

Simple essence of AD

Artur Ezequiel Nelson

Universidade do Minho

26 de Abril

Index

- 1 Categories
- 2 Fork and Join
- 3 Numeric operations
- 4 Generalizing Automatic Differentiation
- 5 Reverse-Mode Automatic Differentiation(RAD)
- 6 Gradient and Duality
- 7 Foward-Mode Automatic Differentiation(FAD)
- 8 Scaling Up
- 9 Related Work and conclusion

Definition of Derivative

Definition

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

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

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

Definition of Derivative

Definition

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

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

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

Definition of Derivative

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

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

Definition of Derivative

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

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

Definition of Derivative

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

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

Generalization and Chain Rule

Let **A** and **B** be two Jacobian matrices.

The chain rule in $\mathbb{R}^m \rightarrow \mathbb{R}^n$ 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 chain rule previously seen, we will define a new generalization:

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \frac{f(x + \varepsilon) - f(x)}{\varepsilon} - f'(x) = 0 &\Leftrightarrow \lim_{\varepsilon \rightarrow 0} \frac{f(x + \varepsilon) - (f(x)) + \varepsilon \cdot f'(x)}{\varepsilon} = 0 \\ &\Leftrightarrow \lim_{\varepsilon \rightarrow 0} \frac{\|f(x + \varepsilon) - (f(x)) + \varepsilon \cdot f'(x)\|}{\|\varepsilon\|} = 0 \end{aligned}$$

Generalization and Chain Rule

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

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \frac{f(x + \varepsilon) - f(x)}{\varepsilon} - f'(x) = 0 &\Leftrightarrow \lim_{\varepsilon \rightarrow 0} \frac{f(x + \varepsilon) - (f(x)) + \varepsilon \cdot f'(x)}{\varepsilon} = 0 \\ &\Leftrightarrow \lim_{\varepsilon \rightarrow 0} \frac{\|f(x + \varepsilon) - (f(x)) + \varepsilon \cdot f'(x)\|}{\|\varepsilon\|} = 0 \end{aligned}$$

Derivate as a linear map

Definition

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

$$\mathcal{D} :: (a \rightarrow b) \rightarrow (a \rightarrow (astob))$$

If we differentiate two times, we have:

$$\mathcal{D}^2 = \mathcal{D} \circ \mathcal{D} :: (a \rightarrow b) \rightarrow (a \rightarrow (astoastob))$$

Rules for Differentiation - Sequential Composition

Theorem

Let $f :: a \rightarrow b$ and $g :: b \rightarrow c$ 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 derivate definition:

$$\begin{aligned}\mathcal{D}_0^+ &:: (a \rightarrow b) \rightarrow ((a \rightarrow b) \times (a \rightarrow (a \multimap b))) \\ \mathcal{D}_0^+ f &= (f, \mathcal{D} f)\end{aligned}$$

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

$$\begin{aligned}&\mathcal{D}_0^+ (g \circ f) \\ &\{\text{definition of } \mathcal{D}_0^+\} \\ &= (g \circ f, \mathcal{D} (g \circ f)) \\ &\{\text{theorem and definition of } g \circ f\} \\ &= (\lambda a \rightarrow g(f a), \lambda a \rightarrow \mathcal{D} g (f a) \circ \mathcal{D} f a)\end{aligned}$$

Rules for Differentiation - Sequential Composition

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

$$\begin{aligned}\mathcal{D}_0^+ &:: (a \rightarrow b) \rightarrow ((a \rightarrow b) \times (a \rightarrow (a \multimap b))) \\ \mathcal{D}_0^+ f &= (f, \mathcal{D} f)\end{aligned}$$

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

$$\begin{aligned}\mathcal{D}_0^+ (g \circ f) & \\ \{\text{definition of } \mathcal{D}_0^+\} & \\ = (g \circ f, \mathcal{D}(g \circ f)) & \\ \{\text{theorem and definition of } g \circ f\} & \\ = (\lambda a \rightarrow g(f a), \lambda a \rightarrow \mathcal{D} g (f a) \circ \mathcal{D} f a) &\end{aligned}$$

