A Computational Model for Multi-Variable Differential Calculus

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Abstract. We introduce a domain-theoretic computational model for multi-variable differential calculus, which for the first time gives rise to data types for differentiable functions. The model, a continuous Scott domain for differentiable functions of n variables, is built as a sub-domain of the product of $n+1$ copies of the function space on the domain of intervals by tupling together consistent information about locally Lipschitz (piecewise differentiable) functions and their differential properties (partial derivatives). The main result of the paper is to show, in two stages, that consistency is decidable on basis elements, which implies that the domain can be given an effective structure. First, a domain-theoretic notion of line integral is used to extend Green's theorem to interval-valued vector fields and show that integrability of the derivative information is decidable. Then, we use techniques from the theory of minimal surfaces to construct the least and the greatest piecewise linear functions that can be obtained from a tuple of $n+1$ rational step functions, assuming the integrability of the n-tuple of the derivative part. This provides an algorithm to check consistency on the rational basis elements of the domain, giving an effective framework for multi-variable differential calculus.

1 Introduction

We introduce a domain-theoretic computational model for multi-variable differential calculus, which for the first time gives rise to data types for differentiable functions. The model is a continuous Scott domain for differentiable functions of n variables. It allows us to deal with differentiable functions in a recursion theoretic setting, and is thus fundamental for applications in computational geometry, geometric modelling, ordinary and partial differential equations and other fields of computational mathematics. The overall aim of the framework is to synthesize differential calculus and computer science, which are two major pillars of modern science and technology.

The basic idea of the model is to collect together the local differential properties of multi-variable functions by developing a generalization of the concept of a Lipschitz constant to an interval vector Lipschitz constant. The collection of these local differentiable properties are then used to define the domain-theoretic derivative of a multi-variable function and the primitives of an interval-valued vector field, which leads to a fundamental theorem of calculus for interval-valued functions, a theorem that has no counterpart in classical analysis. This fundamental theorem is then used to construct the domain of differentiable functions as a sub-domain of the product of $n+1$ copies of the function space on the domain of intervals by tupling together consistent information about locally Lipschitz (piecewise differentiable) functions and their differential properties (partial derivatives). The base of this domain is a finitary data type, given by consistent tuples of $n+1$ step functions, where consistency means that there exists a piecewise differentiable function, equivalently a piecewise linear function, which is approximated, together with its n partial derivatives where defined, by the $n+1$ step functions.

The geometric meaning of the finitary data type and consistency is as follows. Each step function is represented by a finite set of $n+1$ dimensional rational hyper-rectangles in, say, $[0,1]^n \times \mathbb{R}$ such that any two hyper-rectangles have non-empty intersection whenever the interior of their base in $[0,1]^n$ have non-empty intersection. Such a set of hyper-rectangle gives a finitary approximation to a real-valued function on the unit cube $[0,1]^n$ if in the interior of the base of each hyper-rectangle the graph of the function is contained in that hyper-rectangle. A collection of $n+1$ such sets of hyper-rectangles could thus provide a finitary approximation to a function and its n partial derivatives. Consistency of this collection means that there exists a piecewise differentiable function which is approximated together with its partial derivatives, where defined, by the collection. For a consistent tuple, there are a least and a greatest piecewise differentiable function which satisfy the function and the partial derivative constraints. Figure 1 shows two examples of consistent tuples for $n = 2$ and in each case the least and greatest functions consistent with the derivative constraints are drawn. In the first case, on the left, there is a single hyper-rectangle for function approximation and the derivative approximations in the x and y directions over the whole domain of the function are given respectively by the constant intervals $[n, N]$ and $[m, M]$ with $n, m > 0$. In the second case, on the right, there are two intersecting hyper-rectangles for the function approximation and the derivative approximations are the constant intervals $[0, 0]$ and $[m, M]$ with $m > 0$.

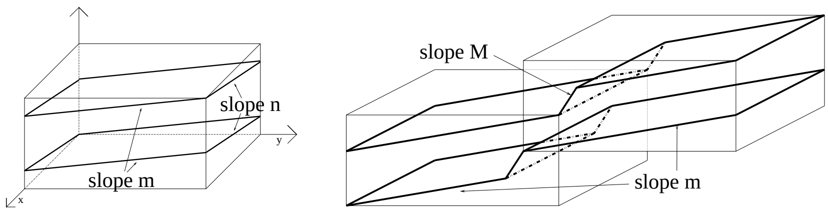

Fig. 1. Two examples of consistent function and derivative approximations

The main question now is whether consistency of the $n+1$ step functions is actually decidable. This problem is, as we have seen, very simple to state but it turns out to be very hard to solve, as it requires developing some new mathematics. The main result of the paper is to show, in two stages, that consistency is decidable on basis elements. As in classical differential multi-variable calculus, an interval-valued function may fail to be integrable. Thus, in the first stage, we introduce a domain-theoretic notion of line integral, which we use to establish a necessary and sufficient condition for an interval-valued Scott continuous vector function to be integrable: zero must be contained in the line integral of the interval-valued vector field with respect to any closed path. This extends the classical Green's Theorem for a vector field to be a gradient [9, pages 286-291] to interval-valued vector fields. We thus obtain a main result of this paper: an algorithm to check integrability for rational step functions, i.e., given n rational step functions, to check if there exists a piecewise differentiable function whose partial derivatives, where defined, are approximated by these step functions.

