Categories of Differentiable Polynomial Circuits for Machine Learning

Paul Wilson*, Fabio Zanasi

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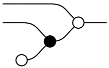
Motivation

- Narrow view: What's in the paper?
- Wide view: Why is what's in the paper in the paper?

This Paper: Narrow View

- A machine learning model class PolyCirc_S
- A graphical account of *reverse derivatives*
- A recipe to construct and extend *reverse derivative categories*
- An extension of PolyCirc to gain *functional completeness*



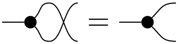
$$x_1 \;\; x_2 \mapsto x_1 \cdot (x_2 + 1)$$

Presentations by Generators and Equations

Generators (example):

Build terms with composition and tensor:

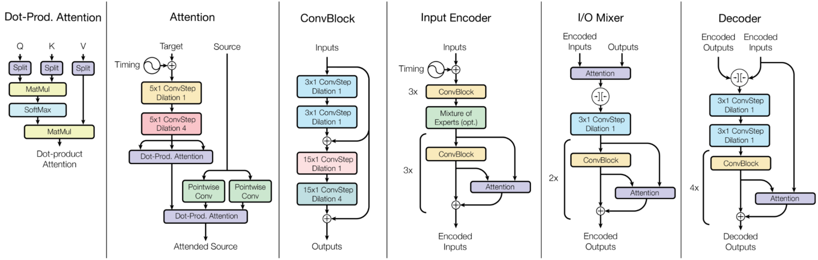
Equations (example):



This Paper: Wide View

Slogan: Machine Learning with String Diagrams

- ML papers often use diagrammatic exposition (below from [KGS+17])
- We want to make this completely formal
- Use string diagrams: gain access to lots of free theoretical tools!



Why is graphical structure important?

Morphisms of PolyCirc will represent machine learning models. We want to...

- ... *represent* terms easily on a computer [WZ21a]
- ... *manipulate* terms (rewriting/optimization) [BGK+20]
- ... *evaluate* and *compile* (to unusual targets!)
- ... *visualise* execution + model internals

Aside from this, we also have an immediate application in mind...

Application: Gradient based learning without $\mathbb{R}$ I

In 5 bullet points:

- Want to learn a function $f : \mathbb{R}^a \to \mathbb{R}^b$
- Define a model $m : \mathbb{R}^p \times \mathbb{R}^a \to \mathbb{R}^b$
- Learning: repeatedly nudge your parameters in the 'direction of best improvement'.
- Final result: parameters $\theta \in \mathbb{R}^p$
- ... giving a function $m(\theta, -) : \mathbb{R}^a \to \mathbb{R}^b$

This paper: what about for arbitrary semirings instead of $\mathbb{R}$?

Application: 'Gradient' Based Learning without $\mathbb{R}$ II

Problems with $\mathbb{R}$:

- We can't *really* represent values of $\mathbb{R}$ on a computer anyway
- Instead, we need to deal with *finite representations*
- Floating-point is relatively expensive: sometimes not available!

Another option:

- An extreme choice: use $\mathbb{Z}_2$ instead of $\mathbb{R}$ [WZ21b]
- 'Nudging an input' = flipping a bit
- We can express any function $\mathbb{B}^a \to \mathbb{B}^b$ in terms of polynomials over $\mathbb{Z}_2$ (functional completeness!)

What about other semirings S? That's where $\mathsf{PolyCirc}_S$ comes in

Summary

So we want categories which …

- … have RDC structure
- … are presented by generators and relations
- … represent a 'suitably expressive' class of models

So that we can …

- … do 'gradient' based learning
- … use computer representations to evaluate/compile them
- … define an appropriate model for a given problem

PolyCirc fits these criteria

Structure of this talk

- ~~Motivation~~
- Reverse Derivatives
- Polynomial Circuits
- Functional Completeness

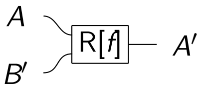
Presentation-Friendly Reverse Derivatives

