

# Categorical Foundations of Gradient-Based Learning

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**Abstract**—We propose a categorical foundation of gradient-based machine learning algorithms in terms of lenses, parametrised maps, and reverse derivative categories. This foundation provides a powerful explanatory and unifying framework: it encompasses a variety of gradient descent algorithms such as ADAM, AdaGrad, and Nesterov momentum, as well as a variety of loss functions such as MSE and Softmax cross-entropy, shedding new light on their similarities and differences. Our approach also generalises beyond neural networks (modelled in categories of smooth maps), accounting for other structures relevant to gradient-based learning such as boolean circuits. Finally, we also develop a novel implementation of gradient-based learning in Python, informed by the principles introduced by our framework.

## 1. Introduction

The last decade has witnessed a surge of interest in machine learning, fuelled by the numerous successes and applications that these methodologies have found in many fields of science and technology. However, we still lack a systematic understanding of *why* certain techniques are effective, why they are correct, and what their limits are. This is widely accepted through academia, industry, policy makers and funding agencies where there is general agreement on the need for a more rigorous approach to the foundations of machine learning [1].

Consider, for example, one of the most common machine learning scenarios: supervised learning with a neural network. This technique trains the model towards a certain task, as for instance the recognition of certain patterns in a data set. Now, as one may expect, there are several different ways of implementing the supervised learning process. Often, at the core there is a *gradient descent*-based algorithm, depending on a given *error function*, which updates in steps the *parameters* of the network. On the top of this, there may be variations and optimisation techniques, such as Adagrad [2], Momentum [3], and Adam [4].

This highlights several questions: can we distill the essential properties that make gradient descent adapted to supervised learning? Can we establish what properties the error function needs to satisfy? Can we develop a unifying picture of the various optimisation techniques, clarifying their limits, their similarities and their differences?

Moreover, it should be noted that supervised learning is not limited to neural networks. Not only there are several variations of this structure (such as recurrent neural networks [5], and Generative Adversarial Networks [6]), but for instance learning techniques are applicable to boolean circuits [7], in the context of binarisation (see e.g., [8]). This paper therefore seeks to answer the question: *what are the fundamental mathematical structures underpinning gradient-based learning?*

We formulate our answer in the language of *category theory*. There are numerous advantages to the categorical language. In particular, (i) it is general enough to cover set-theoretic, topological, metric, domain theoretic and other approaches; and (ii) it naturally enables *compositional reasoning* whereby complex systems can be built up from smaller, and hence easier to understand, components. Compositionality is a fundamental tenet of programming language semantics and, in the last few years, it has found application in the analysis of diverse kinds of computational models, across different fields— see e.g. [9], [10], [11], [12]. Nevertheless, we are careful to ensure that the structure of our model should be inherent to learning and not an artifact of the categorical nature of our model. This is shown by our proof-of-concept code, which uses the same structure to create a working non-trivial neural network model for the MNIST dataset, achieving accuracy on par with an equivalent model in Keras, a mainstream deep learning framework [13].

Our work develops a compositional foundation for gradient based learning, via the following main contributions:

- (I) We provide an abstract framework for gradient-based learning by abstractly treating the key components of gradients, back-propagation, and parameter update.
- (II) We cover a wide range of algorithms, illustrating their similarities and differences. This includes binary circuits whose inherently discrete nature might make one think gradient-based learning is not applicable.
- (III) As a concrete payoff of our approach, we develop a prototype implementation as explained above.

In order to develop (I), differentiation (specifically, the operation of the reverse derivative) is handled by working in the setting of Cartesian reverse differential categories (CRDCs) [14]. Second, parametrised functions are handled by a functorial construction **Para**, which turn a CRDC  $\mathcal{C}$  into one **Para**( $\mathcal{C}$ ) with parametrised arrows.

Third, back-propagation— that is, the backwards flow of information, allowing an algorithm to learn — is captured by the functorial construction  $\mathbf{Lens}(-)$ , which yields a category  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  of *lenses* [10], [15], [16], with parametrised arrows going both forward and backwards.

The composite  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  will define an abstract setting with enough structure to define and perform gradient-based learning. The learning operation itself will be a functor GL of type  $\mathbf{Para}(\mathcal{C}) \rightarrow \mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$ , which intuitively turns a parametrised function into one “with the ability to learn” through training. As with the underlying categories, we also describe GL itself in a modular way, relying on the three ingredients fundamental to gradient descent learning: the parametrised reverse derivative, the error map, and the update map. Each of these ingredients will be treated separately as a functor, whose composite yields GL. Moreover, we identify minimal requirements on  $\mathcal{C}$  allowing one to define the error and update map.

For (II), we show how our framework instantiates to Momentum [3], Nesterov Momentum [17], Adagrad [2], and Adam (Adaptive Moment Estimation) [4] learning on neural networks. Also, we handle gradient-based learning for boolean circuits by considering a different base category  $\mathcal{C}$ .

Finally, for point (III), we show how to implement our ideas in Python, and demonstrate a working convolutional neural network model for the MNIST image-classification problem. We also show that our model achieves comparable accuracy to an equivalent model implemented in Keras.

**Synopsis.** Section 2 develops the categorical structures necessary for our abstract description of gradient descent algorithms. Section 3 uses these structures to abstractly define the gradient descent algorithm. Section 4 illustrates such definition on our case studies. Section 5 briefly presents the implementation. Finally, in Sections 6 and 7, we discuss related and future work, including an extensive comparison with the closely related work of Fong, Spivak and Tuyéras [18].

## 2. Categorical components of gradient descent

In this section, we describe the three categorical components of our framework, each corresponding to an aspect of gradient-based learning. In Section 2.1 we review the **Para** construction which builds a category of parametrised maps from a monoidal category. In Section 2.2, we review Cartesian reverse differential categories, a setting for categories equipped with an abstract gradient operator. In Section 2.3, we review the **Lens** construction, which builds a category of “bidirectional” maps out of a Cartesian category. In Section 2.4, we give an explicit description of the combination of the **Para** and **Lens** constructions and how it can be viewed as a category of generalized “learners”.

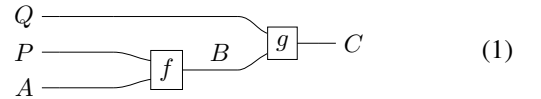
### 2.1. The Para construction

In supervised learning we are often interested in function approximation, i.e. approximating maps  $A \rightarrow B$ . But a

supervised learning algorithm will search only some pre-defined subset of the function space  $A \rightarrow B$ . This can be formalized by choosing a “parameter space”  $P$  and a map  $f' : P \rightarrow [A, B]$ . Given that the main objects of study in machine learning are Euclidean spaces (which are not Cartesian closed), we interpret the the aforementioned map under the tensor-hom adjunction. Namely, we study the map

$$f : P \otimes A \rightarrow B$$

meaning that for every  $p \in P$  we get a function  $f(p, -) : A \rightarrow B$ . This “perspective switching” matches what happens in practice where we often want to consider the map  $f : P \otimes A \rightarrow B$  to have the type  $A \rightarrow B$ . This is central to neural networks: a neural network of type  $\mathbb{R}^n \rightarrow \mathbb{R}^m$  is actually a smooth map of type  $\mathbb{R}^p \times \mathbb{R}^n \rightarrow \mathbb{R}^m$ , where  $\mathbb{R}^p$  is the set of possible weights of that neural network. Composition of two parameterized maps  $f : P \otimes A \rightarrow B$  and  $g : Q \otimes B \rightarrow C$  is done in the only way possible: by holding on to the loose threads of parameters  $P$  and  $Q$  and collecting them in a monoidal product. We will often write maps in this category as string diagrams [19] eg., the composite of  $(P, f)$  and  $(Q, g)$  can be written as



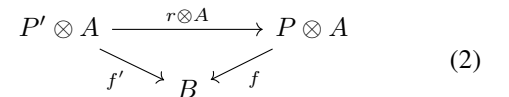
The **Para** construction allows this perspective shift for an arbitrary monoidal category, including categories which already have a potentially complex forward-backward information flow, such as lenses. The **Para** construction is rich in categorical structure. It can be looked at in a myriad of ways: as a bicategory, as a CoKleisli category of a graded comonad, as a 2-monad on  $\mathbf{SMC}_{Str}$ , and as a Grothendieck construction of a particular pseudofunctor. We will not delve into these details here, and instead just present the basic definition. For more details, see [20, Section 3.3.1], or [18] where **Para** was originally introduced in a specialized form.

**Definition 2.1.** Let  $\mathcal{C}$  be a symmetric monoidal category. Then we define  $\mathbf{Para}(\mathcal{C})$  as the bicategory with the following data:

- **Objects/0-cells.** An object is an object of  $\mathcal{C}$ ;
- **Morphisms/1-cells.** A map between  $A$  and  $B$  is a pair  $(P, f)$  where  $P$  is an object of  $\mathcal{C}$  and

$$P \otimes A \xrightarrow{f} B \quad \text{in } \mathcal{C}$$

- **2-cells.** A 2-cell from  $(P, f)$  to  $(P', f')$  is a morphism in  $r : P' \rightarrow P$  in  $\mathcal{C}$  such that the following diagram commutes in  $\mathcal{C}$ :



- **Identity 1-cell.** For an object  $A \in \mathbf{Para}(\mathcal{C})$  the pair  $(I, \lambda_A : I \otimes A \rightarrow A)$  is the identity 1-cell.
- **Horizontal composition of 1-cells.** As in (1).

