Simple essence of AD

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Definition of Derivative

Definition

Let $f : \mathbb{R} \to \mathbb{R}$ be a function. The derivative of f at point $x \in \mathbb{R}$ is defined the following way:

$$f'(x) = \lim_{\varepsilon \to 0} \frac{f(x + \varepsilon) - f(x)}{\varepsilon}$$

This definition will also work with functions of types $\mathbb{C} \to \mathbb{C}$ and $\mathbb{R} \to \mathbb{R}^n$.

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Definition of Derivative

For functions F of types $\mathbb{R}^m \to \mathbb{R}$ and $\mathbb{R}^m \to \mathbb{R}^n$ (with $n > 1$), we need a different definition.

- For functions of type $\mathbb{R}^m \to \mathbb{R}$, it is necessary the introduction of the notion of parcial derivatives, $\frac{\partial F}{\partial x_j}$, with $j \in \{1, ..., m\}$.
- For functions of type $\mathbb{R}^m \to \mathbb{R}^n$ (with $n > 1$), apart from the use of parcial derivatives, it is necessary the use of Jacobian matrices $\mathbf{J}_{i,j} = \frac{\partial F_i}{\partial x_j}$, where $i \in \{1, ..., n\}$ and F_i is a function $\mathbb{R}^m \to \mathbb{R}$.

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Generalization and Chain Rule

Let **A** and **B** be two Jacobian matrices.
The composition rule in $\mathbb{R}^m \to \mathbb{R}^n$ is:

$$(\mathbf{A} \cdot \mathbf{B})_{i,j} = \sum_{k=1}^{m} \mathbf{A}_{i,k} \cdot \mathbf{B}_{k,j}$$

Generalization and Chain Rule

Assuming that the notion of derivatives that we need matches with a linear map, where it is accepted the composition rule previously seen, we will define a new generalization:

$$\lim_{\varepsilon \to 0} \frac{f(x+\varepsilon) - f(x)}{\varepsilon} - f'(x) = 0 \Leftrightarrow \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon) - (f(x)) + \varepsilon \cdot f'(x)}{\varepsilon} = 0$$

$$\Leftrightarrow \lim_{\varepsilon \to 0} \frac{\|f(x+\varepsilon) - (f(x)) + \varepsilon \cdot f'(x)\|}{\|\varepsilon\|} = 0$$

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Derivate as a linear map

Definition

Let $f :: a \to b$ be a function, where a and b are vectorial spaces that share a common underlying field. The first derivative definition is the following:

$$\mathcal{D} :: (a \to b) \to (a \to (a \multimap b))$$

If we differentiate two times, we have:

$$\mathcal{D}^2 = \mathcal{D} \circ \mathcal{D} :: (a \to b) \to (a \to (a \multimap a \multimap b))$$

Rules for Differentiation - Sequential Composition

Theorem

Let $f :: a \to b$ and $g :: b \to c$ be two functions. Then the derivative of the composition of f and g is:

$$\mathcal{D}\ (g \circ f)\ a = \mathcal{D}\ g\ (f\ a) \circ \mathcal{D}\ f\ a$$

Rules for Differentiation - Sequential Composition

Unfortunately the previous theorem isn't a efficient recipe for composition. As such we will introduce a second derivative definition:

$$\mathcal{D}_0^+ :: (a \to b) \to ((a \to b) \times (a \to (a \multimap b)))$$
$$\mathcal{D}_0^+\ f = (f, \mathcal{D}\ f)$$

With this, the chain rule will have the following expression:

$\mathcal{D}_0^+\,(g \circ f)$

{definition of $\mathcal{D}_0^+$}

$= (g \circ f, \mathcal{D}\,(g \circ f))$

{theorem and definition of $g \circ f$}

$= (\lambda a \to g(f\,a), \lambda a \to \mathcal{D}\,g\,(f\,a) \circ \mathcal{D}\,f\,a)$

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Rules for Differentiation - Sequential Composition

Having in mind optimizations, we introduce the third and last derivative definition:

$$\mathcal{D}^+ :: (a \to b) \to (a \to (b \times (a \multimap b)))$$
$$\mathcal{D}^+ \; f \; a = (f \; a, \mathcal{D} \; f \; a)$$

As $\times$ has more priority than $\to$ and $\multimap$, we can rewrite $\mathcal{D}^+$ as:

$$\mathcal{D}^+ :: (a \to b) \to (a \to b \times (a \multimap b))$$
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Rules for Differentiation - Sequential Composition

Corollary

$\mathcal{D}^+$ is compositionally efficient in relation to $(\circ)$, that is, in Haskell:

$$\mathcal{D}^+ \ (g \circ f) \ a = \textbf{let} \ \{(b, f') = \mathcal{D}^+ \ f \ a; (c, g') = \mathcal{D}^+ \ g \ b\} \\ \quad \textbf{in} \ (c, g' \circ f')$$

$$\begin{tikzcd}
(C \times C^B) \times B^A \arrow[d, "(id \times (uncurry\ (\circ))) \circ assocr"'] & B \times B^A \arrow[l, "\mathcal{D}^+ g \times id"'] & A \arrow[l, "\mathcal{D}^+ f"'] \arrow[dll, "\mathcal{D}^+ (g \circ f)"] \\
C \times C^A & &
\end{tikzcd}$$