- Original formulation
- What are reverse derivatives for?
- Alternative ‘presentation-friendly’ axioms
- ‘Extensibility theorem’

Reverse Derivative Categories (2019)
Robin Cockett, Geoffrey Cruttwell, Jonathan Gallagher, Jean-Simon Pacaud Lemay, Benjamin MacAdam, Gordon Plotkin, Dorette Pronk

Defines categories with a reverse derivative combinator:

$$\frac{A \xrightarrow{f} B}{A \times B' \xrightarrow[\mathrm{R}[f]]{} A'}$$



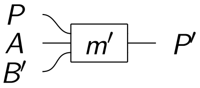
obeying some axioms **RD.1** - **RD.7**, along with some other ‘base’ structure.

Why do we need Reverse Derivatives?

Earlier we said...

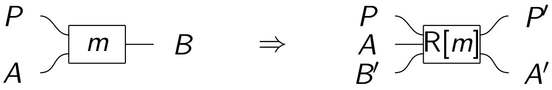
- Want to learn a map $f \colon A \to B$
- Define a model $m : P \times A \to B$
- Learning: repeatedly nudge your parameters in the 'direction of best improvement'.

We need something like this:



Reverse Derivatives

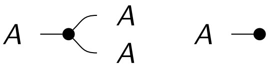
Taking the reverse derivative of our model gets us what we want:



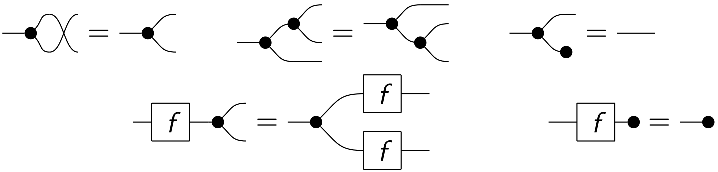
But RDCs have some required 'base' structure...

RDC Requirements I: Cartesian Structure

... means that each object A comes equipped with a *copy* and a *discard* map:



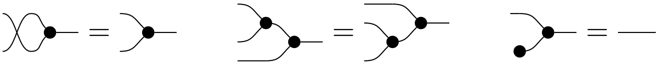
such that...



Cartesian Left Additive Structure I

A **Cartesian Left-Additive Category** ([CCG+19], [BCS09]) is a cartesian category in which each object A is equipped with a commutative monoid and zero map:

so that

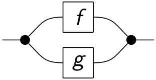


Cartesian Left Additive Structure II: Adding Morphisms

We used the ‘alternative’ definition of cartesian left-additive structure. The original has these axioms:

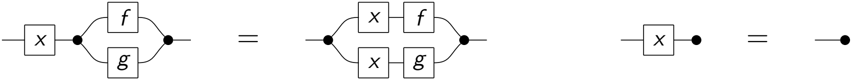
$$x \fatsemi (f + g) = (x \fatsemi f) + (x \fatsemi g) \qquad\qquad x \fatsemi 0 = 0$$

We can recover these by defining addition and zero:

$f + g :=$ 

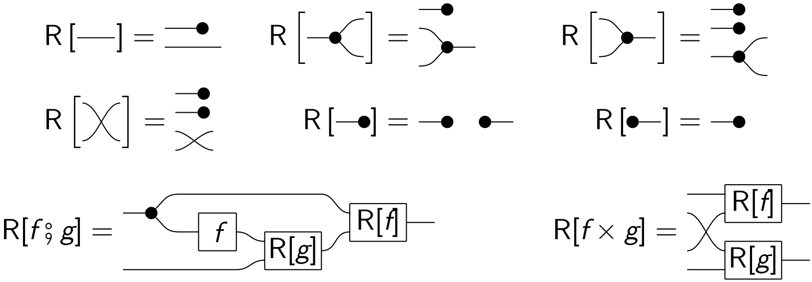
$0 :=$ 

Then the equations above can be written diagrammatically:



