Efficient automatic differentiation made easy via elementary category theory

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What is differentiation? (Fréchet)

On Banach spaces a and b,

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

$f\ a + \mathcal{D}\ f\ a\ \varepsilon$ approximates $f\ (a + \varepsilon)$ for small ε.

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

See *Calculus on Manifolds* by Michael Spivak.

What is *automatic* differentiation?

Differentiation of computable functions is not computable.

Instead, differentiate *recipes*: $[\![\bar{\mathcal{D}}\ p]\!] = \mathcal{D}\ [\![p]\!]$.

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Popular recipe forms: graphs, imperative programs, lambda calculus.

Differentiation composes messily in these forms,

but tidily in language of categories!

Composition

Sequential:

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

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

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Parallel:

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

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

Linear functions

Linear functions

Linear functions are their own derivatives everywhere.

$$
\begin{aligned}
\mathcal{D}\; \mathit{id}\;\; a &= \mathit{id} \\
\mathcal{D}\; \mathit{exl}\; a &= \mathit{exl} \\
\mathcal{D}\; \mathit{exr}\; a &= \mathit{exr} \\
&\ldots
\end{aligned}
$$

Compositionality

Chain rule:

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

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To fix, combine regular result with derivative:

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

so that $\mathcal{D}\ f = \mathit{exr} \circ \hat{\mathcal{D}}\ f$.

Abstract algebra for functions

$$
\begin{array}{l}
\mathbf{class}\ \mathit{Category}\ (\leadsto)\ \mathbf{where} \\
\quad \mathit{id}\ \ :: a \leadsto a \\
\quad (\circ) :: (b \leadsto c) \rightarrow (a \leadsto b) \rightarrow (a \leadsto c)
\end{array}
$$

$$
\begin{array}{l}
\mathbf{class}\ \mathit{Category}\ (\leadsto) \Rightarrow \mathit{Cartesian}\ (\leadsto)\ \mathbf{where} \\
\quad \mathit{exl}\ :: (a \times b) \leadsto a \\
\quad \mathit{exr} :: (a \times b) \leadsto b \\
\quad (\vartriangle)\ :: (a \leadsto c) \rightarrow (a \leadsto d) \rightarrow (a \leadsto (c \times d))
\end{array}
$$

Plus laws and classes for arithmetic etc.

Automatic differentiation (specification)

$$\textbf{newtype}\ D\ a\ b = D\ (a \to b \times (a \multimap b))$$

$$\hat{\mathcal{D}} :: (a \to b) \to D\ a\ b$$
$$\hat{\mathcal{D}}\ f = D\ (f \vartriangle \mathcal{D}\ f) \quad \text{-- not computable}$$

Automatic differentiation (specification)

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$$\hat{\mathcal{D}}\ f = D\ (f \vartriangle \mathcal{D}\ f) \quad \text{-- not computable}$$

Specification: $\hat{\mathcal{D}}$ is a cartesian functor, i.e.,

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

$$\hat{\mathcal{D}}\ exl = exl$$
$$\hat{\mathcal{D}}\ exr = exr$$
$$\hat{\mathcal{D}}\ (f \vartriangle g) = \hat{\mathcal{D}}\ f \vartriangle \hat{\mathcal{D}}\ g$$

The game: solve these equations for the RHS operations.

Automatic differentiation (solution)

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

$$\mathit{linearD}\ f = D\ (\lambda a \rightarrow (f\ a, f))$$

$\textbf{instance}\ \mathit{Category}\ D\ \textbf{where}$

$\quad \mathit{id} = \mathit{linearD}\ \mathit{id}$

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

$\textbf{instance}\ \mathit{Cartesian}\ D\ \textbf{where}$

$\quad \mathit{exl} = \mathit{linearD}\ \mathit{exl}$

$\quad \mathit{exr} = \mathit{linearD}\ \mathit{exr}$

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

$\textbf{instance}\ \mathit{NumCat}\ D\ \textbf{where}$

$\quad \mathit{negateC} = \mathit{linearD}\ \mathit{negateC}$

$\quad \mathit{addC} = \mathit{linearD}\ \mathit{addC}$

$\quad \mathit{mulC} = D\ (\mathit{mulC} \vartriangle (\lambda(a, b) \rightarrow \lambda(da, db) \rightarrow b * da + a * db))$

Generalizing AD

$$\textbf{newtype}\ D\ a\ b = D\ (a \to b \times (a \multimap b))$$

$$linearD\ f = D\ (\lambda a \to (f\ a, f))$$

$$\begin{array}{l}
\textbf{instance}\ Category\ D\ \textbf{where} \\
\quad id = linearD\ id \\
\quad D\ g \circ D\ f = D\ (\lambda a \to \textbf{let}\ \{(b, f') = f\ a; (c, g') = g\ b\}\ \textbf{in}\ (c, g' \circ f'))
\end{array}$$

$$\begin{array}{l}
\textbf{instance}\ Cartesian\ D\ \textbf{where} \\
\quad exl\ = linearD\ exl \\
\quad exr = linearD\ exr \\
\quad D\ f \vartriangle D\ g = D\ (\lambda a \to \textbf{let}\ \{(b, f') = f\ a; (c, g') = g\ a\}\ \textbf{in}\ ((b, c), f' \vartriangle g'))
\end{array}$$

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

Generalize from $(\multimap)$ to other cartesian categories.