Rules for Differentiation - Parallel Composition

Another important way of combining functions is the operation cross, that combines two functions in parallel:

$$(\times) :: (a \to c) \to (b \to d) \to (a \times b \to c \times d)$$
$$f \times g = \lambda(a, b) \to (f\ a, g\ b)$$

Theorem

Let $f :: a \to c$ and $g :: b \to d$ be two function. Then the cross rule is the following:

$$\mathcal{D}(f \times g)(a, b) = \mathcal{D} f\ a \times \mathcal{D} g\ b$$

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$$\mathcal{D}\,(f \times g)\,(a, b) = \mathcal{D}\,f\ a \times \mathcal{D}\,g\ b$$

Rules for Differentiation - Parallel Composition

Corollary

The function $\mathcal{D}^+$ is compositional in relation to $(\times)$

$$\begin{aligned} &\mathcal{D}^+\ (f \times g)\ (a, b) = \textbf{let}\ \{(c, f') = \mathcal{D}^+\ f\ a; (d, g') = \mathcal{D}^+\ g\ b\} \\ &\quad \textbf{in}\ ((c, d), f' \times g') \end{aligned}$$

Derivative and Linear Functions

Definition

A function f is said to be linear when preserves addition and scalar multiplication.

$$f(a + a') = f\,a + f\,a'$$
$$f(s \cdot a) = s \cdot f\,a$$

Theorem

For all linear functions f, $\mathcal{D}\,f\,a = f$.

Corollary

For all linear functions f, $\mathcal{D}^{+}\,f = \lambda a \rightarrow (fa, f)$.

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A short introdution

- We want to calculate $\mathcal{D}^+$.
- However, $\mathcal{D}$ is not computable.
- Solution: reimplement corollaries using category theory.

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A short introdution

Corollary 1.1

$$\mathcal{D}^+ \ (g \circ f) \ a = \mathbf{let} \ \{(b, f') = \mathcal{D}^+ \ f \ a; (c, g') = \mathcal{D}^+ \ g \ b\} \\ \mathbf{in} \ (c, g' \circ f')$$

Corollary 2.1

$$\mathcal{D}^+ \ (f \times g) \ (a, b) = \mathbf{let} \ \{(c, f') = \mathcal{D}^+ \ f \ a; (d, g') = \mathcal{D}^+ \ g \ b\} \\ \mathbf{in} \ ((c, d), f' \times g')$$

Corollary 3.1

For all linear functions f, $\mathcal{D}^+ \ f = \lambda a \to (fa, \ f)$.

Categories

A category is a collection of objects (sets and types) and morphisms (operation between objects), with 2 basic operations (identity and composition) of morfisms, and 2 laws:

- (C.1) $id \circ f = f \circ id = f$
- (C.2) $f \circ (g \circ h) = (f \circ g) \circ h$

Note

For this article, objects are data types and morfisms are functions

class *Category k* **where**
$id :: (a'k'a)$
$(\circ) :: (b'k'c) \to (a'k'b) \to (a'k'c)$

instance *Category* $(\to)$ **where**
$id = \lambda a \to a$
$g \circ f = \lambda a \to g\ (f\ a)$

Functors

A functor F between 2 categories $\mathcal{U}$ *and* $\mathcal{V}$ is such that:

- given any object t $\in \mathcal{U}$ there exists an object F t $\in \mathcal{V}$
- given any morphism m :: a $\rightarrow$ b $\in \mathcal{U}$ there exists a morphism F m :: F a $\rightarrow$ F b $\in \mathcal{V}$
- F id ($\in \mathcal{U}$) = id ($\in \mathcal{V}$)
- F (f $\circ$ g) = F f $\circ$ F g

Note

Given this category properties (objects are data types) functors map types to themselves

Objective

$\mathcal{D}$ definition

newtype $\mathcal{D}\ a\ b = \mathcal{D}\ (a \rightarrow b \times (a \multimap b))$

Adapted definition for $\mathcal{D}$ type

$$\hat{\mathcal{D}} :: (a \rightarrow b) \rightarrow \mathcal{D}\ a\ b$$
$$\hat{\mathcal{D}}\ f = \mathcal{D}\ (\mathcal{D}^{+}\ f)$$

Our objective is to deduce an instance of a Category for $\mathcal{D}$ where $\hat{\mathcal{D}}$ is a functor.

Instance deduction

Using corollaries 3.1 and 1.1 we can determine that

- (DP.1) $\mathcal{D}^{+}\ id = \lambda a \rightarrow (id\ a, id)$
- (DP.2)

$$\mathcal{D}^{+}\ (g \circ f) = \lambda a \rightarrow \textbf{let}\ \{(b, f') = \mathcal{D}^{+}\ f\ a; (c, g') = \mathcal{D}^{+}\ g\ b\}\\ \quad \textbf{in}\ (c, g' \circ f')$$

Saying that $\hat{\mathcal{D}}$ is a functor is equivalent to, for all f and g functions of appropriate types:
$id = \hat{\mathcal{D}}\ id = \mathcal{D}\ (\mathcal{D}^{+}\ id)$
$\hat{\mathcal{D}}\ g \circ \hat{\mathcal{D}}\ f = \hat{\mathcal{D}}\ (g \circ f) = \mathcal{D}\ (\hat{\mathcal{D}}\ (g \circ f))$

Instance deduction

Based on (DP.1) and (DP.2) we'll rewrite the above into the following definition:

$id = \mathcal{D}\ (\lambda a \to (id\ a, id))$

$\hat{\mathcal{D}}\ g \circ \hat{\mathcal{D}}\ f = \mathcal{D}\ (\lambda a \to \textbf{let}\ \{(b, f') = \mathcal{D}^+\ f\ a; (c, g') = \mathcal{D}^+\ g\ b\}\ \textbf{in}\ (c, g' \circ f'))$

The first equation shown above has a trivial solution.