Finally, we use techniques from the theory of minimal surfaces to construct the least and the greatest piecewise linear functions obtained from a tuple of $n + 1$ rational step functions, in which the n-tuple of the derivative part is assumed to be integrable. These surfaces are obtained by, respectively, maximalizing and minimalizing the lower and the upper line integrals of the derivative information over piecewise linear paths. The maximalization and minimization are achieved for a piecewise linear path which can all be effectively constructed. The decidability of consistency is then reduced to checking whether the minimal surface is below the maximal surface, a task that can be done in finite time. This leads to an algorithm to check consistency of an $n + 1$ tuple and to show that consistency is decidable on the rational basis elements of the domain for locally Lipschitz functions, giving an effective framework for multi-variable differential calculus.

In the last section, we mention two applications of our framework, each worked out in detail in a follow-up paper. In the first, the domain for differential functions allows us to develop a domain-theoretic version of the inverse and implicit function theorem, which provides a robust technique for construction of curves and surfaces in geometric modelling and CAD. Our second application is a domain-theoretic adaption of Euler's method for solving ordinary differential equations, where we use the differential properties of the vector field defining the equation to improve the quality of approximations to the solution.

Due to the large number of new concepts in the paper and lack of space, nearly all proofs had to be omitted.

1.1 Related work

This work represents an extension of the domain-theoretic framework for differential calculus of a function of one variable introduced in [6] and its applications in solving initial value problems [5, 8]. The extension to higher dimension is however far more involved than the extension of classical differential calculus to higher dimensions.

The domain-theoretic derivative is closely related to the so-called generalized (or Clarke's) gradient, which is a key tool in nonsmooth analysis, control theory and optimization theory [3, 4]. For any locally Lipschitz function, the domain-theoretic derivative at a point gives the smallest hyper-rectangle, with sides parallel to the coordinate planes, which contains the Clarke's gradient.

In computable analysis, Pour-El and Richards [11] relate the computability of a function with the computability of its derivative. Weihrauch's scheme [13] leads to partially defined representations, but there is no general result on decidability. Interval analysis [10] also provides a framework for verified numerical computation. There, differentiation is performed by symbolic techniques [12] in contrast to our sequence of approximations of the functions.

1.2 Notations and terminology

We use the standard notions of domain theory as in [1]. Let $D^0[0,1]^n = [0,1]^n \to \mathbf{I}\mathbb{R}$ be the domain of all Scott continuous functions of type $[0,1]^n \to \mathbf{I}\mathbb{R}$; we often write D^0 for $D^0[0,1]^n$. A function $f \in D^0$ is given by a pair of respectively lower and upper semi-continuous functions $f^-, f^+ : [0,1]^n \to \mathbb{R}$ with $f(x) = [f^-(x), f^+(x)]$. Given a domain A, we denote by A_s^n the smash product, i.e., $a \in A_s^n$ if $a = (a_1, \cdots, a_n) \in A^n$ with $a_i \neq \bot$ for all $i = 1, \cdots, n$ or $a = \bot$. Let $(\mathbf{I}\mathbb{R})_s^{m\times n}$ denote the set of all $m \times n$ matrices with entries in $\mathbf{I}\mathbb{R}$, where for such a matrix either all components are non-bottom or the matrix itself is bottom. We use standard operations of interval arithmetic on interval matrices. By $a = [\underline{a}, \overline{a}] \in (\mathbf{I}\mathbb{R})^{m\times n}$, where $\underline{a}, \overline{a} \in \mathbb{R}^{m\times n}$, we denote an interval matrix with (i,j) entry given by the interval $[\underline{a}_{ij}, \overline{a}_{ij}]$. We identify the real number $r \in \mathbb{R}$ with the singleton $\{r\} \in \mathbf{I}\mathbb{R}$. And similarly for interval vectors and functions. We will use the *sign* function given by the multiplicative group homomorphism $\sigma : \mathbb{R} \to \{-, 0, +\}$. We write $\|x\| = \sqrt{\sum_{i=1}^n x_i^2}$ for the standard Euclidean norm of $x = (x_1, \cdots, x_n) \in \mathbb{R}^n$. The classical derivative of a map $f : [0,1]^n \to \mathbb{R}$ at $y \in [0,1]$, when it exists, is denoted by $f'(y)$. We will reserve the notation $\frac{df}{dx}$ exclusively in this paper for the domain-theoretic derivative which will be introduced later. The interior of a set $A \subset \mathbb{R}^n$ is denoted by A° and its closure by $\mathrm{cl}(A)$.

2 Ties of functions of several variables

The local differential property of a function is formalized in our framework by the notion of an interval Lipschitz constant.

Definition 1. *The continuous function $f : [0,1]^n \to \mathbf{I}\mathbb{R}$ has* an interval Lipschitz constant $b \in (\mathbf{I}\mathbb{R})_s^{1\times n}$ *in $a \in (\mathbf{I}[0,1])^n$ if for all $x, y \in a^\circ$ we have: $b(x-y) \sqsubseteq f(x)-f(y)$. The* single-step tie $\delta(a,b) \subseteq D^0[0,1]$ *of a with b is the collection of all functions in $D^0[0,1]$ which have an interval derivative b in a.*

For example, if $n = 2$, the information relation above reduces to $b_1(x_1 - y_1) + b_2(x_2 - y_2) \sqsubseteq f(x) - f(y)$. For a single-step tie $\delta(a,b)$, one can think of b as a Lipschitz interval vector constant for the family of functions in $\delta(a,b)$. A classical Lipschitz would require $k = |\overline{b_i}| = |\underline{b_i}| \geq 0$ for all $i = 1 \cdots n$. By generalizing the concept of a Lipschitz constant in this way, we are able to obtain essential information about the differential properties of the function, which includes what the classical Lipschitz constants provide:

Proposition 1. *If $f \in \delta(a,b)$ for $a^\circ \neq \emptyset$ and $b \neq \bot$, then $f(x)$ is maximal for each $x \in a^\circ$ and the induced function $f : a^\circ \to \mathbb{R}$ is Lipschitz: for all $u, v \in a^\circ$ we have $|f(u) - f(v)| \leq k\|u - v\|$, where $k = \max_{1\leq i\leq n}(|\underline{b}_i|, |\overline{b}_i|)$.*

The following proposition justifies our definition of interval derivative.

