Beyond backpropagation: implicit gradients for bilevel optimization

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Abstract

This paper reviews gradient-based techniques to solve bilevel optimization problems. Bilevel optimization is a general way to frame the learning of systems that are implicitly defined through a quantity that they minimize. This characterization can be applied to neural networks, optimizers, algorithmic solvers and even physical systems, and allows for greater modeling flexibility compared to an explicit definition of such systems. Here we focus on gradient-based approaches that solve such problems. We distinguish them in two categories: those rooted in implicit differentiation, and those that leverage the equilibrium propagation theorem. We present the mathematical foundations that are behind such methods, introduce the gradient-estimation algorithms in detail and compare the competitive advantages of the different approaches.

Recent years have witnessed an explosion of breakthroughs fueled by deep learning in many scientific fields such as computer vision (Krizhevsky et al., 2012), natural language processing (Brown et al., 2020), game playing (Mnih et al., 2015) and biology (Jumper et al., 2021). There are many lessons that can be learned from these advances. Among them is the surprising effectiveness of gradient descent: updating the millions, or even billions, of parameters of a deep learning model through greedy gradient-following updates turns out to be extremely powerful and cheap, thanks to the backpropagation of errors algorithm (Linnaemaa, 1976; Werbos, 1982; Rumelhart et al., 1986).

In its standard form, backpropagation provides an efficient way of computing gradients in neural networks, but its applicability is limited to acyclic directed computational graphs whose nodes are explicitly defined. Feedforward neural networks or unfolded-in-time recurrent neural networks are prime examples of such graphs. However, there exists a wide range of computations that are easier to describe through what they achieve, rather than by the exact sequence of calculations that are performed, and

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that thus do not fulfill the requirements of backpropagation. This includes outputs of algorithmic solvers which provably minimize some cost function (Djolonga and Krause, 2017; Wang et al., 2019; Vlastelica et al., 2020), of learning processes that do loss minimization (MacKay et al., 2019; Bengio, 2000) and even of physical systems, such as biological neural networks (Hopfield, 1984) or electrical circuits (Wyatt and Standley, 1989; Kendall et al., 2020; Scellier, 2021), reaching a steady state. These computations therefore cannot be improved by gradient descent based on naive backpropagation, as the algorithm is not directly applicable.

In this article, we frame learning such implicitly-defined systems as a bilevel optimization problem and review how the corresponding gradients can be computed through implicit differentiation methods. We then present an alternative, less explored approach for obtaining such gradients which relies on the equilibrium propagation theorem, found and proved by Scellier and Bengio (2017).

Our article is organized as follows:

- In Section 1 we introduce bilevel optimization along with some examples in which it appears in machine learning. More specifically we present the context in which the methods we are here interested in were introduced and then focus on hyperparameter optimization and meta-learning to give the reader a sense of what are the challenges behind solving bilevel optimization problems.

- At the very basis of the tools of interest for this article is the concept of implicit function and the so-called implicit function theorem. In Section 2 we highlight why this notion is fundamental, present the theorem and give some intuition around its assumptions.

- Section 3 is the core of the paper: we there introduce two gradient-based approaches to solve bilevel optimization problems. We classify them in two categories: the ones that leverage the differentiation formula provided by the implicit function theorem and the ones which make use of an other theorem, the equilibrium propagation theorem. For each type of approach we underline their mathematical foundations and show how to transform them into proper gradient estimation algorithms. We also provide a theoretical analysis of the quality of the gradient they produce as a function of the different sources of approximation made.

- In Section 4 we compare the different algorithms we presented in the last section with each other, showing their qualities and limitations. We then discuss when these methods can be useful by contrasting them to the alternatives that are backpropagation through the optimization process and black-box optimization strategies.

This article has two levels of reading: one for the reader interested in learning new gradient estimation methods and one for the reader who additionally desires to understand in detail the mathematical foundations behind them. For this reason we mark all
1 Bilevel optimization in machine learning

1.1 Bilevel optimization

The high level description of bilevel optimization that we briefly sketched above contains two elements: an inner optimization process which describes what our system does, and an outer-loss function that ultimately measures how good the result of this process is. We now make this formulation more precise.

Let us denote by $\phi$ the inner-parameters that are optimized by the inner process and $\theta$ the outer-parameters that shape the inner-loss function $L^{\text{in}}$. The computation performed by our system can then be described as

$$\phi^*_0 \in \arg \min_{\phi} L^{\text{in}}(\phi, \theta).$$

We use the subscript $\theta$ to underline that $\phi^*_0$ is an implicit function of $\theta$ (as $L^{\text{in}}$ depends on $\theta$), and we use the symbol $\in$ to emphasize that $\phi^*_0$ can be any local minimizer of the inner-loss $L^{\text{in}}$. Note that we do not make any assumption on how we obtain $\phi^*_0$, we only assume that it minimizes a loss function.

The quality of the output $\phi^*_0$ of the system is measured through the outer-loss $L^{\text{out}}$, which plays the usual role of a loss function in machine learning. We can then frame learning of the outer-parameters $\theta$ as the minimization of the outer-loss, which leads to the bilevel optimization problem that we will study in the rest of the article:

$$\min_{\theta} L^{\text{out}}(\phi^*_0, \theta)$$

$$s.t. \quad \phi^*_0 \in \arg \min_{\phi} L^{\text{in}}(\phi, \theta). \quad (1)$$

1.2 Historical perspective

Bilevel optimization was originally introduced in the 1930s by Stackelberg (von Stackelberg, 1934) in the context of two-players games with a leader and a follower, and later extensively studied in the field of optimization as a way to model optimization problems that contain different objectives (Bard, 1998). Closer to the learning formulation of interest to this article is bilevel optimization as introduced for the training of recurrent neural networks in the late 1980s. Instead of describing neural dynamics by their updates and then backpropagating through them, the neural activity is assumed to converge to a steady state. This view led to the introduction of the recurrent backpropagation algorithm (Almeida, 1990; Pineda, 1987) which provides a different way of computing gradients that does not require keeping the trajectory in memory. Often, converging dynamics are described as minimizing an energy function (Hopfield, 1984;
This implicit characterization of entire neural networks, or layers of them, introduced in the early days of deep learning has regained considerable interest recently (Amos and Kolter, 2017; Djolonga and Krause, 2017; Agrawal et al., 2019; Gould et al., 2021). Notably, a class of such implicit networks called deep equilibrium models\(^1\) (Bai et al., 2019, 2020) have achieved state-of-the-art performance in many problem domains. These results demonstrate that the performance of large, deep feedforward neural networks can be matched by neural networks with far fewer parameters, when the computations they perform are iterated repeatedly until equilibrium. As we will later see in more detail, this results in large memory savings not only during inference, but also during learning. Bilevel optimization also appears in many other forms in modern machine learning, going from hyperparameter optimization and meta-learning, to generative adversarial networks (Goodfellow et al., 2014; Metz et al., 2017) and reinforcement learning (Pfau and Vinyals, 2016; Rajeswaran et al., 2020; Nikishin et al., 2022). We zoom in on hyperparameter optimization and meta-learning in the next section as this is the problem for which bilevel optimization is mostly used nowadays. We refer the curious reader to Appendix A for a more extensive presentation of some existing formulations.