Generalized AD

$$\textbf{newtype}\ D_{(\leadsto)}\ a\ b = D\ (a \to b \times (a \leadsto b))$$

$$\mathit{linearD}\ f\ f' = D\ (\lambda a \to (f\ a, f'))$$

$$\begin{array}{l}
\textbf{instance}\ \mathit{Category}\ (\leadsto) \Rightarrow \mathit{Category}\ D_{(\leadsto)}\ \textbf{where} \\
\quad \mathit{id} = \mathit{linearD}\ \mathit{id}\ \mathit{id} \\
\quad D\ g \circ D\ f = D\ (\lambda a \to \textbf{let}\ \{(b, f') = f\ a; (c, g') = g\ b\}\ \textbf{in}\ (c, g' \circ f'))
\end{array}$$

$$\begin{array}{l}
\textbf{instance}\ \mathit{Cartesian}\ (\leadsto) \Rightarrow \mathit{Cartesian}\ D_{(\leadsto)}\ \textbf{where} \\
\quad \mathit{exl}\ = \mathit{linearD}\ \mathit{exl}\ \mathit{exl} \\
\quad \mathit{exr} = \mathit{linearD}\ \mathit{exr}\ \mathit{exr} \\
\quad D\ f \vartriangle D\ g = D\ (\lambda a \to \textbf{let}\ \{(b, f') = f\ a; (c, g') = g\ a\}\ \textbf{in}\ ((b, c), f' \vartriangle g'))
\end{array}$$

$$\begin{array}{l}
\textbf{instance}\ \ldots \Rightarrow \mathit{NumCat}\ D\ \textbf{where} \\
\quad \mathit{negateC} = \mathit{linearD}\ \mathit{negateC}\ \mathit{negateC} \\
\quad \mathit{addC} = \mathit{linearD}\ \mathit{addC}\ \mathit{addC} \\
\quad \mathit{mulC} = ??
\end{array}$$

Numeric operations

Specific to (linear) *functions*:

$$mulC = D\ (mulC \vartriangle (\lambda(a, b) \rightarrow \lambda(da, db) \rightarrow b * da + a * db))$$

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Rephrase:

$$\begin{aligned}
&scale :: Multiplicative\ a \Rightarrow a \rightarrow (a \rightarrow a)\\
&scale\ u = \lambda v \rightarrow u * v
\end{aligned}$$

$$\begin{aligned}
&(\triangledown) :: Additive\ c \Rightarrow (a \rightarrow c) \rightarrow (b \rightarrow c) \rightarrow ((a \times b) \rightarrow c)\\
&(f \triangledown g)\ (a, b) = f\ a + g\ b
\end{aligned}$$

Now

$$mulC = D\ (mulC \vartriangle (\lambda(a, b) \rightarrow scale\ b \triangledown scale\ a))$$

New generalized vocabulary

$$
\begin{array}{l}
\textbf{class}\ \mathit{Category}\ (\leadsto) \Rightarrow \mathit{Cocartesian}_{\times}\ (\leadsto)\ \textbf{where} \\
\quad \mathit{inl}\ :: a \leadsto (a \times b) \\
\quad \mathit{inr} :: b \leadsto (a \times b) \\
\quad (\triangledown) :: (a \leadsto c) \rightarrow (b \leadsto c) \rightarrow ((a \times b) \leadsto c)
\end{array}
$$

$$
\begin{array}{l}
\textbf{class}\ \mathit{ScalarCat}\ (\leadsto)\ a\ \textbf{where} \\
\quad \mathit{scale} :: a \rightarrow (a \leadsto a)
\end{array}
$$

Differentiation:

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

The rest are linear.