To solve the second we'll first solve a more general one:

$\mathcal{D}\ g \circ \mathcal{D}\ f = \mathcal{D}\ (\lambda a \to \textbf{let}\ \{(b, f') = f\ a; (c, g') = g\ b\}\ \textbf{in}\ (c, g' \circ f'))$

This condition also leads us to a trivial solution inside our instance.

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This condition also leads us to a trivial solution inside our instance.

Instance deduction

$\hat{\mathcal{D}}$ definition for linear functions

$$
\begin{aligned}
&\mathit{linearD} :: (a \to b) \to \mathcal{D}\ a\ b \\
&\mathit{linearD}\ f = \mathcal{D}\ (\lambda a \to (f\ a, f))
\end{aligned}
$$

Categorical instance we've deduced

$$
\begin{aligned}
&\mathbf{instance}\ \mathit{Category}\ \mathcal{D}\ \mathbf{where} \\
&\quad \mathit{id} = \mathit{linearD}\ \mathit{id} \\
&\quad \mathcal{D}\ g \circ \mathcal{D}\ f = \\
&\quad \mathcal{D}\ (\lambda a \to \mathbf{let}\ \{(b, f') = f\ a; (c, g') = g\ b\}\ \mathbf{in}\ (c, g' \circ f'))
\end{aligned}
$$

Instance proof

In order to prove that the instance is correct we must check if it follows laws (C.1) and (C.2).
First we must make a concession: that we only use morfisms arising from $\mathcal{D}^+$. If we do, then $\mathcal{D}^+$ is a functor.

(C.1) proof

id $\circ$ $\hat{\mathcal{D}}$ f
{ functor law for id (specification of $\hat{\mathcal{D}}$) }
= $\hat{\mathcal{D}}$ id $\circ$ $\hat{\mathcal{D}}$ f
{ functor law for ($\circ$) }
= $\hat{\mathcal{D}}$ (id $\circ$ f)
{ categorical law }
= $\hat{\mathcal{D}}$ f

Instance proof

(C.2) proof

$\hat{\mathcal{D}}$ h ∘ ($\hat{\mathcal{D}}$ g ∘ $\hat{\mathcal{D}}$ f)
{ 2x functor law for (∘) }
= $\hat{\mathcal{D}}$ (h ∘ (g ∘ f))
{ categorical law }
= $\hat{\mathcal{D}}$ ((h ∘ g) ∘ f)
{ 2x functor law for (∘) }
= ($\hat{\mathcal{D}}$ h ∘ $\hat{\mathcal{D}}$ g) ∘ $\hat{\mathcal{D}}$ f

Note

Those proofs don't require anything from $\mathcal{D}$ *and* $\hat{\mathcal{D}}$ aside from functor laws. As such, all other instances of categories created from a functor won't require further proving like this one did.

Monoidal categories and functors

Generalized parallel composition shall be defined using a monoidal category:

$$
\begin{aligned}
&\textbf{class}\ \mathit{Category}\ k \Rightarrow \mathit{Monoidal}\ k\ \textbf{where}\\
&\quad (\times) :: (a\ {}'\mathtt{k}'\ c) \to (b\ {}'\mathtt{k}'\ d) \to ((a \times b)\ {}'\mathtt{k}'\ (c \times d))\\
&\textbf{instance}\ \mathit{Monoidal}\ (\to)\ \textbf{where}\\
&\quad f \times g = \lambda(a, b) \to (f\ a, g\ b)
\end{aligned}
$$

Monoidal Functor definition

A monoidal functor F between categories $\mathcal{U}$ *and* $\mathcal{V}$ is such that:

- F is a functor
- F (f $\times$ g) = F f $\times$ F g

Instance deduction

From corollary 2.1 we can deduce that:
$\mathcal{D}^+\ (f \times g) = \lambda(a,b) \rightarrow \textbf{let}\ \{(c,f') = \mathcal{D}^+\ f\ a; (d,g') = \mathcal{D}^+\ g\ b\}$
$\textbf{in}\ ((c,d), f' \times g')$

Deriving F from $\hat{\mathcal{D}}$ leaves us with the following definition:
$\mathcal{D}\ (\mathcal{D}^+\ f) \times \mathcal{D}\ (\mathcal{D}^+\ g) = \mathcal{D}\ (\mathcal{D}^+\ (f \times g))$

Using the same method as before, we replace $\mathcal{D}^+$ with its definition and generalize the condition:
$\mathcal{D}\ f \times \mathcal{D}\ g =$
$\mathcal{D}\ (\lambda(a,b) \rightarrow \textbf{let}\ \{(c,f') = f\ a; (d,g') = g\ b\}\ \textbf{in}\ ((c,d), f' \times g'))$
and this is enough for our new instance.