1.3 Hyperparameter optimization and meta-learning

**Hyperparameter optimization.** Let us consider the following problem: we want to find the parameters \( \theta \) of a learning algorithm (its hyperparameters) that generate model parameters \( \phi \) which generalize well, i.e., which perform well on held-out data. As is conventionally done, we assume that model parameters are obtained by maximum a posteriori estimation (MacKay, 1992; Foo et al., 2007) or, alternatively, by regularized empirical risk minimization (Bengio, 2000; Goutte and Larsen, 1998). This leads to the following bilevel optimization problem:

\[
\min_{\theta} L(\phi^*, D^{\text{val}}) \\
\text{s.t. } \phi^* \in \arg\min_{\phi} L(\phi, D^{\text{train}}) + R(\phi, \theta),
\]

where \( L \) is the negative log-likelihood that measures the discrepancy between the predictions of a neural network parameterized by \( \phi \) and the target outputs on a dataset \( D \), \( D^{\text{train}} \) is the training set, \( D^{\text{val}} \) is a held-out dataset and \( R(\phi, \theta) \) is the negative log-prior (in the Bayesian view) or a regularizing term on \( \phi \) (in the frequentist view). For instance, a very common choice is to take \( R(\phi, \theta) = \lambda \| \phi \|^2 \); in this case, the hyperparameters are \( \theta = \{ \lambda \} \). A zoo of different interactions between \( \phi \) and \( \theta \) can be considered, and we mention a few of them in Appendix A.2.

\(^1\)See (Kolter et al., 2021) for a tutorial on the topic.
When $\theta$ is low-dimensional, the best hyperparameters can be found through black-box optimization methods such as grid or random search (Bergstra and Bengio, 2012), but these become intractable for high-dimensional hyperparameters. Alternatively, one could backpropagate through the training trajectory, but this does not scale well with the number of updates, as the entire history of parameters must be stored during training, and then revisited in reverse-time order. The implicit methods we will present in Section 3 do not suffer from these limitations. They can scale to a very large number of hyperparameters and to long training procedures.

**Meta-learning.** The previous formulation can be extended to meta-learning (Schmidhuber, 1987; Finn et al., 2017; Bertinetto et al., 2019) by considering several tasks. The goal is now to learn meta-parameters $\theta$ which yield a learning algorithm that generalizes well on a family of tasks: ideally, the algorithm will achieve low loss on unseen tasks, which are assumed to be similar to those encountered during meta-learning. The corresponding optimization problem is then:

$$\min_\theta \mathbb{E}_\tau \left[ L^{\text{out}}(\phi^*_\tau, \theta, D^{\text{val}_\tau}) \right]$$

s.t. $\phi^*_\tau, \theta \in \arg \min_\phi L^{\text{in}}(\phi, \theta, D^{\text{train}_\tau})$, \hspace{1cm} (3)

where $L^{\text{in}}$ and $L^{\text{out}}$ are the same kind of loss used for hyperparameter optimization with the difference that the data on which they are defined is now dependent on the task $\tau$. In practice this is solved by stochastic gradient descent on the expected outer-loss over the task distribution: one task (or more) is sampled and the gradient corresponding to that task is approximated in the same way it would be for hyperparameter optimization. Thus, blackbox optimization methods and backpropagation through training suffer from the same problems that we highlighted above.

### 2 The implicit function theorem

Studying implicit functions is about understanding the relationship between two variables $y$ and $x$, when they are linked together through an equation $f(x, y) = 0$. The first apparitions of implicit functions can be traced back to Descartes (1637) and Newton (1670) who considered the behavior of some specific curves (Krantz and Parks, 2003). Cauchy (1831) laid down the theoretical foundations behind the implicit functions theorem and the extended modern multivariate version of the theorem was introduced by Ulyss Dini in lecture notes supporting his teaching on infinitesimal analysis at University of Pisa during the academic year 1877-1878 (Scarpello and Ritelli, 2002). We end this historical note with a citation from Euler (1748) (as translated by John D. Blanton) that perfectly captures why implicit functions are relevant in mathematics in general and which particularly relates with the philosophy behind bilevel optimization:

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There is however no trace of the implicit function theorem in the 69 original papers Dini published.
Indeed frequently algebraic functions cannot be expressed explicitly. For example, consider the function $Z$ of $z$ defined by the equation, 
$$z^5 = az^2Z^3 - bZ + cz^2Z - 1.$$ 
Even if this equation cannot be solved, still it remains true that $Z$ is equal to some expression composed of the variable $z$ and constants, and for this reason $Z$ shall be a function of $z$.

Implicit functions are inherent to bilevel optimization as the function $\phi^* \theta$ is defined as $\partial_\theta L^{\text{in}}(\phi^*, \theta) = 0$ whenever $\phi^* \theta \in \arg \min L^{\text{in}}(\phi, \theta)$. Understanding how implicit functions behave is therefore crucial; this is what the implicit function theorem brings. More precisely it contains two statements: first, it ensures $\theta \mapsto \phi^* \theta$ exists and second, it yields an analytical formula for the outer-gradient $\nabla_\theta$ associated to our problem:

$$\nabla_\theta^T := \frac{d}{d\theta} L^{\text{out}}(\phi^*, \theta)$$

$$= \frac{\partial L^{\text{out}}}{\partial \theta}(\phi^*, \theta) - \frac{\partial L^{\text{out}}}{\partial \phi}(\phi^*, \theta) \left( \frac{\partial^2 L^{\text{in}}}{\partial \phi^2}(\phi^*, \theta) \right)^{-1} \frac{\partial^2 L^{\text{in}}}{\partial \theta \partial \phi}(\phi^*, \theta).$$

(4)

We derive this formula in Section 2.2.

The attentive reader will have noticed that we are using two different notations for derivatives in the outer-gradient formula. Let us clarify the convention we follow. We use $\partial_x$ to denote partial derivatives with respect to $x$ and $d_x$ for total derivatives. There is no difference between partial and total derivatives when the function only depends on one variable. In the multivariate case this is different. We there use the $\partial_x$ notation when the derivative is straight-forward to calculate, as for the gradient of a loss function, and the $d_x$ one when the function has some hidden dependency on $x$, as it occurs for implicit functions. We consider both partial and total derivatives of scalar functions to be row vectors, so that $\partial_\phi L^{\text{out}}$ is a row vector of size $|\phi|$, $\partial_\phi L^{\text{in}}$ a squared matrix of size $|\phi| \times |\phi|$ and $\partial_\theta \partial_\phi L^{\text{in}}$ a matrix of size $|\phi| \times |\theta|$.