Note the slightly counter-intuitive contravariance in the 2-cells which arises from the Grothendieck construction. This permits reindexing: given a morphism  $r : P' \rightarrow P$  in  $\mathcal{C}$  we can reparameterize a given  $P$ -parameterized morphism to a  $P'$ -parameterized morphism. We often work with strict monoidal categories whose objects are natural numbers and whose monoidal product is addition. In such settings,

**Corollary 2.2.** If  $\mathcal{C}$  is a strict symmetric monoidal category, then  $\mathbf{Para}(\mathcal{C})$  is a 2-category.

We have shown how  $\mathbf{Para}$  acts on some base category  $\mathcal{C}$ . However,  $\mathbf{Para}$  is also natural with respect to base change, i.e. given a functor  $F : \mathcal{C} \rightarrow \mathcal{D}$ , there is an induced functor  $\mathbf{Para}(F) : \mathbf{Para}(\mathcal{C}) \rightarrow \mathbf{Para}(\mathcal{D})$ :

**Proposition 2.3.** Let  $\mathcal{C}$  and  $\mathcal{D}$  be strict symmetric monoidal categories. Let  $F : \mathcal{C} \rightarrow \mathcal{D}$  be a lax symmetric monoidal functor. Then there is an induced 2-functor

$$\mathbf{Para}(F) : \mathbf{Para}(\mathcal{C}) \rightarrow \mathbf{Para}(\mathcal{D})$$

which agrees with  $F$  on objects.

This 2-functor is straightforward: for a 1-cell  $(P, f) : A \rightarrow B$ , it applies  $F$  to  $P$  and  $f$  and uses the (lax) comparison to get a map of the correct type.

Lastly, we mention that  $\mathbf{Para}(\mathcal{C})$  inherits the symmetric monoidal structure from  $\mathcal{C}$  and that the induced 2-functor  $\mathbf{Para}(F)$  respects that structure. This will allow us to compose learners not only in series, but also in parallel.

## 2.2. Cartesian reverse differential categories

Fundamental to all gradient-based learning is, of course, the gradient operation. In most cases this gradient operation is performed in the category of smooth maps between Euclidean spaces. However, recent work [7] has shown that gradient-based learning can also work well in other categories; for example, in a category of boolean circuits. Thus, to encompass these examples in a single framework, it is helpful to work in a category with an abstract gradient operation. Specifically, we will work in a Cartesian reverse differential category (first defined in [14]), a category in which every map has an associated reverse derivative. The reverse derivative is a generalization of the gradient operation: for example, in the category of smooth maps, the reverse derivative of a map of type  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  is essentially its derivative.

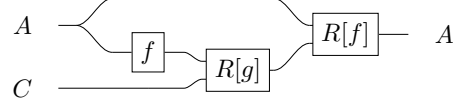
**Definition 2.4.**

- [14, Defn. 1] A **Cartesian left additive category** consists of a category  $\mathcal{C}$  with chosen finite products (including a terminal object), and an addition operation in each homset, satisfying various axioms.
- [14, Defn. 13] A **Cartesian reverse differential category** (CRDC) consists of a Cartesian left additive category  $\mathcal{C}$ , together with an operation which provides, for each map  $f : A \rightarrow B$  in  $\mathcal{C}$ , a map

$$R[f] : A \times B \rightarrow A$$

satisfying seven axioms (for full details, see the appendix).

For example, one of the key axioms is the reverse chain rule: for any maps  $f : A \rightarrow B, g : B \rightarrow C$ ,  $R[f;g]^1$  is equal to the map



Similarly, the other axioms capture additional important properties of the derivative (such as the linearity of the derivative in its vector variable, and the independence of order of partial differentiation). For another perspective on the CRDC axioms, see the comment after Proposition 2.12.

**Example 2.5.** The category **Smooth** has as objects natural numbers and maps  $n \rightarrow m$  are  $m$ -tuples of smooth maps  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ . **Smooth** is Cartesian with product given by addition. **Smooth** is a Cartesian reverse differential category: given a smooth map  $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ .

$$R[f] : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n$$

sends a pair  $(x, v)$  to  $J[f]^T(x) \cdot v$ : the transpose of the Jacobian of  $f$  at  $x$  in the direction  $v$ .

For example, if  $f : \mathbb{R}^2 \rightarrow \mathbb{R}^3$  is defined as

$$f(x_1, x_2) := (x_1^3 + 2x_1x_2, x_2, \sin(x_1)),$$

then  $R[f] : \mathbb{R}^2 \times \mathbb{R}^3 \rightarrow \mathbb{R}^2$  is given by

$$(x, v) \mapsto \begin{bmatrix} 3x_1 + 2x_2 & 0 & \cos(x_1) \\ 2x_1 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$

Using the reverse derivative (as opposed to the forward derivative) is well-known to be much more computationally efficient for functions  $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$  when  $m \ll n$  (for example, see [21]), as is the case in most supervised learning situations (where often  $m = 1$ ).

**Example 2.6.** Another RDC is the PROP  $\mathbf{POLY}_{\mathbb{Z}_2}$  [14, Example 14], whose morphisms  $f : A \rightarrow B$  are  $B$ -tuples of polynomials  $\mathbb{Z}_2[x_1 \dots x_A]$ . When presented by generators and relations these morphisms can be viewed as a syntax for boolean circuits, with learners for such circuits described in [7].

## 2.3. Lenses

The final piece of abstract categorical machinery we will need is the construction of the category of lenses. In machine learning, it is fundamental that information flows both forwards and backwards. One determines what one's model outputs on a given input (forward information flow), and then, using how this information compares to the

1. In this paper we write  $f;g$  for the composite of  $f$  followed by  $g$ .

correct output, modifies the model appropriately (backward information flow). The category of lenses is the ideal setting to capture this type of structure, as it is a category consisting of maps with both a “forward” and a “backward” part.

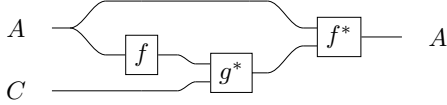
There are a number of variants of the categories of lenses (including generalizations to structures such as optics [22]); here we work with the particular version which is most appropriate for use with reverse derivative categories.

**Definition 2.7.** Let  $\mathcal{C}$  be a Cartesian category. Define  $\mathbf{Lens}(\mathcal{C})$  to be the category with:

- Objects are those of  $\mathcal{C}^2$
- A map from  $A$  to  $B$  is a pair of maps  $(f, f^*)$  with  $f : A \rightarrow B$  and  $f^* : A \times B \rightarrow A$ . From the discussion above, the map  $f$  can be thought of as the “forward” part of the map and  $f^*$  the “backward” part of the map. However, following standard terminology, we will refer to  $f$  as the get part of the map and  $f^*$  as the put part of the map.
- The identity from  $A$  to  $A$  is the pair  $(1_A, \pi_1)$ .
- The composite of  $(f, f^*) : A \rightarrow B$  and  $(g, g^*) : B \rightarrow C$  is given by  $f; g : A \rightarrow C$ , together with

$$A \times C \xrightarrow{\langle \pi_0, \pi_0; f, \pi_1 \rangle} A \times B \times C \xrightarrow{1 \times g^*} A \times B \xrightarrow{f^*} A$$

which we render as the string diagram



As we shall see, many important components of gradient descent algorithms can be interpreted as lenses, and this perspective is crucial to our setup. One key example is the reverse derivative of a map:

**Example 2.8.** If  $f : A \rightarrow B$  is a map in a CRDC  $\mathcal{C}$ , then the pair  $(f, R[f])$  is a map in  $\mathbf{Lens}(\mathcal{C})$ .

In fact, comparing the reverse chain rule (see the discussion after Definition 2.4) to the rule of composition in  $\mathbf{Lens}(\mathcal{C})$  (given above) one immediately sees that the reverse chain rule is precisely expressing the functoriality of the map  $f \mapsto (f, R[f])$ . Later on, we shall see how loss functions and optimization algorithms can also be interpreted as lenses (see Sections 3.3 and 3.4, respectively).

The pair  $(f, R[f])$  lands in the subcategory of *linear* lenses:

**Definition 2.9.**

- If  $\mathcal{C}$  is a Cartesian left-additive category, define  $\mathbf{Lens}_A(\mathcal{C})$  to be the subcategory of  $\mathbf{Lens}(\mathcal{C})$  which consists of maps whose put part  $f^* : A \times B \rightarrow A$  is additive in its second argument.