Rules for Differentiation - Sequential Composition

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

$$\begin{aligned}\mathcal{D}^+ &:: (a \rightarrow b) \rightarrow (a \rightarrow (b \times (a \multimap b))) \\ \mathcal{D}^+ f a &= (f a, \mathcal{D} f a)\end{aligned}$$

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

$$\begin{aligned}\mathcal{D}^+ &:: (a \rightarrow b) \rightarrow (a \rightarrow b \times (a \multimap b)) \\ \mathcal{D}^+ f a &= (f a, \mathcal{D} f a)\end{aligned}$$

Rules for Differentiation - Sequential Composition

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

$$\begin{aligned}\mathcal{D}^+ &:: (a \rightarrow b) \rightarrow (a \rightarrow (b \times (a \multimap b))) \\ \mathcal{D}^+ f a &= (f a, \mathcal{D} f a)\end{aligned}$$

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

$$\begin{aligned}\mathcal{D}^+ &:: (a \rightarrow b) \rightarrow (a \rightarrow b \times (a \multimap b)) \\ \mathcal{D}^+ f a &= (f a, \mathcal{D} f a)\end{aligned}$$

Rules for Differentiation - Sequential Composition

Corollary

\mathcal{D}^+ is efficiently compositional in relation to (\circ) , that is, in Haskell:

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

Rules for Differentiation - Parallel Composition

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

$$(\times) :: (a \rightarrow c) \rightarrow (b \rightarrow d) \rightarrow (a \times b \rightarrow c \times d)$$

$$f \times g = \lambda(a, b) \rightarrow (f\ a, g\ b)$$

Theorem

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

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

Rules for Differentiation - Parallel Composition

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

$$(\times) :: (a \rightarrow c) \rightarrow (b \rightarrow d) \rightarrow (a \times b \rightarrow c \times d)$$

$$f \times g = \lambda(a, b) \rightarrow (f\ a, g\ b)$$

Theorem

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

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

Rules for Differentiation - Parallel Composition

Corollary

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

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

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

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

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 , $\mathcal{D}^+ f = \lambda a \rightarrow (f a, f)$.

A short introduction

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

A short introduction

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

A short introduction

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

A short introduction

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

Categories

A category is a collection of objects (sets and types) and morphisms (operation between objects), with 2 basic operations (identity and composition) of morphisms, 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 paper, objects are data types and morphisms are functions

class *Category* *k* **where**

$id :: (a' k' a)$

$(\circ) :: (b' k' c) \rightarrow (a' k' b) \rightarrow (a' k' c)$

instance *Category* (\rightarrow) **where**

$id = \lambda a \rightarrow a$

$g \circ f = \lambda a \rightarrow g (f a)$

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 $F m :: F a \rightarrow F b \in \mathcal{V}$
- $F \text{ id } (\in \mathcal{U}) = \text{id } (\in \mathcal{V})$
- $F (f \circ g) = F f \circ F g$

Note

Given this papers 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)

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

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:

$$\begin{aligned} id &= \mathcal{D} (\lambda a \rightarrow (id \ a, id)) \\ \hat{\mathcal{D}} \ g \circ \hat{\mathcal{D}} \ f &= \mathcal{D} (\lambda a \rightarrow \mathbf{let} \ \{ (b, f') = \mathcal{D}^+ \ f \ a; (c, g') = \\ &\mathcal{D}^+ \ g \ b \} \ \mathbf{in} \ (c, g' \circ f')) \end{aligned}$$

The first equation shown above has a trivial solution.

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

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

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

Instance deduction

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

$$\begin{aligned}
 id &= \mathcal{D} (\lambda a \rightarrow (id \ a, id)) \\
 \hat{\mathcal{D}} \ g \circ \hat{\mathcal{D}} \ f &= \mathcal{D} (\lambda a \rightarrow \mathbf{let} \ \{(b, f') = \mathcal{D}^+ \ f \ a; (c, g') = \\
 &\mathcal{D}^+ \ g \ b\} \ \mathbf{in} \ (c, g' \circ f'))
 \end{aligned}$$

The first equation shown above has a trivial solution.

