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The simple essence of automatic differentiation

Conal Elliott

Target

January/June 2018

Conal Elliott January/June 2018 1 / 48

What's a derivative?

- Number
- Vector
- Covector
- Matrix
- Higher derivatives

Chain rule for each.

What's a derivative?

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

where

$$\lim_{\varepsilon \to 0} \frac{\|f(a+\varepsilon) - (fa + \mathcal{D} f a \varepsilon)\|}{\|\varepsilon\|} = 0$$

See Calculus on Manifolds by Michael Spivak.

Composition

Sequential:

$$(\circ) :: (b \to c) \to (a \to b) \to (a \to c)$$
$$(g \circ f) \ a = g \ (f \ a)$$

$$\mathcal{D}(g \circ f) a = \mathcal{D}g(f a) \circ \mathcal{D}f a$$
 -- "chain rule"

What's a derivative?

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where

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$$\mathcal{D}(g \circ f) \ a = \mathcal{D} \ g \ (f \ a) \circ \mathcal{D} \ f \ a$$
 -- "chain rule"

Parallel:

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

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

Compositionality

Chain rule:

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

To fix, combine regular result with derivative:

$$\hat{\mathcal{D}}$$
:: $(a \to b) \to (a \to (b \times (a \multimap b)))$
 $\hat{\mathcal{D}} f = f \land \mathcal{D} f$ -- specification

Often much work in common to f and $\mathcal{D} f$.

Linear functions

Linear functions are their own perfect linear approximations.

$$\mathcal{D}$$
 id $a = id$ \mathcal{D} fst $a = fst$ \mathcal{D} snd $a = snd$...

For linear functions f,

$$\hat{\mathcal{D}} f \ a = (f \ a, f)$$

Abstract algebra for functions

class
$$Category (\sim)$$
 where
 $id :: a \sim a$
 $(\circ) :: (b \sim c) \rightarrow (a \sim b) \rightarrow (a \sim c)$

class $Category (\sim) \Rightarrow Cartesian (\sim)$ where
 $exl :: (a \times b) \sim a$
 $exr :: (a \times b) \sim b$
 $(\triangle) :: (a \sim c) \rightarrow (a \sim d) \rightarrow (a \sim (c \times d))$

Plus laws and classes for arithmetic etc.

Linear functions

Linear functions are their own perfect linear approximations.

$$\mathcal{D} id \quad a = id$$
 $\mathcal{D} fst \quad a = fst$
 $\mathcal{D} snd \quad a = snd$
...

For linear functions f,

$$\hat{\mathcal{D}} f \ a = (f \ a, f)$$

Abstract algebra for functions

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 $(\triangle) :: (a \sim c) \rightarrow (a \sim d) \rightarrow (a \sim (c \times d))$

Plus laws and classes for arithmetic etc.

Automatic differentiation

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

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

$$\hat{\mathcal{D}} f = D (f \triangle \mathcal{D} f)$$
 -- not computable

Require $\hat{\mathcal{D}}$ to preserve Category and Cartesian structure:

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

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

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

$$\hat{\mathcal{D}} (f \triangle g) = \hat{\mathcal{D}} f \triangle \hat{\mathcal{D}} g$$

The game: solve these equations for the RHS operations.

Solution: simple automatic differentiation

```
newtype D a b = D (a \rightarrow b \times (a \multimap b))
linearD f = D (\lambda a \rightarrow (f a, a))
instance Category D where
   id = linearD id
   D g \circ D f = D (\lambda a \to \text{let } \{(b, f') = f \ a; (c, g') = g \ b\} \text{ in } (c, g' \circ f'))
instance Cartesian D where
   exl = linearD \ exl
   exr = linearD \ exr
   D \ f \triangle D \ g = D \ (\lambda a \to \text{let} \ \{(b, f') = f \ a; (c, g') = g \ a\} \ \text{in} \ ((b, c), f' \triangle g'))
instance NumCat D where
   negate = linearD negate
   add = linearD \ add
   mul = D (mul \triangle (\lambda(a,b) \rightarrow \lambda(da,db) \rightarrow b * da + a * db))
```