Linear maps as functions

$$\textbf{newtype}\ a \multimap b = \mathit{LFun}\ (a \to b) \quad \text{-- } \mathit{linear}$$

$$\begin{array}{l}
\textbf{instance}\ \mathit{Category}\ (\multimap)\ \textbf{where} \\
\quad \mathit{id}\ \ = \mathit{LFun}\ \mathit{id} \\
\quad (\circ) = \mathit{inNew}_2\ (\circ)
\end{array}$$

$$\begin{array}{l}
\textbf{instance}\ \mathit{Cartesian}\ (\multimap)\ \textbf{where} \\
\quad \mathit{exl}\ \ = \mathit{LFun}\ \mathit{exl} \\
\quad \mathit{exr} = \mathit{LFun}\ \mathit{exr} \\
\quad (\vartriangle)\ = \mathit{inNew}_2\ (\vartriangle)
\end{array}$$

$$\begin{array}{l}
\textbf{instance}\ \mathit{Cocartesian}_{\times}\ (\multimap)\ \textbf{where} \\
\quad \mathit{inl}\ \ = \mathit{LFun}\ (\lambda a \to (a, 0)) \\
\quad \mathit{inr} = \mathit{LFun}\ (\lambda b \to (0, b)) \\
\quad (\triangledown) = \mathit{inNew}_2\ (\lambda f\ g\ (a, b) \to f\ a + g\ b)
\end{array}$$

$$\begin{array}{l}
\textbf{instance}\ \mathit{Multiplicative}\ s \Rightarrow \mathit{ScalarCat}\ (\multimap)\ s\ \textbf{where} \\
\quad \mathit{scale}\ s = \mathit{LFun}\ (s\ *)
\end{array}$$

Extracting a data representation

- Finally, extract a matrix or gradient vector.
- Very inefficient for gradient-based optimization!
- Alternatively, represent as "generalized matrices" ($M_s\ a\ b$).
  Then solve more homomorphisms.

Efficiency of composition

- 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.

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  - 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 $a \leadsto b$ by $(b \leadsto r) \to (a \leadsto r)$.
- Meaning: $f' \mapsto (\lambda h \to h \circ f')$.
- Construct $h \circ \mathcal{D}\ f\ a$ directly, without $\mathcal{D}\ f\ a$.

Old technique (Cayley 1854), vastly generalized by Yoneda.

Continuation category (specification)

$$\textbf{newtype}\ \mathit{ContC}\ ({\leadsto})\ r\ a\ b = \mathit{Cont}\ ((b \leadsto r) \rightarrow (a \leadsto r))$$

$$\begin{array}{l} \mathit{cont} :: \mathit{Category}\ ({\leadsto}) \Rightarrow (a \leadsto b) \rightarrow \mathit{ContC}\ ({\leadsto})\ r\ a\ b \\ \mathit{cont}\ f = \mathit{Cont}\ ({\circ}\, f) \end{array}$$

Specification: *cont* is a cartesian functor.

Continuation category (specification)

$$\mathbf{newtype}\ ContC\ (\leadsto)\ r\ a\ b = Cont\ ((b \leadsto r) \to (a \leadsto r))$$

$$\begin{aligned} &cont :: Category\ (\leadsto) \Rightarrow (a \leadsto b) \to ContC\ (\leadsto)\ r\ a\ b \\ &cont\ f = Cont\ (\circ\ f) \end{aligned}$$

Specification: *cont* is a cartesian functor.

We'll use an isomorphism:

$$\begin{aligned} &join\ \ \ \ :: Cocartesian\ (\leadsto) \Rightarrow (c \leadsto a) \times (d \leadsto a) \to ((c \times d) \leadsto a) \\ &unjoin :: Cocartesian\ (\leadsto) \Rightarrow ((c \times d) \leadsto a) \to (c \leadsto a) \times (d \leadsto a) \end{aligned}$$

$$\begin{aligned} &join\ (f, g) = f \triangledown g \\ &unjoin\ h\ \ \ = (h \circ inl, h \circ inr) \end{aligned}$$

Continuation category (solution)

$$
\begin{aligned}
&\textbf{instance } \mathit{Category}\ (\leadsto) \Rightarrow \mathit{Category}\ (\mathit{ContC}\ (\leadsto)\ r)\ \textbf{where}\\
&\quad \mathit{id} = \mathit{Cont}\ \mathit{id}\\
&\quad \mathit{Cont}\ g \circ \mathit{Cont}\ f = \mathit{Cont}\ (f \circ g)
\end{aligned}
$$

$$
\begin{aligned}
&\textbf{instance } \mathit{Cartesian}\ (\leadsto) \Rightarrow \mathit{Cartesian}\ (\mathit{ContC}\ (\leadsto)\ r)\ \textbf{where}\\
&\quad \mathit{exl}\ = \mathit{Cont}\ (\mathit{join} \circ \mathit{inl})\\
&\quad \mathit{exr} = \mathit{Cont}\ (\mathit{join} \circ \mathit{inr})\\
&\quad (\vartriangle) = \mathit{inNew}_2\ (\lambda f\ g \rightarrow (f \triangledown g) \circ \mathit{unjoin})
\end{aligned}
$$

