Data Types for Differentiable Functions

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Computational Models

Suppose $M = (M, d)$ is a metric space.

Idea: A computational model adds approximations to elements $x \in M$.

Computational Model for M:

An ω-continuous effective domain $(D, \sqsubseteq)$ with a *topological embedding*

$$\mathbf{I} : M \to D$$

s.t. $\mathbf{I}(x)$ is maximal for all $x \in M$.

Derived Notion of **Computability:**

$$x \in M \text{ computable} \quad \Longleftrightarrow \quad \mathbf{I}(x) \text{ computable}$$

Topological Embedding: Continuous w.r.t. the *metric* topology on M and the *Scott* topology on D.

Computational Models

Computational Model for **Real Numbers**:

$$\mathbf{I}\mathbb{R} = \{[\underline{a}, \overline{a}] \mid \underline{a}, \overline{a} \in \mathbb{R}, \underline{a} \leq \overline{a}\} \cup \{\mathbb{R}\}$$

with topological embedding

$$\mathbb{R} \to \mathbf{I}\mathbb{R}, r \mapsto [r, r]$$

Computational Model for **Continuous Functions**:

$$D^0([0,1]^n) = \{f : [0,1]^n \to \mathbf{I}\mathbb{R} \mid f \text{ Scott continuous}\}$$

with topological embedding

$$C^0([0,1]^n) \to D^0([0,1]^n), f \mapsto \mathbf{I}f = \lambda x.\{f(x)\}$$

Applications: Ordinary differential equations(!), root finding, solid modelling etc.

This talk: Computational Model for **Differentiable Functions**

A Domain for Differentiable Functions

Fact: If f is a limit of f_n's, then the f_n's tell us nothing about the derivative of f.

This Talk: A computational model for differentiable functions, i.e. a domain D^1 and a topological embedding

$$\begin{array}{ccc} C^1([0,1]^n) & \xrightarrow{\Gamma^1} & D^1([0,1]^n) \\ \lambda f.f' \Big\downarrow & & \Big\downarrow \lambda f.f' \\ C^0([0,1]^n)^n & \xrightarrow{\Gamma^0} & D^0([0,1]^n)^n \end{array}$$

Main Results:

- Generalisation of the Gradient Theorem
- Effectiveness of D^1

Applications: Inverse and Implicit Functions, ODEs.

Step Ties and Step Functions

Unless otherwise stated, all functions elements of $D^0([0,1]^n) = [0,1]^n \to \mathbf{I}\mathbb{R}$.

Step Functions: finitary information about the values of a function.

$$a \searrow b(x) = \begin{cases} b & x \in a^o \\ \perp & \text{o/w} \end{cases}$$

where $a \in \mathbf{I}[0,1]^n$, $b \in \mathbf{I}\mathbb{R}$ and $a^o =$ interior of a.

Step Ties: finitary information about differential properties.

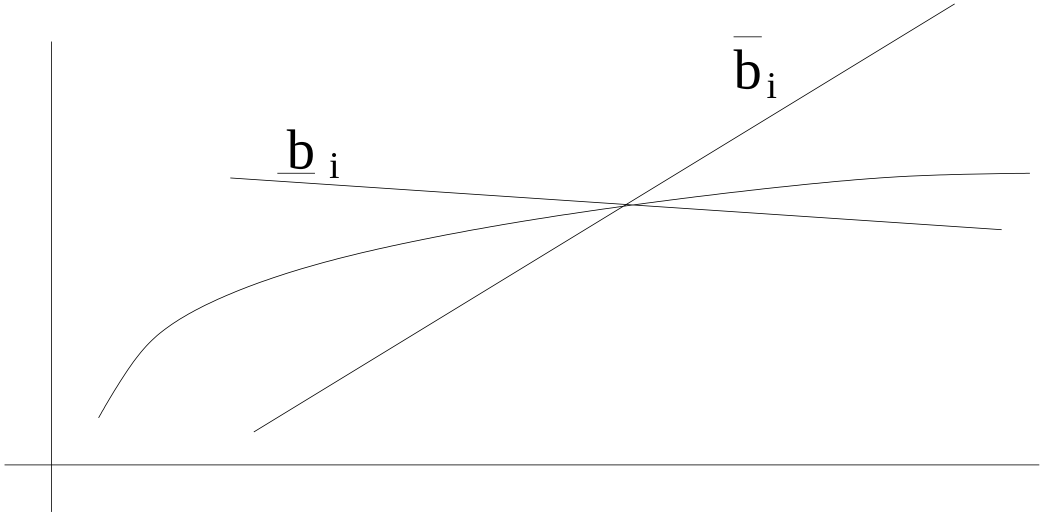
$$f \in \delta(a,b) \iff b(x-y) \sqsubseteq f(x) - f(y)$$