Proposition 2. *For $f \in C^1[0,1]^n$, the following three conditions are equivalent: (i) $f \in \delta(a,b)$, (ii) $\forall z \in a^\circ.\ f'(z) \in b$ and (iii) $a \searrow b \sqsubseteq f'$.*

When the components of a and b are rational intervals $\delta(a,b)$ is a family of functions in D^0 with a finitary differential property. For the rest of this section, we assume we are in dimension $n \geq 2$.

Definition 2. *A* step tie *of D^0 is any finite intersection $\bigcap_{1\leq i\leq n} \delta(a_i, b_i) \subset D^0$. A* tie *of D^0 is any intersection $\Delta = \bigcap_{i\in I} \delta(a_i, b_i) \subset D^0$. The* domain *of a non-empty tie Δ is defined as dom$(\Delta) = \bigcup_{i\in I}\{a_i^\circ \mid b_i \neq \bot\}$.*

A non-empty step tie with rational intervals gives us a family of functions with a *finite* set of consistent differential properties, and a non-empty general tie gives a family of functions with a consistent set of differential properties. The following result sums up the main relation between step ties and step functions.

Proposition 3. *For any indexing set I, the family of step functions $(a_i \searrow b_i)_{i\in I}$ is consistent if $\bigcap_{i\in I} \delta(a_i, b_i) \neq \emptyset$.*

Let $(T^1[0,1], \supseteq)$ be the dcpo of ties of D^0 ordered by reverse inclusion. We are finally in a position to define the primitives of a Scott continuous function; in fact now we can do more and define:

Definition 3. *The* primitive map $\int : ([0,1]^n \to (\mathbf{I}\mathbb{R})_s^{1\times n}) \to T^1$ *is defined by $\int(\bigsqcup_{i\in I} a_i \searrow b_i) = \bigcap_{i\in I} \delta(a_i, b_i)$. We usually write $\int(f)$ as $\int f$ and call it the* primitives *of f.*

Proposition 4. *The primitive map is well-defined and continuous.*

For $n \geq 2$, as we are assuming here, the primitive map will have the empty tie in its range, a situation which does not occur for $n = 1$. Therefore, we have the following important notion in dimensions $n \geq 2$.

Definition 4. *A map $g \in [0,1]^n \to (\mathbf{I}\mathbb{R})_s^{1\times n}$ is said to be* integrable *if $\int g \neq \emptyset$.*

Example 1. Let $g \in [0,1]^2 \to (\mathbf{I}\mathbb{R})_s^{1\times 2})$ be given by $g = (g_1, g_2) = (\lambda x_1.\lambda x_2.1, \lambda x_1.\lambda x_2.x_1)$. Then $\frac{\partial g_1}{\partial x_2} = 0 \neq 1 = \frac{\partial g_2}{\partial x_1}$, and it will follow that $\int g = \emptyset$.

3 Domain-theoretic derivative

Given a Scott continuous function $f : [0,1]^n \to \mathbf{I}\mathbb{R}$, the relation $f \in \delta(a,b)$, for some intervals a and b, provides, as we have seen, finitary information about the local differential properties of f. By collecting all such local information, we obtain the complete differential properties of f, namely its derivative.

Definition 5. *The* derivative *of a continuous function $f : [0,1]^n \to \mathbf{I}\mathbb{R}$ is the map*

$$\frac{df}{dx} = \bigsqcup_{f\in\delta(a,b)} a \searrow b : [0,1]^n \to (\mathbf{I}\mathbb{R})_s^{1\times n}.$$

Theorem 1. (i) $\frac{df}{dx}$ *is well-defined and Scott continuous.*
(ii) *If* $f \in C^1[0,1]^n$ *then* $\frac{df}{dx} = f'$.
(iii) $f \in \delta(a,b)$ *iff* $a \searrow b \sqsubseteq \frac{df}{dx}$.

We obtain the generalization of Theorem 1(iii) to ties, which provides a duality between the domain-theoretic derivative and integral and can be considered as a variant of the fundamental theorem of calculus.

Corollary 1. $f \in \int g$ *iff* $g \sqsubseteq \frac{df}{dx}$.

The following proposition relates the domain theoretic derivative to its classical counterpart.

Proposition 5. (i) *Let* $f : [0,1]^n \to \mathbf{I}\mathbb{R}$ *be Scott continuous. Suppose for some* $z \in [0,1]^n$, $f(z)$ *is not maximal, then* $\frac{df}{dx}(z) = \bot$.
(ii) *If* $\frac{df}{dx}(y) = c \in (\mathbf{I}\mathbb{R})_s^{1\times n}$ *is maximal, then* f *sends elements to maximal elements in a neighborhood* U *of* y *and the derivative of the induced restriction* $f : U \to \mathbb{R}$ *exists at* y *and* $f'(y) = c$.

In the full version of the paper, we formulate the relation between the domain-theoretic derivative with two other notions of derivative, namely Dini's derivative and Clarke's gradient. We express the domain-theoretic derivative in terms of lower and upper limits of the Dini's derivatives and we show that, for Lipschitz functions, the domain-theoretic derivative gives the smallest hyper-rectangle containing the Clarke's gradient.