Automatic differentiation

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

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

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$$\hat{\mathcal{D}} (f \land g) = \hat{\mathcal{D}} f \land \hat{\mathcal{D}} g$$

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```

Running examples

```
sqr :: Num \ a \Rightarrow a \rightarrow a

sqr \ a = a * a

magSqr :: Num \ a \Rightarrow a \times a \rightarrow a

magSqr \ (a, b) = sqr \ a + sqr \ b

cosSinProd :: Floating \ a \Rightarrow a \times a \rightarrow a \times a

cosSinProd \ (x, y) = (cos \ z, sin \ z) where z = x * y
```

In categorical vocabulary:

$$sqr = mul \circ (id \triangle id)$$
 $magSqr = add \circ (mul \circ (exl \triangle exl) \triangle mul \circ (exr \triangle exr))$
 $cosSinProd = (cos \triangle sin) \circ mul$

Solution: simple automatic differentiation

```
newtype D a b = D (a \rightarrow b \times (a \multimap b))
linearD f = D (\lambda a \rightarrow (f a, a))
instance Category D where
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   mul = D (mul \triangle (\lambda(a,b) \rightarrow \lambda(da,db) \rightarrow b * da + a * db))
```

Running examples

$$sqr :: Num \ a \Rightarrow a \rightarrow a$$

 $sqr \ a = a * a$
 $magSqr :: Num \ a \Rightarrow a \times a \rightarrow a$
 $magSqr \ (a, b) = sqr \ a + sqr \ b$
 $cosSinProd :: Floating \ a \Rightarrow a \times a \rightarrow a \times a$
 $cosSinProd \ (x, y) = (cos \ z, sin \ z)$ where $z = x * y$

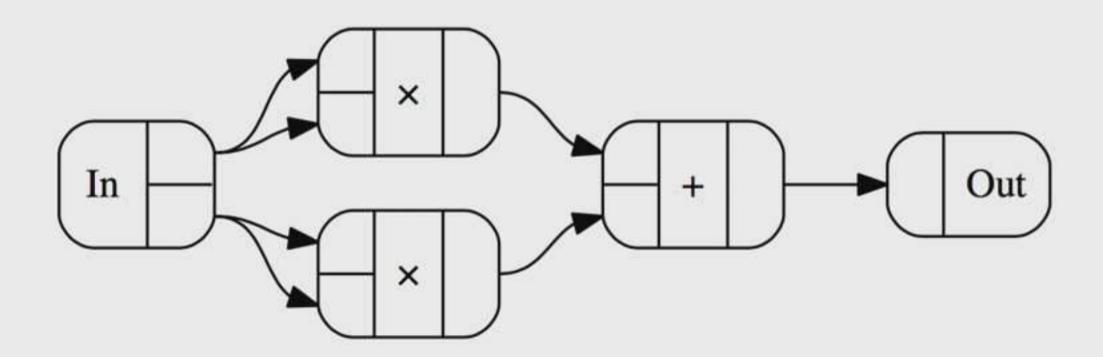
In categorical vocabulary:

$$sqr = mul \circ (id \triangle id)$$
 $magSqr = add \circ (mul \circ (exl \triangle exl) \triangle mul \circ (exr \triangle exr))$
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Visualizing computations

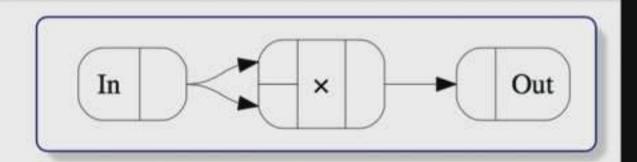
$$magSqr(a,b) = sqr(a + sqr(b))$$

$$magSqr = add \circ (mul \circ (exl \triangle exl) \triangle mul \circ (exr \triangle exr))$$