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

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

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

Instance deduction

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

$$\begin{aligned} id &= \mathcal{D} (\lambda a \rightarrow (id\ a, id)) \\ \hat{\mathcal{D}}\ g \circ \hat{\mathcal{D}}\ f &= \mathcal{D} (\lambda a \rightarrow \mathbf{let}\ \{(b, f') = \mathcal{D}^+ f\ a; (c, g') = \\ &\mathcal{D}^+ g\ b\} \mathbf{in}\ (c, g' \circ f')) \end{aligned}$$

The first equation shown above has a trivial solution.

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

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

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

Instance deduction

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

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

Categorical instance we've deduced

instance *Category* \mathcal{D} **where**

$$\text{id} = \text{linearD id}$$

$$\mathcal{D} \ g \circ \mathcal{D} \ f =$$

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

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

$$\text{id} \circ \hat{\mathcal{D}}$$

{ functor law for id (specification of $\hat{\mathcal{D}}$) }

$$= \hat{\mathcal{D}} \text{id} \circ \hat{\mathcal{D}} f$$

{ functor law for (\circ) }

$$= \hat{\mathcal{D}} (\text{id} \circ f)$$

{ categorical law }

$$= \hat{\mathcal{D}} f$$

Instance proof

(C.2) proof

$$\begin{aligned} & \hat{\mathcal{D}} h \circ (\hat{\mathcal{D}} g \circ \hat{\mathcal{D}} f) \\ & \{ 2x \text{ functor law for } (\circ) \} \\ & = \hat{\mathcal{D}} (h \circ (g \circ f)) \\ & \{ \text{categorical law} \} \\ & = \hat{\mathcal{D}} ((h \circ g) \circ f) \\ & \{ 2x \text{ functor law for } (\circ) \} \\ & = (\hat{\mathcal{D}} h \circ \hat{\mathcal{D}} g) \circ \hat{\mathcal{D}} f \end{aligned}$$

Note

This 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:

class *Category* $k \Rightarrow \text{Monoidal } k$ **where**

$(\times) :: (a \text{ ' } k \text{ ' } c) \rightarrow (b \text{ ' } k \text{ ' } d) \rightarrow ((a \times b) \text{ ' } k \text{ ' } (c \times d))$

instance *Monoidal* (\rightarrow) **where**

$f \times g = \lambda(a, b) \rightarrow (f \ a, g \ b)$

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:

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

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 it's definition and generalize the condition:

$$\mathcal{D} f \times \mathcal{D} g =$$

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

and this is enough for our new instance.

Instance deduction

From corollary 2.1 we can deduce that:

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

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 it's definition and generalize the condition:

$$\mathcal{D} f \times \mathcal{D} g =$$

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

and this is enough for our new instance.

Instance deduction

From corollary 2.1 we can deduce that:

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

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 it's definition and generalize the condition:

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

and this is enough for our new instance.

Instance deduction

Categorical instance we've deduced

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

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

Cartesian categories and functors

class *Monoidal* $k \Rightarrow \text{Cartesian } k$ **where**

$\text{exl} :: (a, b) \rightarrow k \rightarrow a$

$\text{exr} :: (a, b) \rightarrow k \rightarrow b$

$\text{dup} :: a \rightarrow k \rightarrow (a, a)$

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

$\text{exl} = \lambda(a, b) \rightarrow a$

$\text{exr} = \lambda(a, b) \rightarrow b$

$\text{dup} = \lambda a \rightarrow (a, a)$

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

- F is a monoidal functor
- $F \text{ exl} = \text{exl}$
- $F \text{ exp} = \text{exp}$
- $F \text{ dup} = \text{dup}$

Instance deduction

From corollary 3.1 and from exl , exr and dup being linear functions we can deduce that:

$$\mathcal{D}^+ exl = \lambda p \rightarrow (exl\ p, exl)$$

$$\mathcal{D}^+ exr = \lambda p \rightarrow (exr\ p, exr)$$

$$\mathcal{D}^+ dup = \lambda p \rightarrow (dup\ a, dup)$$

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 it's definition and remembering linearD's definition we can obtain:

$exl = \text{linearD } exl$

$exr = \text{linearD } exr$

$dup = \text{linearD } dup$

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 paper coproducts are categorical products, i.e., biproducts

Definition

```
class Category  $k \Rightarrow \text{Cocartesian } k$  where
  inl ::  $a \text{ ' } k \text{ ' } (a, b)$ 
  inr ::  $b \text{ ' } k \text{ ' } (a, b)$ 
  jam ::  $(a, a) \text{ ' } k \text{ ' } a$ 
```