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$\mathcal{D}^{+}\ (f \times g) = \lambda(a, b) \rightarrow \textbf{let}\ \{(c, f') = \mathcal{D}^{+}\ f\ a; (d, g') = \mathcal{D}^{+}\ g\ b\}$
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and this is enough for our new instance.

Instance deduction

Categorical instance we've deduced

instance *Monoidal* $\mathcal{D}$ **where**

$\mathcal{D}\ f \times \mathcal{D}\ g = \mathcal{D}\ (\lambda(a,b) \rightarrow \textbf{let}\ \{(c,f') = f\ a; (d,g') = g\ b\}$

$\quad \textbf{in}\ ((c,d), f' \times g'))$

Cartesian categories and functors

class *Monoidal k* $\Rightarrow$ *Cartesian k* **where**

$exl :: (a, b)$ `'k'` a

$exr :: (a, b)$ `'k'` b

$dup :: a$ `'k'` (a, a)

instance *Cartesian* $(\rightarrow)$ **where**

$exl = \lambda(a, b) \rightarrow a$

$exr = \lambda(a, b) \rightarrow b$

$dup = \lambda a \rightarrow (a, a)$

A cartesian functor F between categories $\mathcal{U}$ *and* $\mathcal{V}$ is such that:

- F is a monoidal functor
- F exl = exl
- F exp = exp
- F dup = dup

Instance deduction

From corollary 3.1 and from exl, exr and dup being linear functions we can deduce that:
$\mathcal{D}^+\ exl = \lambda p \to (exl\ p, exl)$
$\mathcal{D}^+\ exr = \lambda p \to (exr\ p, exr)$
$\mathcal{D}^+\ dup = \lambda p \to (dup\ a, dup)$

With this in mind we can arrive at our instance:
$exl = \mathcal{D}\ (\mathcal{D}^+\ exl)$
$exr = \mathcal{D}\ (\mathcal{D}^+\ exr)$
$dup = \mathcal{D}\ (\mathcal{D}^+\ dup)$

Instance deduction

Replacing $\mathcal{D}^{+}$ with its definition and remembering linearD's definition we can obtain:

exl = linearD exl

exr = linearD exr

dup = linearD dup

and convert this directly into a new instance:

Categorical instance we've deduced

instance *Cartesian D* **where**

$exl = linearD\ exl$

$exr = linearD\ exr$

$dup = linearD\ dup$

Cocartesian category

This type of categories is the dual of the cartesian type of categories.

Note

In this article coproducts are categorical products, i.e., biproducts

Definition

$$
\begin{array}{l}
\textbf{class } \mathit{Category}\ k \Rightarrow \mathit{Cocartesian}\ k \textbf{ where} \\
\quad \mathit{inl} :: a\ `\mathtt{k}`\ (a, b) \\
\quad \mathit{inr} :: b\ `\mathtt{k}`\ (a, b) \\
\quad \mathit{jam} :: (a, a)\ `\mathtt{k}`\ a
\end{array}
$$

Cocartesian functors

Cocartesian functor definition

A cocartesian functor F between categories $\mathcal{U}$ *and* $\mathcal{V}$ is such that:

- F is a functor
- F inl = inl
- F inr = inr
- F jam = jam

Fork and Join

- $\triangle :: \mathit{Cartesian}\ k \Rightarrow (a\ '\mathtt{k}'\ c) \to (a\ '\mathtt{k}'\ d) \to (a\ '\mathtt{k}'\ (c \times d))$

$$
\begin{tikzcd}
 & c \\
a \arrow[ur] \arrow[dr] & \\
 & d
\end{tikzcd}
$$

- $\nabla :: \mathit{Cartesian}\ k \Rightarrow (c\ '\mathtt{k}'\ a) \to (d\ '\mathtt{k}'\ a) \to ((c \times d)\ '\mathtt{k}'\ a)$

$$
\begin{tikzcd}
c \arrow[dr] & \\
 & a \\
d \arrow[ur] &
\end{tikzcd}
$$

Instance of $\rightarrow^{+}$

newtype $a \rightarrow^{+} b = \mathit{AddFun}\ (a \rightarrow b)$

instance $\mathit{Category}\ (\rightarrow^{+})$ **where**

  type $\mathit{Obj}\ (\rightarrow^{+}) = \mathit{Additive}$

  $\mathit{id} = \mathit{AddFun}\ \mathit{id}$

  $\mathit{AddFun}\ g \circ \mathit{AddFun}\ f = \mathit{AddFun}\ (g \circ f)$

instance $\mathit{Monoidal}\ (\rightarrow^{+})$ **where**

  $\mathit{AddFun}\ f \times \mathit{AddFun}\ g = \mathit{AddFun}\ (f \times g)$

instance $\mathit{Cartesian}\ (\rightarrow^{+})$ **where**

  $\mathit{exl} = \mathit{AddFun}\ \mathit{exl}$

  $\mathit{exr} = \mathit{AddFun}\ \mathit{exr}$

  $\mathit{dup} = \mathit{AddFun}\ \mathit{dup}$

Instance of $\rightarrow^+$

instance *Cocartesian* $(\rightarrow^+)$ **where**
  $inl = AddFun\ inlF$
  $inr = AddFun\ inrF$
  $jam = AddFun\ jamF$