Using the outer-gradient $\nabla_\theta$ for gradient descent would in principle yield an efficient algorithm to solve our bilevel optimization problem with the nice property that it only requires knowing $\phi^* \theta$. Unlike backpropagation-through-time, storing the sequence of intermediate parameter values generated by the learning algorithm is no longer needed. However, computing the outer-gradient requires computing the Hessian $\partial_\phi^2 L^{\text{in}}(\phi^*, \theta)$, which is a second-order derivative, and inverting it. Those two operations are costly and often intractable in large-scale machine learning problems. We therefore need to approximate the outer-gradient $\nabla_\theta$ if we want to use it for practical purposes. This is what the methods we present in Section 3 do.

The rest of the section is dedicated to explaining in further detail the statements and consequences of the implicit function theorem for our bilevel optimization problem. It can be skipped on a first reading without impairing the understanding of the rest of the article.

The usual formulation of the theorem (Dontchev and Rockafellar, 2009) encompasses both the existence statement and the differentiation formula. We present and discuss
next the two parts separately for the sake of clarity.

2.1 Existence of implicit functions †

In the bilevel optimization formulation (1), we used the implicit function $\phi^*_\theta$ without ensuring that it is correctly defined. The first part of the implicit function theorem ensures that such a function exists.

**Theorem 2.1.1** (Existence of implicit functions (Dontchev and Rockafellar, 2009)). Let $f$ be continuously differentiable and $(\phi, \theta)$ be such that $f(\phi, \theta) = 0$. If $\partial f(\phi, \theta)$ is invertible, there exists a unique continuous implicit function $\theta \mapsto \phi^*_\theta$ defined in a neighborhood of $\theta$ such that $\phi^*_\theta = \phi$ and which verifies $f(\phi^*_\theta, \theta) = 0$ for all $\theta$ in that neighborhood.

Once applied to the constraint $f = \partial L^\text{in}$ that follows from the local minimality constraint, the invertibility condition becomes an invertibility condition on the Hessian $\partial^2 L^\text{in}(\phi^*_\theta, \theta)$ and the implicit function verifies $\partial L^\text{in}(\phi^*_\theta, \theta) = 0$ on the neighborhood on which it is defined. Note that if $\hat{\phi}$ is a minimizer of $L^\text{in}(\cdot, \hat{\theta})$ then $\phi^*_\theta$ will also be as long as $L^\text{in}$ is twice continuously differentiable\(^3\). The implicit function theorem is purely local in the sense that several implicit functions can cohabit for a given $\theta$ but in different regions of the $\phi$ space, as shown on Figure 1.B for $\theta > 0$. This why we use the notation $\phi^*_\theta \in \arg \min \phi L^\text{in}(\phi, \theta)$ in (1): the problem is still well defined even if there exists several local minimums for the same $\theta$.

The main assumption of Theorem 2.1.1 applied to bilevel optimization is the invertibility of the Hessian at $(\hat{\phi}, \hat{\theta})$. Without this assumption, the graph associated to the minimizers can split, as illustrated in the following example. Let $L^\text{in}(\phi, \theta) := \phi^4 - \theta \phi^2$ for $\phi$ and $\theta$ real variables. We plot the graph of this function for several $\theta$ values on Figure 1.A. The Hessian, here a second-order derivative, is null when $(\phi, \theta) = (0, 0)$ (hence not invertible). A branching behavior occurs at this point, since there exists a unique minimizer (which is also the only stationary point) of the function at $\phi = 0$ when $\theta$ is negative and three otherwise, see Figure 1.B. The graph associated to the implicit functions therefore splits into 3 branches at $\theta = 0$, making it impossible to properly define an implicit function in this neighborhood.

2.2 Analytical formula for the outer-gradient †

Once we know that an implicit function exists, we would like to know how it locally reacts to changes in $\theta$, i.e., if it is differentiable, and if so, what is its derivative. This is what the second part of the implicit function theorem brings.

**Theorem 2.2.1** (Differentiating implicit functions (Dontchev and Rockafellar, 2009)).

\(^3\)This can be obtained by remarking that 1. the smallest eigenvalue of an invertible Hessian is strictly positive and 2. the smallest eigenvalue of $\partial^2 L^\text{in}(\phi^*_\theta, \theta)$ is a continuous function of $\theta$. This implies that for $\theta$ in the neighborhood of $\hat{\theta}$ considered in Theorem 2.1.1, the smallest eigenvalue of $\partial^2 L^\text{in}(\phi^*_\theta, \theta)$ is strictly positive and hence that $\phi^*_\theta$ is a local minimizer of $L^\text{in}$ for every $\theta$ in this neighborhood.
Figure 1: (A) Visualization of the function $L^{\text{in}}: (\phi, \theta) \mapsto \phi^4 - \theta \phi^2$ for several $\theta$ values. (B) When $\theta$ equals 0, the Hessian at $\phi = 0$ is non-invertible which implies that there is no implicit function defined around $\phi = 0$, as shown on the graph of the solution mapping $S(\theta) := \{ \phi | \partial_{\phi} L^{\text{in}}(\phi, \theta) = 0 \}$ associated to the equilibrium condition $\partial_{\phi} L^{\text{in}}(\phi, \theta) = 0$.

Under the assumptions of Theorem 2.1.1, the implicit function $\phi^*_\theta$ defined in Theorem 2.1.1 is differentiable and

$$
\frac{d \phi^*_\theta}{d \theta} = - \left( \frac{\partial f}{\partial \phi}(\phi^*_\theta, \theta) \right)^{-1} \frac{\partial f}{\partial \theta}(\phi^*_\theta, \theta).
$$

Proof. The derivation of the previous formula is relatively straight-forward once we know the differentiable implicit function exists as it only requires differentiating through the constraint using the chain rule: as $f(\phi^*_\theta, \theta) = 0$ for all $\theta$ on which $\phi^*_\theta$ is defined, we have

$$
0 = \frac{d}{d \theta} f(\phi^*_\theta, \theta) = \frac{\partial f}{\partial \theta}(\phi^*_\theta, \theta) + \frac{\partial f}{\partial \phi}(\phi^*_\theta, \theta) \frac{d \phi^*_\theta}{d \theta},
$$

which yields the desired formula after rearranging the different terms. \hfill \square

We can then use this formula to obtain $d_{\theta} \phi^*_\theta$ for our bilevel optimization problem

$$
\frac{d \phi^*_\theta}{d \theta} = - \left( \frac{\partial^2 L^{\text{in}}}{\partial \phi^2}(\phi^*_\theta, \theta) \right)^{-1} \frac{\partial^2 L^{\text{in}}}{\partial \theta \partial \phi}(\phi^*_\theta, \theta).
$$