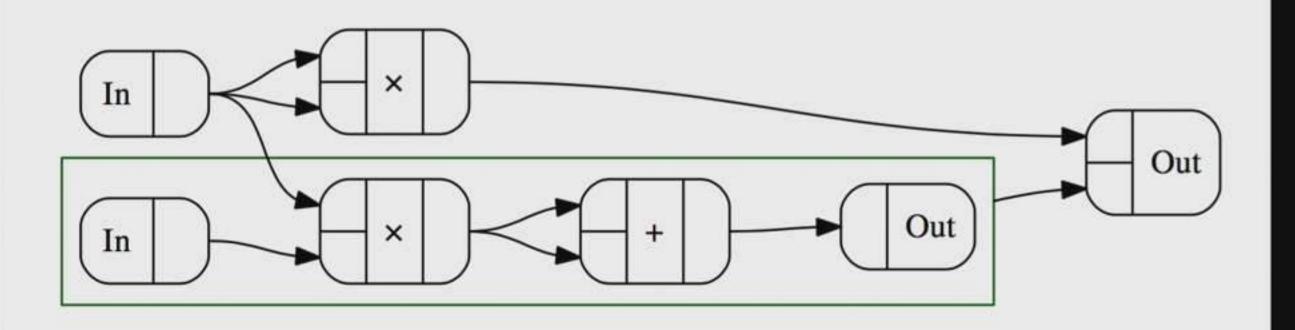
Auto-generated from Haskell code. See Compiling to categories.

AD example

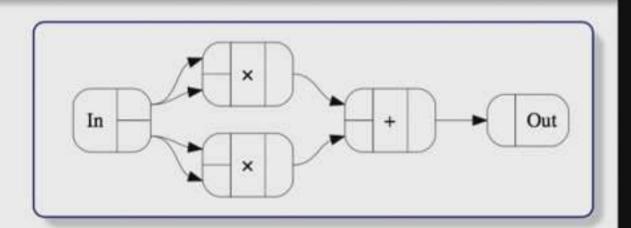


$$sqr \ a = a * a$$

$$sqr = mul \circ (id \land id)$$

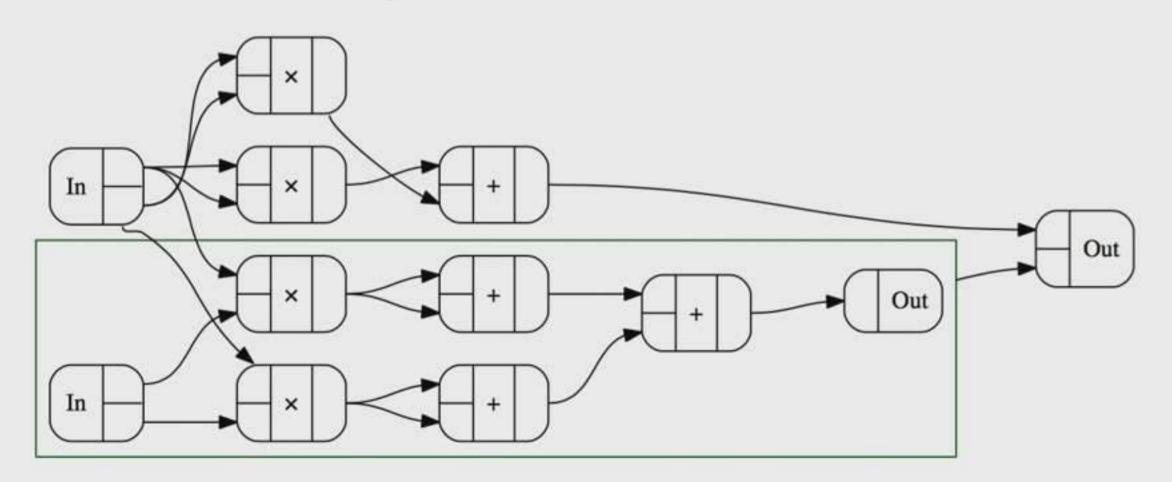


AD example

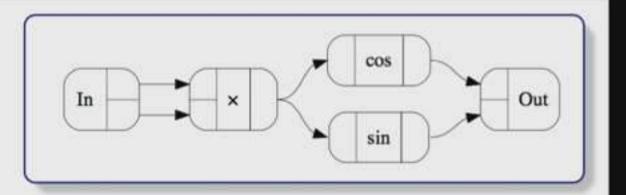


magSqr(a,b) = sqr(a + sqr(b))