$$
\begin{aligned}
&\textbf{instance } \mathit{Cocartesian}_{\times}\ (\leadsto) \Rightarrow \mathit{Cocartesian}_{\times}\ (\mathit{ContC}\ (\leadsto)\ r)\ \textbf{where}\\
&\quad \mathit{inl}\ = \mathit{Cont}\ (\mathit{exl} \circ \mathit{unjoin})\\
&\quad \mathit{inr} = \mathit{Cont}\ (\mathit{exr} \circ \mathit{unjoin})\\
&\quad (\triangledown) = \mathit{inNew}_2\ (\lambda f\ g \rightarrow \mathit{join} \circ (f \vartriangle g))
\end{aligned}
$$

$$
\begin{aligned}
&\textbf{instance } \mathit{ScalarCat}\ (\leadsto)\ a \Rightarrow \mathit{ScalarCat}\ (\mathit{ContC}\ (\leadsto)\ r)\ a\ \textbf{where}\\
&\quad \mathit{scale}\ s = \mathit{Cont}\ (\mathit{scale}\ s)
\end{aligned}
$$

Reverse-mode AD without tears

$$D_{ContC\ M_s\ r}$$

Duality

- Vector space dual: $u^* = u \multimap s$, with u a vector space over s.
- If u has finite dimension, then $u^* \cong u$.
- Represent $a \multimap b$ by $b^* \to a^*$ by $b \to a$.
- *Ideal* for extracting gradient vector. Just apply to 1 (id).

Duality (specification)

$$\textbf{newtype}\ Dual_{(\leadsto)}\ a\ b = Dual\ (b \leadsto a)$$

$$\begin{aligned} &asDual :: ContC\ (\leadsto)\ s\ a\ b \rightarrow Dual_{(\leadsto)}\ a\ b \\ &asDual\ (Cont\ f) = Dual\ (dot^{-1} \circ f \circ dot) \end{aligned}$$

where

$$\begin{aligned} dot &:: u \rightarrow (u \multimap s) \\ dot^{-1} &:: (u \multimap s) \rightarrow u \end{aligned}$$

Specification: *asDual* is a cartesian functor.

Duality (solution)

$$\mathbf{newtype}\ \mathit{Dual}_{(\leadsto)}\ a\ b = \mathit{Dual}\ (b \leadsto a)$$

$$\begin{aligned}
&\mathbf{instance}\ \mathit{Category}\ (\leadsto) \Rightarrow \mathit{Category}\ \mathit{Dual}_{(\leadsto)}\ \mathbf{where} \\
&\quad \mathit{id}\ \ = \mathit{Dual}\ \mathit{id} \\
&\quad (\circ) = \mathit{inNew}_2\ (\mathit{flip}\ (\circ))
\end{aligned}$$

$$\begin{aligned}
&\mathbf{instance}\ \mathit{Cocartesian}_{\times}\ (\leadsto) \Rightarrow \mathit{Cartesian}\ \mathit{Dual}_{(\leadsto)}\ \mathbf{where} \\
&\quad \mathit{exl}\ \ = \mathit{Dual}\ \mathit{inl} \\
&\quad \mathit{exr} = \mathit{Dual}\ \mathit{inr} \\
&\quad (\vartriangle)\ = \mathit{inNew}_2\ (\triangledown)
\end{aligned}$$

$$\begin{aligned}
&\mathbf{instance}\ \mathit{Cartesian}\ (\leadsto) \Rightarrow \mathit{Cocartesian}_{\times}\ \mathit{Dual}_{(\leadsto)}\ \mathbf{where} \\
&\quad \mathit{inl}\ \ = \mathit{Dual}\ \mathit{exl} \\
&\quad \mathit{inr} = \mathit{Dual}\ \mathit{exr} \\
&\quad (\triangledown)\ = \mathit{inNew}_2\ (\vartriangle)
\end{aligned}$$

$$\begin{aligned}
&\mathbf{instance}\ \mathit{ScalarCat}\ (\leadsto)\ s \Rightarrow \mathit{ScalarCat}\ \mathit{Dual}_{(\leadsto)}\ s\ \mathbf{where} \\
&\quad \mathit{scale}\ s = \mathit{Dual}\ (\mathit{scale}\ s)
\end{aligned}$$

Backpropagation

Backpropagation

$$D_{Dual_{\multimap}}$$

Conclusions

- Simple AD algorithm, specializing to forward, reverse, mixed.
- No graphs, tapes, tags, partial derivatives, or mutation.
- Parallel-friendly and possibly low memory use.
- Calculated from simple, regular algebra problems.
- Generalizes to derivative categories other than linear maps.
- Differentiate regular Haskell code (via plugin).
- ICFP 2018 paper: pictures, proofs, incremental computation.