4 Domain for Lipschitz functions

We will construct a domain for locally Lipschitz functions and for $C^1[0,1]^n$. The idea is to use D^0 to represent the function and $[0,1]^n \to (\mathbf{I}\mathbb{R})_s^{1\times n}$ to represent the differential properties (partial derivatives) of the function. Note that the domain $[0,1]^n \to (\mathbf{I}\mathbb{R})_s^{1\times n}$ is isomorphic to the smash product $(D^0)_s^n$; we can write $g \in [0,1]^n \to (\mathbf{I}\mathbb{R})_s^{1\times n}$ as $g = (g_1, \cdots, g_n) \in (D^0)_s^n$ with $\text{dom}(g) = \text{dom}(g_i)$ for all $i = 1, \cdots, n$. Consider the *consistency* relation

$$\mathsf{Cons} \subset D^0 \times (D^0)_s^n,$$

defined by $(f, g) \in \mathsf{Cons}$ if $\uparrow\! f \cap \int g \neq \emptyset$. For a consistent (f, g), we think of f as the *function part* or the *function approximation* and g as the *derivative part* or the *derivative approximation*. We will show that the consistency relation is Scott closed.

Proposition 6. *Let* $g \in (D^0)_s^n$ *and* $(f_i)_{i\in I}$ *be a non-empty family of functions* f_i : *dom*$(g) \to \mathbb{R}$ *with* $f_i \in \int g$ *for all* $i \in I$. *If* $h_1 = \inf_{i\in I} f_i$ *is real-valued then* $h_1 \in \int g$. *Similarly, if* $h_2 = \sup_{i\in I} f_i$ *is real-valued, then* $h_2 \in \int g$.

Let $R[0,1]$ be the set of partial maps of $[0,1]$ into the extended real line. Consider the two dcpo's $(R[0,1], \leq)$ and $(R[0,1], \geq)$. Define the maps $s : D^0 \times (D^0)_s^n \to (R, \leq)$ and $t : D^0 \times (D^0)_s^n \to (R, \geq)$ by

$$s : (f, g) \mapsto \inf\{h : \text{dom}(g) \to \mathbb{R} \mid h \in \int g \;\&\; h \geq f^-\}$$

$$t : (f, g) \mapsto \sup\{h : \text{dom}(g) \to \mathbb{R} \mid h \in \int g \;\&\; h \leq f^+\}.$$

We use the convention that the infimum and the supremum of the empty set are ∞ and $-\infty$, respectively. Note that given a connected component A of dom(g) with $A \cap$ dom$(f) = \emptyset$, then $s(f, g)(x) = -\infty$ and $t(s, f)(x) = \infty$ for $x \in A$. In words, $s(f, g)$ is the least primitive map of g that is greater than the lower part of f, whereas $t(f, g)$ is greatest primitive map of g less that the upper part of f.

Proposition 7. *The following are equivalent:*

(i) $(f, g) \in \mathsf{Cons}$.
(ii) $s(f, g) \leq t(f, g)$.
(iii) *There exists a continuous function h : dom$(g) \to \mathbb{R}$ with $g \sqsubseteq \frac{dh}{dx}$ and $f \sqsubseteq h$ on dom(g).*

Moreover, s and t are well-behaved:

Proposition 8. *The maps s and t are Scott continuous.*

This enables us to deduce:

Corollary 2. *The relation* Cons *is Scott closed.*

We can now sum up the situation for a consistent pair of function and derivative information.

Corollary 3. *Let $(f, g) \in \mathsf{Cons}$. Then in each connected component O of the domain of definition of g which intersects the domain of definition of f, there exist two locally Lipschitz functions $s : O \to \mathbb{R}$ and $t : O \to \mathbb{R}$ such that $s, t \in \uparrow f \cap \int g$ and for each $u \in \uparrow f \cap \int g$, we have with $s(x) \leq u(x) \leq t(x)$ for all $x \in O$.*

We now can define a central notion of this paper:

Definition 6. *Define*

$$D^1 = \{(f, g) \in D^0 \times (D^0)^n_s : (f, g) \in \mathsf{Cons}\}.$$

From Corollary 2, we obtain our first major result:

Corollary 4. *The poset D^1 is a continuous Scott domain, i.e. a bounded complete countably based continuous dcpo.*

The collection of step functions of the form $(f, g) \in D^0 \times (D^0)^n_s$, where $f \in D^0$ and $g \in (D^0)^n_s$ are step functions, forms a basis of D^1. The *rational* basis of D^1 is the collection of all rational step functions (f, g), i.e., those whose domains and values are defined over rational numbers.We will show in Section 6 that for rational step functions $f \in D^0$ and $g \in (D^0)^n_s$, the maps s and t will be piecewise linear, and can be effectively constructed to test the consistency of (f, g).

Let $C^0[0, 1]^n$ and $C^1[0, 1]^n$ be, respectively, the collection of real-valued C^0 and C^1 functions. Let $\Gamma : C^0[0, 1]^n \to D^1[0, 1]^n$ be defined by $\Gamma(f) = (f, \frac{df}{dx})$ and let Γ^1 be the restriction of Γ to $C^1[0, 1]^n$.

Theorem 2. *The maps Γ and Γ^1 are respectively embeddings of $C^0[0,1]^n$ and $C^1[0,1]^n$ into the set of maximal elements of D^1.*

Furthermore, Γ restricts to give an embedding for locally Lipschitz functions (where $\frac{df}{dx} \neq \bot$ for all x) and it restricts to give an embedding for piecewise C^1 functions (where $\frac{df}{dx}$ is maximal except for a finite set of points).

5 Integrability of derivative information

In this section, we will derive a necessary and sufficient condition for integrability and show that on rational basis elements integrability is decidable.