2. While in this paper we denote objects of  $\mathbf{Lens}(\mathcal{C})$  as objects of  $\mathcal{C}$ , it can be helpful to think of them as pairs of objects  $(A, A)$ . The first  $A$  is the “input” used by both get and put maps, while the second  $A$  is the “output” produced by the put. This can be useful for understanding the graphical language of lenses, but also for generalizations where the pair contains different objects, or has one of the objects depend on the other.

- If  $\mathcal{C}$  is a CRDC, define  $\mathbf{Lens}_L(\mathcal{C})$  to be the subcategory of  $\mathbf{Lens}_A(\mathcal{C})$  consisting of maps whose put part  $f^* : A \times B \rightarrow A$  is linear in its second argument (for details of additive and linear maps, see the appendix).

As we shall see in Definition 3.6, to be able to describe “update” data in an axiomatic way, we need to be able to talk about lenses which are invertible in a particular variable, and for this need our categories of lenses to be at least weak Cartesian. (Recall that a category is said to be **weak Cartesian** if it satisfies the existence, but not necessarily uniqueness, requirements of finite products.) However, for an arbitrary Cartesian  $\mathcal{C}$ ,  $\mathbf{Lens}(\mathcal{C})$  is not (weak) Cartesian. Given that the forward get maps are those of the base category  $\mathcal{C}$ , Cartesian structure of the objects and forward maps will have to be that of  $\mathcal{C}$ . The problem is the put maps: given lenses

$$f = (f, f^*) : A \rightarrow B \text{ and } g = (g, g^*) : A \rightarrow C,$$

we need a lens  $\langle f, g \rangle : A \rightarrow B \times C$ . We have

$$f^* : A \times B \rightarrow A \text{ and } g^* : A \times C \rightarrow A$$

but we need  $\langle f, g \rangle^* : A \times B \times C \rightarrow A$ , and in general there is no way to use both  $f^*$  and  $g^*$  to define such a map.

However, if  $\mathcal{C}$  is Cartesian *left-additive* (as is the case when  $\mathcal{C}$  is a CRDC) then there is a natural choice for such a map:

$$\langle \pi_0, \pi_1 \rangle; f^* + \langle \pi_0, \pi_2 \rangle; g^*.$$

And there is a natural choice of projections using the zero maps: define a lens  $p_0 : A \times B \rightarrow A$  with get map the ordinary projection  $\pi_0$  and put map

$$\langle \pi_2, 0 \rangle : A \times B \times A \rightarrow A \times B.$$

and similarly define  $p_1 : A \times B \rightarrow B$  with get map  $\pi_1$  and with put map

$$\langle 0, \pi_2 \rangle : A \times A \times B \rightarrow A \times B$$

It is easily checked that these choices of pairing and projections make the necessary diagrams commute. In general, however, these pairings will not be unique. Thus, we have

**Proposition 2.10.** If  $\mathcal{C}$  is Cartesian left-additive, then  $\mathbf{Lens}(\mathcal{C})$  is weak Cartesian.

However, the situation improves if we restrict to the subcategories  $\mathbf{Lens}_A(\mathcal{C})$  and  $\mathbf{Lens}_L(\mathcal{C})$ . In these cases, the requirement that the put part of the lenses be additive or linear in the second argument forces uniqueness of the pairing maps. Thus, we have:

**Proposition 2.11.** If  $\mathcal{C}$  is Cartesian left-additive, then  $\mathbf{Lens}_A(\mathcal{C})$  is Cartesian, and if  $\mathcal{C}$  is a CRDC, then  $\mathbf{Lens}_L(\mathcal{C})$  is Cartesian (both with pairings and projections as defined above).

The following appears as Proposition 31 in [14] (albeit with different notation for  $\mathbf{Lens}_L(\mathcal{C})$ ):

**Proposition 2.12.** If  $\mathcal{C}$  is a CRDC, then there is a product-preserving functor  $R$  from  $\mathcal{C}$  to  $\mathbf{Lens}_L(\mathcal{C})$  which is the identity on objects, and sends  $f$  to the pair  $(f, R[f])$ .

In fact, this result gives an alternative perspective on some of the CRDC axioms: one can prove that  $R$  is a product-preserving functor from  $\mathcal{C}$  to  $\mathbf{Lens}_A(\mathcal{C})$  if and only if the first 5 CRDC axioms hold.

Since the subcategories  $\mathbf{Lens}_A(\mathcal{C})$  and  $\mathbf{Lens}_L(\mathcal{C})$  are Cartesian (as opposed to merely weak Cartesian), one might wonder why we have bothered discussing the weak Cartesian structure of  $\mathbf{Lens}(\mathcal{C})$  at all. The issue is that some of the update lenses that occur in practice (such as those arising from Adagrad and Adam - see Examples 3.18 and 3.19) do not live in  $\mathbf{Lens}_A(\mathcal{C})$  but in the more general category  $\mathbf{Lens}(\mathcal{C})$  (see Remark 3.20). Thus, we need to be able to work with this more general category (with its merely weak Cartesian structure) to handle these examples.

## 2.4. Models and learners

Now let us recap what these constructions give us. For any Cartesian category  $\mathcal{C}$ , we can construct the (2-)categories

$$\mathbf{Para}(\mathcal{C}) \text{ and } \mathbf{Para}(\mathbf{Lens}(\mathcal{C})).$$

The first category can be thought of as a category of *models*: as described in section 2.1, a map in this category from an object  $A$  to an object  $B$  consists of a parameter space  $P$  and a map  $f : P \times A \rightarrow B$ , which we can think of as a family of possible functions from  $A$  to  $B$  which we hope search. For example, such a map is in machine learning terminology called a *neural network architecture*.

On the other hand, the category  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  can be thought of as a category of *learners*. Let us work out explicitly what it looks like:

**Lemma 2.13.** For any Cartesian category  $\mathcal{C}$ , the category  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  has:

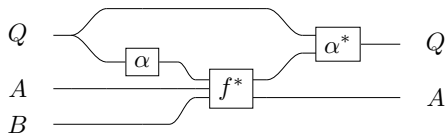
- Objects/0-cells are the same as those of  $\mathcal{C}$ .
- A morphism/1-cell from  $A$  to  $B$  consists of a triple  $(P, f, f^*)$  where  $P$  is an object of  $\mathcal{C}$ ,  $f : P \times A \rightarrow B$ , and  $f^* : P \times A \times B \rightarrow P \times A$ .
- A 2-cell from  $(P, f, f^*)$  to  $(Q, g, g^*)$  consists of a lens  $(\alpha, \alpha^*) : Q \rightarrow P$  such that  $(1 \times \alpha); f = g$  in  $\mathbf{Lens}(\mathcal{C})$ ; explicitly, this means that

$$g(p, a) = f(\alpha(p), a)$$

and

$$g^*(q, a, b) = (\alpha^*(q, p), a')$$

where  $(q, a') = f(\alpha(p), a, b)$ . Diagrammatically, this last equality says that



is equal to  $g^*$ .

The key point is that a morphism from  $A$  to  $B$  has a parameter space  $P$ , a map  $f : P \times A \rightarrow B$  (as in  $\mathbf{Para}(\mathcal{C})$ ), but also, in addition, a map

$$f^* : P \times A \rightarrow B \rightarrow P \times A$$

which one can think of as “a way that  $f$  can learn”. Ideally, given a parameter  $p \in P$ , an input  $a \in A$ , and a “desired output”  $b \in B$ , the  $P$  component of  $f^*(p, a, b)$  would give a better parameter to use for the model  $f$ . While not used much in machine learning, the  $A$  component of  $f^*(p, a, b)$  is interesting in its own right: one can think of it as “the input  $f$  would have preferred to see given that the output was supposed to be  $b$ ”.

Following simply from the definition of the monoidal structure and 2-cells for a category  $\mathbf{Para}(\mathcal{C})$  for an arbitrary category  $\mathcal{C}$ , the monoidal structure and the 2-cells of  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  are automatically defined for us, and play an important role. The former allows us to compose learners in parallel, while the latter allows us to reindex learners on their parameter spaces, now not by precomposition with morphisms in  $\mathcal{C}$ , but by precomposition with morphisms in  $\mathbf{Lens}(\mathcal{C})$ , i.e. lenses.

Readers familiar with [18] may recognize the similarity of  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  to the category  $\mathbf{Learn}$  of that paper (when  $\mathcal{C} = \mathbf{Smooth}$ ). While similar, there are key differences between the structure of their 2-cells, and this has an important effect when defining (2-)functors related to these categories. For more details, see Section 6.