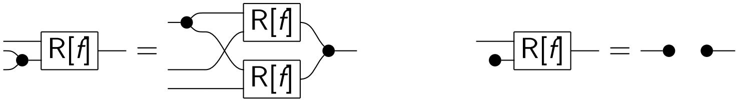
RDC Axioms I: Structural Axioms

[ARD.1] (Structural axioms, equivalent to RD.1, RD.3-5 in [CCG+19])



RDC Axioms II: Additivity of Change

[ARD.2] (Additivity of change, equivalent to RD.2 in [CCG+19])

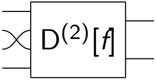


RDC Axioms III: Higher Derivatives

[ARD.3] (Linearity of change, equivalent to RD.6 in [CCG$^+$19])

$D_B[R[f]] =$ 

[ARD.4] (Symmetry of partials, equivalent to RD.7 in [CCG$^+$19])

$D^{(2)}[f] =$ 

Equivalence to Original Definition

- Original formulation had axioms **RD.1** - **RD.7**
- Our formulation has axioms **ARD.1** - **ARD.4**
- These are equivalent (Theorem 1)

Now let's use our formulation to show how to extend RDCs...

Extending RDC Presentations: A Theorem

How to extend an RDC $\mathscr{C}$ presented by generators Σ and equations E (Theorem 2):

- Add a new generator s and equations e.g. $l = r$
- Define $R[s]$
- Check R is well-defined $(\mathrm{R}[l] = \mathrm{R}[r])$
- Check R satisfies **ARD.2** - **ARD.4**

Formally:

Theorem

Let $\mathscr{C}$ be the cartesian left-additive category presented by generators (Obj, Σ) and equations E. If for each $s \in \Sigma$ there is some $\mathrm{R}[s]$ which is well-defined with respect to E, and which satisfies axioms ARD.1-4, then $\mathscr{C}$ is a reverse derivative category.

Summary

We've done this:

- Redefined the RDC axioms in a 'presentation friendly' way
- Showed how we can extend an RDC with new generators and equations

Now we can slowly build up PolyCirc from parts

Polynomial Circuits

- Definition
- Relationship to POLY_S
- Examples

Defining PolyCirc$_S$

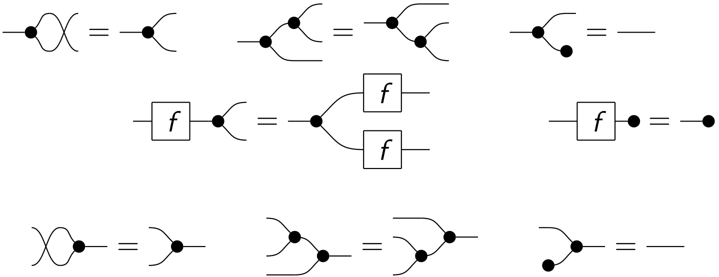
Piece-by-piece:

- Cartesian left-additive structure
- A multiplication operation
- Constants and equations

Cartesian Left Additive Structure

Generators:

Equations:

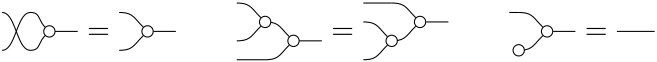


The reverse derivative is fixed by **ARD.1**

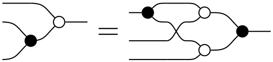
Cartesian Distributive Categories

Now add a multiplication  and 1 constant  to get a **Cartesian Distributive Category**:

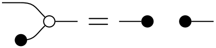
Satisfying cartesian left-additive and *multiplicativity* equations



and the *distributivity* and *annihilation* equations



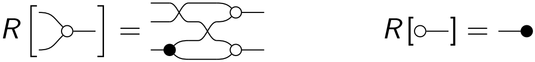
$$x_1 \cdot (x_2 + x_3) = x_1 \cdot x_2 + x_1 \cdot x_3$$



$$x_1 \cdot 0 = 0$$

Cartesian Distributive Categories II: Reverse Derivative

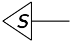
- Take an RDC
- Add the generators and equations of Cartesian Distributive categories
- Give it a reverse derivative:

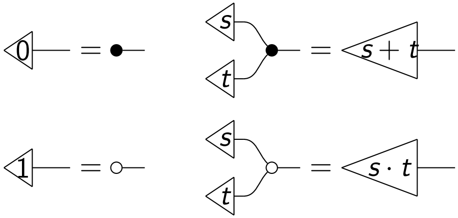


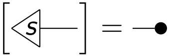
This is well-defined and satisfies ARD.1-4.