Let $g = (g_1, \ldots, g_n) \in (D^0)^n_s$ be a step function. Recall that a *crescent* is the intersection of an open set and a closed set. The domain $\mathrm{dom}(g)$ of g is partitioned into a finite set of disjoint crescents $\{C_j : j \in I_i\}$, in each of which the value of g_i is constant, where we assume that the indexing sets I_i are pairwise disjoint for $i = 1, \ldots, n$. The collection

$$\{ \bigcap_{1\leq i\leq n} C_{k_i} : k_i \in I_i, 1 \leq i \leq n\}$$

of crescents partition $\mathrm{dom}(g)$ into regions in which the value of g is a constant interval vector; they are called the *associated crescents* of g, which play a main part in deciding integrability as we will see later in this section. Each associated crescent has boundaries parallel to the coordinate planes and these boundaries intersect at points, which are called the *corners* of the crescent. A point of the boundary of an associated crescent is a *coaxial point* of a point in some associated crescent if the two points have precisely $n-1$ coordinates in common. Clearly, each point has a finite number of coaxial points. In Figure 2, an example of a step function g is given with its associated crescents, the interval in each crescent gives the value of g in that crescent. A solid line on the boundary of a crescent indicates that the boundary is in the crescent, whereas a broken line indicates that it is not. The coaxial points of the corners are illustrated on the picture on the right.

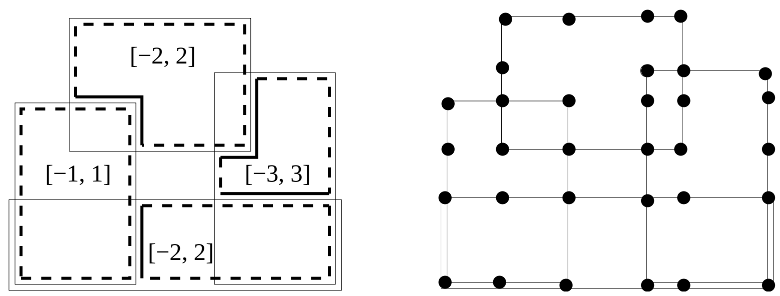

Fig. 2. Crescents of a step function (left); the corners and their coaxial points (right)

A path in a connected region $R \subset \mathbb{R}^n$ is a continuous map $p : [0,1] \to R$ with endpoints $p(0)$ and $p(1)$. If p is piecewise C^1, respectively piecewise linear, then the path is called a piecewise C^1, respectively piecewise linear. The space $P(R)$ of piecewise C^1 paths in R is equipped with the C^1 norm. A path p is *non-self-intersecting* if $p(r) = p(r')$ for $r < r'$ implies $r = 0$ and $r' = 1$. We will be mainly concerned with piecewise linear paths in this paper. For these paths, there exists a strictly increasing sequence of points $(r_i)_{0 \le i \le k}$ for some $k \in \mathbb{N}$ with $0 = r_0 < r_1 < \cdots r_{k-1} < r_k = 1$ such that p is linear in $[r_i, r_{i+1}]$ for $0 \le i \le k-1$. The points $p(r_i)$ for $i = 0, \cdots, k$, are said to be the *nodes* of p; the nodes $p(r_i)$ for $i = 1, \cdots, k-1$ are called the *inner* nodes. The line segment $\{p(r) : r_i \le r \le r_{i+1}\}$ is denoted by $p([r_i, r_{i+1}])$. If $p(0) = p(1)$, the path is said to be *closed*.

A *simple* path in a region $R \subset \mathbb{R}^n$ is a non-self-intersecting piecewise linear map. We now consider simple paths in the closure $\text{cl}(O)$ of a connected component $O \subseteq \text{dom}(g)$.

Recall that given a vector field $F : R \to \mathbb{R}^n$ in a region $R \subset R^n$ and a piecewise C^1 path $p : [0,1] \to R$, the line integral of F with respect to p from 0 to $w \in [0,1]$ is defined as $\int_0^1 F(p(r)) \cdot p'(r)\, dr$, when the integral exists. Here, $u \cdot v = \sum_{i=1}^n u_i v_i$ denotes the usual scalar product of two vectors $u, v \in \mathbb{R}^n$.

We define a generalization of the notion of scalar product for vectors of type: $u \in (\mathbf{I}\mathbb{R})^n$ and $v \in \mathbb{R}^n$. For $a = [\underline{a}, \overline{a}] \in (\mathbf{I}\mathbb{R})^n_s$, let $a^- = \underline{a}$, $a^+ = \overline{a}$ and $a^0 = 1$. We define the *direction dependent scalar product* as the strict map

$$- \odot - : (\mathbf{I}\mathbb{R})^n_s \times \mathbb{R}^n \to \mathbb{R}_\perp$$

with $u \odot v = \sum_{i=1}^n u_i^{\sigma(v_i)} v_i$ for $u \neq \perp$. The extension of the usual dot product to the interval dot product i.e. $u \cdot v = \{w \cdot v \mid w \in u\}$ then satisfies: $(u \cdot v)^- = -u \odot (-v)$ and $(u \cdot v)^+ = u \odot v$. We can now define a notion of line integral of the interval-valued vector function $g = [g^-, g^+] \in (D^0)^n_s$ with respect to any piecewise C^1 path from y to x in $\text{cl}(O)$, where O is a connected component of $\text{dom}(g)$. For each $i = 1, \cdots n$, the ith component of g is given by $g_i = [g_i^-, g_i^+]$.