## 3. The gradient learner (2-)functor

This section culminates (Section 3.5) in our main categorical construction: in any CRDC  $\mathcal{C}$  with *update data* (data to calculate parameter updates) and *displacement maps* (maps to compute error), there is a functor  $\mathbf{GL}$  from  $\mathbf{Para}(\mathcal{C})$  to  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  which generates for every parameterized function, a gradient based learner for that function. Many variants of gradient-based learning will fit into this framework. Concretely, this functor takes a parameterized function  $P \times A \rightarrow B$  (for example, coming from some neural network architecture) and turn it into a learner, ie a lens  $P \times A \rightarrow B$  with backwards component  $P \times A \times B \rightarrow P \times A$ . That means, intuitively, that back-propagation takes a parameter  $p$ , an input  $a$ , and a “desired” output  $b$ , and return (in its output  $P$  component) a better parameter for the model to use, given how far off the model’s output was. How the functor does this will vary based on which update data and displacement maps are chosen: one could choose momentum as one’s update with the ordinary displacement map coming from mean-squared loss, or Adagrad as one’s update, with Softmax cross entropy as the displacement, etc. Our setup allows one to vary these components as desired. The fact that the result is functorial, no matter which update data or displacement map is chosen, tells us that we get the same result if i) we first use the entire network to create training data for each of its individual parts, and then train each part separately, or ii) we train the entire network at once. This is an instance of compositionality.

We will construct the functor in three steps:

- 1) The *parametrised reverse derivative functor*: for any CRDC  $\mathcal{C}$ , define a functor from  $\mathbf{Para}(\mathcal{C})$  to  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  which makes use of the reverse derivative  $R$ . This functor alone is not the required learner: all it does is compute the reverse derivative of the model. A full machine learning algorithm will additionally use two functors:
- 2) The *error endofunctor*: given any collection of “displacement maps” in  $\mathcal{C}$ , we define an endofunctor on  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  which turns the desired output into the error signal used by the previous functor.
- 3) The *update endofunctor*: given any sufficiently well-behaved collection of “update data” in  $\mathcal{C}$ , we define an endofunctor on  $\mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$  which uses the computed parameter error signal together with the current parameter to compute a new parameter value. The update data will vary depending on the algorithm used: it is quite straightforward for basic gradient descent, but, for example, more involved when working with Nesterov momentum.

### 3.1. Parametrised reverse derivative functor

Given the results of the previous sections, the first functor is completely straightforward. Recall from Proposition 2.12 that for any CRDC  $\mathcal{C}$ , there is a product-preserving functor  $R : \mathcal{C} \rightarrow \mathbf{Lens}_L(\mathcal{C})$  which is the identity on objects, and sends a map  $f : A \rightarrow B$  to the lens  $(f, R[f])$ . Thus, we simply apply the 2-functor  $\mathbf{Para}$  to this functor:

**Corollary 3.1.** For any CRDC  $\mathcal{C}$ , there is a monoidal 2-functor

$$\mathbf{Para}(R) : \mathbf{Para}(\mathcal{C}) \rightarrow \mathbf{Para}(\mathbf{Lens}_L(\mathcal{C})).$$

Specifically, this functor is the identity on objects, and sends a parametrised map  $(P, f : P \times A \rightarrow B)$  to the triple  $(P, f, R[f])$ , where now  $R[f] : P \times A \times B \rightarrow P \times A$ .

### 3.2. Towards error and update endofunctors

This section develops the categorical structures necessary to define the remaining two components of a learner, “error” and “update”, which will be finalised in Sections 3.3–3.4. They can be seen as specific instances of some very basic constructions one can perform on any category of the form  $\mathbf{Para}(\mathcal{C})$ . Moreover, both have their origin in a very simple construction one can perform on any category:

**Lemma 3.2.** If  $\mathcal{C}$  is a category, and  $\{i_A : A \rightarrow A\}$  is a family of isomorphisms (one for each object  $A$  of  $\mathcal{C}$ ), then one can define a monoidal endofunctor  $F : \mathcal{C} \rightarrow \mathcal{C}$  by setting  $F$  to be the identity on objects, and for an  $f : A \rightarrow B$  in  $\mathcal{C}$ , setting  $F(f)$  to be the composite

$$A \xrightarrow{i_A^{-1}} A \xrightarrow{f} B \xrightarrow{i_B} B$$

Note that no compatibilities between the  $i_A$ ’s are needed: functoriality immediately follows by definition of

isomorphism. In fact, note that this functor is very trivial from the point of view of general category theory, as it is naturally isomorphic to the identity.

In the case of  $\mathbf{Para}(\mathcal{C})$ , there are two variants of this construction which we can perform: given a parametrised map  $(P, f) : A \rightarrow B$ , one in which the isomorphisms apply to the “data”  $A$ , and one in which the isomorphisms apply to the “parameter”  $P$ . Neither is the same as applying the 2-functor  $\mathbf{Para}$  to the construction of Lemma 3.2, as this would involve modifying both the data and the parameter simultaneously. As far as we are aware, while the construction of lemma 3.2 is standard, the two constructions we will describe here are new.

The first construction modifies the data:

**Proposition 3.3.** Suppose  $\mathcal{C}$  is a monoidal category, and we have, for each object  $A$ , an isomorphism  $i_A : A \rightarrow A$  such that  $i_{A \otimes B} = i_A \otimes i_B$  and  $i_I = 1_I$ . Then we can define a monoidal endo-2-functor  $I$  on  $\mathbf{Para}(\mathcal{C})$  as follows:

- $I$  is the identity on objects.
- $I$  maps a 1-cell  $(P, f) : A \rightarrow B$  to  $P$  with the map

$$P \otimes A \xrightarrow{1 \otimes i_A^{-1}} P \otimes A \xrightarrow{f} B \xrightarrow{i_B} B$$

- $I$  maps a 2-cell  $r : (P, f) \rightarrow (P', f')$  to  $r$ .

In Section 3.3, we will use this particular construction with the “error” or “loss” functions associated to a machine learning algorithm.

The second endofunctor we will construct updates the parameter part of a map in  $\mathbf{Para}(\mathcal{C})$ . We begin with a basic version:

**Proposition 3.4.** Suppose  $\mathcal{C}$  is a monoidal category, and we have, for each object  $P$ , an isomorphism  $u_P : P \rightarrow P$  such that for any  $P, Q$ ,  $u_{P \otimes Q} = u_P \otimes u_Q$ , and  $u_I = 1_I$ . Then we can define a monoidal endofunctor  $U$  on  $\mathbf{Para}(\mathcal{C})$  as follows:

- $U$  is the identity on objects.
- $U$  maps a 1-cell  $(P, f) : A \rightarrow B$  to  $P$  with the map

$$P \otimes A \xrightarrow{u_P \otimes 1} P \otimes A \xrightarrow{f} B$$

- $U$  maps a 2-cell  $R : (P, f) \rightarrow (P', f')$  to the composite

$$P' \xrightarrow{u_{P'}} P' \xrightarrow{r} P \xrightarrow{u_P^{-1}} P$$

**PROOF:** This is essentially immediate: functoriality on 1-cells follows from the monoidal product compatibility requirement, while well-definedness and 2-functoriality of 2-cells follows as in Lemma 3.2.  $\square$

Note something subtle in the above construction: the use of the inverses appears at the level of 2-cells, but not at the level of 1-cells. As noted above, 1-functoriality follows from the monoidal product compatibility, not the existence of the inverse.

As we shall see in Section 3.4, the above basic version will be sufficient to handle standard gradient descent. However, more sophisticated machine learning algorithms (such as momentum and Adagrad) need to keep track of previous updates, and for this, we need our parameter update endofunctor to keep track of this data in some way. To do this, we add an additional endofunctor  $S$  on the base category mapping parameters to states: applied to an object  $P$ ,  $S(P)$  can be thought of as “the object of states that the update needs to keep track of”.

First, we need to recall the following definition:

**Definition 3.5.** If  $\mathcal{C}$  is (weak) Cartesian, a map  $f : A \times B \rightarrow C$  is said to be **invertible in its second variable** if there is a map  $g : A \times C \rightarrow B$  so that

$$\langle \pi_0, f \rangle g = \pi_1 \text{ and } \langle \pi_0, g \rangle f = \pi_1.$$

We can then define what sort of data can let us build a more sophisticated parameter update endofunctor. The key point is that the update will now be of the form  $u_P : S(P) \times P \rightarrow P$ : updating the parameter  $P$  given not just its current state but also potentially past states as well. In this more general case, to get functoriality it is sufficient to ask that  $u_P$  be invertible in its second variable.

**Definition 3.6.** Suppose that  $\mathcal{C}$  is weak Cartesian. We define **parameter update data** to consist of the following:

- a product-preserving endofunctor  $S : \mathcal{C} \rightarrow \mathcal{C}$ ;
- for each object  $P$  of  $\mathcal{C}$ , a map

$$u_P : S(P) \times P \rightarrow P$$

which is invertible in its second variable;

- such that this data respects products: for each pair of objects  $P, Q$ ,  $u_{Q \times P}$  the following commutes:

$$\begin{array}{ccc} S(Q \times P) \times Q \times P & \xrightarrow{u_{Q \times P}} & Q \times P \\ \downarrow & & \uparrow u_Q \times u_P \\ S(Q) \times S(P) \times Q \times P & \longrightarrow & S(Q) \times Q \times S(P) \times P \end{array}$$

From such data, we can define an endofunctor:

**Proposition 3.7.** Suppose  $\mathcal{C}$  is a weak Cartesian category with update data  $\{u_P : P \in \mathcal{C}\}$ . Then we can define a monoidal endofunctor  $U$  on  $\mathbf{Para}(\mathcal{C})$  as follows:

- $U$  is the identity on objects.
- $U$  maps a 1-cell  $(P, f) : A \rightarrow B$  to  $S(P) \times P$ , with the map

$$S(P) \times P \times A \xrightarrow{u_P \times 1} P \times A \xrightarrow{f} B$$

- $U$  maps a 2-cell  $r : (P, f) \rightarrow (P', f')$  to the composite

$$\begin{aligned} S(P') \times P' &\xrightarrow{\langle \pi_0, u_{P'} \rangle} S(P') \times P' \xrightarrow{S(r) \times r} S(P) \times P \\ &\xrightarrow{\langle \pi_0, u_P^{-1} \rangle} S(P) \times P \end{aligned}$$

PROOF: Follows essentially as in Proposition 3.4, using product-preservation of  $S$  when checking functoriality.  $\square$

As noted above, this more sophisticated version will be needed to handle machine learning algorithms that update their parameters based on previous states. For examples, see Section 3.4 and Section 4.

