, (l+m) \rangle \rightarrow_* [c_1, d_1] + [c'_1, d'_1]\varepsilon$ and $[c, d] + [c', d']\varepsilon \sqsubseteq [c_1, d_1] + [c'_1, d'_1]\varepsilon$, from which the implication follows.

We now show that $[a, b] + [a', b']\varepsilon \ll Eval(Yf x_1 \dots x_n)$ implies $[a, b] + [a', b']\varepsilon \ll E[Yf x_1 \dots x_n]$. We start from

$$[a, b] + [a', b']\varepsilon \ll Eval(Yf x_1 \dots x_n).$$

This implies that there is some n such that

$$[a, b] + [a', b']\varepsilon \ll Eval(f^n \perp x_1 \dots x_n).$$

By the computability of f , we have that

$$[a, b] + [a', b']\varepsilon \ll E[f^n \perp x_1 \dots x_n] \sqsubseteq E[Yf x_1 \dots x_n].$$

And we are done.

9.4 Proofs of Section 5

Solving initial value problems.

We recall Picard's theorem on the existence and uniqueness of the solution of the initial value problem. Suppose that v maps $[-K, K]$ to $[-M, M]$ with $a > 0$ such that $aM \leq K$. Define an integral operator on $C[-a, a]$, the collection of real-valued continuous functions on the compact interval $[-a, a]$, by

$$y \mapsto \lambda x. \int_0^x v(y(t)) dt$$

This integral operator is a contraction for sufficiently small a provided v satisfies a Lipschitz condition [37]. By Banach's theorem then we obtain a unique solution of the initial value problem.

A domain-theoretic version of Picard's theorem has been presented for dimension n in [21], which we now describe here in dimension one by extending it to time intervals. .

Consider the two function spaces $V = (\mathbb{I}[-K, K] \rightarrow \mathbb{I}[-2M, 2M])$, and $S = (\mathbb{I}[-a, a] \rightarrow \mathbb{I}[-K, K])$, of Scott continuous functions. For $u \in V$, the domain-theoretic Picard operator is given by $P_u : S \rightarrow S$ with $P_u(y) = \lambda x. \int_0^x u(y(t)) dt$. By Kleene's theorem, the least fixed point y of P_u satisfies $y = P_u(y)$. In addition, if u is an extension function v and f is a solution of the IVP in Equation (7) then y contains f i.e., $y \sqsubseteq f$, whereas if y is maximal then it is the maximal extension of the unique solution of the initial value theorem; cf. [21, Proposition 3.7].

In our language the solution of the initial value problem can be expressed in the following way. Let $e_v : \pi \rightarrow \pi$, be an expression defining the function v in its domain of definition. Then, the solution of the initial value problem is given by the expression:

$$Y(\lambda f. \lambda x. \text{int } \lambda t. x * \text{pr}_M(e_v(f(t * x))))$$

where pr_M is a function projecting the real line onto the interval $[-M, M]$ and defined as $\lambda x. (\text{in}_\pi M) * \text{pr } x/M$, with M a rational constant. The expression $\lambda f. \lambda x. \text{int } \lambda t. x * \text{pr}_M(e_v(f(t * x)))$ needs to contain the projection function pr_M in order to define a functional mapping the bottom function to a function f_1 that maps the interval $[-a, a]$ to the interval $[-K, K]$. Notice that $e_v(f_1([0, 1] * [-a, a]))$ denotes an interval containing $[-M, M]$; it follows that, in the evaluation of the fixed point obtained by functional iteration, after the first iteration, pr_M is applied to points in $[-M, M]$ and therefore acts as the identity function. Moreover, recall from Equation (6) that using variable substitution, $\int_0^x f(t) dt$ can be evaluated by the expression $\text{int } \lambda t. x * f(x * t)$.

By using currying, the above construction can be easily extended to solve the initial value problem in \mathbb{R}^n .

Lemma 3. Suppose $F : \mathbb{D}_{\vec{\tau} \rightarrow \delta}$ is a standard-robust and standard maximal preserving continuous functional. If $L(F)^s((\vec{d})^s, (\vec{d}')^s)$ is bounded for some pair (\vec{d}, \vec{d}') of lists of locally consistent and standard preserving elements, then the restriction of $(F)^s$ to the space of maximal preserving elements is locally Lipschitzian at $((\vec{d})^s, (\vec{d}')^s)$.