Definition 7. *Given a step function $g \in (D^0)^n_s$ and a piecewise C^1 path p in the closure of connected component O of the domain of g, the* upper line integral *of g over p from 0 to $w \in [0,1]$ is defined as:*

$$\mathsf{U}\int_{p[0,w]} g(r)\, dr = \int_0^w g(p(r)) \odot p'(r)\, dr.$$

The lower line integral *of g over p from 0 to $w \in [0,1]$ is similarly defined as*

$$\mathsf{L}\int_{p[0,w]} g(r)\, dr = -\int_0^w g(p(r)) \odot (-p'(r))\, dr.$$

Thus, if the jth component of the path, for some j with $1 \le j \le n$, is increasing locally at some $r \in [0,1]$, i.e. $p_j' > 0$ in a neighborhood of r, then $g_j^{-\sigma(p_j(r))} = g_j^-$ will contribute locally to the jth component of the sum in the lower integral, while if $p_j' < 0$ in a neighborhood of r, then $g_j^{-\sigma(p_j(r))} = g_j^+$ will contribute. In case the path is locally perpendicular to the jth axis at r, i.e. $p_j'(r) = 0$ in a local neighborhood of r, then there will be zero contribution for the jth component in the sum. For the upper integral the contributions of g_i^- and g_i^+ are reversed. Note that for all $w \in [0, 1]$ we have from the definitions: $\mathsf{L} \int_{p[0,w]} g(r)\, dr \sqsubseteq \mathsf{U} \int_{p[0,w]} g(r)\, dr$.

The geometric interpretation of the lower and upper line integrals is as follows. We regard $g \in (D^0)_s^n$ as an interval-valued vector field in $[0, 1]^n$. For any continuous vector field $F : \text{dom}(g) \to \mathbb{R}^n$ with $F(x) \in g(x)$ for all $x \in \text{dom}(g)$ and any piecewise C^1 path $p \in P(O)$ in a connected component O of dom(g), the classical line integral is always bounded below and above by the lower and upper line integrals respectively.

We now introduce the domain-theoretic generalization of Green's celebrated condition for the integrability of a vector field.

Definition 8. *Given a step function $g \in (D^0)_s^n$ and a closed simple path p in the closure of a connected component of dom(g), we say that g satisfies the* zero-containment loop condition for p *if*

$$0 \in \int_{p[0,1]} g(r)\, dr.$$

We say that $g \in (D^0)_s^n$ satisfies the zero-containment loop condition *if it satisfies the zero-containment loop condition for any closed simple path p in the closure of any connected component of dom(g).*

For simplicity, we have only defined the zero-loop condition for step functions as required in this paper. By using piecewise differentiable closed paths instead of closed simple paths, the definition can be easily extended to any Scott continuous interval-valued vector field. If g only takes point (maximal) values, then the zero-containment loop condition is simply the standard condition for g to be a gradient i.e., that the line integral of g vanishes on any closed path. Figure 3 gives an example of a step function $g = (g_1, g_2)$, with dom$(g) = ((0, 3) \times (0, 3)) \setminus ([1, 2] \times [1, 2])$ which does not satisfy the zero-containment loop condition. The values of g_1 (left) and g_2 (right) are given for each of the four single-step functions. Denote the dashed path by p; it has nodes at $p(0) = p(1) = (1/2, 1/2)$, $p(1/4) = (5/2, 0)$, $p(1/2) = (5/2, 5/2)$ and $p(3/4) = (1/2, 5/2)$. The lower line integral of g over p gives a strictly positive value:

$$\begin{aligned}
&\mathsf{L} \textstyle\int_p g(r)dr = \sum_{i=0}^{3} \int_{\frac{i}{4}}^{\frac{i+1}{4}} -g(p(r)) \odot (-p'(r))dr \\
&= -\textstyle\int_0^{\frac{1}{4}} g(p(r)) \odot (-8, 0)dr - \int_{\frac{1}{4}}^{\frac{1}{2}} g(p(r)) \odot (0, -8)dr \\
&- \textstyle\int_{\frac{1}{2}}^{\frac{3}{4}} g(p(r)) \odot (8, 0)dr - \int_{\frac{3}{4}}^{1} g(p(r)) \odot (0, 8)dr \\
&= 1/4(8 \cdot 1 + 8 \cdot 1 + 8 \cdot 1 + 8 \cdot 1) = 8 > 0.
\end{aligned}$$

Recall that $g \in (D^0)_s^n$ is called integrable if $\int g \neq \emptyset$. The following is an extension of Green's Theorem also called the Gradient Theorem in classical differential calculus [9].

Theorem 3. *Suppose $g \in (D^0)_s^n$ is an integrable step function. Then g satisfies the zero-containment loop condition.*

We will now show that if a step function $g \in (D^0)_s^n$ satisfies the zero-containment loop condition, then it is integrable. Let O be a connected component of dom(g). Note

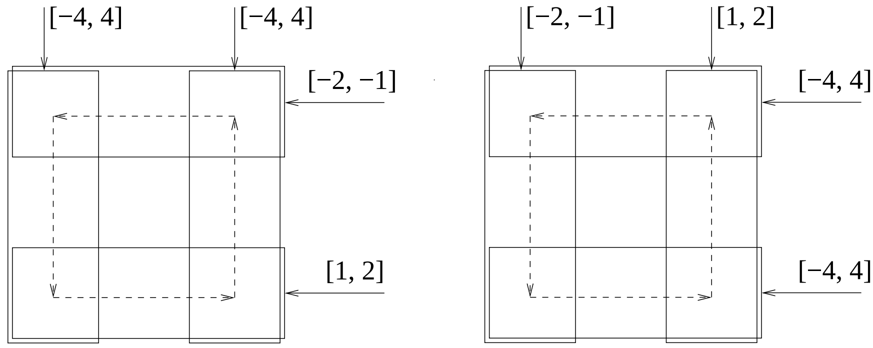

Fig. 3. Failure of zero-containment: g_1 (left) and g_2 (right)

that any step function g can be extended to the boundary of dom(g) by the lower and upper semi continuity of g^- and g^+ respectively. We adopt the following convention. If two crescents have a common boundary, we consider their common boundary as infinitesimally separated so that they have distinct boundaries. This means that a line segment of a simple path on a common boundary of two different crescents is always regarded as the limit of a sequence of parallel segments contained on one side of this boundary.