$inlF :: Additive\ b \Rightarrow a \rightarrow a \times b$
$inrF :: Additive\ a \Rightarrow b \rightarrow a \times b$
$jamF :: Additive\ a \Rightarrow a \times a \rightarrow a$

$inlF = \lambda a \rightarrow (a, 0)$
$inrF = \lambda b \rightarrow (0, b)$
$jamF = \lambda(a, b) \rightarrow a + b$

NumCat definition

$$
\begin{array}{l}
\textbf{class}\ \mathit{NumCat}\ k\ a\ \textbf{where} \\
\quad \mathit{negateC} :: a\ `k`\ a \\
\quad \mathit{addC} :: (a \times a)\ `k`\ a \\
\quad \mathit{mulC} :: (a \times a)\ `k`\ a \\
\quad \ldots \\
\textbf{instance}\ \mathit{Num}\ a \Rightarrow \mathit{NumCat}\ (\rightarrow)\ a\ \textbf{where} \\
\quad \mathit{negateC} = \mathit{negate} \\
\quad \mathit{addC} = \mathit{uncurry}\ (+) \\
\quad \mathit{mulC} = \mathit{uncurry}\ (*) \\
\quad \ldots
\end{array}
$$

$$\mathcal{D}\ (negate\ u) = negate\ (\mathcal{D}\ u)$$
$$\mathcal{D}\ (u + v) = \mathcal{D}\ u + \mathcal{D}\ v$$
$$\mathcal{D}\ (u * v) = u * \mathcal{D}\ v + v * \mathcal{D}\ u$$

- Imprecise on the nature of u and v.
- A precise and simpler definition would be to differentiate the operations themselves.

class $Scalable\ k\ a$ **where**
  $scale :: a \rightarrow (a \text{ ` } k \text{ ` } a)$

instance $Num\ a \Rightarrow Scalable\ (\rightarrow^{+})\ a$ **where**
  $scale\ a = AddFun\ (\lambda da \rightarrow a * da)$

instance $NumCat\ D$ **where**
  $negateC = linearD\ negateC$
  $addC = linearD\ addC$
  $mulC = D\ (\lambda(a, b) \rightarrow (a * b, scale\ b \triangledown scale\ a))$

instance $FloatingCat\ D$ **where**
  $sinC = D\ (\lambda a \rightarrow (sin\ a, scale\ (cos\ a)))$
  $cosC = D\ (\lambda a \rightarrow (cos\ a, scale\ (-sin\ a)))$
  $expC = D\ (\lambda a \rightarrow \textbf{let}\ e = exp\ a\ \textbf{in}\ (e, scale\ e))$
  ...

Examples

$$
\begin{aligned}
&sqr :: Num\ a \Rightarrow a \to a\\
&sqr\ a = a * a\\
&magSqr :: Num\ a \Rightarrow a \times a \to a\\
&magSqr\ (a, b) = sqr\ a + sqr\ b\\
&cosSinProd :: Floating\ a \Rightarrow a \times a \to a \times a\\
&cosSinProd\ (x, y) = (cos\ z, sin\ z)\ \textbf{where}\ z = x * y
\end{aligned}
$$

With a compiler plugin we can obtain

$$
\begin{aligned}
&sqr = mulC \circ (id \vartriangle id)\\
&magSqr = addC \circ (mulC \circ (exl \vartriangle exl) \vartriangle mulC \circ (exr \vartriangle exr))\\
&cosSinProd = (cosC \vartriangle sinC) \circ mulC
\end{aligned}
$$

Generalizing Automatic Differentiation

$$\textbf{newtype}\ D_k\ a\ b = D\ (a \to b \times (a\ \text{`}\ k\ \text{`}\ b))$$

$$linearD :: (a \to b) \to (a\ \text{`}\ k\ \text{`}\ b) \to D_k\ a\ b$$
$$linearD\ f\ f' = D\ (\lambda a \to (f\ a, f'))$$

$$\textbf{instance}\ Category\ k \Rightarrow Category\ D_k\ \textbf{where}$$
$$\quad \textbf{type}\ Obj\ D_k = Additive \land Obj\ k\ ...$$

$$\textbf{instance}\ Monoidal\ k \Rightarrow Monoidal\ D_k\ \textbf{where}\ ...$$

$$\textbf{instance}\ Cartesian\ k \Rightarrow Cartesian\ D_k\ \textbf{where}\ ...$$

$$\textbf{instance}\ Cocartesian\ k \Rightarrow Cocartesian\ D_k\ \textbf{where}$$
$$\quad inl = linearD\ inlF\ inl$$
$$\quad inr = linearD\ inrF\ inr$$
$$\quad jam = linearD\ jamF\ jam$$

$$
\begin{aligned}
&\textbf{instance } \mathit{Scalable}\ k\ s \Rightarrow \mathit{NumCat}\ D_k\ s \textbf{ where}\\
&\quad \mathit{negateC} = \mathit{linearD}\ \mathit{negateC}\ \mathit{negateC}\\
&\quad \mathit{addC} = \mathit{linearD}\ \mathit{addC}\ \mathit{addC}\\
&\quad \mathit{mulC} = D\ (\lambda(a, b) \to (a * b, \mathit{scale}\ b \triangledown \mathit{scale}\ a))
\end{aligned}
$$

Matrices

There exists three, non-exclusive, possibilities for a nonempty matrix W:

- width W = height W = 1;
- W is the horizontal juxtaposition of two matrices U and V, where height W = height U = height V and width W = width U + width V;
- W is the vertical juxtaposition of two matrices U and V, where width W = width U = width V and height W = height U + height V.