Running examples

$$sqr :: Num\ a \Rightarrow a \to a$$
$$sqr\ a = a * a$$

$$magSqr :: Num\ a \Rightarrow a \times a \to a$$
$$magSqr\ (a, b) = sqr\ a + sqr\ b$$

$$cosSinProd :: Floating\ a \Rightarrow a \times a \to a \times a$$
$$cosSinProd\ (x, y) = (cos\ z, sin\ z)\ \mathbf{where}\ z = x * y$$

Running examples

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In categorical vocabulary:

$$sqr = mulC \circ (id \vartriangle id)$$

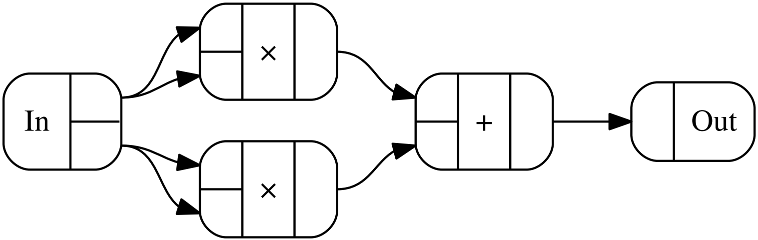
$$magSqr = addC \circ ((sqr \circ exl) \vartriangle (sqr \circ exr))$$

$$cosSinProd = (cosC \vartriangle sinC) \circ mulC$$

Visualizing computations

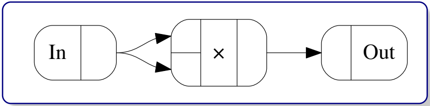
$$magSqr\ (a, b) = sqr\ a + sqr\ b$$

$$magSqr = addC \circ ((sqr \circ exl) \vartriangle (sqr \circ exr))$$



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

AD example



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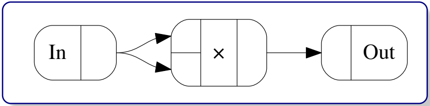

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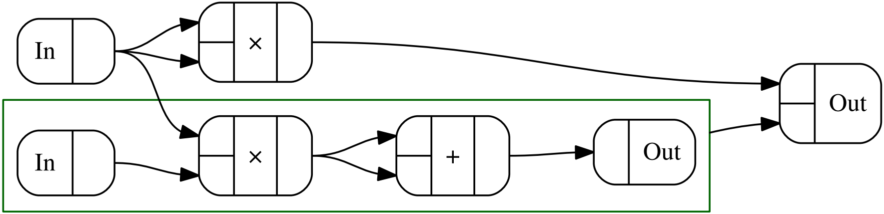
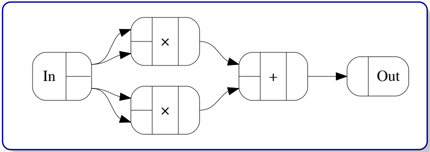


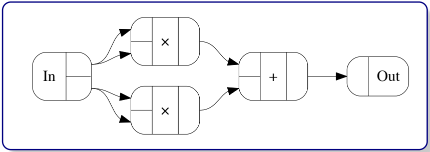
AD example



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

$$magSqr = addC \circ ((sqr \circ exl) \vartriangle (sqr \circ exr))$$

AD example



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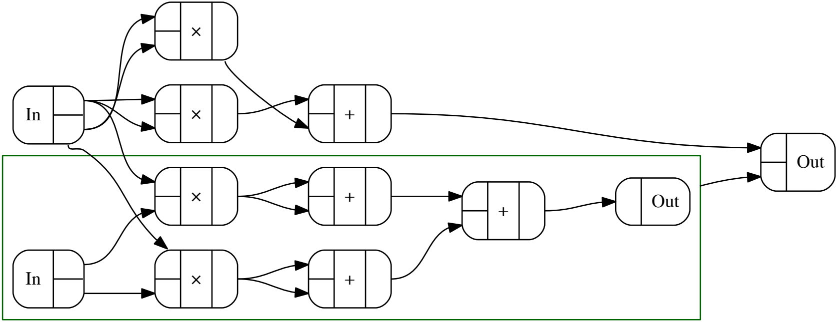

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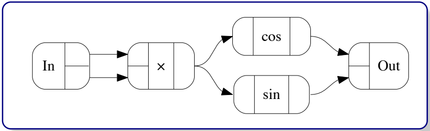

$$cosSinProd\ (x, y) = (cos\ z, sin\ z)\ \mathbf{where}\ z = x * y$$

$$cosSinProd = (cosC \vartriangle sinC) \circ mulC$$

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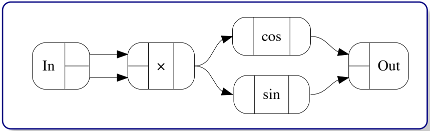