Coupled to the chain rule, this is just what we need to obtain the outer-gradient formula:

$$
\nabla^T_{\theta} = \frac{d}{d \theta} L^{\text{out}}(\phi^*_\theta, \theta) = \frac{\partial L^{\text{out}}}{\partial \theta}(\phi^*_\theta, \theta) + \frac{\partial L^{\text{out}}}{\partial \phi}(\phi^*_\theta, \theta) \frac{d \phi^*_\theta}{d \theta} = \frac{\partial L^{\text{out}}}{\partial \theta}(\phi^*_\theta, \theta) - \frac{\partial L^{\text{out}}}{\partial \phi}(\phi^*_\theta, \theta) \left( \frac{\partial^2 L^{\text{in}}}{\partial \phi^2}(\phi^*_\theta, \theta) \right)^{-1} \frac{\partial^2 L^{\text{in}}}{\partial \theta \partial \phi}(\phi^*_\theta, \theta).
$$
Note that for the implicit function theorem, and for all the methods that will be presented here, we only require the stationarity condition $\partial \phi L^\text{in}(\phi^*_g, \theta) = 0$ and not the more restrictive minimality assumption $\phi^*_g \in \text{arg min}_\phi L^\text{in}(\phi, \theta)$. The methods we introduce in the next section can therefore be easily be extended to solve any optimization problem of the form

$$\min_{\theta} L^\text{out}(\phi^*_g, \theta)$$

$$\text{s.t. } \partial \phi L^\text{in}(\phi^*_g, \theta) = 0.$$  

(7)

3 Approximations of the outer-gradient

As we mentioned in the last section, computing the outer-gradient using its analytical formula

$$\nabla_{\theta} = \frac{\partial L^\text{out}(\phi^*_g, \theta)}{\partial \theta} - \frac{\partial L^\text{out}(\phi^*_g, \theta)}{\partial \phi}(\phi^*_g, \theta) - \frac{1}{2} \frac{\partial^2 L^\text{in}(\phi^*_g, \theta)}{\partial \phi \partial \theta}(\phi^*_g, \theta)$$

(8)

is not feasible in most of practical applications of bilevel optimization: we need approximations. Different methods exist to do so. We classify them in two different categories: implicit differentiation methods that approximate the outer-gradient by directly using the analytical formula (8) obtained with the implicit function theorem and equilibrium propagation which leverages an alternative formulation for the outer-gradient that we will later present. Note that we have here written the derivative with respect to outer-parameters $\theta$ but everything can be transposed to derivatives with respect to inputs, thus allowing to backpropagate through implicitly defined layers in deep architectures (Amos and Kolter, 2017; Gould et al., 2021).

In the following, we provide intuition behind the different methods, exhibit their fundamental similarities and differences, and compare their theoretical guarantees.

3.1 Implicit differentiation

Gradient computation as minimization of a quadratic form. Computing and inverting Hessians are costly operations (respectively quadratic and cubic in the size of the differentiated parameter) so the inverse Hessian term must often be approximated in practice. The first key insight needed for those methods is to iteratively approximate the row vector

$$\pi^* := \frac{\partial L^\text{out}(\phi^*_g, \theta)}{\partial \phi}(\phi^*_g, \theta)^{-1}$$

(9)

by minimizing the quadratic form

$$\pi \mapsto \frac{1}{2} \pi \frac{\partial^2 L^\text{in}(\phi^*_g, \theta)}{\partial \phi^2}(\phi^*_g, \theta)^{-1} - \pi \frac{\partial L^\text{out}(\phi^*_g, \theta)}{\partial \phi}. $$

(10)

It is worth noting that as we are using row vectors the quantity $\pi \partial \phi L^\text{out}(\phi^*_g, \theta)^\top$ corresponds to a dot product. If $\phi^*_g$ is a non-flat local minimizer of $L^\text{in}$ then the invertible
Algorithm 1: Side-by-side comparison of implicit differentiation (Section 3.1) and equilibrium propagation (Section 3.2) methods

**Result:** Approximate solution $\theta$ of the bilevel optimization problem (1)

```
for $i = 1, \ldots, n$
    Minimize $L^{\text{in}}(\phi, \theta)$ with respect to $\phi$ and note $\hat{\phi}$ the result;

    **Implicit differentiation**
    Minimize the quadratic form
    $$
    \pi \mapsto \frac{1}{2} \pi \frac{\partial^2 L^{\text{in}}}{\partial \phi^2}(\hat{\phi}, \theta) \pi^\top - \pi \frac{\partial L^{\text{out}}}{\partial \phi}(\hat{\phi}, \theta)^\top
    $$
    through e.g. gradient descent or conjugate gradient and note $\hat{\pi}$ the approximated result;
    Estimate the outer-gradient with
    $$
    \hat{\nabla}_\theta := \frac{\partial L^{\text{out}}}{\partial \theta}(\hat{\phi}, \theta) - \pi \frac{\partial^2 L^{\text{in}}}{\partial \theta \partial \phi}(\hat{\phi}, \theta);
    $$

    **Equilibrium propagation**
    Minimize $L(\phi, \theta, \beta) = L^{\text{in}}(\phi, \theta) + \beta L^{\text{out}}(\phi, \theta)$ with respect to $\phi$ for some small non-zero $\beta$ value (potentially for more $\beta$ values if needed), starting from $\hat{\phi}$, and note $\hat{\phi}_\beta$ the result;
    Estimate the outer-gradient with
    $$
    \hat{\nabla}_\theta := \frac{1}{\beta} \left( \frac{\partial L}{\partial \theta}(\hat{\phi}_\beta, \theta, \beta) - \frac{\partial L}{\partial \theta}(\hat{\phi}, \theta, 0) \right)
    $$
    or with an estimator that uses more points;
    Update $\theta$ using $\hat{\nabla}_\theta$;
```

Hessian condition needed in Theorem 2.1.1 is satisfied and the quadratic form (10) is positive definite so it has a unique minimizer, which is $\pi^*$. 

**Choice of the optimizer.** Naively minimizing the quadratic form (10) does not yet lead to a practical algorithm. Let us take the example of gradient descent. An update would take the form

$$
\pi \leftarrow \pi - \alpha \left( \pi \frac{\partial^2 L^{\text{in}}}{\partial \phi^2}(\phi^*_\theta, \theta) - \frac{\partial L^{\text{out}}}{\partial \phi}(\phi^*_\theta, \theta) \right)
$$

(11)

with $\alpha$ the learning rate. This appears to require computing the Hessian $\frac{\partial^2 L^{\text{in}}}{\partial \phi^2}$, and then multiplying it with the vector $\pi$, an operation with quadratic complexity which would render the method impractical. However, there is a way of obtaining the update above without ever having to explicitly calculate the Hessian: a cleverer implementation exploits the fact that all we need is a Hessian-vector product. Remarkably, such products
can be computed at approximately the same cost as computing gradients (Pearlmutter, 1994). Gradient descent, and in fact many other optimization procedures, can therefore be executed efficiently. We call this process the second phase, when the first phase consists in computing $\phi^*_\theta$.