Proof. Let $I = L(F)^{\mathbf{s}}((\vec{d})^{\mathbf{s}}, (\vec{d}')^{\mathbf{s}})$ be a compact interval for some $(\vec{d})^{\mathbf{s}}$ and $(\vec{d}')^{\mathbf{s}}$. Put $a = 1 + \max(|I^-|, |I^+|)$. Recall that $\vec{\tau} \rightarrow \delta$ denotes the type $\tau_1 \rightarrow (\dots \rightarrow (\tau_n \rightarrow \delta) \dots)$. By the Scott continuity of $L(F)^{\mathbf{s}}$ at $((\vec{d})^{\mathbf{s}}, (\vec{d}')^{\mathbf{s}})$, there exist open sets O_j and O'_j for $1 \leq j \leq n$ with $(d_j)^{\mathbf{s}} \in O_j$ and $[-(d'_j)^{\mathbf{s}}, (d'_j)^{\mathbf{s}}] \subset O'_j$ such that $L(F)^{\mathbf{s}}[\times_{j=1}^n O_j \times O'_j] \subset (-a, a)$. The result follows.

Proposition 10. A standard-robust and standard maximal preserving continuous functional $F : \mathbb{D}_{\vec{\tau} \rightarrow \delta}$ is locally consistent if and only if for any pair of lists of locally consistent and standard maximal preserving elements \vec{d} and \vec{d}' , we have:

$$\text{In}(F(\vec{d} + \varepsilon \vec{d}')) \sqsubseteq L(F)^{\mathbf{s}}((\vec{d})^{\mathbf{s}}, (\vec{d}')^{\mathbf{s}}). \quad (13)$$

Proof. To prove the “only if” part, let F be locally consistent. Let \vec{d}_n and \vec{d}'_n , $n \in \mathbb{N}$ be two chains such that $\vec{d}_n \ll \vec{d}$, $\vec{d}'_n \ll \vec{d}'$ and $\bigsqcup_n \vec{d}_n = \vec{d}$, $\bigsqcup_n \vec{d}'_n = \vec{d}'$, and let $r_n > 0$ be a sequence rational numbers converging to 0.

We have $\vec{d} + \varepsilon \vec{d}' = \bigsqcup_n (\vec{d}_n \sqcap (\vec{d}_n + r_n \vec{d}'_n)) + \varepsilon \vec{d}'_n$.

For any $n \in \mathbb{N}$, for each rational number r' such that $0 < r' < r_n$, and for each pair of lists of locally consistent, standard maximal preserving elements \vec{e}, \vec{e}' such that $\vec{d}_n \ll \vec{e}$, $\vec{d}'_n \ll \vec{e}'$, we have:

$$\text{In}(F((\vec{d}_n \sqcap (\vec{d}_n + r_n \vec{d}'_n)) + \varepsilon \vec{d}'_n)) \uparrow \frac{\text{St}(F(\vec{e} + r' \vec{e}') - F(\vec{e}))}{r'}$$

This relation follows immediately from the local consistency of F, \vec{e}, \vec{e}' , from the monotonicity of F and from the fact that the consistent relation \uparrow is downward closed.

Because $\frac{\text{St}(F(\vec{e} + r' \vec{e}') - F(\vec{e}))}{r'}$ is a maximal element in \mathbb{DR} , we have:

$$\text{In}(F((\vec{d}_n \sqcap (\vec{d}_n + r_n \vec{d}'_n)) + \varepsilon \vec{d}'_n)) \sqsubseteq \frac{\text{St}(F(\vec{e} + r' \vec{e}') - F(\vec{e}))}{r'}.$$

Note that for $n \in \mathbb{N}$,

$$O_n := \{(\vec{e})^{\mathbf{s}} \mid \vec{d}_n \ll \vec{e}, \vec{e} \text{ standard maximal preserving} \}$$

$$O'_n := \{(\vec{e}')^{\mathbf{s}} \mid \vec{d}'_n \ll \vec{e}', \vec{e}' \text{ standard maximal preserving} \}$$

are systems of open neighbourhoods for $(\vec{d})^{\mathbf{s}}$ and $(\vec{d}')^{\mathbf{s}}$ respectively. Thus, by the definition of $L(F)^{\mathbf{s}}((\vec{d})^{\mathbf{s}}, (\vec{d}')^{\mathbf{s}})$, we obtain:

$$\text{In}(F((\vec{d}_n \sqcap (\vec{d}_n + r_n \vec{d}'_n)) + \varepsilon \vec{d}'_n)) \sqsubseteq L(F)^{\mathbf{s}}((\vec{d})^{\mathbf{s}}, (\vec{d}')^{\mathbf{s}})$$

and, hence, Relation (8) follows by the continuity of F .