Cocartesian functors

Cocartesian functor definition

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

- F is a functor
- $F \text{ inl} = \text{inl}$
- $F \text{ inr} = \text{inr}$
- $F \text{ jam} = \text{jam}$

Fork and Join

- $\Delta :: \textit{Cartesian } k \Rightarrow (a' \text{ k}' c) \rightarrow (a' \text{ k}' d) \rightarrow (a' \text{ k}' (c \times d))$
- $\nabla :: \textit{Cartesian } k \Rightarrow (c' \text{ k}' a) \rightarrow (d' \text{ k}' a) \rightarrow ((c \times d)' \text{ k}' a)$

Instance of \rightarrow^+

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

instance *Category* (\rightarrow^+) **where**

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

$\text{id} = \text{AddFun id}$

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

instance *Monoidal* (\rightarrow^+) **where**

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

instance *Cartesian* (\rightarrow^+) **where**

$\text{exl} = \text{AddFun exl}$

$\text{exr} = \text{AddFun exr}$

$\text{dup} = \text{AddFun dup}$

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

class *NumCat* *k a* **where**

negateC :: *a* ' *k* ' *a*

addC :: (*a* × *a*) ' *k* ' *a*

mulC :: (*a* × *a*) ' *k* ' *a*

...

instance *Num a* ⇒ *NumCat* (→) *a* **where**

negateC = *negate*

addC = *uncurry* (+)

mulC = *uncurry* (*)

...

$$\mathcal{D}(\text{negate } u) = \text{negate } (\mathcal{D} u)$$

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

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

- 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* ' *k* ' *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* ($\lambda(a, b) \rightarrow (a * b, \text{scale } b \nabla \text{scale } a)$)

instance *FloatingCat* *D* **where**

sinC = *D* ($\lambda a \rightarrow (\sin a, \text{scale } (\cos a))$)

cosC = *D* ($\lambda a \rightarrow (\cos a, \text{scale } (-\sin a))$)

expC = *D* ($\lambda a \rightarrow \text{let } e = \exp a \text{ in } (e, \text{scale } e)$)

...

Examples

$$\text{sqr} :: \text{Num } a \Rightarrow a \rightarrow a$$

$$\text{sqr } a = a * a$$

$$\text{magSqr} :: \text{Num } a \Rightarrow a \times a \rightarrow a$$

$$\text{magSqr } (a, b) = \text{sqr } a + \text{sqr } b$$

$$\text{cosSinProd} :: \text{Floating } a \Rightarrow a \times a \rightarrow a \times a$$

$$\text{cosSinProd } (x, y) = (\cos z, \sin z) \textbf{ where } z = x * y$$

With a compiler plugin we can obtain

$$\text{sqr} = \text{mulC} \circ (\text{id} \Delta \text{id})$$

$$\text{magSqr} = \text{addC} \circ (\text{mulC} \circ (\text{exl} \Delta \text{exl}) \Delta \text{mulC} \circ (\text{exr} \Delta \text{exr}))$$

$$\text{cosSinProd} = (\text{cosC} \Delta \text{sinC}) \circ \text{mulC}$$

Generalizing Automatic Differentiation

newtype $D_k a b = D (a \rightarrow b \times (a' k' b))$

linearD :: $(a \rightarrow b) \rightarrow (a' k' b) \rightarrow D_k a b$

linearD $f f' = D (\lambda a \rightarrow (f a, f'))$

instance *Category* $k \Rightarrow \text{Category } D_k$ **where**

type *Obj* $D_k = \text{Additive} \wedge \text{Obj } k \dots$

instance *Monoidal* $k \Rightarrow \text{Monoidal } D_k$ **where** ...

instance *Cartesian* $k \Rightarrow \text{Cartesian } D_k$ **where** ...

instance *Cocartesian* $k \Rightarrow \text{Cocartesian } D_k$ **where**

inl = *linearD inlF inl*

inr = *linearD inrF inr*

jam = *linearD jamF jam*

instance *Scalable* $k\ s \Rightarrow \text{NumCat } D_k\ s$ **where**
 negateC = *linearD negateC negateC*
 addC = *linearD addC addC*
 mulC = $D\ (\lambda(a, b) \rightarrow (a * b, \text{scale } b \nabla \text{scale } a))$

Matrices

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

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

Extracting a Data Representation

In machine learning, a Gradient-based optimization works by searching for local minima in the domain of a differentiable function $f :: a \rightarrow s$. 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 .