We are now ready to introduce a key concept of this paper. For $x, y \in \text{cl}(O))$, we put

$$V_g(x,y) = \sup\{\mathsf{L}\int_{p[0,1]} g(r)\,dr : p \text{ a piecewise linear path in cl}(O) \text{ from } y \text{ to } x\},$$

$$W_g(x,y) = \inf\{\mathsf{U}\int_{p[0,1]} g(r)\,dr : p \text{ a piecewise linear path in cl}(O) \text{ from } y \text{ to } x\}.$$

Proposition 9. *Suppose g satisfies the zero-containment loop condition and $x, y \in$ cl(O), then there are simple paths p and q from y to x such that:*

$$V_g(x,y) = \mathsf{L}\int_{p[0,1]} g(r)\,dr \qquad W_g(x,y) = \mathsf{U}\int_{q[0,1]} g(r)\,dr.$$

Moreover, for each $y \in$ cl(O), the two maps given by $V_g(\cdot, y), W_g(\cdot, y)$: cl$(O) \to \mathbb{R}$ are continuous, piecewise linear and satisfy $V_g(y,y) = W_g(y,y) = 0$,

$$g \sqsubseteq \frac{dV_g(\cdot,y)}{dx} \qquad \textit{and} \qquad g \sqsubseteq \frac{dW_g(\cdot,y)}{dx}.$$

Thus, we obtain the following main result:

Theorem 4. *A function $g \in (D^0)^n_s$ is integrable iff it satisfies the zero-containment loop condition.*

Proposition 10. *For a rational step function $g \in (D^0)^n_s$ defined over rational numbers, the zero-containment loop condition is decidable.*

Proof. There are a finite number of connected components of $\mathrm{dom}(g)$. In each connected component O of $\mathrm{dom}(g)$, the values of $\mathsf{L}\int_{p[0,1]} g(r)\,dr$ and $\mathsf{U}\int_{p[0,1]} g(r)\,dr$, for a closed simple path in $\mathrm{cl}(O)$ depend piecewise linearly on the coordinates of any given node of the path. It follows that the maximum value of the lower integral and the minimum value of the upper integral are reached for a path p with nodes at the corners of the crescents of O and their coaxial points. Since the number of such closed simple paths is finite and since for each such path $\mathsf{L}\int_{p[0,1]} g(r)\,dr$ is a rational number, we can decide in finite time if the zero-containment loop condition holds for g. □

For an associated crescent a of a step function g we write $v(a)$ for the value of g on a, i.e. $v(a) = g(x)$ where $x \in a^o$ is some point in the interior of a. To check whether a rational step function g is integrable, the proof of Proposition 10 shows that it suffices to check that g satisfies the zero-containment loop condition on all paths with nodes in the finite set of corners of the associated crescents and their coaxial points. This gives rise to the following algorithm:

```
input: a rational step function g : [0,1]^n → IR^n
output: true, if g is integrable and false otherwise
D := connected components of dom(g)
for each C ∈ D do
   A := associated crescents of C
   R := corners and coaxial points of A
   /* P represents the closed paths */
   P := all lists (p_0 --a_0--> ... --a_{k-1}--> p_k) where a_i ∈ A, p_i ∈ R, p_i, p_{i+1} ∈ cl(a_i)
      and p_i = p_j ⟹ i = 0 and j = k
   for each p = (p_0 --a_0--> ... --a_{k-1}--> p_k) ∈ P do
      /* compute upper and lower line integral */
      L := Σ_{i=0}^{k-1} v(a_i) ⊙ (p_{i+1} - p_i)
      U := Σ_{i=0}^{k-1} v(a_i) ⊙ (p_i - p_{i+1})
      if L > 0 or U < 0 then output false; end
   enddo
enddo; output true
```

6 Consistency of function and derivative information

We will now show that for a pair of rational step functions $(f, g) \in D^1$, with g integrable, the consistency relation $(f, g) \in \mathsf{Cons}$ is decidable. For this, we explicitly construct $s(f, g)$ and $t(f, g)$, which will be piecewise linear functions that enable us to decide if $s(f, g) \leq t(f, g)$. Let x and y be in the same connected component O of $\mathrm{dom}(g)$ with $O \cap \mathrm{dom}(f) \neq \emptyset$.

Theorem 5. *The maps $V_g(\cdot, y), W_g(\cdot, y) : cl(O) \to \mathbb{R}$ are respectively the least and the greatest continuous maps $L, G : O \to \mathbb{R}$ with $L(y) = 0$ and $G(y) = 0$ such that $g \sqsubseteq \frac{dL}{dx}$ and $g \sqsubseteq \frac{dG}{dx}$.*

Let $S_{(f,g)}(x,y) = V_g(x,y) + \underline{\lim} f^-(y)$.

Corollary 5. *Let O be a connected component of dom(g) with non-empty intersection with dom(f). For $x \in O$, we have:*

$$s(f,g)(x) = \sup_{y \in O \cap \textit{dom(f)}} S_{(f,g)}(x,y). \tag{1}$$

Proposition 11. *There exist a finite number of points $y_0, y_1, \ldots, y_i \in$ cl$(O \cap$ dom(f)$)$ with*

$$s(f,g)(x) = \max\{S_{(f,g)}(x, y_j) : j = 0, 1, \ldots, i\}$$

for $x \in O$.