To prove the “if” part, let F be a functional satisfying

$$\forall \vec{d}, \vec{d}'. \text{In}(F(\vec{d} + \varepsilon \vec{d}')) \sqsubseteq L(F)^{\mathbf{s}}((\vec{d})^{\mathbf{s}}, (\vec{d}')^{\mathbf{s}}).$$

We aim to prove that F is locally consistent. Given two locally consistent, standard maximal preserving \vec{d}, \vec{d}' , if $\text{In}(F((\vec{d} \sqcap (\vec{d} + r\vec{d}')) + \varepsilon\vec{d}')) = 0 + \varepsilon(-\infty, \infty)$, then one can immediately deduce local consistency:

$$\text{In}(F((\vec{d} \sqcap (\vec{d} + r\vec{d}')) + \varepsilon\vec{d}')) \uparrow \frac{\text{St}(F(\vec{d} + r\vec{d}') - F(\vec{d}))}{r}$$

Otherwise, $L(F)^s((\vec{d} \sqcap (\vec{d} + r\vec{d}'))^s, (\vec{d}')^s)$ is bounded, and by Lemma 3, $L(F)^s$ is locally Lipschitzian at $((\vec{d} + r\vec{d}'), (\vec{d}')^s)$. We let $g : [0, r] \rightarrow \mathbb{R}$ be the function defined for $t \in [0, r]$ by

$$g(t) = (F)^s((\vec{d})^s + t(\vec{d}')^s).$$

By monotonicity and the chain rule (Proposition 6), for $t \in [0, r]$, we have:

$$\begin{aligned} L(F)^s((\vec{d} \sqcap (\vec{d} + r\vec{d}'))^s, (\vec{d}')^s) &\subseteq \\ L(F)^s((\vec{d} + t\vec{d}')^s, (\vec{d}')^s) &\subseteq (Lg)(t, 1) \end{aligned}$$

Therefore $(Lg)(t, 1)$ is bounded and g is a locally Lipschitzian function. By the Mean Value Theorem 2, there exists $r_1 \in \mathbb{R}$ with $0 < r_1 < r$ such that $(g(r) - g(0))/r \in (Lg)(r_1, 1)$. Hence, by the previous equality

$$L(F)^s((\vec{d} + r_1\vec{d}')^s, (\vec{d}')^s) \subseteq \frac{(F(\vec{d} + r\vec{d}') - F(\vec{d}))^s}{r}.$$

Multiplying both terms by ε and using the initial hypothesis, one derives

$$\text{In}(F((\vec{d} \sqcap (\vec{d} + r\vec{d}')) + \varepsilon\vec{d}')) \uparrow \frac{\text{St}(F(\vec{d} + r\vec{d}') - F(\vec{d}))}{r}$$

as required.

9.5 Proofs of Section 7

To prove Proposition 12 the following technical lemma is necessary:

Lemma 4. *For any pair of logically consistent first-order functions f, g in $\mathbb{D}_{\delta \rightarrow \dots \rightarrow \delta}$ and any rational number $r > 0$, we have:*

$$R_{\delta \rightarrow \dots \rightarrow \delta}^r(f, f + rg, (f \sqcap (f + rg)) + \varepsilon g).$$

Proof. Let $(x_1, y_1, z_1) \dots (x_n, y_n, z_n)$ be triples of elements in \mathbb{IR} such that $R_{\delta}^r(x_i, y_i, z_i)$ for $1 \leq i \leq n$ for some rational number $r > 0$. The relation

$$\begin{aligned} R_{\delta}^r(f(x_1) \dots (x_n), (f + rg)(y_1) \dots (y_n), \\ ((f \sqcap (f + rg)) + \varepsilon g)(z_1) \dots (z_n)) \end{aligned}$$

needs to be proved.

The first condition for R_δ^r is implied by the following chain of relations:

$$\begin{aligned}
& \text{St}((f \sqcap (f + rg)) + \varepsilon g)(z_1) \dots (z_n) \\
&= \text{St}(f \sqcap (f + rg))(z_1) \dots (z_n) \\
&= \text{St}(f)(z_1) \dots (z_n) \sqcap \text{St}(f + rg)(z_1) \dots (z_n) \\
&\sqsubseteq \text{St}(f)(x_1) \dots (x_n) \sqcap \text{St}(f + rg)(y_1) \dots (y_n)
\end{aligned}$$

To prove the second condition, note that the following chain of relations holds:

$$\begin{aligned}
& (f \sqcap (f + rg) + \varepsilon g)(z_1) \dots (z_n) \\
&\sqsubseteq (f + \varepsilon g)(z_1) \dots (z_n) \\
&\sqsubseteq f(z_1) \dots (z_n) + \varepsilon g(y_1) \dots (y_n) \\
&\uparrow \frac{\text{St}(f(y_1) \dots (y_n) - f(x_1) \dots (x_n))}{r} + \varepsilon g(y_1) \dots (y_n) \\
&= \frac{\text{St}((f + rg)(y_1) \dots (y_n) - f(x_1) \dots (x_n))}{r}
\end{aligned}$$

Since the consistency relation is downward closed, the first and the last element in the chain are consistent, proving the claim.