for all $x, y \in a^o$, where $a \in \mathbf{I}[0,1]^n$, $b \in \mathbf{I}\mathbb{R}^n$. We call $\delta(a,b)$ a *single step tie*.

Simple Properties

Suppose $b = (b_1, \ldots, b_n) \in \mathbf{I}\mathbb{R}^n$ with $b_i = [\underline{b}_i, \overline{b}_i]$.

Geometric Intuition I: If $f \in \delta(a, b)$, then $\underline{b}_i$, $\overline{b}_i$ are lower and upper Lipschitz constants for f in a^o in the direction of the i-th coordinate axis.



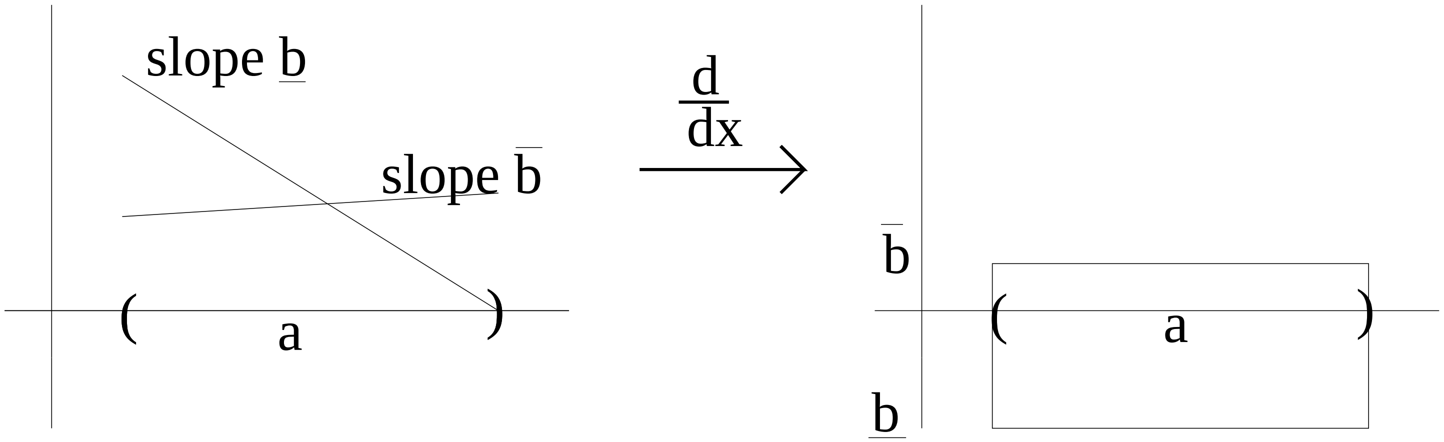
If $x = y + he_i$ we have

$$h \cdot b_i \sqsubseteq f(y + he_i) - f(y), \text{ i.e. } h \cdot \underline{b}_i \leq f(y + he_i) - f(y) \leq h \cdot \overline{b}_i$$

for all $x, y \in a^o$.

Primitive Maps

Geometric Intuition II: $\delta(a, b)$ are the primitive maps of $a \searrow b$.



Ties and Primitive Functions

Correspondence and Consistency:

(*i*) Correspondence: $a \searrow b \sqsubseteq c \searrow d \iff \delta(a,b) \supseteq \delta(c,d)$

(*ii*) Consistency: If $(\delta(a_i, b_i))_{i\in I}$ is consistent, then so is $(a_i \searrow b_i)_{i\in I}$.

Ties and the Primitives Map:

(*i*) A *(step) tie* is a (finite) intersection of ties. The dcpo of ties is $(T^1, \supseteq)$.