Polynomial Circuits

We define $\mathsf{PolyCirc}_S$ as the cartesian distributive category presented by:

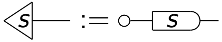
- one generating object 1 (so the objects are natural numbers)
- for each $s \in S$, a generating morphism  $: 0 \to 1$,
- the 'constant' equations (below)

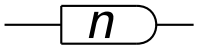


$\mathsf{PolyCirc}_S$ is an RDC with R  .

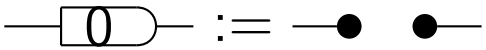
Polynomial Circuits Examples I: $\mathrm{PolyCirc}_{\mathbb{N}}$

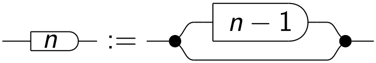
define each constant $s \in S$ as repeated addition:



where we define 

inductively as

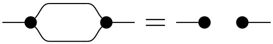




$\mathrm{PolyCirc}_{\mathbb{N}}$ is the free Cartesian Distributive Category on one generating object

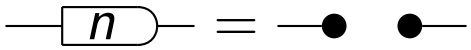
Polynomial Circuits Examples II: $\mathrm{PolyCirc}_{\mathbb{Z}_n}$

$\mathrm{PolyCirc}_{\mathbb{Z}_2}$ is the same, but we need one additional equation:



This says that $1 + 1 = 0$ (it's XOR)

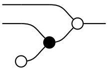
More generally for $\mathrm{PolyCirc}_{\mathbb{Z}_n}$:



$\mathrm{PolyCirc}_S$ and POLY_S

- Take a morphism $f : m \to n$ of $\mathrm{PolyCirc}_S$
- It's the same as an n-tuple of m-variable polynomials...
- i.e. an element of the free module over polynomial ring $S[x_1 \ldots x_m]^n$
- This makes $\mathrm{PolyCirc}_S \cong \mathrm{POLY}_S$ (POLY_S is from [CCG+19])

Recall our first example:



$$x_1 \;\; x_2 \mapsto x_1 \cdot x_2 + x_1$$

Except something is missing for functional completeness: we need to extend $\mathrm{PolyCirc}_S$ by adding a new operation (and we'll no longer have polynomials)

Functional Completeness

- Why do we want it?
- How do we define it?
- When do we have it?
- Extending $\mathsf{PolyCirc}_S$ to get it

Why do we want it?

- We want to use morphisms of PolyCirc_S as ML models
- Interpreting morphisms $m \to n$ gives us functions $S^m \to S^n$
- We would like to be able to express *any* function using our syntax
- If we can do this, we have functional completeness
- This is like a discrete analog of "Universal Approximator" theorems for NNs
- We will now be working only with **finite** semirings!

How do we define it?

More formally...

- We want to interpret morphisms $f : m \to n$ of $\mathrm{PolyCirc}_S$ as functions between sets.
- Define FinSet_S as the PROP whose morphisms are functions $S^m \to S^n$
- When any function in FinSet_S has a corresponding morphism $f \in \mathrm{PolyCirc}_S$, then $\mathrm{PolyCirc}_S$ is functionally complete.

Definition

We say a category $\mathscr{C}$ is **functionally complete** with respect to a finite set S when there a full identity-on-objects functor $\mathrm{F} : \mathscr{C} \to \mathrm{FinSet}_S$.

For some S, $\mathsf{PolyCirc}_S$ is *already* functionally complete

Example: $\mathsf{PolyCirc}_{\mathbb{Z}_2}$...

- Addition as XOR
- Multiplication as AND

...is functionally complete

... but not always!