### 3.3. Error endofunctor

As we saw in Proposition 3.3, any family of isomorphisms in  $\mathcal{C}$  also gives an endofunctor on  $\mathbf{Para}(\mathcal{C})$ . Applying this to the category  $\mathbf{Lens}(\mathcal{C})$ , we have:

**Corollary 3.8.** If  $\{d_a : A \rightarrow A\}$  is a family of isomorphisms in  $\mathbf{Lens}(\mathcal{C})$ , then we get a monoidal endofunctor

$$D : \mathbf{Para}(\mathbf{Lens}(\mathcal{C})) \rightarrow \mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$$

as described in Proposition 3.3.

But what does it mean for a lens  $d_A : A \rightarrow A$  to be an isomorphism? We'll focus on the case when the get part of the lens is the identity (all our examples will be of this type). In this case, if we have a lens  $(1_A, f^*) : A \rightarrow A$ , then it suffices to have a lens  $(1_A, g^*) : A \rightarrow A$  such that

$$\langle \pi_0, f^* \rangle g^* = \pi_1 \text{ and } \langle \pi_0, g^* \rangle f^* = \pi_1.$$

In other words, the put part  $f^*$  must be invertible in its second variable. We call such data a “displacement map”:

**Definition 3.9.** If  $A$  is any object of a (weak) Cartesian category, a **displacement map** on  $A$  is a map

$$d_A : A \times A \rightarrow A$$

which is invertible in its second variable.

The above discussion then gives us the following:

**Proposition 3.10.** If  $\mathcal{C}$  is weak Cartesian, and for every object  $A$  we have a displacement map  $d_A : A \times A \rightarrow A$  such that  $d_{A \times B} \cong d_A \times d_B$ , then we get a family of isomorphisms  $(1_A, d_A) : A \rightarrow A$  in  $\mathbf{Lens}(\mathcal{C})$  and hence an endofunctor

$$D : \mathbf{Para}(\mathbf{Lens}(\mathcal{C})) \rightarrow \mathbf{Para}(\mathbf{Lens}(\mathcal{C}))$$

as described in Proposition 3.3.

The most basic example in **Smooth** is very simple:

**Example 3.11.** In  $\mathcal{C} = \mathbf{Smooth}$ , an example of displacement maps are the maps  $A \times A \rightarrow A$  defined by  $(a, a') \mapsto a - a'$ . The inverse of  $d_A(a, -)$  is  $d_A(a, -)$  itself.

More generally, any “error function”  $e : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$  as described in [18] will give an appropriate family of displacement maps. Given such a map, if  $A = \mathbb{R}^n$ , one first defines  $E_A : A \times A \rightarrow \mathbb{R}$  by

$$E_A(a, a') = \sum_{i=1}^n e(a_i, a'_i).$$

Its reverse derivative is thus a map

$$R[E_a] : A \times A \times \mathbb{R} \rightarrow A \times A$$

Evaluating this at the number  $1 \in \mathbb{R}$  and taking the second projection thus gives a map which we write as  $d_A$ :

$$d_A : A \times A \rightarrow A$$

which is the required displacement map. The perspective of “error functions” is the one taken in machine learning community: a choice of the error function is made first, and then the displacement map is constructed via the procedure above.

The requirement in [18] that the derivative of  $e$  be invertible in its second variable ensures that the displacement maps are invertible in their second variable. Applying the above procedure to the quadratic error  $e(x, y) = \frac{1}{2}(x - y)^2$  gives the map  $(a, a') \mapsto a - a'$  as described above.

While the mentioned quadratic loss is often used for regression problems, for classification problems a different loss function is used: Softmax cross entropy.

**Example 3.12 (Softmax cross entropy).** The Softmax cross entropy loss is a map of type  $\mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$  defined by

$$(x, q) \mapsto \frac{1}{N} \sum_{i:N} q_i(x_i - \log(\text{Softmax}(x)_i))$$

where  $\text{Softmax}(x) = \frac{\exp(x_i)}{\sum_{j:N} \exp(x_j)}$  is defined componentwise for  $i : N$ .

This error function effectively interprets the output of the neural network as a probability distribution - by normalizing it via the Softmax function - and then compares it to the desired probability distribution  $q$  by using the cross entropy loss.

This loss function gives rise to the displacement map of the same type whose implementation is  $(x, q) \mapsto \text{Softmax}(x) - q$ . The seemingly surprising reduction of both the Softmax cross entropy error and the mean squared error to a similar displacement map form can be confirmed with some elementary calculation [23].

Finally, we give an example for a base category other than **Smooth**.

**Example 3.13 (Boolean Circuit Displacement).** The displacement map  $(a, a') \mapsto a - a'$  of Example 3.11 can be directly translated to the setting  $\text{POLY}_{\mathbb{Z}_2}$ , as used in the boolean circuit learners of [7]. Since elements  $a \in \mathbb{Z}_2^n$  are self-inverse (i.e.,  $-a = a$ ), we can instead write  $d_A = (a, a') \mapsto a + a'$ , with  $+$  the pointwise XOR operation. As with Example 3.11, the inverse of  $d_A(a, -)$  is  $d_A(a, -)$ .

### 3.4. Update endofunctor

As seen in Proposition 3.7, update data on a weak Cartesian category yields an endofunctor. Applying this result to the weak Cartesian category **Lens**( $\mathcal{C}$ ) gives:

**Corollary 3.14.** If  $S : \mathcal{C} \rightarrow \mathcal{C}$  is a product-preserving endofunctor, and  $\{u_P : S(P) \times P \rightarrow P\}$  is update data in **Lens**( $\mathcal{C}$ ), then by applying Proposition 3.7, we get a monoidal endofunctor

$$U : \text{Para}(\text{Lens}_L(\mathcal{C})) \rightarrow \text{Para}(\text{Lens}_L(\mathcal{C}))$$

In **Lens**( $\mathcal{C}$ ), update data will consist of a choice of product-preserving functor  $S : \text{Lens}(\mathcal{C}) \rightarrow \text{Lens}(\mathcal{C})$ , as well as a “update map” lens

$$u_P : S(P) \times P \rightarrow P \quad (3)$$

(which is invertible in its second variable) for every object  $P \in \text{Lens}(\mathcal{C})$ . In the category  $\mathcal{C} = \text{Smooth}$ , each of the various gradient descent algorithms has such data. The object  $S(P)$ , in particular, is used to hold data from previous updates.

**Example 3.15 (Basic gradient descent).** Given any fixed  $\epsilon > 0$ , basic gradient descent [24, Algorithm 8.1] is given by  $S(P) = T$  (the terminal object) with  $u_P : P \rightarrow P$  the lens whose get part is the identity, and whose put part is the map  $P \times P \rightarrow P$  defined by  $(p, p') \mapsto p - \epsilon p'$ .

Thus, in the most basic form of gradient descent, no past data is kept, and the get part of the lens is trivial.

**Example 3.16 (Momentum).** Given any fixed  $\epsilon, \gamma > 0$ , momentum gradient descent [3] is given by  $S(P) = P$ , with  $u_P : S(P) \times P \rightarrow P$  the lens whose get part is the second projection, and whose put part is the map

$$S(P) \times P \times P \rightarrow S(P) \times P$$

defined by  $(v, p, p') \mapsto (v', p - v')$ , where  $v' = \gamma v + \epsilon p'$ .

Thus, in momentum gradient descent, we keep track of the previous gradient and use this to inform our next update. However, again the get part of the lens is trivial.

**Example 3.17 (Nesterov Momentum).** Fix  $\epsilon, \gamma > 0$ . Nesterov momentum [17] is given by  $S(P) = P$ , with  $u_P : S(P) \times P \rightarrow P$  the lens whose get part is  $(v, p) \mapsto p - \gamma v$  and whose put part is as in Example 3.16.