Proposition 11. Any first-order function $f : \mathbb{D}_\tau$ is locally consistent if and only if it is logically consistent.

Proof. Consider first the “if” part. Assume $f : \mathbb{D}_\tau$ is logically consistent. Let $\vec{I}, \vec{J}, \vec{K}$ be three arbitrary lists of rational intervals where, for any index i , I_i is not a single point. For any rational $r > 0$ sufficiently small such that \vec{I} is consistent with $\vec{I} + r\vec{K}$, the relation $R_\delta^r(I_i + \varepsilon J_i, I_i + \varepsilon J_i, I_i + \varepsilon K_i)$ therefore holds for any index i . Hence, we have $R_\delta^r(f(\vec{I} + \varepsilon \vec{J}), f(\vec{I} + \varepsilon \vec{J}), f(\vec{I} + \varepsilon \vec{K}))$ from which it follows that $\text{St}(f(\vec{I} + \varepsilon \vec{K})) \sqsubseteq \text{St}(f(\vec{I} + \varepsilon \vec{J}))$. Since $\vec{I}, \vec{J}, \vec{K}$ are arbitrary, it follows that f is standard-robust.

For given \vec{I}, \vec{I}' and rational $r > 0$, suppose, for all indices i , the relation

$$R_\delta^r(I_i, I_i + rI'_i, (I_i \sqcap (I_i + rI'_i) + \varepsilon I'_i))$$

holds. Then, by logical consistency of f , we can deduce the relation:

$$R_\delta^r(f(\vec{I}), f(\vec{I} + r\vec{I}'), f((\vec{I} \sqcap (\vec{I} + r\vec{I}')) + \varepsilon \vec{I}'));$$

therefore $\text{In}(f((\vec{I} \sqcap (\vec{I} + r\vec{I}')) + \varepsilon \vec{I}')) \uparrow \frac{\text{St}(f(\vec{I} + r\vec{I}') - f(\vec{I}))}{r}$. Thus, f is locally consistent.

Next consider the “only if” part. Assume that f is locally consistent. Take any real value r and lists on dual numbers $\vec{I} + \varepsilon \vec{I}', \vec{J} + \varepsilon \vec{J}', \vec{K} + \varepsilon \vec{K}'$, such that for all indices i , we have:

$$R^r(I_i + \varepsilon I'_i, J_i + \varepsilon J'_i, K_i + \varepsilon K'_i)$$

Since $r\vec{K}' \uparrow \vec{J} - \vec{I}$, there exist $\vec{I}_0 \sqsupseteq \vec{I}$ and $\vec{K}'_0 \sqsupseteq \vec{K}'$ such that $\vec{J} \sqsubseteq \vec{I}_0 + r\vec{K}'_0$. By local consistency we get

$$\text{In}(f(\vec{I}_0 \sqcap (\vec{I}_0 + r\vec{K}'_0) + \varepsilon \vec{K}'_0)) \uparrow \frac{\text{St}(f(\vec{I}_0 + r\vec{K}'_0) - f(\vec{I}_0))}{r},$$

and, by the monotonicity of f and the downward closure of the consistency relation we get $\text{In}(f(\vec{K} + \varepsilon \vec{K}')) \uparrow \frac{\text{St}(f(\vec{J}) - f(\vec{I}))}{r}$. Finally by the standard-robustness of f , we have $\text{In}(f(\vec{K} + \varepsilon \vec{K}')) \uparrow \frac{\text{St}(f(\vec{J} + \varepsilon \vec{J}') - f(\vec{I} + \varepsilon \vec{I}'))}{r}$; therefore the first condition for logical consistency holds for f . The second condition holds immediately by the monotonicity of f .

Proposition 12. Any second-order function $F : D_{\vec{\tau} \rightarrow \delta}$ is locally consistent if it is logically consistent.

Proof. Let F be a logically consistent functional. Let $f_1, g_1, \dots, f_n, g_n$ be a chain of locally consistent functions or dual numbers. By Proposition 11, all f_i, g_i are logically consistent. From Lemma 4 it follows that for any rational number $r > 0$ we have: $R_{\vec{\tau}}^r(f_i, f_i + rg_i, (f_i \sqcap (f_i + rg_i)) + \varepsilon g_i)$, from which the result follows.