Implicit differentiation methods take different forms depending on the choice of the optimizer. When gradient descent is chosen as in (11), this leads to recurrent backpropagation, also known as the Almeida-Pineda algorithm (Almeida, 1990; Pineda, 1987)\(^4\). The very same update of recurrent backpropagation can be obtained from different perspectives. For example, it can be derived starting from the Neumann series formulation of the inverse of a matrix (Liao et al., 2018; Lorraine et al., 2020): we have

$$\left( \frac{\partial^2 L_{\text{in}}}{\partial \phi^2} (\phi^*_\theta, \theta) \right)^{-1} = \alpha \left( \frac{\partial^2 L_{\text{in}}}{\partial \phi^2} (\phi^*_\theta, \theta) \right)^{-1}$$

$$= \alpha \sum_{i=0}^{\infty} \left( \text{Id} - \alpha \frac{\partial^2 L_{\text{in}}}{\partial \phi^2} (\phi^*_\theta, \theta) \right)^i \quad (12)$$

whenever the absolute eigenvalues of $(\text{Id} - \alpha \frac{\partial^2 L_{\text{in}}}{\partial \phi^2} (\phi^*_\theta, \theta))$ are strictly smaller than one (which requires $\alpha$ small enough). We cannot use this formula alone as it still requires computing the Hessian but we can use it to iteratively approximate $\pi^*$ using

$$\pi \leftarrow \pi \left( \text{Id} - \alpha \frac{\partial^2 L_{\text{in}}}{\partial \phi^2} (\phi^*_\theta, \theta) \right) + \alpha \frac{\partial L_{\text{out}}}{\partial \phi} (\phi^*_\theta, \theta), \quad (13)$$

which is exactly the same update than (11). This is why we used the same notation for the learning rate and the rescaling parameter even though we introduced those two parameters from different contexts. Alternatively, this update also appears in truncated backpropagation (Williams and Peng, 1990) when gradient descent on $L_{\text{in}}$ has reached a minimum for several steps (Shaban et al., 2019). Backpropagating through the last iteration takes exactly the same form than (11), but it requires storing the intermediate states in memory as opposed to recurrent backpropagation.

Gradient descent is a very general algorithm. Since we want to minimize a specific kind of function, one may ask whether more tailored optimization procedures might be more efficient. This is what the conjugate gradient method (Shewchuk, 1994) provides (details of the algorithm can be found in Appendix B), while still only requiring Hessian-vector products.

Note that we can obtain first-order approximations of the outer-gradient by limiting the number of steps in the second phase. If we skip the second minimization and approximate the result by $\pi = 0$, the corresponding approximate outer-gradient will be

\[^4\]The usual way of deriving recurrent backpropagation is by using iterative updates to find the solution of the linear system $\pi \frac{\partial^2 L_{\text{in}}}{\partial \phi^2} (\phi, \theta) = \frac{\partial L_{\text{out}}}{\partial \phi} (\phi, \theta)$. Although this is equivalent to gradient descent on the quadratic form when applied to bilevel optimization, this view allows considering the more general case in which equilibrium states are not necessarily minimizers of a loss function. Here, we use the quadratic form minimization view as it makes the comparison to other methods easier.
equal to the direct gradient $\partial_\theta L^{\text{out}}(\phi^*_\theta, \theta)$. If we perform only one step and take $\alpha = 1$, we approximate the Hessian with the identity (Luketina et al., 2016). The amount of compute attributed to the second phase therefore progressively transforms a first-order approximation towards the true value of the gradient.

**Some practical considerations.** In practice we almost never directly minimize (10) as we do not have access to an exact minimizer $\phi^*_\theta$ of the inner loss, but only to an estimate $\hat{\phi}$. Instead, we use the estimated version of the quadratic form (replacing $\phi^*_\theta$ by $\hat{\phi}$) as shown in Algorithm 1.

In many applications, $L^{\text{in}}$ is the empirical risk, that is the average of some loss evaluated on many different data samples. In this case, it might not be possible to compute Hessian-vector products for all the data at once. To work around this issue we can resort to stochastic updates on the quadratic (taking a random subset of the data for each step), as noted in the lecture notes of Grosse (2021).

**Robustness to non-optimality †.** As mentioned above, the local minimizer $\phi^*_\theta$ is almost always approximated in practice. A natural question to ask is whether the methods introduced above are robust to this approximation. In other words, we may ask how good $\hat{\nabla}_\theta$ is compared to $\nabla_\theta$, with

$$\hat{\nabla}^\top_\theta = \frac{\partial L^{\text{out}}}{\partial \theta}(\hat{\phi}, \theta) - \hat{\pi} \frac{\partial^2 L^{\text{in}}}{\partial \theta \partial \phi}(\hat{\phi}, \theta),$$

as in Algorithm 1. In the last equation, $\hat{\pi}$ is obtained by iteratively minimizing the estimated version of the quadratic form (10), that consists in replacing $\phi^*_\theta$ by $\hat{\phi}$. Its estimation will therefore be the other source of approximation.

We are doing approximate gradient descent at the outer-level, which will result in approximate solutions of the bilevel optimization problem. d’Aspremont (2008) and Friedlander and Schmidt (2012) have shown that the error made in solving a convex optimization problem with inexact gradients can be linked to the gradient approximation error $\|\hat{\nabla}_\theta - \nabla_\theta\|$. Motivated by those results we present a theoretical bound on the error made in estimating the outer-gradient $\nabla_\theta$ with $\hat{\nabla}_\theta$ depending on the quality of $\hat{\phi}$ and $\hat{\pi}$.

**Assumption 3.1.1.** Suppose that there exists positive real numbers ($\mu, \rho, B, L, M$) such that:

i. $L^{\text{in}}$ is twice continuously differentiable and $L^{\text{out}}$ is continuously differentiable.

ii. $L^{\text{in}}$ is $\mu$-strongly convex as a function of $\phi$.

iii. The second-order derivatives (Hessian and cross derivatives) of $L^{\text{in}}$ are $\rho$-Lipschitz as functions of $\phi$.

iv. As functions of $\phi$, $L^{\text{out}}$ is $B$-Lipschitz, $L$-smooth and $\partial_\theta L^{\text{out}}$ is $M$-Lipschitz,
Theorem 3.1.2 (Error bound for implicit differentiation methods (Pedregosa, 2016)).

Let $\phi^*_{\theta}$ be a minimizer of $L_{\text{in}}$ and $\hat{\phi}$ be its approximated value. Let $\delta \in [0, \frac{1}{2}]$ be an upper bound on the corresponding approximation error:

$$\|\phi^*_{\theta} - \hat{\phi}\| \leq \delta.$$  

Let $\tilde{\pi}$ be an approximation of $\pi^*$ computed by one of the implicit differentiation methods and $\delta' > 0$ be an upper bound of its approximation error:

$$\|\tilde{\pi} - \partial_{\phi} L_{\text{out}}(\hat{\phi}, \theta) \partial^2_{\phi} L_{\text{in}}(\hat{\phi}, \theta)^{-1}\| \leq \delta'.$$

Then, under Assumption 3.1.1, there exists a constant $C$ such that

$$\|\nabla_{\theta} - \hat{\nabla}_{\theta}\| \leq C(\delta + \delta').$$

The quantities $\delta$ and $\delta'$ measure the error made in the two phases of the algorithms, where the first phase consists in finding a minimum of $L_{\text{in}}$ and the second one in minimizing the local quadratic form. Theorem 3.1.2 shows that the approximation error in the outer-gradient grows linearly with those two errors. Assumption 3.1.1 ensures that the problem we are considering and its derivatives are well defined (i. and ii.) and that $L_{\text{in}}$ and $L_{\text{out}}$ are regular enough (iii. and iv.).