In Nesterov momentum, we again keep track of previous data, but now also use a non-trivial get part of the lens. This progression of examples thus shows how the full generality of update data is necessary to handle some of the more interesting forms of gradient descent. Two other commonly used optimization algorithms are Adagrad and Adam:

**Example 3.18 (Adagrad).** Given any fixed  $\epsilon > 0$  and  $\delta \sim 10^{-7}$ , Adagrad [2] is given by  $S(P) = P$ , with  $u_P : S(P) \times P \rightarrow P$  the lens whose get part is  $(g, p) \mapsto p$ . The put is  $(g, p, p') \mapsto (g', p - \frac{\epsilon}{\delta + \sqrt{g'}} \odot p')$  where  $g' = g + p' \odot p'$  and  $\odot$  is the elementwise (Hadamard) product.

Unlike with other optimization algorithms where the learning rate is the same for all parameters, Adagrad divides the learning rate of each individual parameter with the square root of the past accumulated gradients.

**Example 3.19 (Adam).** Fix  $\beta_1, \beta_2 \in [0, 1)$ ,  $\epsilon > 0$ , and  $\delta \sim 10^{-8}$ . Adam [4] is given by  $S(P) = P \times P$ , with  $u_P : S(P) \times P \rightarrow P$  the lens whose get part is  $(m, v, p) \mapsto p$  and whose put part is

$$\text{put}(m, v, p, p') = (\hat{m}', \hat{v}', p - \frac{\epsilon}{\delta + \sqrt{\hat{v}'}} \odot \hat{m}')$$



where  $m' = \beta_1 m + (1 - \beta_1)p'$ ,  $v' = \beta_2 v + (1 - \beta_2)p'^2$ , and

$$\hat{m}' = \frac{m'}{1 - \beta_1^t}, \hat{v}' = \frac{v'}{1 - \beta_2^t}.$$

Adaptive Moment Estimation (Adam) is another method that computes adaptive learning rates for each parameter by storing exponentially decaying average of past gradients ( $m$ ) and past squared gradients ( $v$ ).

**Remark 3.20.** While the lenses for basic gradient descent, momentum, and Nesterov momentum all live in the subcategory of *linear* lenses (Definition 2.9), the lenses for Adagrad and Adam do not (their put part is not linear in the  $p'$  variable). This is the reason we work with the weak Cartesian category of arbitrary lenses as opposed to the Cartesian categories of additive or linear lenses.

Finally, to accompany Example 3.13, we give an example for the base category  $\text{POLY}_{\mathbb{Z}_2}$ .

**Example 3.21 (Boolean Circuit Update).** The boolean circuit parameter update used in [7] is given by  $S(P) = T$  with  $u_P : P \rightarrow P$  the lens  $(1_A, +)$ , where  $+$  is pointwise addition in  $\mathbb{Z}_2$ —the XOR operation.

That all of these diverse examples fall within our framework was a surprising discovery.

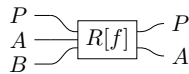
### 3.5. Gradient learner functor

We are now in a position to describe our complete functor. Given displacement and update data as described above, we simply apply each of the above 3 functors in turn (along with one application of the inclusion functor  $i : \text{Para}(\text{Lens}_L(\mathcal{C})) \rightarrow \text{Para}(\text{Lens}(\mathcal{C}))$ ):

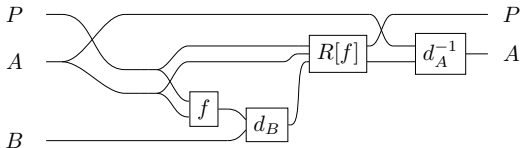
$$\text{GL} := \text{Para}(R); i; D; U$$

giving a monoidal functor from  $\text{Para}(\mathcal{C})$  to  $\text{Para}(\text{Lens}(\mathcal{C}))$ ; that is, a functor from a category of parametrised functions to a category of learners.

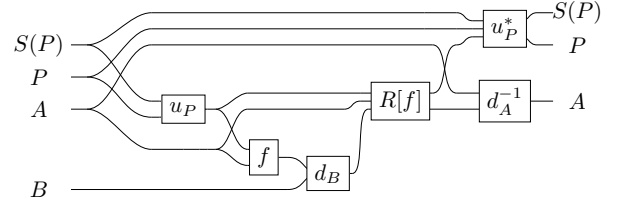
However, it will be helpful to see the effect of each functor in turn and focus on the put part (where back-propagation occurs) of the resulting lens. As noted earlier, the first functor is very simple: it takes a parametrised function  $f : P \times A \rightarrow B$  and gives the lens whose put part is the reverse derivative of  $f$  (in the standard case of  $\mathcal{C} = \text{Smooth}$  and  $B = \mathbb{R}$ , this will simply be the gradient of  $f$ ). Graphically, we can represent this as the following:



In the next step we apply the displacement endofunctor  $D$ . This gives us the lens whose put part can be graphically represented as



In the final step, we apply the update endofunctor  $U$ , giving the complete learner



Note:

- The output of the  $P$  wire is the key component for machine learning: it first applies  $f$  to the given input data, then checks how far off it is from the required output (via the  $d_B$  map) feeds this data into the reverse derivative, then uses the appropriate update algorithm to calculate the new value of the parameter  $P$ .
- The output of the  $S(P)$  wire stores some data based on the algorithm chosen (eg., the previous step's gradient).
- As noted in [18], the output of the  $A$  wire is not obvious. It is not typically used in a machine learning algorithm, but reflects “what the algorithm would have preferred to see as input, given the desired output”. As such, it may be useful to monitor during training to get an insight for “how well the algorithm is learning”. More research in this area is required, however.

Overall, however, note that while the final complete learner can look somewhat complicated, part of what this paper has demonstrated is how it can be built up using smaller, simpler pieces. Moreover, it is not necessarily obvious that the resulting map which takes an  $f$  and gives the above diagram is functorial; again, however, breaking down the overall diagram into the result of several smaller parts shows that is indeed functorial, and hence compositional with respect to sequential composition.

## 4. Case studies

In this section we illustrate our approach on a series of case studies drawn from the machine learning literature, showing how in each case the parameters of our framework (in particular, displacement and update maps) instantiate to familiar concepts. This presentation has the advantage of treating all these case studies uniformly in terms of our basic constructs, highlighting their similarities and differences.

First recall that any chosen families of displacement  $((d_A)_{A:\mathcal{C}})$  and update  $((u_P)_{P:\mathcal{C}})$  maps (as introduced in Defn. 3.9 and 3.6) can be assembled into the gradient descent 2-functor which maps a differentiable, parameterized map  $f : P \times A \rightarrow B$  to a lens of type  $SP \times P \times A \rightarrow B$ .

First, we unpack the content of the aforementioned lens in the general case. Its get map unpacks to the composite  $SP \times P \times A \xrightarrow{u \times A} P \times A \xrightarrow{f} B$ , where  $u : SP \times P \rightarrow P$  is the get part of the update lens  $(u, u^*) : SP \times P \rightarrow P$ . The put map unpacks to

$$\text{put}(s, p, a, b) = (u^*(s, p, p'), d_A^{-1}(a, a'))$$

where  $(p', a') = f^*(u(s, p), a, d_B(f(u(s, p), a), b))$ .

While this formulation might look daunting, we justify its complexity by showing a series of examples. Most of the examples are in the base category **Smooth**, and the last example is instantiated when the base category is  $\text{POLY}_{\mathbb{Z}_2}$  - a syntax for boolean circuits. In all of the cases we fix some map  $f : P \times A \rightarrow B$  in the base category.

For **Smooth**, we start by looking at regression: we fix the displacement map corresponding to the mean squared error (3.11). Then we show how the GL functor behaves on  $f$  as we vary the update endofunctor.

**Example 4.1 (Mean squared error, basic gradient descent).**

Fix the basic gradient descent update rule described in Ex. 3.15. Then the aforementioned takes on the following form. Since there is no state, its type reduces to  $P \times A \rightarrow B$ . The get map of that lens is  $f$  itself, and the put map reduces to

$$\text{put}(p, a, b) = (p - \epsilon p', a - a')$$

where  $(p', a') = f^*(p, a, f(p, a) - b)$ .

This functor gives us a variety of *regression* algorithms solved iteratively by gradient descent: it takes some map in  $(\mathbb{R}^p, f) : \mathbf{Para}(\mathbf{Smooth})(\mathbb{R}^n, \mathbb{R})$  to the corresponding learner which performs regression on input data. If the corresponding map  $f$  is linear, we recover linear regression. If the codomain is additionally multi-dimensional, i.e. we're predicting multiple scalars, then we recover multivariate linear regression.

**Example 4.2 (Mean squared error, momentum).** Fix the momentum update rule described in Ex. 3.16. The type of the learner lens reduces to  $P \times P \times A \rightarrow B$ , since the state space for each parameter is the space  $P$  itself. Similar to the previous example, the get map is still just  $f$  - but with the added difference that we first have to forget the momentum state. That is, the get map reduces to  $\text{get}(v, p, a) = f(p, a)$ . The put map takes on the following form:

$$\text{put}(v, p, a, b) = (v', p - v', a - a')$$

where  $v' = \gamma v + \epsilon p'$  and  $(p', a') = f^*(p, a, f(p, a) - b)$ .