9.6 Proofs of Section 8

Recall that by the Riesz representation theorem [27] any classical continuous linear functional $F : ([0, 1] \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ can be expressed as the difference of two Riemann-Stieljes integrals:

$$F(f) = \int_0^1 f dg_1 - \int_0^1 f dg_2$$

where g_1 and g_2 are non-decreasing and right continuous. Then there exist Borel measures μ_1 and μ_2 on $[0, 1]$ (called Lebesgue-Stieljes measures) such that

$$F(f) = \int_{[0,1]} f d\mu_1 - \int_{[0,1]} f d\mu_2.$$

Proposition 14 follows from the following lemma.

Lemma 5. Let $g : [a, b] \rightarrow \mathbb{R}$ be non-decreasing and right-continuous and put $c = g(a)$ and $d = g(b)$. Then there exists a non-decreasing right continuous map $g^\dagger : [c, d] \rightarrow [a, b]$ such that for any continuous function $f : [a, b] \rightarrow \mathbb{R}$, we have $\int_a^b f(x) dg(x) = \int_c^d (f \circ g^\dagger)(x) dx$.

(This lemma was stated by Lebesgue in [40] and a generalisation of it is proved in [25]. We give an elementary proof here which explicitly constructs the function g^\dagger .)

Proof. First note that both integrals exist. If $J \subset [a, b]$ is a non-trivial interval (i.e., with positive length), denote its left and right end points by J^- and J^+ . If $g^{-1}(\{y\}) = \emptyset$ for some $y \in [c, d]$, then there exists a unique $x_0 \in [a, b]$ such that $\lim_{x \rightarrow x_0^-} g(x) \leq y < \lim_{x \rightarrow x_0^+} g(x)$ and put $g^\dagger(y) := x_0$ and extend g^\dagger to a map $g^\dagger : [c, d] \rightarrow [a, b]$ as follows:

$$g^\dagger(y) \mapsto \begin{cases} x & \text{if } g^{-1}(\{y\}) = \{x\} \\ J^+ & \text{if } g^{-1}(\{y\}) = J \text{ non-trivial interval} \end{cases}$$

Then $g^\dagger : [c, d] \rightarrow [a, b]$ is non-decreasing and right continuous.

Let's denote the lower sum with respect to partition P of $[a, b]$ for the Riemann Stieljes integral $\int_a^b f dg$ by $S^\ell(f, g, P)$ and the lower sum with respect to the partition Q of $[c, d]$ for the Riemann integral $\int_c^d f \circ g^\dagger dx$ by $S^\ell(f \circ g^\dagger, Q)$. Similarly, for the upper sums $S^u(f, g, P)$ and $S^u(f \circ g^\dagger, Q)$.

We will show that

$$\begin{aligned} \int_a^b f dg &= \sup_P S^\ell(f, g, P) \leq \sup_Q S^\ell(f \circ g^\dagger, Q) \\ &= \int_c^d f \circ g^\dagger(x) dx. \end{aligned}$$

Let $\varepsilon > 0$ be given. By the uniform continuity of f on $[a, b]$, there exists $\delta_1 > 0$ such that $|x_1 - x_2| < \delta_1$ implies $|f(x_1) - f(x_2)| < \varepsilon/(2(d-c))$. In addition, since $\int_a^b f dg$ exists, there exists $\delta_2 > 0$ such that for all partition P on $[a, b]$ with $\|P\| < \delta_2$, we have

$$S^\ell(f, g, P) > \int_a^b f dg - \varepsilon/2. \quad (14)$$

Let P be such a partition. Since the lower sum increases if we refine P and the refinement still satisfies the Inequality (14), we apply the following scheme to each non-trivial interval $J \subset [a, b]$ on which g is constant and $P \cap J^\circ \neq \emptyset$. For each such non-trivial interval J , refine P by adding three points to it: the two end points J^- and J^+ of J and a point J^0 such that $J^- < J^0 < J^+$, $|J^0 - J^+| < \delta_1$ and $(J^0, J^+) \cap P = \emptyset$. Note that by right continuity of g we have $g(J^-) = u$, where u is the constant value of g on J . Having refined P in this way with respect to J , we can now remove all partition points $p \in P \cap J$ with $J^- < p < J^0$ since the contributions of these points at which g is constant vanish in the lower or upper sum $S^\ell(f, g, P)$.