Extracting a Data Representation

In machine learning, a Gradient-based optimization works by searching for local minima in the domain of a differentiable function $f :: a \rightarrow s$. 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 .

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:

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

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:

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

A short introduction

- In chapter 4 we've derived an AD algorithm that was generalized in figure 6 of the document
- With fully right-associated compositions this algorithm becomes a forward-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?

A short introduction

- In chapter 4 we've derived an AD algorithm that was generalized in figure 6 of the document
- With fully right-associated compositions this algorithm becomes a forward-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?

A short introduction

- In chapter 4 we've derived an AD algorithm that was generalized in figure 6 of the document
- With fully right-associated compositions this algorithm becomes a forward-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?

A short introduction

- In chapter 4 we've derived an AD algorithm that was generalized in figure 6 of the document
- With fully right-associated compositions this algorithm becomes a forward-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

$f :: a' \rightarrow k' \rightarrow b \Rightarrow (\circ f) :: (b' \rightarrow k' \rightarrow r) \rightarrow (a' \rightarrow k' \rightarrow r)$ 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

newtype $\text{Cont}_r^k a b = \text{Cont} ((b \text{ ' k' } r) \rightarrow (a \text{ ' k' } r))$

Functor derived from type

$\text{cont} :: \text{Category } k \Rightarrow (a \text{ ' k' } b) \rightarrow \text{Cont}_r^k a b$
 $\text{cont } f = \text{Cont } (\circ f)$

Instance deduction

instance *Category* $k \Rightarrow \text{Category } \text{Cont}_r^k$ **where**
 $\text{id} = \text{Cont id}$
 $\text{Cont } g \circ \text{Cont } f = \text{Cont } (f \circ g)$

instance *Monoidal* $k \Rightarrow \text{Monoidal } \text{Cont}_r^k$ **where**
 $\text{Conf } f \times \text{Cont } g = \text{Cont } (\text{join} \circ (f \times g) \circ \text{unjoin})$

instance *Cartesian* $k \Rightarrow \text{Cartesian } \text{Cont}_r^k$ **where**
 $\text{exl} = \text{Cont } (\text{join} \circ \text{inl}); \text{exr} = \text{Cont } (\text{join} \circ \text{inr})$
 $\text{dup} = \text{Cont } (\text{jam} \circ \text{unjoin})$

instance *Cocartesian* $k \Rightarrow \text{Cocartesian } \text{Cont}_r^k$ **where**
 $\text{inl} = \text{Cont } (\text{exl} \circ \text{unjoin}); \text{inr} = \text{Cont } (\text{exr} \circ \text{unjoin})$
 $\text{jam} = \text{Cont } (\text{join} \circ \text{dup})$

instance *Scalable* $k \ a \Rightarrow \text{Scalable } \text{Cont}_r^k \ a$ **where**
 $\text{scale } s = \text{Cont } (\text{scale } s)$

A short introduction

Due to it's 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 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 instantiation

```
class HasDot (S) u where dot :: u → (u → s)
instance HasDot (IR) IR where dot = scale
instance (HasDot (S) a, HasDot (S) b)
  ⇒ HasDot (S) (a × b)
where dot (u, v) = dot u Δ dot v
```

Instance deduction

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

Type definition for duality

```
newtype Dual (K) a b = Dual (b ' K' 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

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

where

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

Instance deduction

instance *Category* $k \Rightarrow$ *Category* $Dual_k$ **where**
id = *Dual id*

Dual g \circ *Dual f* = *Dual (f* \circ *g)*

instance *Monoidal* $k \Rightarrow$ *Monoidal* $Dual_k$ **where**
Dual f \times *Dual g* = *Dual (f* \times *g)*

instance *Cartesian* $k \Rightarrow$ *Cartesian* $Dual_k$ **where**
exl = *Dual inl*; *exr* = *Dual inr*
dup = *Dual jam*

instance *Cocartesian* $k \Rightarrow$ *Cocartesian* $Dual_k$ **where**
inl = *Dual exl*; *inr* = *Dual exr*
jam = *Dual dup*

instance *Scalable* $k \Rightarrow$ *Scalable* $Dual_k$ **where**
scale s = *Dual (scale s)*

Final notes

- (∇) and (Δ) mutually dualize
 $(Dual\ f\ \nabla\ Dual\ g) = Dual\ (f\ \Delta\ g)$ and $Dual\ f\ \Delta\ Dual\ g = Dual\ (f\ \nabla\ g)$
- Using the definition from chapter 8 we can determine that the duality of a matrix corresponds to it's 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 apropiated for low dimention domains.

Type definition and functor from type