(*ii*) The *primitives map* $\int : ([0,1]^n \to \mathbf{I}\mathbb{R}^n) \to T^1$ is given by
$\int(\bigsqcup_i a_i \searrow b_i) = \bigcap_i \delta(a_i, b_i)$.

Continuity and Surjectivity: The primitives map is continuous and onto.

The Domain-Theoretic Derivative

Domain Theoretic Derivative: Suppose $f : [0,1]^n \to \mathbf{I}\mathbb{R}$. Put

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

Simple Properties:

(*i*) $\frac{df}{dx}$ is well defined and continuous.

(*ii*) For $f \in C^1([0,1]^n)$, $\frac{df}{dx} = f'$.

(*iii*) $f \in \delta(a,b)$ iff $a \searrow b \sqsubseteq \frac{df}{dx}$.

Corollary (The Fundamental Theorem in Domain Theory):

$$f \in \int g \text{ iff } g \sqsubseteq \frac{df}{dx}.$$

Examples

Example 1:

Let $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ with $f(x_1, x_2) = a|x_1| + b|x_2|$ where $a \geq 0$ and $b \geq 0$.

Then

$$\frac{df}{dx} = \begin{cases} (\sigma(x_1)a, \sigma(x_2)b) & x_1 \neq 0, x_2 \neq 0 \\ (\sigma(x_1)a, [-b, b]) & x_1 \neq 0, x_2 = 0 \\ ([-a, a], \sigma(x_2)b) & x_1 = 0, x_2 \neq 0 \\ ([-a, a], [-b, b]) & x_1 = 0, x_2 = 0. \end{cases}$$

Towards D^1: Consistency

Problem: Differentiation $f \mapsto \frac{df}{dx}$ is not continuous.

The D^1 Domain: An element of D^1 comprises (possibly partial) information on a function *and* its derivative.

In more detail: We consider $n+1$-tuples $(f_0, f_1, \ldots, f_n)$ where f approximates a function and $f_1, \ldots, f_n$ its n partial derivatives.

Examples:

(*i*) $h : [0,1]^n \to \mathbf{I}\mathbb{R}$, $f = h$ and $g_i = \frac{\partial h}{\partial x_i}$

(*ii*) $f = \lambda x.x$ and $g_1 = \lambda x.[0,1]$ for $n = 1$

(*iii*) $f = \lambda x.[0,1]$ and $g = g_1 = \lambda x.1$

(*iv*) $f = \lambda x.0$ and $g = g_1 = \lambda x.1$??

So there is an issue of *consistency* of approximations.

Consistency

Idea: An $n+1$-tuple $(f, f_1, \ldots, f_n)$ is consistent iff there is a Lipschitz function h s.t. $f \sqsubseteq h$ and $(f_1, \ldots, f_n) \sqsubseteq \frac{dh}{dx}$.

Consistency: Suppose $f : [0,1]^n \to \mathbf{I}\mathbb{R}$ and $g : [0,1]^n \to \mathbf{I}\mathbb{R}^n$. Let

$$(f, g) \in \mathsf{Cons} \iff \uparrow f \cap \int g \neq \emptyset$$

and call f and g *consistent* if $(f, g) \in \mathsf{Cons}$.

Definition of D^1:

$$D^1([0,1]^n) = \{(f,g) \in ([0,1]^n \to \mathbf{I}\mathbb{R}) \times ([0,1]^n \to \mathbf{I}\mathbb{R}^n) \mid (f,g) \in \mathsf{Cons}\}$$

with pointwise ordering.

D^1 as Continuous Scott Domain

Existence of directed suprema: Consider

- $s(f,g) =$ least h : dom$(g) \to \mathbb{R}$ s.t. $h \in \int g$ s.t. $h \geq f^-$
- $t(f,g) =$ greatest h : dom$(g) \to \mathbb{R}$ s.t. $h \in \int g$ s.t. $h \leq f^+$.

Then $(f,g) \in \mathsf{Cons}$ iff $s(f,g) \leq t(f,g)$.

Corollary: Cons is Scott closed. In particlar, D^1 has directed suprema.