Now consider the partition $Q := g[P]$ of $[c, d]$ where the partition $P : p_1 < p_2 < \dots < p_n$ of $[a, b]$ satisfies the above conditions and Inequality (14). We claim that $|S^\ell(f \circ g^\dagger, Q) - \int_a^b f dg| < \varepsilon$. Consider $I \subset \{1, 2, \dots, n\}$ such that $i \in I$ iff $p_i \neq J^-$ and $p_i \neq J^0$ for any nontrivial interval J on which g is constant. Then g takes the subinterval $[p_i, p_{i+1}]$ for $i \in I$ to distinct non-trivial subinterval $[g(p_i), g(p_{i+1})]$. This implies:

$$\begin{aligned} &\sum_{i \in I} (g(p_{i+1}) - g(p_i)) \inf_{x \in [p_i, p_{i+1}]} f(x) \\ &= \sum_{i \in I} (g(p_{i+1}) - g(p_i)) \inf_{y \in [g(p_i), g(p_{i+1})]} f(g^\dagger(y)) \end{aligned}$$

Thus, the difference between $S^\ell(f \circ g^\dagger, Q)$ and $S^\ell(f, g, P)$ can only arise from non-trivial intervals J on which g is constant. Consider now a non-trivial interval J on which g is constant. If g is actually continuous at J^+ , then the contribution to the lower sum $S^\ell(f, g, P)$ from the two subintervals $[J^-, J^0]$ and $[J^0, J^+]$

vanish as g is constant on $[J^-, J^+]$; and since $g(J^-) = g(J^0) = g(J^+)$ the image of the two subintervals collapse to a single point in $[c, d]$ with no contribution to the lower sum $S^\ell(f \circ g^\dagger, Q)$. Consider now those intervals J on which g is constant with $g(J^-) = g(J^0) < g(J^+)$. Note that we always have $g^\dagger(g(J^+)) = J^+$. In fact, if J^+ is the left end of an interval on which g is constant, by the right continuity of g^\dagger , then we have $g^\dagger(g(J^+)) = J^+$. If on the other hand, $\{J^+\} = g^{-1}(g(J^+))$, then by definition we again have $g^\dagger(g(J^+)) = J^+$. Now, since $g(J^0) = g(J^-)$, the contribution to $S^\ell(f, g, P)$ from J is

$$\begin{aligned} & \inf_{x \in [J^-, J^0]} f(x)(g(J^0) - g(J^-)) \\ & + \inf_{x \in [J^0, J^+]} f(x)(g(J^+) - g(J^0)) \\ & = \inf_{x \in [J^0, J^+]} f(x)(g(J^+) - g(J^0)) \end{aligned} \quad (15)$$

On the other hand, the contribution to $S^\ell(f, g^\dagger, g[P])$ from J is

$$\begin{aligned} & \inf_{y \in [g(J^-), g(J^+)]} f \circ g^\dagger(y)(g(J^+) - g(J^-)) \\ & = f(J^+)(g(J^+) - g(J^0)). \end{aligned} \quad (16)$$

Comparing the Expressions (15) and (16), we infer that the difference between the contributions of J to $S^\ell(f, g, P)$ and $S^\ell(f \circ g^\dagger, g[P])$ is bounded by $\varepsilon((g(J^+) - g(J^0)))/(2(d - c))$ by the uniform continuity condition since $J^+ - J^0 < \delta_1$.

It follows that the absolute value of the sum of the difference of the contributions from all such non-trivial intervals J to $S^\ell(f \circ g^\dagger, Q)$ and $S^\ell(f, g, P)$ is given by:

$$\begin{aligned} & \left| \sum_{g(J^-) < g(J^+)} \inf_{y \in [g(J^-), g(J^+)]} f \circ g^\dagger(y)(g(J^+) - g(J^-)) \right. \\ & \quad \left. - \inf_{x \in [J^0, J^+]} f(x)(g(J^+) - g(J^0)) \right| \\ & \leq \sum_{g(J^-) < g(J^+)} \left| \inf_{x \in [J^0, J^+]} f(x) - f(J^+) \right| (g(J^+) - g(J^-)) \\ & \leq \sum_{g(J^-) < g(J^+)} (g(J^+) - g(J^-)) \varepsilon / (2(d - c)) \leq \varepsilon / 2. \end{aligned}$$

Hence, by using Inequality (14), we get

$$\begin{aligned} & |S^\ell(f \circ g^\dagger, Q) - \int_a^b f dg| \leq |S^\ell(f \circ g^\dagger, Q) - S^\ell(f, g, P)| \\ & + |S^\ell(f, g, P) - \int_a^b f dg| < \varepsilon / 2 + \varepsilon / 2 = \varepsilon. \end{aligned}$$

Since $\varepsilon > 0$ is arbitrary, it follows that $\int_c^d f \circ g^\dagger(x) dx \geq \int_a^b f dg$. By using the upper sums, we similarly obtain $\int_c^d f \circ g^\dagger(x) dx \leq \int_a^b f dg$.