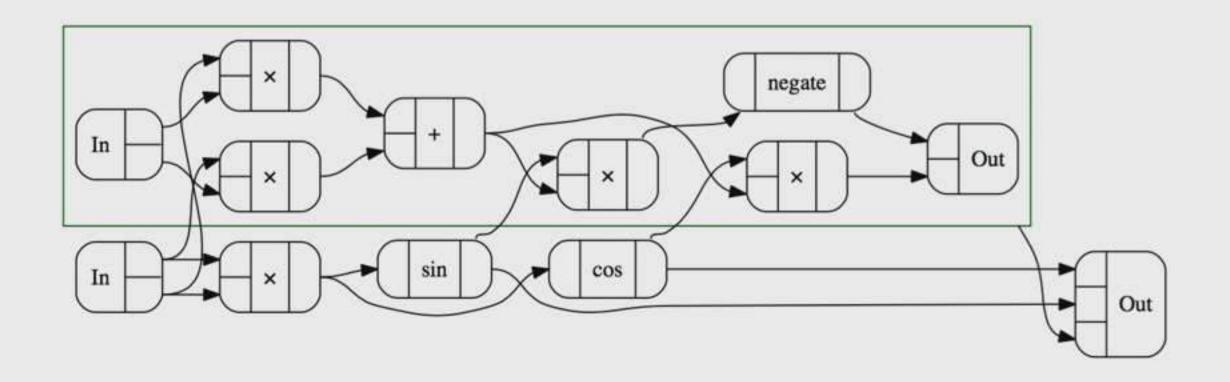
 $magSqr = add \circ (m\mu l \circ (exl \vartriangle exl) \vartriangle mul \circ (exr \vartriangle exr))$



AD example



 $cosSinProd\ (x,y) = (cos\ z, sin\ z)$ where z = x * y $cosSinProd = (cos \triangle sin) \circ mul$



Generalizing AD

```
newtype D a b = D (a \rightarrow b \times (a \multimap b))
linearD f = D (\lambda a \rightarrow (f a, f))
instance Category D where
   id = linearD id
   D g \circ D f = D (\lambda a \to \text{let } \{(b, f') = f \ a; (c, g') = g \ b\} \text{ in } (c, g' \circ f'))
instance Cartesian D where
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```

Each D operation just uses corresponding (\multimap) operation.

Generalize from $(-\circ)$ to other cartesian categories.

Generalized AD

```
newtype D_{(\sim)} a \ b = D \ (a \rightarrow b \times (a^* \sim b))
linearD f f' = D (\lambda a \rightarrow (f a, f'))
instance Category (\sim) \Rightarrow Category D_{(\sim)} where
   id = linearD id id
   D g \circ D f = D (\lambda a \to \text{let } \{(b, f') = f \ a; (c, g') = g \ b\} \text{ in } (c, g' \circ f'))
instance Cartesian (\sim) \Rightarrow Cartesian D_{(\sim)} where
   exl = linearD \ exl \ exl
   exr = linearD \ exr \ exr
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instance... \Rightarrow NumCat\ D where
   negate = linearD negate negate
   add = linearD \ add \ add
   mul = ??
```

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instance... \Rightarrow NumCat D where
   negate = linearD negate negate
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   mul = ??
```

Numeric operations

Specific to (linear) functions:

$$mul = D \ (mul \triangle (\lambda(a,b) \rightarrow \lambda(da,db) \rightarrow b * da + a * db))$$

Rephrase:

scale :: Multiplicative
$$a \Rightarrow a \rightarrow (a \multimap a)$$

scale $u = \lambda v \rightarrow u * v$
 $(\triangledown) :: (a \multimap c) \rightarrow (b \multimap c) \rightarrow ((a \times b) \multimap c)$
 $f \triangledown g = \lambda(a, b) \rightarrow f \ a + g \ b$

Now

$$mul = D \ (mul \triangle (\lambda(a, b) \rightarrow scale \ b \triangledown scale \ a))$$