Example: For $\mathbb{B}$ the boolean semiring with:

- Addition as OR
- Multiplication as AND

$\mathsf{PolyCirc}_{\mathbb{B}}$ is *not* functionally complete (you need a NOT gate!)

The missing piece

$$\text{compare}(x, y) = \begin{cases} 1 & \text{if } x = y \\ 0 & \text{otherwise} \end{cases}$$

Function Tables

The idea is that because S is finite, we can simply encode the function table of any function $f : S^m \to S$.

e.g., for $f(x_1, x_2) = x_1 \cdot (x_2 + 1)$ in $\mathbb{Z}_2$:

x_1	x_2	$f(x_1, x_2)$
0	0	0
0	1	0
1	0	1
1	1	0

How do we encode this?

Function Tables II

We can encode function tables using only constants, addition, and multiplication:

$$x \mapsto \sum_{s \in S^m} \text{compare}(s, x) \cdot f(s)$$

- f is 'syntactic' above- we only use it to build the expression
- compare is 1 only when $s = x$ (i.e. exactly once!)

Example: $S = \mathbb{Z}_3,\ m = 1,\ f(x) = x + 2$

$$\begin{aligned} x \mapsto \quad & \text{compare}(0, x) \cdot 2 \\ & + \text{compare}(1, x) \cdot 0 \\ & + \text{compare}(2, x) \cdot 1 \end{aligned}$$

Theorem

Let S be a finite commutative semiring. A category $\mathscr{C}$ is functionally complete with respect to S iff. there is a monoidal functor $\mathsf{F} : \mathscr{C} \to \mathsf{FinSet}_S$ in whose image are the following functions:

- $\langle\rangle \mapsto s$ *for each* $s \in S$ *(constants)*
- $\langle x, y \rangle \mapsto x + y$ *(addition)*
- $\langle x, y \rangle \mapsto x \cdot y$ *(multiplication)*
- compare

Example: $\text{PolyCirc}_{\mathbb{Z}_p}$

$\text{PolyCirc}_{\mathbb{Z}_p}$ is functionally complete for prime p. Fermat's Little Theorem says:

$$a^{p-1} \equiv 1 (\text{mod } p)$$

for $a > 0$. In other words, this is the 'nonzero indicator' function. We can construct the 'zero indicator' function like this:

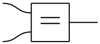
$$\delta(a) := (p-1) \cdot a^{p-1} + 1 = \begin{cases} 1 & \text{if } a = 0 \\ 0 & \text{otherwise} \end{cases}$$

Now we can construct compare (because S is finite):

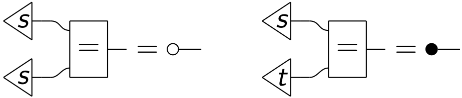
$$\text{compare}(x_1, x_2) = \sum_{s \in S} \delta(x_1 + s) \cdot \delta(x_2 + s)$$

$\mathsf{PolyCirc}_S^{=}$

To get functional completeness, we just add one more widget, which we will interpret as the compare function

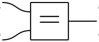


and equations



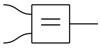
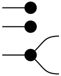
for $s, t \in S$ with $s \neq t$.

The Reverse Derivative of Comparison

To make $\mathrm{PolyCirc}_S^{=}$ an RDC, we need to define R[] in a way that:

- Is consistent with its equations
- Satisfies axioms **ARD.2** - **ARD.4**

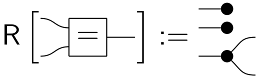
We choose this:

R [] := 

This satisfies the conditions, but is it reasonable?

The Straight-Through Estimator

- DNN architectures sometimes use functions with zero derivatives
- Example: ‘Thresholding’ function $\delta_{x \geq 0}$
- Instead of using the zero derivative, just ‘pass through’ the gradients to not lose information
- This is called the *straight through estimator*



Summary

- We defined PolyCirc in an 'extensible' way
- We showed how RDCs can be defined in a 'presentation friendly' way too
- We used our definition to extend PolyCirc with an additional operation (comparison)
- We ended up with a useful model class for machine learning

Thanks for listening!

Questions?

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