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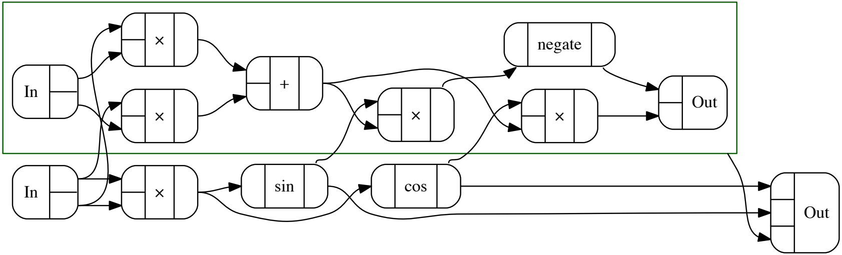
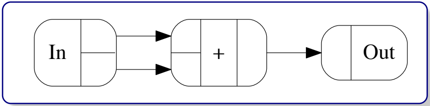
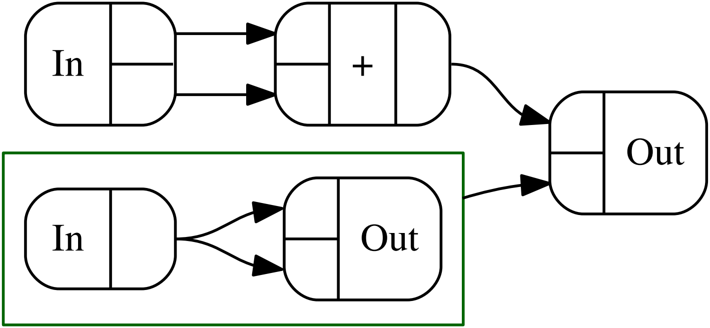
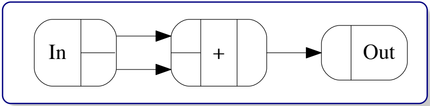


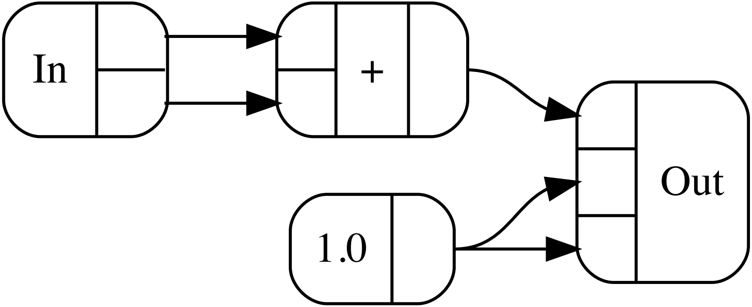
RAD example (dual function)





RAD example (dual vector)





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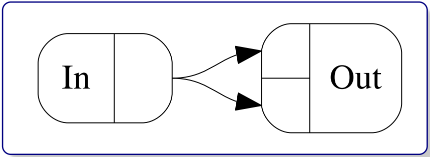
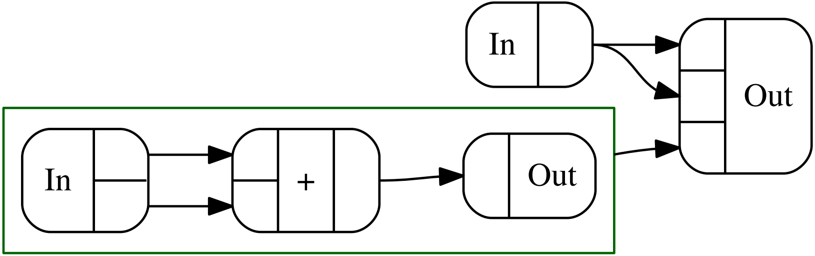
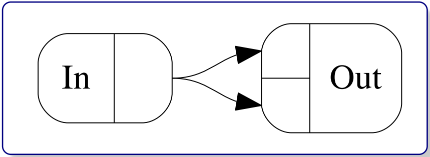
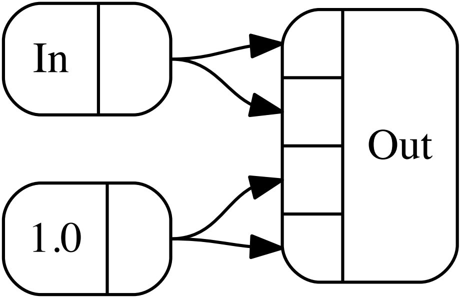




RAD example (vector)





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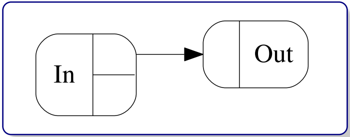