Linear arrow vocabulary

```
class Category (\sim) where
   id :: a \sim a
   (\circ)::(b \leadsto c) \to (a \leadsto b) \to (a \leadsto c)
class Category (\sim) \Rightarrow Cartesian (\sim) where
   exl :: (a \times b) \sim a
   exr :: (a \times b) \rightsquigarrow b
   (\triangle) :: (a \leadsto c) \to (a \leadsto d) \to (a \leadsto (c \times d))
class Category(\sim) \Rightarrow Cocartesian(\sim) where
   inl :: a \leadsto (a \times b)
   inr::b \leadsto (a \times b)
   (\triangledown) :: (a \leadsto c) \to (b \leadsto c) \to ((a \times b) \leadsto c)
class ScalarCat (\sim) a where
   scale :: a \rightarrow (a \rightsquigarrow a)
```

Linear transformations as functions

```
newtype a \rightarrow^+ b = AddFun (a \rightarrow b)
instance Category (\rightarrow^+) where
   id = AddFun id
   (\circ) = inNew_2 (\circ)
instance Cartesian (\rightarrow^+) where
   exl = AddFun \ exl
   exr = AddFun \ exr
   (\triangle) = inNew_2(\triangle)
instance Cocartesian (\rightarrow^+) where
   inl = AddFun(0)
   inr = AddFun(0,)
   (\triangledown) = inNew_2 \ (\lambda f \ q \ (x,y) \rightarrow f \ x + q \ y)
instance Multiplicative s \Rightarrow ScalarCat (\rightarrow^+) s where
   scale \ s = AddFun \ (s *)
```

Extracting a data representation

- How to extract a matrix or gradient vector?
- Sample over a domain basis (rows of identity matrix).
- For *n*-dimensional *domain*,
 - Make n passes.
 - Each pass works on *n*-D sparse ("one-hot") input.
 - Very inefficient.
- For gradient-based optimization,
 - High-dimensional domain.
 - Very low-dimensional (1-D) codomain.

Generalized matrices

newtype
$$M_s$$
 a $b = L (V_s b (V_s a s))$

$$applyL :: M_s \ a \ b \rightarrow (a \rightarrow b)$$

Require applyL to preserve structure. Solve for methods.

Core vocabulary

Sufficient to build arbitrary "matrices":

Types guarantee rectangularity.

Efficiency of composition

- Arrow composition is associative.
- Some associations are more efficient than others, so
 - Associate optimally.
 - Equivalent to matrix chain multiplication $O(n \log n)$.
 - Choice determined by types, i.e., compile-time information.
- All-right: "forward mode AD" (FAD).
- All-left: "reverse mode AD" (RAD).
- RAD is much better for gradient-based optimization.

Left-associating composition (RAD)

- CPS-like category:
 - Represent $a \rightsquigarrow b$ by $(b \rightsquigarrow r) \rightarrow (a \rightsquigarrow r)$.
 - Meaning: $f \mapsto (\circ f)$.
 - Results in left-composition.
 - Initialize with $id :: r \leadsto r$.
 - Construct $h \circ \mathcal{D} f$ a directly, without $\mathcal{D} f$ a.

Continuation category

newtype
$$Cont_{(\sim)}^r$$
 a $b = Cont ((b \sim r) \rightarrow (a \sim r))$

$$cont :: Category (\sim) \Rightarrow (a \sim b) \rightarrow Cont_{(\sim)}^r a b$$

 $cont f = Cont (\circ f)$

Require *cont* to preserve structure. Solve for methods.