We present a proof of Theorem 3.1.2 along with a discussion on how to transform the global convexity assumptions into local ones in Appendix C.2.

3.2 Equilibrium propagation

Instead of differentiating through the implicit functions, we can resort to another mathematical result known as equilibrium propagation (Scellier and Bengio, 2017), which reformulates the outer-gradient in a way that is easier to estimate numerically. While equilibrium propagation was originally presented in the context of energy-based recurrent neural network learning, the result is far more general. As we discuss next, equilibrium propagation can in fact be applied to solve general bilevel optimization problems.

Equilibrium propagation theorem. The first step in equilibrium propagation consists in breaking up the hierarchy of losses and mixing $L_{\text{in}}$ and $L_{\text{out}}$ in an augmented loss

$$\mathcal{L}(\phi, \theta, \beta) := L_{\text{in}}(\phi, \theta) + \beta L_{\text{out}}(\phi, \theta).$$

The nudging strength $\beta$ is a scalar that controls the strength of the mix; when it is equal to 0, we retrieve the inner learning problem. We denote by $\phi^*_{\theta, \beta} \in \arg \min_{\phi} \mathcal{L}(\phi, \theta, \beta)$ the different minimizers of $\mathcal{L}$. The equilibrium propagation result can now be introduced.

Theorem 3.2.1 (Equilibrium propagation (Scellier and Bengio, 2017; Scellier, 2021)). Let $L_{\text{in}}$ and $L_{\text{out}}$ be two twice continuously differentiable functions. Let $\hat{\phi}$ be a stationary point of $\mathcal{L}(\cdot, \bar{\theta}, \beta)$, i.e.,

$$\frac{\partial \mathcal{L}}{\partial \phi}(\hat{\phi}, \bar{\theta}, \beta) = 0,$$
such that $\partial^2_\phi L(\tilde{\phi}, \tilde{\theta}, \tilde{\beta})$ is invertible. Then, there exists a neighborhood of $(\tilde{\theta}, \tilde{\beta})$ and a continuously differentiable function $(\theta, \beta) \mapsto \phi^*_\theta$ such that $\phi^*_\theta = \tilde{\phi}$ and for every $(\theta, \beta)$ in this neighborhood we have

$$\frac{\partial L}{\partial \phi} (\phi^*_\theta, \theta, \beta) = 0$$

and

$$\frac{d}{d\theta} \frac{d}{d\beta} L (\phi^*_\theta, \theta, \beta) = \frac{d}{d\beta} \frac{d}{d\theta} L (\phi^*_\theta, \theta, \beta)^\top.$$ 

**Proof.** The existence part in the equilibrium propagation theorem directly follows from Theorem 2.1.1 using $f = \partial_\phi L$. Obtaining the differentiation formula is not as complicated as it may appear at first glance. The first step consists in applying the symmetry of second-order derivatives result, also known as Schwartz theorem:

$$\frac{d}{d\theta} \frac{d}{d\beta} L (\phi^*_\theta, \theta, \beta) = \frac{d}{d\beta} \frac{d}{d\theta} L (\phi^*_\theta, \theta, \beta)^\top.$$ 

We then apply the chain rule on both sides of the previous equation and use the equilibrium condition $\partial L (\phi^*_\theta, \theta, \beta) = 0$ to simplify the derivatives. For the left-hand side of the previous equation, it yields

$$\frac{d}{d\theta} \frac{d}{d\beta} L (\phi^*_\theta, \theta, \beta) = \frac{d}{d\beta} \left[ \frac{dL}{d\beta} (\phi^*_\theta, \theta, \beta) + \frac{dL}{d\phi} (\phi^*_\theta, \theta, \beta) \frac{d\phi^*_\theta}{d\beta} \right]$$

$$= \frac{d}{d\beta} \left( \phi^*_\theta, \theta, \beta \right).$$ 

The right-hand side can be simplified in the same way, which gives the desired formula. 

The equilibrium propagation result can be used to reformulate the outer-gradient $\nabla_\theta$ by remarking that $\partial_\beta L = \mathcal{L}_{\text{out}}$ and $\phi^*_\theta |_{\beta=0} = \phi^*_\theta$. We then have

$$\nabla_\theta = \frac{d}{d\beta} \left. \frac{dL}{d\phi} (\phi^*_\theta, \theta, \beta) \right|_{\beta=0}. \quad (16)$$ 

Theorem 3.2.1 uses a stationary condition on the vector $\phi$ but more general versions of equilibrium propagation exist for stationary distributions or trajectories (see Scellier (2021) for more details). A very similar gradient estimate has also been derived when $\phi$ is a discrete quantity and the inner- and outer-losses are expectations measured over a continuous distribution (Hazan et al., 2010; Song et al., 2016).

There is a deep connection between the equilibrium propagation and implicit differentiation approaches: the quantity $\pi^*$ that we defined in Equation 9 is actually indirectly computed in equilibrium propagation, since $\pi^* = \frac{d_\beta \phi^*_\theta}{d_\beta} |_{\beta=0}$. The trajectories in the second phases of equilibrium propagation and implicit differentiation methods can also be shown to be closely related, when gradient descent is used in the second phase for the two methods (Scellier and Bengio, 2019).
Numerical estimation of $\nabla_\theta$. The formula provided by the equilibrium propagation theorem might not appear useful at first. Closer inspection, however, reveals that it offers a new way of numerically estimating the outer-gradient that we seek. The outer-gradient is a derivative of a scalar function with respect to a vector $\theta$, and is thus hard to estimate numerically, in particular when $\theta$ is high-dimensional. By contrast, the right-hand side of (16) is the derivative of a vector-valued function with respect to a scalar, which can be readily estimated with finite difference techniques. The simplest finite difference estimator is:

$$
\hat{\nabla}_\theta^\top := \frac{1}{\beta} \left( \frac{\partial L}{\partial \theta} (\hat{\phi}_\beta, \theta, \beta) - \frac{\partial L}{\partial \theta} (\hat{\phi}_0, \theta, 0) \right),
$$

where $\hat{\phi}_0$ and $\hat{\phi}_\beta$ are the approximated values of $\phi_{*,0}$ and $\phi_{*,\beta}$. This formula yields a two-phase algorithm that is detailed in Algorithm 1. The approximation of the outer-gradient can be refined by adding more points to the estimator, for instance by resorting to the central or forward finite difference estimators. The idea is to collect the value of $\partial_\theta L$ at different values, e.g. $-\beta$ and $\beta$ for the central one with three points (as in Laborieux et al. (2021)) or $0, \beta, 2\beta, \ldots$, for the forward ones. We provide more details to the interested reader in Appendix D.3.

Robustness to non-optimality †. As for implicit differentiation methods, it is possible to bound the error made by the two-point equilibrium propagation estimator (17). There are two sources of error: the approximation of the minimizers in the two phases and the one rooted in the finite difference scheme. When $\beta$ gets smaller, the finite difference error gets smaller. On the other side, decreasing $\beta$ increases the sensitivity of the estimation to noise or inaccurate minimizations. Theorem 3.2.3 quantifies it; we highlight the main elements of the proof in Appendix D.1 and visualize the result on Figure 2.