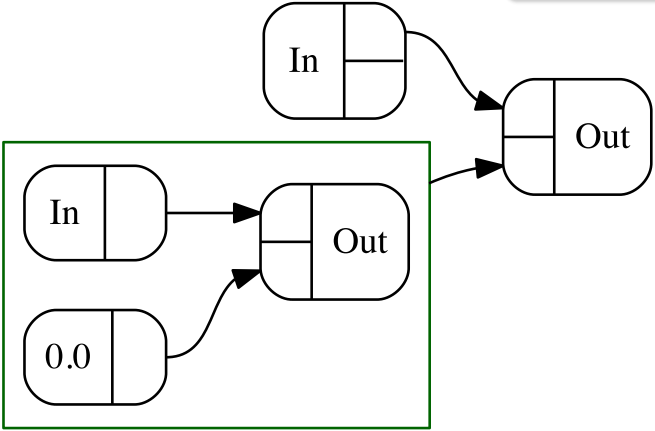

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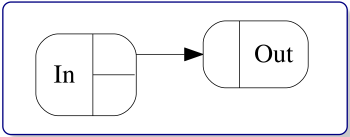

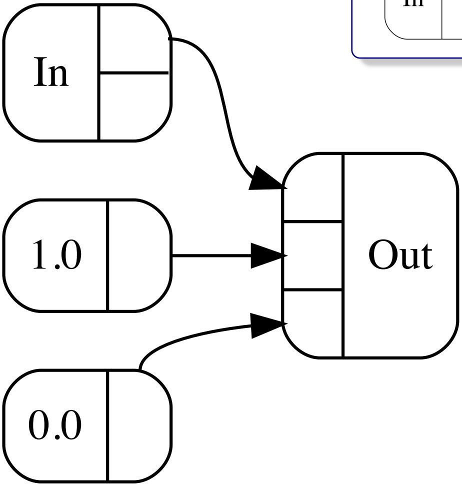

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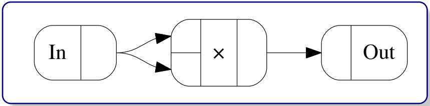

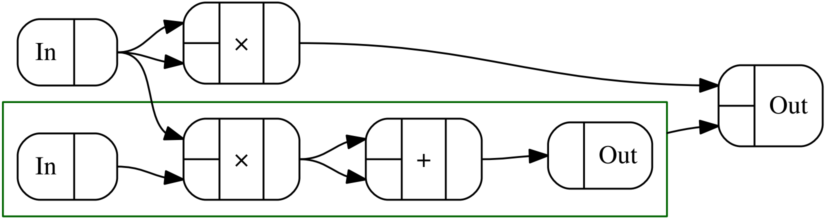

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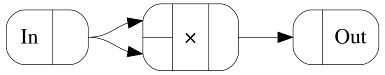

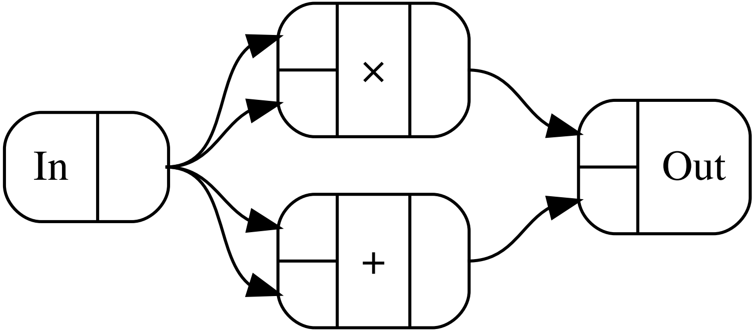

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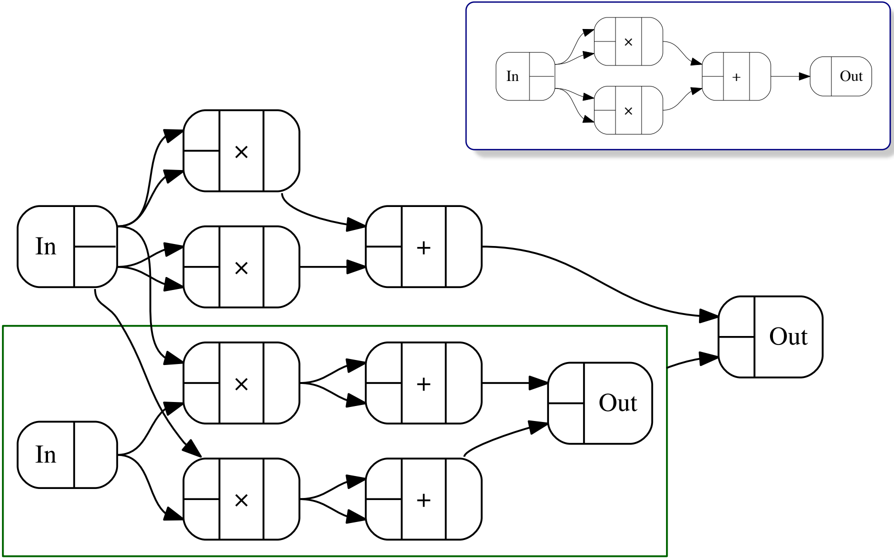