Extracting a Data Representation

In machine learning, a Gradient-based optimization works by searching for local minima in the domain of a differentiable function $f :: a \to s$. Each step in the search is in the direction opposite of the gradient of f, which is a vector form of $\mathcal{D}\ f$.

Given a linear map $f' :: U \multimap V$ represented as a function, it is possible to extract a Jacobian matrix by applying f to every vector in a basis of U.

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Generalized Matrices

Given a scalar field s, a free vector space has the form $p \rightarrow s$ for some p, where the cardinality of p is the dimension of the vector space and there exists a finite number of values for p.

In particular, we can represent vector spaces over a given field as a representable functor, i.e., a functor F such that:

$$\exists p \, \forall s \; F\, s \;\cong\; p \rightarrow s$$

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A short introdution

- We've derived and generalized an AD algorithm using categories.
- With fully right-associated compositions this algorithm becomes a foward-mode AD and with fully left-associated becomes a reverse-mode AD.
- We want to obtain generalized FAD and RAD algorithms.
- How do we describe this in Categorical notation?

Converting morfisms

Given a category k we can represent its morfisms the following way:

Left-Compose functions

$f :: a \, {}'\mathrm{k}{}' \, b \Rightarrow (\circ f) :: (b \, {}'\mathrm{k}{}' \, r) \rightarrow (a \, {}'\mathrm{k}{}' \, r)$ where r is any object of k.

If h is the morfism we'll compose with f then h is the continuation of f.

Instance deduction

Defining new type

$$\textbf{newtype}\ \mathit{Cont}_k^r\ a\ b = \mathit{Cont}\ ((b\ `\mathtt{k}`\ r) \to (a\ `\mathtt{k}`\ r))$$

Functor derived from type

$$\mathit{cont} :: \mathit{Category}\ k \Rightarrow (a\ `\mathtt{k}`\ b) \to \mathit{Cont}_k^r\ a\ b$$
$$\mathit{cont}\ f = \mathit{Cont}\ (\circ f)$$

Instance deduction

$$
\begin{array}{l}
\textbf{instance } \mathit{Category}\ k \Rightarrow \mathit{Category}\ \mathit{Cont}^r_k \textbf{ where} \\
\quad \mathit{id} = \mathit{Cont}\ \mathit{id} \\
\quad \mathit{Cont}\ g \circ \mathit{Cont}\ f = \mathit{Cont}\ (f \circ g) \\
\textbf{instance } \mathit{Monoidal}\ k \Rightarrow \mathit{Monoidal}\ \mathit{Cont}^r_k \textbf{ where} \\
\quad \mathit{Conf}\ f \times \mathit{Cont}\ g = \mathit{Cont}\ (\mathit{join} \circ (f \times g) \circ \mathit{unjoin}) \\
\textbf{instance } \mathit{Cartesian}\ k \Rightarrow \mathit{Cartesian}\ \mathit{Cont}^r_k \textbf{ where} \\
\quad \mathit{exl} = \mathit{Cont}\ (\mathit{join} \circ \mathit{inl}); \mathit{exr} = \mathit{Cont}\ (\mathit{join} \circ \mathit{inr}) \\
\quad \mathit{dup} = \mathit{Cont}\ (\mathit{jam} \circ \mathit{unjoin}) \\
\textbf{instance } \mathit{Cocartesian}\ k \Rightarrow \mathit{Cocartesian}\ \mathit{Cont}^r_k \textbf{ where} \\
\quad \mathit{inl} = \mathit{Cont}\ (\mathit{exl} \circ \mathit{unjoin}); \mathit{inr} = \mathit{Cont}\ (\mathit{exr} \circ \mathit{unjoin}) \\
\quad \mathit{jam} = \mathit{Cont}\ (\mathit{join} \circ \mathit{dup}) \\
\textbf{instance } \mathit{Scalable}\ k\ a \Rightarrow \mathit{Scalable}\ \mathit{Cont}^r_k\ a \textbf{ where} \\
\quad \mathit{scale}\ s = \mathit{Cont}\ (\mathit{scale}\ s)
\end{array}
$$

A short introdution

Due to its widespread use in ML we'll talk about a specific case of RAD: computing gradients (derivatives of functions with scalar codomains).
A vector space A over a scalar field s has A $\multimap$ s as its dual.
Each linear map in A $\multimap$ s can be represented in the form of dot u for some u :: A where

Definition and instanciation

$$\textbf{class } \mathit{HasDot}\ (S)\ u\ \textbf{where } \mathit{dot} :: u \to (u \multimap s)$$

$$\textbf{instance } \mathit{HasDot}\ (\mathit{IR})\ \mathit{IR}\ \textbf{where } \mathit{dot} = \mathit{scale}$$

$$\begin{aligned}&\textbf{instance } (\mathit{HasDot}\ (S)\ a, \mathit{HasDot}\ (S)\ b)\\ &\quad \Rightarrow \mathit{HasDot}\ (S)\ (a \times b)\\ &\quad \textbf{where } \mathit{dot}\ (u, v) = \mathit{dot}\ u\ \Delta\ \mathit{dot}\ v\end{aligned}$$

Instance deduction

The internal representation of $Cont^{s}_{\multimap}$ a b is (b $\multimap$ s) $\rightarrow$ (a $\multimap$ s) which is isomorfic to (a $\rightarrow$ b).