Assumption 3.2.2. Assume that $L^\text{in}$ and $L^\text{out}$ are three-times continuously differentiable. Additionally, suppose that there exists positive real numbers $(B_\text{in}, B_\text{out}, L, \mu, \rho, \sigma)$ such that $L^\text{in}$ and $L^\text{out}$, as functions of $\phi$, verify the following properties:

1. $\partial_\theta L^\text{in}$ is $B_\text{in}$-Lipschitz and $\partial_\theta L^\text{out}$ is $B_\text{out}$-Lipschitz.
2. $L^\text{in}$ and $L^\text{out}$ are $L$-smooth and $\mu$-strongly convex.
3. their Hessians are $\rho$-Lipschitz.
4. $\partial_\phi \partial_\theta L^\text{in}$ and $\partial_\phi \partial_\theta L^\text{out}$ are $\sigma$-Lipschitz.

Theorem 3.2.3 (Error bound for equilibrium propagation (Zucchet et al., 2021)). Let $\beta > 0$ and $(\delta, \delta')$ be such that

$$
\|\hat{\phi}_0 - \phi_{*,0}^*\| \leq \delta
$$

and

$$
\|\hat{\phi}_\beta - \phi_{*,\beta}^*\| \leq \delta'.
$$
Then, under Assumption 3.2.2, there exists a \( \theta \)-dependent constant \( C \) such that

\[
\| \hat{\nabla}_\theta - \nabla \theta \| \leq \frac{B_{\text{in}}(\delta + \delta')}{\beta} + B_{\text{out}} \delta' + C \frac{\beta}{1 + \beta} =: B(\delta, \delta', \beta).
\]

Figure 2: Visualization of the bound \( B \) from Theorem 3.2.3 (\( C = 1, B_{\text{in}} = B_{\text{out}} = 1 \)), as a function of \( \beta \) (A) and as a function of \( \delta = \delta' \) (B) (figure taken from Zucchet et al. (2021)).

As for implicit differentiation methods, a more local version of Theorem 3.2.3 can be obtained if we replace the strong convexity assumption of \( L_{\text{in}} \) by a non-flat minimum assumption. The behavior of the estimator when the Hessian of \( L_{\text{in}} \) at \( \hat{\phi} \) is not positive definite is however quite different from the other kind of methods. Assuming that \( L_{\text{in}} \) is bounded from below, the second phase ends up in a nearby basin of attraction in the worse case. The gradient estimator will then converge to some finite value, as opposed to implicit differentiation methods that will diverge.

Comparison with implicit differentiation methods †. It is not yet possible to compare the bounds from Theorem 3.1.2 and Theorem 3.2.3 as the bound for equilibrium propagation is still \( \beta \)-dependent. We can remove this dependency through the following corollary, that we prove in Appendix D.2.

**Corollary 3.2.4 (Corollary of Theorem 3.2.2 (Zucchet et al., 2021)).** Under Assumption 3.2.2, if we suppose that for every \( \beta > 0 \) we approximate the two equilibrium points with precision \( \delta \) and \( \delta' \) and if \( (\delta + \delta') < C/B_{\text{in}} \), the best achievable bound in Theorem 3.2.3 is smaller than

\[
B_{\text{out}} \delta' + 2 \sqrt{C B_{\text{in}}(\delta + \delta')}.
\]

The error made in the two-point equilibrium propagation estimator is therefore \( O(\sqrt{\delta + \delta'}) \), which implies that implicit differentiation methods are theoretically less sensitive to approximations in the two phases than equilibrium propagation. We compare in more details the two approaches in the next section.
4 Comparison of the different approaches

Having introduced implicit methods for bilevel optimization, the questions that come next are in which conditions they are useful, and which one to pick. The purpose of this section is not to give a definitive answer to such questions, but to help the reader understand where the different methods shine.

4.1 Implicit methods vs. the rest

When the process used to estimate $\phi^*_\theta$ can be written as a sequence of differentiable operations, backpropagation through time (Werbos, 1990) can be used to compute gradients. In most settings, it is impossible to store the entire sequence of intermediate parameters produced by the algorithm in memory. The standard workaround to this problem is to run (truncate) the backward pass for a limited number of steps (Jaeger, 2002; Shaban et al., 2019) or to use a checkpointing strategy (Gruslys et al., 2016). Whenever backpropagation or its truncated version is applicable, it is often a strong alternative to the implicit methods studied here; it is difficult to rule out a priori one class of methods over the other without experimenting with both.

There is, however, a number of clearly identifiable scenarios in which the methods discussed in this article may be preferable. Perhaps most importantly, it is not always possible to write the underlying optimization algorithm as a differentiable program. For example, an algorithmic solver can provably minimize a smooth loss function, but its inner process is not necessarily differentiable. In such cases, automatic differentiation is not an option, and implicit methods are in general the only gradient-based methods available. Furthermore, even when the learning algorithm is technically differentiable, it may generate chaotic sequences of parameters, which render gradients extremely noisy (Metz et al., 2019). In such situations, the methods studied here may lead to an implicit form of regularization of the learning process, by selecting outer-parameters that are less prone to inducing chaos. More work is needed to investigate this hypothesis.

There is growing interest in physically-plausible learning algorithms, where optimization is performed by a physical system evolving in time (Millar, 1951; Kendall et al., 2020; Stern et al., 2021). It is generally impossible to implement backpropagation in such systems, as this would entail going back in (physical) time; even for reversible processes it is difficult to conceive backpropagation through time, since the computations performed in the forward and backward phases of this algorithm are not the same. Provided that the process which governs the time evolution of the parameters is differentiable, forward differentiation (also known as real-time recurrent learning, cf. Williams and Zipser, 1989) is the classic alternative to backpropagation which avoids going backwards in time. However, in its original form, this algorithm is typically infeasible to implement as well. First, its memory requirements scale with the dimension of $\theta$ multiplied by the dimension of $\phi$, which results in a huge memory cost. This is in fact a concern for most standard computer implementations as well. Second, the algorithm requires computing Jacobian-vector products, which may or may not be difficult to calculate.
in physical systems. Most of the concerns outlined above apply equally when looking at backpropagation or forward differentiation as biological learning algorithms. Some approximations have been developed to circumvent these limitations (Sutton, 1992; Tallec and Ollivier, 2018; Bellec et al., 2020; Marschall et al., 2020; Menick et al., 2021).

4.2 Comparison of the different implicit methods

Finally, we compare the methods presented in the previous sections. More concretely, we consider methods which use first-order (FO) approximations of the outer-gradient\(^5\), equilibrium propagation (EP), recurrent backpropagation (RBP), and the conjugate gradient (CG) method. We determine use cases for the different methods based on three criteria: efficiency when all the assumptions are met, robustness to violation of the assumptions, and simplicity of the methods in terms of the computational elements involved. The result of the comparison is summarized in Table 1.