Similarly as before, this functor gives us a variety of regression algorithms solved by more advanced variant of gradient descent: momentum.

The difference here is that the update map takes the previous momentum value  $v$ , discounts it by some factor  $\gamma$  and computes the updated momentum by summing it up with the  $\epsilon$ -rescaled parameter. This computed momentum value is then used to compute the next parameter step.

**Example 4.3 (Mean squared error, Nesterov momentum).**

Fix the Nesterov momentum update rule described in Ex. 3.17. Here the get unpacks to  $\text{get}(v, p, a) = f(p - \gamma v, a)$ . The put map takes on the following form:

$$\text{put}(v, p, a, b) = (v', p - v', a - a')$$

where  $v' = \gamma v + \epsilon p'$  and

$$(p', a') = f^*(p - \gamma v, a, f(p - \gamma v, a) - b).$$

Instead of discarding the accumulated momentum value like in standard momentum, we see that in the Nesterov momentum the get map does something nontrivial: it computes the “lookahead” parameter value by moving in the direction of the already accumulated momentum. This is important since Nesterov momentum is in practice handled in an ad-hoc way. Usually, an extra function is added somewhere in the code to perform this lookahead computation.

We see here that the framework of lenses handles this case naturally by using the get map which was a seemingly trivial, unused piece of data for the previous two optimizers.

**Example 4.4 (Mean squared error, Adagrad).** Fix the Adagrad update rule described in Ex. 3.18. Similar to momentum, the learner lens reduces to the type  $P \times P \times A \rightarrow B$ . Its get is  $\text{get}(g, p, a) = f(p, a)$ . The put map reduces to

$$\text{put}(g, p, a, b) = (g', p - \frac{\epsilon}{\delta + \sqrt{g'}} \odot p', a - a')$$

where  $g' = g + p' \odot p'$  and  $(p', a') = f^*(p, a, f(p, a) - b)$ .

**Example 4.5 (Mean squared error, Adam).** Fix the Adam update rule described in Ex. 3.19. The Adam lens reduces to the type  $P \times P \times P \times A \rightarrow B$ , since the state remembered consists of the accumulated first and second moment variables. The get map reduces to  $(m, v, p, a) \mapsto f(p, a)$ . The put map is

$$\text{put}(m, v, p, a, b) = (\hat{m}', \hat{v}', p - \frac{\epsilon}{\delta + \sqrt{\hat{v}'}} \odot \hat{m}')$$

where  $m' = \beta_1 m + (1 - \beta_1)p'$ ,  $v' = \beta_2 v + (1 - \beta_2)p'^2$ ,

$$\hat{m}' = \frac{m'}{1 - \beta_1^t}, \quad \hat{v}' = \frac{v'}{1 - \beta_2^t}$$

$$(p', a') = f^*(p, a, f(p, a) - b).$$

This shows how our framework handles a variety of update maps. In a similar way this can be extended to the ones not covered with these examples, such as Nesterov Adam [25].

We now show that loss functions can be varied as well. By fixing the Softmax cross entropy loss, we recover learners which perform classification.

**Example 4.6 (Cross-entropy loss, basic gradient descent).**

Fix the displacement map given by the Softmax cross-entropy loss described in Ex. 3.12. Fix basic gradient descent in Ex. 3.15. In this case the learner reduces to just the lens of type  $P \times A \rightarrow B$  whose get is  $f$  itself. The put map reduces to

$$\text{put}(p, a, b) = (p - \epsilon p', \text{Softmax}(a) - a')$$

where  $(p', a') = f^*(p, a, \text{Softmax}(f(p, a)) - b)$ .

Being quite similar in form to Example 4.1, we see that the learner here in addition routes its outputs - the unnormalized logits - through the Softmax map. The details of all the Softmax cross entropy learners with any of the

other update maps are analogous to the already worked out examples with the mean squared error.

We finish off these examples with a different base category:  $\text{POLY}_{\mathbb{Z}_2}$ .

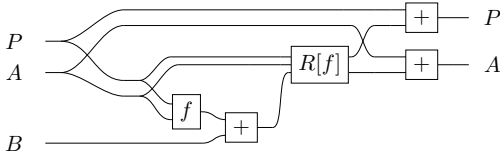
**Example 4.7 (Boolean circuits).** Fix displacement and update maps as in Examples 3.13 and 3.21, so the learner lens reduces to the type  $P \times A \rightarrow B$ . The get map is  $f$ , and the put map reduces to

$$\text{put}(p, a, b) = (p + p', a + a')$$

where

$$(p', a') = f^*(p, a, f(p, a) + b)$$

We additionally write the put map of this example as the string diagram



This allows us to easily compare it to [7], where boolean circuit learning was originally introduced: this composite is almost identical to the  $\text{rdaStep}_f$  map of [7, Equation 7]; the only difference is that the output data  $A$  is not discarded.

## 5. Implementation

We provide a proof-of-concept implementation as a Python library.<sup>3</sup> We validate our library with empirical tests, including a neural network classifier for the MNIST [26] image classification benchmark dataset. We also ensure that the accuracy of our models is on par with an equivalent implementation in an existing deep learning framework. In doing so, we demonstrate the advantages of our approach. Firstly, computing the gradients of the network is greatly simplified through the use of lens composition. Secondly, model architectures can be expressed in a principled, mathematical language; as morphisms of a monoidal category. Finally, the modularity of our approach makes it easy to define new optimization algorithms: the user need only define an appropriate update map.

### 5.1. Lenses

We model a lens  $(f, f^*)$  in our library with the `Lens` class, which consists of a pair of maps `fwd` and `rev` corresponding to  $f$  and  $f^*$ , respectively. For example, we write the identity lens  $(1_A, \pi_2)$  as follows:

```
identity = Lens(lambda x: x, lambda x_dy: x_dy[1])
```

Our library provides a number of lenses as primitives. For example, the `linear` lens computes a matrix-vector product, `add` computes pointwise addition of arrays, and `sigmoid` applies the sigmoid function pointwise to each

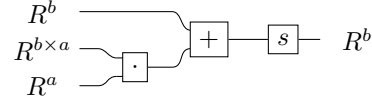
3. Full usage examples, source code, and experiments of our proof-of-concept can be found at <https://github.com/lics2021-submission-208/code>.

element in an array. In all three cases, the `rev` maps correspond to reverse derivatives of these functions.

In addition to primitives, a new `Lens` can be constructed using composition  $f \gg g$  and monoidal product  $f @ g$ . For example, one can define a neural network dense layer with sigmoid activation as follows, with `add` playing the role of the network's biases:

```
dense_lens = (identity @ linear) >> add >> sigmoid
```

We depict this as the following string diagram, with  $\cdot$  denoting matrix-vector product,  $+$  as addition, and  $s$  as sigmoid activation:



Constructing model architectures in this way simplifies the computation of reverse derivatives, which are given by lens composition. Furthermore, adding new primitives is also simplified: the user need simply provide a function and its reverse derivative in the form of a `Lens`.

### 5.2. Para & Learner

Just as `Lens` models morphisms of  $\text{Lens}(\mathcal{C})$ , `Para` models morphisms of  $\text{Para}(\text{Lens}(\mathcal{C}))$ . Pseudocode for the `Para` class is given below, with composition  $\gg$  and monoidal product  $@$  defined as in Section 2.1.

```
class Para:
    param : P
    arrow : P @ A -> B
```

As with `Lens`, our library provides several ways to construct morphisms of `Para`. One of these is `dense`, which we can use to construct simple neural network with a 10 node hidden layer:

```
model = dense((input_dimensions, 10), sigmoid) \
    >> dense((10, output_dimensions), sigmoid)
```

Once a model has been defined, we usually want to optimize its parameters with respect to some data. To do this, we use the gradient learner functor as defined in Section 3.5. Since this functor is defined for a particular choice of model, update, and displacement map, our library provides the `Learner` class, which represents specific choices of each. For example, if we choose the standard gradient descent update `gd` (Example 3.15) with learning rate 0.01 and mean squared error displacement map `mse` (Example 3.11) we can construct a learner as follows:

```
learner = Learner(model, gd(0.01), mse)
```

To compute the action of the gradient learner functor of Section 3.5, the `Learner` class provides the `to_lens` method. However, the user of our library is not typically expected to call this function directly; instead, we provide a function `train`, which applies the resulting map iteratively to a dataset in order to optimize some choice of initial parameters.

## 6. Related Work

The work [18] is closely related to ours, in that it provides abstract categorical model of back-propagation. However, we give a complete lens-theoretic explanation of *what* is back-propagated via (i) the use of CRDCs to model gradients; and (ii) the **Para** construction to model parameterized functions and parameter update. We thus can go well beyond [18] in terms of examples - their example of smooth functions and basic gradient descent is our Example 4.1. We also explain some of the constructions of [18] in a more structured way. For example, rather than considering the category **Learn** of [18] as primitive, here we construct it as a composite of two more basic constructions (the **Para** and **Lens** constructions). Similarly, we view the gradient learner functor as a composite of three separate functors, making it more clear which parts are used at which times. The flexibility could be used, for example, to compositionally replace **Para** with a variant allowing parameters to come from a different category.