To prove Theorem 4, we need two lemmas. For any map $h : [c, d] \rightarrow [a, b] \subset \mathbb{I}[a, b]$, its envelope $h^* : \mathbb{I}[c, d] \rightarrow \mathbb{I}[a, b]$ is given by $h^*(J) = h[J]$ for any non-empty compact interval $J \subset [c, d]$. If h is non-decreasing, then h has at most a countable number of discontinuities and since the left and right limits, $\lim_{x \rightarrow x_0^-} h(x)$ and $\lim_{x \rightarrow x_0^+} h(x)$, exist at any point of discontinuity $x_0 \in [c, d]$, it follows easily that we then have $h^*(x_0) = [\lim_{x \rightarrow x_0^-} h(x), \lim_{x \rightarrow x_0^+} h(x)]$, i.e., h^* simply closes the discontinuous gap at x_0 . We immediately have:

Lemma 6. *Suppose $h : [c, d] \rightarrow \mathbb{R}$ is non-decreasing with $a = h(c)$ and $b = h(d)$. Assume $f : [a, b] \rightarrow \mathbb{R}$ is continuous. Then the three extensions $h^* : \mathbb{I}[c, d] \rightarrow \mathbb{I}[a, b]$, $f^* : \mathbb{I}[a, b] \rightarrow \mathbb{I}\mathbb{R}$ and $(f \circ h)^* : \mathbb{I}[c, d] \rightarrow \mathbb{I}\mathbb{R}$ satisfy: $f^* \circ h^* = (f \circ h)^*$.*

Lemma 7. *Suppose $h : [c, d] \rightarrow \mathbb{R}$ is non-decreasing with $a = h(c)$ and $b = h(d)$, and suppose $f : [a, b] \rightarrow \mathbb{R}$ is continuous. Then,*

$$\int_c^d f \circ h(x) dx = \int_{[c, d]} f^* \circ h^*(x) dx.$$

(We note that the integral on the left is a classical Riemann integral while the integral on the right is an interval valued integral of an interval variable. The lemma says that the interval on the right is the singleton real number given by the left hand side.)

Proof. For any partition $P : 0 = x_0 < x_1 < \dots < x_n = 1$ of the interval $[0, 1]$, we check that the Darboux lower sums $S^\ell(f \circ h, P)$ and $S^\ell(f^* \circ h^*, P)$ of the two integrands are the same. By Lemma 6, we simply show that the Darboux lower sums $S^\ell(f \circ h, P)$ and $S^\ell((f \circ h)^*, P)$ are the same. Since at each point of discontinuity $x \in [c, d]$, the envelope $(f \circ h)^*$ at x is the closed interval gap $[\lim_{y \rightarrow x^-} f(h(y)), \lim_{y \rightarrow x^+} f(h(y))]$, it follows that in each partition interval $[x_{i-1}, x_i]$ of P , we have

$$\inf_{y \in [x_{i-1}, x_i]} f \circ h(y) = \inf_{y \in [x_{i-1}, x_i]} (f \circ h)^*(y).$$

Thus, the Darboux lower sums are the same. Similarly, the Darboux upper sums are the same; the result follows.

In order to extend the continuous linear functional to the domain-theoretic setting, we use the notion of the envelope of a map as in Proposition 1 and consider the envelopes $(g_1^\dagger)^*$ and $(g_2^\dagger)^*$ of the two non-decreasing maps g_1^\dagger and g_2^\dagger in Proposition 14.

Theorem 4 . The continuous linear functional $F : ([0, 1] \rightarrow \mathbb{R}) \rightarrow \mathbb{R}$ has a conservative extension $F^* : (\mathbb{I}[0, 1] \rightarrow \mathbb{I}\mathbb{R}) \rightarrow \mathbb{I}\mathbb{R}$ given by

$$\begin{aligned} & F^*(f) \\ &= \int_{[c_1, d_1]} f \circ (g_1^\dagger)^*(x) dx - \int_{[c_2, d_2]} f \circ (g_2^\dagger)^*(x) dx. \end{aligned}$$

Similarly the embedding $(F)^{\mathbf{d}}$ of F in the dual domain $\mathbb{D}_{(\delta \rightarrow \delta) \rightarrow \delta}$ is given by:

$$\begin{aligned} & (F)^{\mathbf{d}}(f) \\ &= \int_{[c_1, d_1]}^{\mathbf{d}} f((g_1^\dagger)^\star(x)^{\mathbf{s}})^{\mathbf{d}} dx - \int_{[c_2, d_2]}^{\mathbf{d}} f((g_2^\dagger)^\star(x)^{\mathbf{s}})^{\mathbf{d}} dx \end{aligned}$$

Proof. The first part follows from Lemma 7.