Corollary: $D^1([0,1]^n)$ is a continuous Scott domain (i.e. bounded complete with countable base) and

$$\begin{array}{ccc}
C^1([0,1]^n) & \xrightarrow{\lambda f.(\mathbf{I}f,\frac{d\mathbf{I}f}{dx})} & D^1([0,1]^n) \\
\Big\downarrow{\scriptstyle \lambda f.f'} & & \Big\downarrow{\scriptstyle \lambda (f,g).g} \\
C^0([0,1]^n)^n & \xrightarrow{\lambda f.\mathbf{I}f} & D^0([0,1]^n)^n
\end{array}$$

commutes, where $\mathbf{I}f(x) = \lambda x.\{f(x)\}$.

D^1 as Effective Domain

Clearly: D^1 is an effective domain $\iff$ consistency is decidable on a base.

Deciding Consistency: Suppose $f : [0,1]^n \to \mathbf{I}\mathbb{R}$ and $g : [0,1]^n \to \mathbf{I}\mathbb{R}^n$ are rational step functions.

(*i*) Decide whether $\int g = \emptyset$, i.e. whether g is *integrable*.

(*ii*) Decide whether $\uparrow f \cap \int g = \emptyset$.

For (i) we use a generalised version of the *Gradient Theorem:*

$g : [0,1]^n \to \mathbf{I}\mathbb{R}^n$ is integrable iff $0 \in \int_p g$ for all closed paths p.

Item (ii) follows by constructing a minimal and maximal surface.

Corollary: $D^1([0,1]^n)$ is an effective continuous Scott domain.

A 2nd Order Method for ODEs

Consider the initial value problem

$$\dot{y} = v(y) \text{ with initial condition } y(0) = 0$$

where $v : [-K, K]^n \to [-M, M]^n$ and $y : [0, a] \to \mathbb{R}$.

Idea: Given $p \leq q$ and $y : [0, p] \to \mathbf{I}\mathbb{R}$, use Taylor's formula to extend y to $[0, q]$.

This needs

A priory bounds. Suppose $z : [0, a] \to \mathbb{R}$ solves the IVP. Then

$$z(t) = z(p) + \int_p^t v(z(x))dx \sqsubseteq z(p) + \underbrace{[-(q-p)M, (q-p)M]^n}_{C_{p,q}}$$

for $t \in [p, q]$.

Continuation of Solutions

Suppose $y : [0,p] \to \mathbf{I}\mathbb{R}$ and $y \sqsubseteq z\restriction_{[0,p]}$ where $z : [0,a] \to \mathbb{R}$ is a solution.

Continuation of y to $[0,q]$ where $p \leq q$:

Continuous Case: $v \in C^0([-K,K]^n)$. Then, for some $\phi \in [p,q]$

$$z(t) = z(p) + (t-p) \cdot \dot{z}(\phi) \sqsubseteq y(p) + (t-p) \cdot \mathbf{I}v(y(p) + C_{p,q}).$$

Differentiable Case: $v \in C^1([-K,K]^n)$. Then, for some $\phi \in [p,q]$

$$\begin{aligned} z(t) &= z(p) + (t-p) \cdot \dot{z}(p) + \frac{(t-p)^2}{2}\ddot{z}(\phi) \\ &\sqsubseteq y(p) + (t-p) \cdot \mathbf{I}v(y(p)) + \frac{(t-p)^2}{2}\mathbf{I}v' \cdot \mathbf{I}v(y(p) + C_{p,q}) \end{aligned}$$

In general, the information on v' allows for a *much* tighter approximation.

Convergence of Solutions

Recall $\Gamma : C^1([-K, K]^n) \to D^1([-K, K]^n)$ and suppose that $\Gamma(v) = \bigsqcup_k v_k$.

For a partition $Q_k = (q_0, \ldots, q_l)$ of $[0, a]$ define $y_k(0) = 0$ and

$$y_k(q_i) + (q_{i+1} - t) \cdot \mathbf{I}v_k(y(q_i)) + \frac{(q_{i+1} - t)^2}{2}\mathbf{I}v_k' \cdot \mathbf{I}v_k(y(q_i) + C_{q_i, q_{i+1}})$$

for $t \in (q_i, q_{i+1}]$.