We also correct a small issue in Theorem III.2 of [18]. There, the morphisms of **Learn** were defined up to an equivalence (pg. 4 of [18]) but, unfortunately, the functor defined in Theorem III.2 does not respect this equivalence relation. Our approach instead uses 2-cells which comes from the universal property of **Para** — a 2-cell from  $(P, f) : A \rightarrow B$  to  $(Q, g) : A \rightarrow B$  is a lens, and hence has two components: a map  $\alpha : Q \rightarrow P$  and  $\alpha^* : Q \times P \rightarrow Q$ . By comparison, we can see the equivalence relation of [18] as being induced by map  $\alpha : Q \rightarrow P$ . Our approach not only highlights the importance of the 2-categorical structure of learners, but also gives a more flexible definition of the (2-)category of learners that makes gradient descent algorithms correctly (2-)functorial.

Other than [18], there are a few more relevant papers. Lenses and Learners are studied in the eponymous work of [27] which observes that lenses are parameterised learners. They do not explore any of the relevant **Para** or CRDC structure, but make the distinction between *symmetric* and *asymmetric lenses*, studying how they are related to learners defined in [18]. A lens-like implementation of automatic differentiation is the focus of [28], but learning algorithms aren't studied. Lastly, usage of Cartesian differential categories to study learning is found in [29]. They extend the differential operator to work on stateful maps, but do not study lenses, parameterisation nor update maps.

## 7. Conclusions and Future directions

We give a categorical foundation of gradient-based learning algorithms, which supports a number of different desiderata. (i) A first, basic requirement is that the foundations should cover the core features of gradient-based learning such as how a gradient is computed, how gradients are back-propagated and how parameter update occurs: we achieved this, and did so via three separate constructions, to allow us to compositionally vary them should this be desired. (ii) A second desiderata is that a foundation ought to

be principled and mathematically clean, which we pursued by founding each of the above three components on the theory of lenses. Lenses are achieving ever greater uses and - as we discuss below - our use of lenses as a framework for gradient-based learning opens the way to relating gradient-based learning to other structures. (iii) A third desiderata is that our foundation should include a number of previous examples and explain how these examples are related to each other. We fulfill this by covering learning over smooth functions with a wide range of different techniques, as well as the very different learning over boolean circuits— which is simply obtained by switching to a different CRDC. (iv) A final desiderata is that the structure of our framework should be inherent to learning and not a mere expression of categorification. We demonstrate this by developing a Python library, which we use to create the same structures to create a working non-trivial neural network model for the MNIST dataset. This network achieves accuracy on par with an equivalent model in Keras [13].

In terms of future work, we have a number of key directions which are possible to explore because of this work. As noted in Section 2.2, we have not made use of the full power of the CRDC axioms; in particular, we did not explicitly need axioms RD.6 or RD.7, which deal with the behaviour of higher-order derivatives. However, some supervised learning algorithms do use the higher-order derivatives (for example, the Hessian) for additional optimisations; as such, future work includes exploring how to use those axioms to capture these optimisations. Taking this idea in a different direction, one can see that much of our work can be applied to any functor of the form  $F : \mathcal{C} \rightarrow \mathbf{Lens}(\mathcal{C})$  -  $F$  does not necessarily have to be of the form  $f \mapsto (f, R[f])$  for a CRDC  $R$ . Moreover, by working with more generalised forms of the lens category (such as dependent lenses), we may be able to capture ideas related to supervised learning on manifolds. And, of course, we can vary the parameter space to endow it with different structure from the functions we wish to learn. In this vein, we wish to use fibrations/dependent types to model the use of tangent bundles: this would foster the extension of the *correct by construction* paradigm to machine learning, and thereby addressing the widely acknowledged problem of trusted machine learning. The possibilities are made much easier by the compositional nature of our framework. Finally, another key topic for future work is to link gradient-based learning with game theory. At a high level, the former takes little incremental steps to achieve an equilibrium while the latter aims to do so in one fell swoop. Formalising this intuition is possible with our lens-based framework and the lens-based framework for game theory [10].

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## Appendix

Here we briefly review the definitions of Cartesian left additive category (CLAC), Cartesian reverse differential category (CRDC) and additive and linear maps in these categories.

**Definition A.1.** A category  $\mathcal{C}$  is said to be **Cartesian** when there are chosen binary products  $\times$ , with projection maps  $\pi_i$  and pairing operation  $\langle -, - \rangle$ , and a chosen terminal object  $T$ , with unique maps  $!$  to the terminal object.

**Definition A.2.** A **left additive category** [30, Definition 1.1.1] (CLAC) is a category  $\mathcal{C}$  such that each hom-set has commutative monoid structure, with addition operation  $+$  and zero maps  $0$ , such that composition on the left preserves the additive structure: for any appropriate  $f, g, h$ ,  $f; (g + h) = f; g + f; h$  and  $f; 0 = 0$ .

**Definition A.3.** A map  $h : X \rightarrow Y$  in a CLAC is **additive** if it has the property that it preserves additive structure by composition on the right: for any maps  $x, y : Z \rightarrow X$ ,  $(x + y); h = x; h + y; h$ , and  $0; h = 0$ .

**Definition A.4.** A **Cartesian left additive category** [30, Definition 1.2.1] is a left additive category  $\mathcal{C}$  which is Cartesian and such that all projection maps  $\pi_i$  are additive.

The central definition of [14] is the following:

**Definition A.5.** A **Cartesian reverse differential category** (CRDC) is a Cartesian left additive category  $\mathcal{C}$  which has, for each map  $f : A \rightarrow B$  in  $\mathcal{C}$ , a map

$$R[f] : A \times B \rightarrow A$$

satisfying seven axioms:

**[RD.1]**  $R[f + g] = R[f] + R[g]$  and  $R[0] = 0$ .

**[RD.2]**  $\langle a, b + c \rangle R[f] = \langle a, b \rangle R[f] + \langle a, c \rangle R[f]$  and  $\langle a, 0 \rangle R[f] = 0$ .

**[RD.3]**  $R[1] = \pi_1$ , while for the projections, the following diagrams commute:

$$\begin{array}{ccc} (A \times B) \times A & \xrightarrow{R[\pi_0]} & A \times B \\ & \searrow \pi_1 & \nearrow \iota_0 \\ & A & \end{array}$$

$$\begin{array}{ccc} (A \times B) \times B & \xrightarrow{R[\pi_1]} & A \times B \\ & \searrow \pi_1 & \nearrow \iota_1 \\ & B & \end{array}$$

where  $\iota_0 = \langle 1, 0 \rangle$  and  $\iota_1 = \langle 0, 1 \rangle$ .

**[RD.4]** For a tupling of maps  $f$  and  $g$ , the following equality holds:

$$R[\langle f, g \rangle] = (1 \times \pi_0); R[f] + (1 \times \pi_1); R[g]$$

And if  $!_A : A \rightarrow T$  is the unique map to the terminal object,  $R[!_A] = 0$ .

**[RD.5]** For composable maps  $f$  and  $g$ , the following diagram commutes:

$$\begin{array}{ccc} A \times C & \xrightarrow{R[f;g]} & A \\ \langle \pi_0, \langle \pi_0 f, \pi_1 \rangle \rangle \downarrow & & \uparrow R[f] \\ A \times (B \times C) & \xrightarrow{1 \times R[g]} & A \times B \end{array}$$

**[RD.6]**  $\langle 1 \times \pi_0, 0 \times \pi_1 \rangle; (\iota_0 \times 1); R[R[R[f]]]; \pi_1 = (1 \times \pi_1); R[f]$ .

**[RD.7]**  $(\iota_0 \times 1); R[R[(\iota_0 \times 1)R[R[f]]\pi_1]]; \pi_1 = \text{ex}; (\iota_0 \times 1); R[R[(\iota_0 \times 1)R[R[f]]\pi_1]]; \pi_1$  (where  $\text{ex}$  is the map that exchanges the middle two variables).

As discussed in [14], these axioms correspond to familiar properties of the (reverse) derivative:

- **[RD.1]** says that differentiation preserves addition of maps, while **[RD.2]** says that differentiation is additive in its vector variable.
- **[RD.3]** and **[RD.4]** handle the derivatives of identities, projections, and tuples.
- **[RD.5]** is the (reverse) chain rule.
- **[RD.6]** says that the reverse derivative is linear in its vector variable.
- **[RD.7]** expresses the independence of order of mixed partial derivatives.

Moreover, as noted in the discussion after Proposition 2.12, the first 5 axioms of a CRDC are equivalent to asking for a functor from  $\mathcal{C}$  to  $\mathbf{Lens}_A(\mathcal{C})$ .

**Definition A.6.** [14, 22] A map  $f : A \rightarrow B$  in a CRDC is said to be **linear** if

$$\iota_1(\iota_0 \times 1); R[R[f]]; \pi_1 = f.$$

See [14, Section 3.2] for more discussion of this abstract definition of linearity in a CRDC.