For the second part, by definition: $(F)^{\mathbf{d}} = G^\star$ with

$$G(f) = F((f)^{\mathbf{s}}) + \varepsilon((LF)^\star((f)^{\mathbf{s}}, (f)^{\mathbf{i}})).$$

By linearity of F , we obtain:

$$\begin{aligned} G(f) &= F((f)^{\mathbf{s}}) + \varepsilon F((f)^{\mathbf{i}}) \text{ (by Proposition 14)} \\ &= \int_{c_1}^{d_1} (f)^{\mathbf{s}} \circ g_1^\dagger(x) dx - \int_{c_2}^{d_2} (f)^{\mathbf{s}} \circ g_2^\dagger(x) dx \\ &\quad + \varepsilon \int_{c_1}^{d_1} (f)^{\mathbf{i}} \circ g_1^\dagger(x) dx - \varepsilon \int_{c_2}^{d_2} (f)^{\mathbf{i}} \circ g_2^\dagger(x) dx \\ &= \int_{c_1}^{d_1} (f)^{\mathbf{s}} \circ g_1^\dagger(x) dx + \varepsilon \int_{c_1}^{d_1} (f)^{\mathbf{i}} \circ g_1^\dagger(x) dx \\ &\quad - \int_{c_2}^{d_2} (f)^{\mathbf{s}} \circ g_2^\dagger(x) dx - \varepsilon \int_{c_2}^{d_2} (f)^{\mathbf{i}} \circ g_2^\dagger(x) dx. \end{aligned}$$

The result now follows by the definition of envelope and integration on the dual domain.

We can now extend Lemma 5 and then Theorem 4 to continuous linear functionals on $C_0(\mathbb{R})$ equipped with its sup norm topology. Recall the following extension of Riesz's representation theorem, referred to as Riesz-Markov representation theorem.

Theorem 5 (See [6, Theorem 1.4].) If $F : C_0(\mathbb{R}) \rightarrow \mathbb{R}$ is a continuous linear functional, then there exists a finite signed measure ν , such that $F(f) = \int_{-\infty}^{\infty} f d\nu$.

By Hahn decomposition, let ν_1 and ν_2 be, respectively, the positive and negative parts of the finite measure ν , i.e., $F(f) = \int_{-\infty}^{\infty} f d\nu_1 - \int_{-\infty}^{\infty} f d\nu_2$. Let $g_i : \mathbb{R} \rightarrow \mathbb{R}$ ($i = 1, 2$) with

$$g_i(x) = \begin{cases} \nu_i((0, x]) & x > 0 \\ -\nu_i(\{0\}) & x = 0 \\ -\nu_i((x, 0]) & x < 0. \end{cases}$$

Then g_i is non-decreasing and right continuous on \mathbb{R} for $i = 1, 2$. Put

$$\tilde{c}_i := -\nu_i((-\infty, 0]) = \lim_{x \rightarrow -\infty} g_i(x) \quad (17)$$

$$\tilde{d}_i := \nu_i((0, \infty]) = \lim_{x \rightarrow \infty} g_i(x), \quad (18)$$

for $i = 1, 2$. In addition, the construction of g^\dagger in Lemma 5 extends to $g_i^\dagger : [\tilde{c}_i, \tilde{d}_i] \rightarrow \mathbb{R}$ for $i = 1, 2$.

Corollary 5. . For $i = 1, 2$:

$$\int_{-\infty}^{\infty} f dg_i = \int_{\tilde{c}_i}^{\tilde{d}_i} f \circ g_i^\dagger(x) dx$$

Proof. By Lemma 5, we have for any pair of real numbers $a < b$, the following equality:

$$\int_a^b f dg_i = \int_{c_i}^{d_i} f \circ g_i^\dagger(x) dx$$

with $c_i = g_i(a)$ and $d_i = g_i(b)$ for $i = 1, 2$. The result now follows by taking the limits $a \rightarrow -\infty$ and $b \rightarrow \infty$ and observing Equations (17) and (18).

It follows that, for any continuous linear functional F on $C_0(\mathbb{R})$ equipped with the sup norm topology, we have the extension:

$$F(f) = \int_{\tilde{c}_1}^{\tilde{d}_1} f \circ g_1^\dagger(x) dx - \int_{\tilde{c}_2}^{\tilde{d}_2} f \circ g_2^\dagger(x) dx.$$

Thus, Theorem 4 can be extended to continuous linear functionals on $C_0(\mathbb{R})$.