Proof. For fixed (f,g) and x, the value of $S_{(f,g)}(x,y)$ depends piecewise linearly on the coordinates of y, and thus its maximum value is reached for a simple path with modes at the corners of the crescents of O and x and their coaxial points. □

Results dual to those above are obtained for $t(f,g)$ as follows. We put $T_{(f,g)}(x,y) = W_g(x,y) + \overline{\lim} f^+(y)$. Then, we have

$$t(f,g)(x) = \inf_{y \in O \cap \text{dom(f)}} T_{(f,g)}(x,y),$$

and there exist $y_0, y_1, \ldots, y_i \in \text{cl}(O \cap \text{dom(f)})$ with

$$t(f,g)(x) = \min\{T_{(f,g)}(x, y_j) : j = 0, 1, \ldots, i\},$$

for $x \in O$.

Corollary 6. *The predicate Cons is decidable on basis elements (f,g) consisting of rational step functions.*

The algorithm for deciding consistency of a rational step function $f : [0,1]^n \to \mathbf{I}\mathbb{R}$ and a rational step function $g : [0,1]^n \to (\mathbf{I}\mathbb{R})^n_s$ works as follows: Recall that f and g are consistent iff $s(f,g) \le t(f,g)$. By the proof of Proposition 11, both functions can be constructed by evaluating line integrals over simple paths with inner nodes in the set of corners of the crescents of g, the endpoint of the line integrals and the coaxial points of these. This is achieved by the following algorithm:

```
input: a rational step functions f : [0,1]^n → IR
       an integrable rational step function g : [0,1]^n → (IR)^n_s
output: true, if f is consistent with g, false otherwise.
D := connected components of dom(g)
for each C ∈ D do
   A := associated crescents of C; K := corners of C
   /* x = (x_1,...,x_n) represents the varying endpoint */
   R(x) := K ∪ { coaxial points of K ∪ {x}}
   /* P(x) represents the paths to x */
   P := all lists (p_0 --a_0--> ... --a_{k-1}--> p_k) where p_i ∈ R(x) are pairwise
```

```
      distinct, p_k = x and p_i, p_{i+1} ∈ cl(a_i) for all i = 1,...,k-1.
   for each p = (p_0 -a_0-> ... -a_{k-1}-> p_k), q = (q_0 -a_0-> ... -a_{l-1}-> q_l) ∈ P(x) do
      /* compute upper and lower line integral */
      s(x) := lim_ f^-(p_0) + Σ_{i=0}^{k-1} v(a_i) ⊙ (p_{i+1} - p_i)
      t(x) := lim‾ f^+(q_0) + Σ_{i=0}^{l-1} v(a_i) ⊙ (q_i - q_{i+1})
      if s(x) > t(x) for some x ∈ a‾ then output false; end
   enddo
enddo; output true
```

Note that $s(x)$ and $t(x)$ are piecewise linear functions in x with rational coefficients, hence we can decide $s(x) \leq t(x)$ on $\mathrm{cl}(a)$ by first computing the rectangles on which both s and t are linear and then checking for $s \leq t$ on the corners of those.

Theorem 6. *The domain D^1 can be given an effective structure using a standard enumeration of its rational basis.*

7 Applications

The construction of an effective domain for differentiable functions paves the road for applications of domain theory in a number of areas of numerical analysis and computational mathematics. Here, we make a start on this by mentioning two fields of applications which have been worked out in detail in two follow-up papers.

7.1 Robust construction of curves and surfaces

In geometric modelling, as in CAD, the standard method to construct curves and surfaces is to use the implicit function theorem to define these geometric objects implicitly [2]. For example a C^1 surface $g : [0,1]^2 \to \mathbb{R}$ can be specified as the zero set $\{g(x,y) : f(x,y,g(x,y)) = 0\}$ where $f : [0,1]^3 \to \mathbb{R}$ is a C^1 function with $\frac{\partial f}{\partial z} \neq 0$. The domain for differential functions allows us to develop a domain-theoretic version of the implicit function theorem, in which the implicit function together with its derivative are approximated by step functions. This means that from an increasing sequence of step functions converging to f and its derivative in the domain of differentiable functions we can effectively obtain an increasing sequence of step functions converging in this domain to the desired surface g and its derivative. Combined with the domain-theoretic model for computational geometry developed in [7], this provides a robust technique for geometric modelling and CAD.

7.2 A Second Order Method for Solving Differential Equations

We consider the initial value problem given by the system of differential equations

$$y' = v(y), \qquad y(0) = (0, \ldots, 0)$$

where $v \in C^1([-K,K]^n, [-M,M]^n)$ is a differentiable function defined on a rectangle containing the origin. A first-order method for solving this equation usually postulates that the vector field v is Lipschitz, and uses the Lipschitz constant to conservatively approximate a solution. Assuming that v is differentiable, we can locally replace the Lipschitz constant by the derivative, giving rise to tighter approximations. Extending the present framework to functions of interval variables, we can approximate vector fields along with their derivatives by a pair of functions (v, v') where $v : \mathbf{I}\mathbb{R}^n \to \mathbf{I}\mathbb{R}^n$ approximates the vector field and $v' : \mathbf{I}\mathbb{R}^n \to \mathbf{I}\mathbb{R}^{(n \times n)}$ approximates the matrix of partial derivatives. Compared to the approach of interval analysis [10], we are in particular able to give guarantees on this improved speed of convergence, thus providing a sound and complete framework for solving the initial value problem.

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