```
newtype  $Begin_r^k$   $a\ b = Begin\ ((r\ 'k'\ a) \rightarrow (r\ 'k'\ b))$   

 $begin :: Category\ k \Rightarrow (a\ 'k'\ b) \rightarrow Begin_r^k\ a\ b$   

 $begin\ f = Begin\ (f \circ)$ 
```

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 .

- Practical applications often involves 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 Category  $k \Rightarrow \text{Monoidall } k \ h$  where  
  crossI ::  $h \ (a' \ k' \ b) \rightarrow (h \ a' \ k' \ h \ b)$   
instance Zip  $h \Rightarrow \text{Monoidall } (\rightarrow) \ h$  where  
  crossI = zipWith id
```

```
class Monoidall k h  $\Rightarrow$  CartesianI k h where
```

```
  exl  :: h (h a ' k ' a)
```

```
  repl :: a ' k ' h a
```

```
class (Representable h, Zip h, Pointed h)  $\Rightarrow$ 
```

```
  CartesianI ( $\rightarrow$ ) h where
```

```
  exl = tabulate (flip index)
```

```
  repl = point
```

- The following is not the class the author was thinking

```
class Representable h where
```

```
  type Rep h :: *
```

```
  tabulate :: (Rep h  $\rightarrow$  a)  $\rightarrow$  h a
```

```
  index :: h a  $\rightarrow$  Rep h  $\rightarrow$  a
```

class *Monoidall* *k h* \Rightarrow *Cocartesian1* *k h* **where**

inl :: *h* (*a* ' *k* ' *h a*)

jaml :: *h a* ' *k* ' *a*

instance (*Monoidall* *k h*, *Zip h*) \Rightarrow *Monoidall* *D_k h* **where**

crossl *fs* = *D* ((*id* \times *crossl*) \circ *unzip* \circ *crossl* (*fmap unD fs*))

instance (*Cocartesian1* (\rightarrow) *h*, *Cartesian1* *k h*, *Zip h*) \Rightarrow

Cartesian1 *D_k h* **where**

exl = *linearD* *exl* *exl*

repll = *zipWith linearD repll repll*

instance (*Cocartesian1* *k h*, *Zip h*) \Rightarrow *Cocartesian1* *D_k h* **where**

inl = *zipWith linearD inlF inl*

jaml = *linearD* *sum jaml*

class *Monoidall* *k h* \Rightarrow *Cocartesian1* *k h* **where**

inl :: *h* (*a* ' *k* ' *h a*)

jaml :: *h a* ' *k* ' *a*

instance (*Monoidall* *k h*, *Zip h*) \Rightarrow *Monoidall* *D_k h* **where**

crossl *fs* = *D* ((*id* \times *crossl*) \circ *unzip* \circ *crossl* (*fmap unD fs*))

instance (*Cocartesian1* (\rightarrow) *h*, *Cartesian1* *k h*, *Zip h*) \Rightarrow

Cartesian1 *D_k h* **where**

exl = *zipWith linearD exl exl*

repll = *linearD repll repll*

instance (*Cocartesian1* *k h*, *Zip h*) \Rightarrow *Cocartesian1* *D_k h* **where**

inl = *zipWith linearD inlF inl*

jaml = *linearD sum jaml*

- Suggests that some of the work referred to does just a part of this paper.
- This paper was a continuation of the [Elliot 2017]
- Suggests that this implementation is simple, efficient, it can free memory dynamically (RAD) and is naturally parallel.
- Future work are detailed performance analysis; higher-order differentiation and automatic incrementation (continuing previous work [Elliot 2017])