We'll use an isomorphism:

$$join$$
 :: $Cocartesian (\leadsto) \Rightarrow (c \leadsto a) \times (d \leadsto a) \rightarrow ((c \times d) \leadsto a)$
 $unjoin$:: $Cocartesian (\leadsto) \Rightarrow ((c \times d) \leadsto a) \rightarrow (c \leadsto a) \times (d \leadsto a)$
 $join (f,g) = f \triangledown g$
 $unjoin \ h = (h \circ inl, h \circ inr)$

Continuation category (solution)

```
instance Category (\sim) \Rightarrow Category\ Cont_{(\sim)}^r where
   id = Cont id
   Cont\ g\circ Cont\ f=Cont\ (f\circ g)
instance Cartesian (\sim) \Rightarrow Cartesian Cont_{(\sim)}^r where
   exl = Cont (join \circ inl)
   exr = Cont (join \circ inr)
   (\triangle) = inNew_2 \ (\lambda f \ g \rightarrow (f \lor g) \circ unjoin)
instance Cocartesian (\sim) \Rightarrow Cocartesian Cont_{(\sim)}^r where
   inl = Cont (exl \circ unjoin)
   inr = Cont (exr \circ unjoin)
   (\triangledown) = inNew_2 \ (\lambda f \ g \rightarrow join \circ (f \triangle g))
instance ScalarCat (\sim) a \Rightarrow ScalarCat Cont_{(\sim)}^r a where
   scale \ s = Cont \ (scale \ s)
```

Reverse-mode AD without tears

 $D_{Cont_{M_s}^r}$

Duality

- Vector space dual: $u \multimap s$, with u a vector space over s.
- If u has finite dimension, then $u \multimap s \cong u$.
- For $f :: u \multimap s$, f = dot v for some v :: u.
- Gradients are derivatives of functions with scalar codomain.
- Represent $a \multimap b$ by $(b \multimap s) \to (a \multimap s)$ by $b \to a$.
- *Ideal* for extracting gradient vector. Just apply to 1 (id).

Duality

newtype
$$Dual_{(\sim)}$$
 $a \ b = Dual \ (b \sim)$ $asDual :: Cont_{(\sim)}^s \ a \ b \rightarrow Dual_{(\sim)} \ a \ b$ $asDual \ (Cont \ f) = Dual \ (dot^{-1} \circ f \circ dot)$

where

$$dot :: u \to (u \multimap s)$$
$$dot^{-1} :: (u \multimap s) \to u$$

Require asDual to preserve structure. Solve for methods.

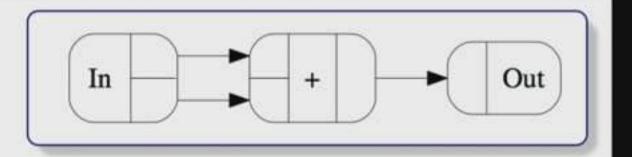
Duality (solution)

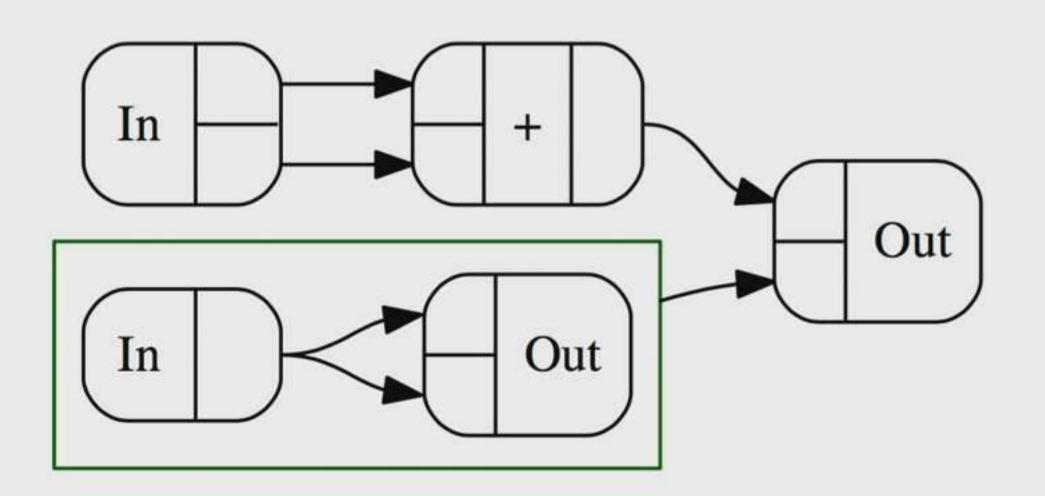
```
newtype Dual_{(\sim)} a \ b = Dual \ (b \sim a)
instance Category (\sim) \Rightarrow Category Dual_{(\sim)} where
   id = Dual id
   (\circ) = inNew_2 (flip (\circ))
instance Cocartesian (\sim) \Rightarrow Cartesian Dual_{(\sim)} where
   exl = Dual inl
   exr = Dual inr
   (\triangle) = inNew_2(\nabla)
instance Cartesian (\sim) \Rightarrow Cocartesian Dual_{(\sim)} where
   inl = Dual \ ext
   inr = Dual \ exr
   (\triangledown) = inNew_2 (\triangle)
instance ScalarCat (\sim) s \Rightarrow ScalarCat Dual_{(\sim)} s where
   scale \ s = Dual \ (scale \ s)
```