Type definition for duality

$$\textbf{newtype}\ \mathit{Dual}_k\ a\ b = \mathit{Dual}\ (b\ \text{'}\mathtt{k}\text{'}\ a)$$

Instance deduction

All we need to do to create dual representations of linear maps is to convert from $Cont_k^S$ to $Dual_k$ using a functor:

Functor definition

$$
\begin{aligned}
&asDual :: (HasDot\ (S)\ a, HasDot\ (S)\ b) \Rightarrow \\
&\quad ((b \multimap s) \to (a \multimap s)) \to (b \multimap a) \\
&asDual\ (Cont\ f) = Dual\ (onDot\ f)
\end{aligned}
$$

where

$$
\begin{aligned}
&onDot :: (HasDot\ (S)\ a, HasDot\ (S)\ b) \Rightarrow \\
&\quad ((b \multimap s) \to (a \multimap s)) \to (b \multimap a) \\
&onDot\ f = dot^{-1} \circ f \circ dot
\end{aligned}
$$

Instance deduction

$$
\begin{array}{l}
\textbf{instance } \mathit{Category}\ k \Rightarrow \mathit{Category}\ \mathit{Dual}_k \textbf{ where} \\
\quad \mathit{id} = \mathit{Dual}\ \mathit{id} \\
\quad \mathit{Dual}\ g \circ \mathit{Dual}\ f = \mathit{Dual}\ (f \circ g) \\
\textbf{instance } \mathit{Monoidal}\ k \Rightarrow \mathit{Monoidal}\ \mathit{Dual}_k \textbf{ where} \\
\quad \mathit{Dual}\ f \times \mathit{Dual}\ g = \mathit{Dual}\ (f \times g) \\
\textbf{instance } \mathit{Cartesian}\ k \Rightarrow \mathit{Cartesian}\ \mathit{Dual}_k \textbf{ where} \\
\quad \mathit{exl} = \mathit{Dual}\ \mathit{inl};\ \mathit{exr} = \mathit{Dual}\ \mathit{inr} \\
\quad \mathit{dup} = \mathit{Dual}\ \mathit{jam} \\
\textbf{instance } \mathit{Cocartesian}\ k \Rightarrow \mathit{Cocartesian}\ \mathit{Dual}_k \textbf{ where} \\
\quad \mathit{inl} = \mathit{Dual}\ \mathit{exl};\ \mathit{inr} = \mathit{Dual}\ \mathit{exr} \\
\quad \mathit{jam} = \mathit{Dual}\ \mathit{dup} \\
\textbf{instance } \mathit{Scalable}\ k \Rightarrow \mathit{Scalable}\ \mathit{Dual}_k \textbf{ where} \\
\quad \mathit{scale}\ s = \mathit{Dual}\ (\mathit{scale}\ s)
\end{array}
$$

Final notes

- (∇) *and* (Δ) mutually dualize
  $(\mathit{Dual}\ f\ \nabla\ \mathit{Dual}\ g) = \mathit{Dual}\ (f\ \Delta\ g)$ *and* $\mathit{Dual}\ f\ \Delta\ \mathit{Dual}\ g = \mathit{Dual}\ (f\ \nabla\ g))$
- Using the definition from chapter 8 we can determine that the duality of a matrix corresponds to its transposition

Fowards-mode Automatic Differentiation(FAD)

We can use the same deductions we've done in Cont and Dual to derive a category with full right-side association, thus creating a generized FAD algorithm.
This algorithm is far more appropriate for low dimension domains.

Type definition and functor from type

$$\textbf{newtype}\ \mathit{Begin}_k^r\ a\ b = \mathit{Begin}\ ((r\ `\mathtt{k}`\ a) \rightarrow (r\ `\mathtt{k}`\ b))$$
$$\mathit{begin} :: \mathit{Category}\ k \Rightarrow (a\ `\mathtt{k}`\ b) \rightarrow \mathit{Begin}_k^r\ a\ b$$
$$\mathit{begin}\ f = \mathit{Begin}\ (f \circ)$$

We can derive categorical instances from the functor above and we can choose r to be the scalar field s, noting that s $\multimap$ a is isomorfic to a.

Scaling Up

- Practical applications often involve high-dimensional spaces.
- Binary products are a very inefficient and unwieldy way of encoding high-dimensional spaces.
- A practical alternative is to consider n-ary products as representable functors.