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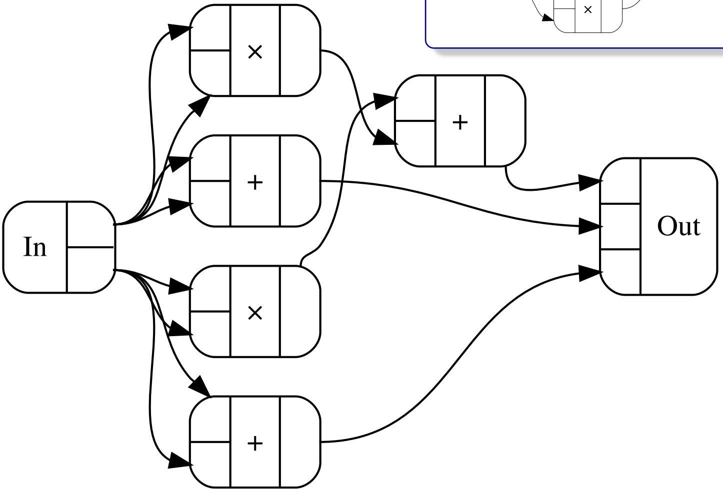

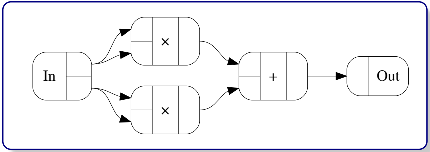

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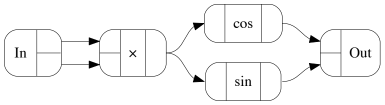
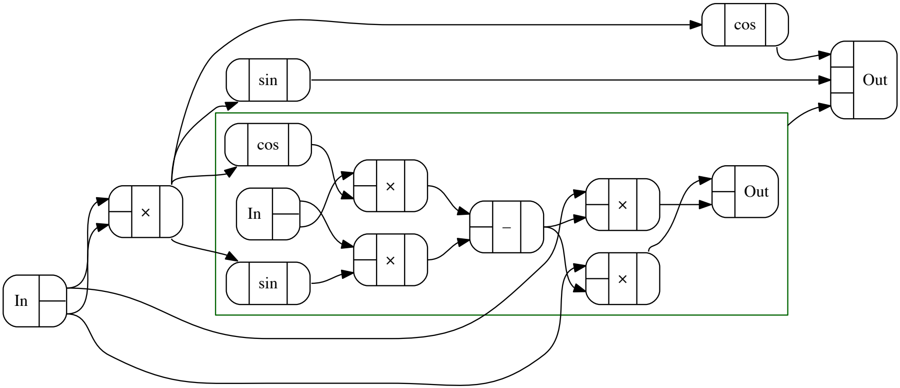
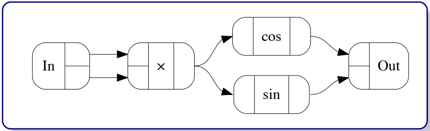
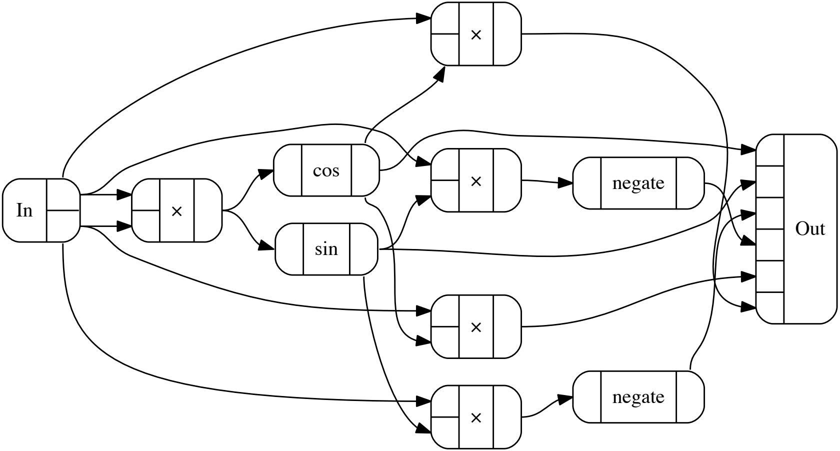




RAD example (matrix)





Reflections: recipe for success

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Key principles:

- Capture main concepts as first-class values.
- Focus on abstract notions, not specific representations.
- Calculate efficient implementation from simple specification.

Not previously applied to AD (afaik).

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Quandary: Most programming languages poor for function-like things.

Solution: *Compiling to categories*.

Symbolic vs automatic differentiation

Often described as opposing techniques:

- *Symbolic*:
  - Apply differentiation rules symbolically.
  - Can duplicate much work.
  - Needs algebraic manipulation.
- *Automatic*:
  - FAD: easy to implement but often inefficient.
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My view: *AD is SD done by a compiler.*

Compilers already work symbolically and preserve sharing.