Backpropagation

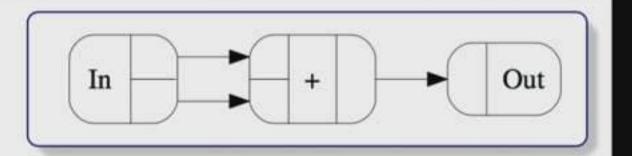
$$D_{Dual}$$

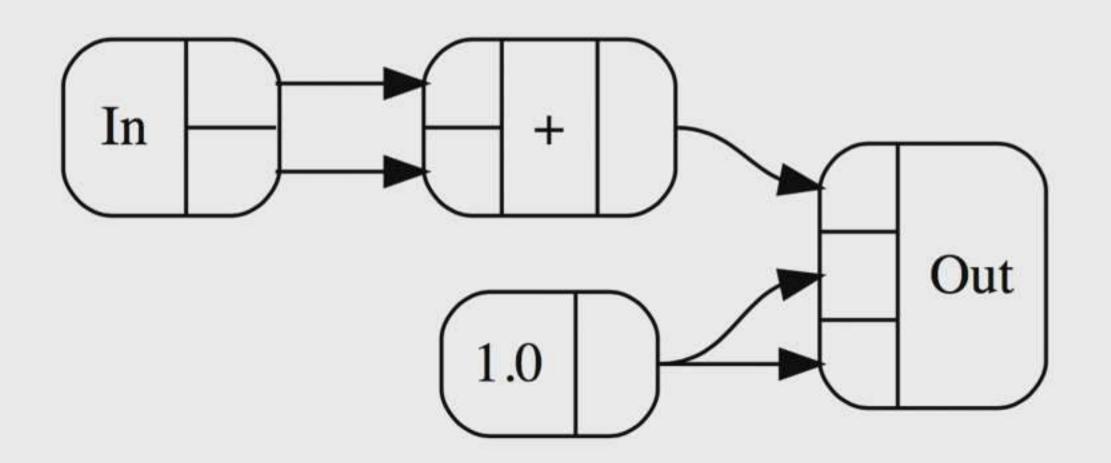
RAD example (dual function)





RAD example (dual vector)





Solution: simple automatic differentiation

```
newtype D a b = D (a \rightarrow b \times (a \multimap b))
linearD f = D (\lambda a \rightarrow (f a, a))
instance Category D where
   id = linearD id
   D g \circ D f = D (\lambda a \to \text{let } \{(b, f') = f \ a; (c, g') = g \ b\} \text{ in } (c, g' \circ f'))
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   negate = linearD negate
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   mul = D (mul \triangle (\lambda(a,b) \rightarrow \lambda(da,db) \rightarrow b * da + a * db))
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Generalizing AD

```
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linearD f = D (\lambda a \rightarrow (f a, f))
instance Category D where
   id = linearD id
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instance Cartesian D where
   exl = linearD \ exl
   exr = linearD \ exr
   D f \triangle D g = D (\lambda a \to \text{let } \{(b, f') = f \ a; (c, g') = g \ a\} \text{ in } ((b, c), f' \triangle g'))
```

Each D operation just uses corresponding (\multimap) operation.

Generalize from $(-\circ)$ to other cartesian categories.