class $\mathit{Category}\ k \Rightarrow \mathit{MonoidalI}\ k\ h$ **where**
    $\mathit{crossI} :: h\ (a\ `k`\ b) \rightarrow (h\ a\ `k`\ h\ b)$
instance $\mathit{Zip}\ h \Rightarrow \mathit{MonoidalI}\ (\rightarrow)\ h$ **where**
    $\mathit{crossI} = \mathit{zipWith}\ \mathit{id}$

$$\begin{array}{l}
\textbf{class}\ \mathit{MonoidalI}\ k\ h \Rightarrow \mathit{CartesianI}\ k\ h\ \textbf{where} \\
\quad \mathit{exI}\ \ :: h\ (h\ a\ `k`\ a) \\
\quad \mathit{replI} :: a\ `k`\ h\ a
\end{array}$$

$$\begin{array}{l}
\textbf{instance}\ (\mathit{Representable}\ h, \mathit{Zip}\ h, \mathit{Pointed}\ h) \Rightarrow \\
\quad \mathit{CartesianI}\ (\to)\ h\ \textbf{where} \\
\quad \mathit{exI} = \mathit{tabulate}\ (\mathit{flip}\ \mathit{index}) \\
\quad \mathit{replI} = \mathit{point}
\end{array}$$

- The following is not the class the author was thinking

$$\begin{array}{l}
\textbf{class}\ \mathit{Representable}\ h\ \textbf{where} \\
\quad \textbf{type}\ \mathit{Rep}\ h :: * \\
\quad \mathit{tabulate} :: (\mathit{Rep}\ h \to a) \to h\ a \\
\quad \mathit{index} :: h\ a \to \mathit{Rep}\ h \to a
\end{array}$$

$$
\begin{array}{l}
\textbf{class}\ \mathit{MonoidalI}\ k\ h \Rightarrow \mathit{CocartesianI}\ k\ h\ \textbf{where} \\
\quad \mathit{inI} :: h\ (a\ `k`\ h\ a) \\
\quad \mathit{jamI} :: h\ a\ `k`\ a
\end{array}
$$

$$
\begin{array}{l}
\textbf{instance}\ (\mathit{MonoidalI}\ k\ h, \mathit{Zip}\ h) \Rightarrow \mathit{MonoidalI}\ D_k\ h\ \textbf{where} \\
\quad \mathit{crossI}\ \mathit{fs} = D\ ((\mathit{id} \times \mathit{crossI}) \circ \mathit{unzip} \circ \mathit{crossI}\ (\mathit{fmap}\ \mathit{unD}\ \mathit{fs}))
\end{array}
$$

$$
\begin{array}{l}
\textbf{instance}\ (\mathit{CocartesianI}\ (\rightarrow)\ h, \mathit{CartesianI}\ k\ h, \mathit{Zip}\ h) \Rightarrow \\
\quad \mathit{CartesianI}\ D_k\ h\ \textbf{where} \\
\quad \mathit{exI} = \mathit{linearD}\ \mathit{exI}\ \mathit{exI} \\
\quad \mathit{replI} = \mathit{zipWith}\ \mathit{linearD}\ \mathit{replI}\ \mathit{replI}
\end{array}
$$

$$
\begin{array}{l}
\textbf{instance}\ (\mathit{CocartesianI}\ k\ h, \mathit{Zip}\ h) \Rightarrow \mathit{CocartesianI}\ D_k\ h\ \textbf{where} \\
\quad \mathit{inI} = \mathit{zipWith}\ \mathit{linearD}\ \mathit{inIF}\ \mathit{inI} \\
\quad \mathit{jamI} = \mathit{linearD}\ \mathit{sum}\ \mathit{jamI}
\end{array}
$$

$$
\begin{array}{l}
\textbf{class}\ \mathit{MonoidalI}\ k\ h \Rightarrow \mathit{CocartesianI}\ k\ h\ \textbf{where} \\
\quad \mathit{inI} :: h\ (a\ `k`\ h\ a) \\
\quad \mathit{jamI} :: h\ a\ `k`\ a \\
\textbf{instance}\ (\mathit{MonoidalI}\ k\ h, \mathit{Zip}\ h) \Rightarrow \mathit{MonoidalI}\ D_k\ h\ \textbf{where} \\
\quad \mathit{crossI}\ \mathit{fs} = D\ ((\mathit{id} \times \mathit{crossI}) \circ \mathit{unzip} \circ \mathit{crossI}\ (\mathit{fmap}\ \mathit{unD}\ \mathit{fs})) \\
\textbf{instance}\ (\mathit{CocartesianI}\ (\to)\ h, \mathit{CartesianI}\ k\ h, \mathit{Zip}\ h) \Rightarrow \\
\quad \mathit{CartesianI}\ D_k\ h\ \textbf{where} \\
\quad \mathit{exI} = \mathit{zipWith}\ \mathit{linearD}\ \mathit{exI}\ \mathit{exI} \\
\quad \mathit{replI} = \mathit{linearD}\ \mathit{replI}\ \mathit{replI} \\
\textbf{instance}\ (\mathit{CocartesianI}\ k\ h, \mathit{Zip}\ h) \Rightarrow \mathit{CocartesianI}\ D_k\ h\ \textbf{where} \\
\quad \mathit{inI} = \mathit{zipWith}\ \mathit{linearD}\ \mathit{inIF}\ \mathit{inI} \\
\quad \mathit{jamI} = \mathit{linearD}\ \mathit{sum}\ \mathit{jamI}
\end{array}
$$

Conclusion

- Suggests that some of the work referred to does just a part of this article.
- This article ([Elliott 2018][2]) is a follow up of [Elliott 2017][1]
- Suggests that this implementation is simple, efficient, it can free memory dinamically (RAD) and is naturally parallel.
- Future work are detailed performace analysis; higher-order differentiation and automatic incrementation (continuing previous work [Elliott 2017][1])

ELLIOTT, C.
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