Theorem: Suppose $Q_0 \subseteq Q_1 \subseteq Q_2 \subseteq \ldots$ are increasing.

(*i*) The y_k are monotone, i.e. $y_k \sqsubseteq y_{k+1}$

(*ii*) $\bigsqcup_k y_k$ is real-valued and solves the IVP.

(*iii*) If (Q_k) and (v_k) are effectively given, then so is (y_k).

Convergence Speed: proportional to that of (Q_k) and (v_k).

Construction of Inverse Functions

Classical Inverse Function Theorem:

Suppose $0 \in D \subseteq \mathbb{R}^n$ and $f : D \to \mathbb{R}^n$ is C^1 and $f'(0)$ is invertible.

Then there exists $V \subseteq D, W \subseteq \mathbb{R}^n$ and a C^1-function $g : W \to V$ s.t.

(*i*) $V\restriction_V : V \to W$ is a diffeomorphism with smooth inverse g

(*ii*) $g'(f(x)) = f'(x)^{-1}$

Proof Sketch: Construct g as a fixpoint using Banach's Theorem.

Wlog assume that $f'(0) = I$; otherwise consider $\tilde{f} = f'(0)^{-1} \circ f$.

In a neighbourhood O of 0 the functional

$$T_f : C^1(O, O) \to C^1(O, O), h \mapsto -f \circ (\mathrm{id} + h)$$

is well defined and contracting. Put $f^{-1} = \mathrm{id} + g$ where $T_f(g) = g$.

Applications: Implicit Differential Equations, Implicit Surfaces

Domain-Theoretic Inverse Function Theorem

Idea: Use the fixpoint construction $h \mapsto -f \circ (\mathrm{id} + h)$ *on* $D^1(O)$

Needs: Operations $+$, $-$, $\circ$, etc. on D^1.

Composition: $(\cdot \circ \cdot) : D^1(\mathbb{R}^m \to \mathbf{I}\mathbb{R}^k) \times D^1([0,1]^n \to \mathbf{I}\mathbb{R}^m)$

$$((f_0, f_1), (g_0, g_1)) \mapsto (I f_0 \circ g_0, (\mathbf{I} f_1 \circ g) \cdot g_1)$$

Proposition: Composition is well-defined.

As $+, -, *, / \in D^1(\mathbb{R}^2 \to \mathbf{I}\mathbb{R})$ we obtain:

Corollary: Addition, Subtraction, Multiplication, Division are well-defined as operators $D^1([0,1]^n) \times D^1([0,1]^n) \to D^1([0,1]^n)$

Inverse Functions in Domain Theory

Suppose $f : [-1,1]^n \to \mathbb{R}^n$ is Lipschitz, i.e. $(f, \frac{df}{dx}) \in D^1([0,1]^n)$ is maximal.

Mean Differential: Midpoint-Matrix M of $\frac{df}{dx}(0)$.

Theorem: Suppose $f(0) = 0$ and $\|M^{-1}\frac{df}{dx} - E\| \leq \min\{\frac{1}{2}, \frac{1}{n}\}$.

(*i*) f has a Lipschitz inverse g in a neighbourhood of 0

(*ii*) If $f \in C^1([0,1]^n)$, then so is g.

(*iii*) If f is effectively given, then so is g and, if $f \in C^1([0,1]^n)$, also g'.

Proof Sketch: Put $\tilde{f} = M^{-1} \circ f$. The functional

$$T_f : D^1(O) \to D^1(O), h \mapsto -\tilde{f} \circ (\mathrm{id} + g)$$

is well-defined in a neighbourhood of 0 and admits a least fixpoint $\tilde{g}$.

Then $g = M(\mathrm{id} + g)$ satisfies the above requirements.

Related and Future Work

Related Work:

- Interval Analysis (exact solutions of ODE's – no convergence guarantee)
- Computability for Differentiable functions: Ad-hoc treatment in TTE
- Inverse Function Theorem in BISH (non-apparent algorithm)

Differential Equations:

- Generalisation to Boundary Value Problems (shooting, finite differences)
- Ultimate Goal: PDE's

Computational Geometry:

- Construction of Implicit Surfaces
- Domain for Closed Manifolds
- Surface Intergrals