### Table 1: Summary of the comparison between methods rooted in implicit differentiation

| Method                  | Efficiency | Robustness | Simplicity |
|-------------------------|------------|------------|------------|
| First-order approximation| +          | +++        | +++        |
| Recurrent backpropagation| ++         | ++         | +          |
| Conjugate gradients     | +++        | +          | +          |
| Equilibrium propagation | ++         | ++         | ++         |

Note that, as we mentioned in Section 3.1, those methods can be seen as implicit differentiation methods with extremely short second phases.
Robustness to violated assumptions. In the last paragraph we assumed that we are sufficiently close to minimizing the inner loss so that all implicit methods are properly justified. We now look at how they behave when those conditions are not met. First-order methods here shine as they just perform a crude approximation and do not rely on those assumptions. In principle both CG and RBP would have a diverging second phase if the Hessian is not positive definite but in practice it seems that CG is much more unstable (Liao et al., 2018; Lorraine et al., 2020; Grosse, 2021). EP does not have diverging second phase as long as $\beta \geq 0$ and the inner- and outer-losses are bounded from below.

Simplicity of the computational elements. The methods we compare here require different computational elements. While every method requires computing partial derivatives with respect to the outer-parameters, approximate first-order methods stand out in their simplicity of implementation. In particular, these methods do not even require storing the result of the first phase. On the other hand, implicit differentiation methods are the most complex to implement as they involve calculating Hessian-vector products. In digital computers, automatic differentiation software offers efficient implementations of this operation (e.g., (Abadi et al., 2016; Paszke et al., 2019; Bradbury et al., 2018)). However, implementing Hessian-vector products can be challenging in large-scale distributed systems, neuromorphic hardware, or more exotic analog physical systems. Arguably, it is also hard to conceive such operation as being biologically-plausible.

Which method to choose? First-order methods tend to work best off-the-shelf, without extensive tuning, so they are a good choice if performance is not the most important criterion. When performance is important and inner-optimization is easy enough so that it is possible to closely approximate a local minimum of the inner loss function, the conjugate gradient method is the best one. If it reveals to be too unstable, recurrent backpropagation might solve those instability issues. Finally, if computing Hessian-vector-products is not an option, but performance is still important, equilibrium propagation is worth being considered.

5 Conclusion

We have presented bilevel optimization in a broad machine learning context and discussed gradient-based methods to solve such problems. Framing learning through bilevel optimization generalizes the traditional cost-minimization view of learning to computations that are not necessarily explicitly described, and that therefore cannot be learned through gradient descent with backpropagated errors. The implicit methods we reviewed here, either rooted in implicit differentiation or in equilibrium propagation, allow computing gradients for such problems using local information, and sometimes using only elementary operations. These properties may turn out to be of particular importance for the development of biological theories of learning, as well as for the development of
next-generation learning machines.

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A Some bilevel optimization formulations

A.1 Energy-based neural networks

Energy-based are neural networks whose internal states are implicitly defined as minimizers of some energy function. This fundamentally differs from the classical description of feedforward neural networks where the computations perform by each layer are explicitly described. We here compare both formulations as it nicely highlights the differences between the two paradigms.

**Explicit description of neural networks.** Neural networks are usually described through the computations that they perform to process an input signal $x$. For a feedforward neural network it usually takes the following form:

$$
\phi^0 = x, \quad \phi^{l+1} = \rho(W^l \phi^l + b^l)
$$

where $\phi^l$ corresponds to the activity of the neurons from the $l$-th layer, $\rho$ to a non-linear activation function, $W^l$ to the weights connecting layer $l$ to layer $l+1$ and $b^l$ to the biases of layer $l$. In the supervised learning framework, the activity $\phi^L$ at the very last layer is compared to a desired output $y$ through a cost function $C(\phi^L, y)$. Learning is then done by minimizing the expected cost averaged over all the training samples through stochastic gradient descent (Bottou, 2010) on the parameters $\theta = \{W, b\}$. The backpropagation algorithm (Linmainmaa, 1976; Werbos, 1982; Rumelhart et al., 1986) which propagates the error measured at the last layer towards the first layers of the network to compute gradients. It is very efficient as is it particularly suited to the way information is processed.

**Energy-based description.** An alternative description of neural networks is to consider that the activity is an equilibrium point of some energy function $E$. Going from an explicit to an implicit description is easy for the feedforward neural network$^6$: the energy function

$$
E(\phi, \theta, x) := \frac{1}{2} \|\phi^0 - x\|^2 + \frac{1}{2} \sum_{l=0}^{L-1} \|\phi^{l+1} - \rho(W^l \phi^l + b^l)\|^2
$$

has only one global minimizer which is the neuronal activity $\phi^*_\theta$, as computed through the feedforward processing described above. Interestingly the same energy has been extensively studied in the predictive coding framework (Rao and Ballard, 1999; Whittington and Bogacz, 2017) where it is derived from an approximate probabilistic approach.

The energy formulation is more general as many other type of energy functions can be used, such as the Hopfield energy (Hopfield, 1984; Scellier and Bengio, 2017), thus describing different form of computations. Although the term *energy* has a physical

---

$^6$Similar manipulations can be done in general to obtain an implicit description of a system from an explicit one.
meaning, physical networks can minimize other quantities than the physical energy, such as the co-content for electrical circuits (Millar, 1951; Kendall et al., 2020).

Under this paradigm, learning under supervision can be formulated as the following bilevel optimization:

\[
\min_\theta \mathbb{E}_{(x,y)}[C(\phi^*_\theta, y)] \\
\text{s.t. } \phi^*_\theta \in \arg \min_\phi E(\phi, \theta, x). \tag{20}
\]

### A.2 Hyperparameter optimization and meta-learning

We have briefly introduced bilevel optimization for hyperparameter optimization and meta-learning in Section 1.3. Recall that in this context bilevel optimization generally takes the form

\[
\min_\theta \mathbb{E}_\tau \left[ L^{\text{out}}(\phi^*_\tau, \theta, D^{\text{val}}_\tau) \right] \\
\text{s.t. } \phi^*_\tau, \theta \in \arg \min_\phi L^{\text{in}}(\phi, \theta, D^{\text{train}}_\tau), \tag{21}
\]

where expectation is taken over multiple tasks for meta-learning and over a single one for hyperparameter optimization (the expectation then disappears).

The purpose of this section is to underline the diversity of interactions between inner and outer-parameters. We have mentioned in Section 1.3 that the outer-parameters can be the parameters of a quadratic regularization in the context of hyperparameter optimization (Goutte and Larsen, 1998; Bengio, 2000) but the very same regularizer can be used in meta-learning (Rajeswaran et al., 2020; Zucchet et al., 2021). An other example is when the outer-parameters are the weights of a hypernetwork (Ha et al., 2017) that take the inner-parameters as input to produce the weights of the network that processes incoming data (Lorraine and Duvenaud, 2018; MacKay et al., 2019; Zhao et al., 2020). The task-specific modification can also be done at the neurons level (Zintgraf et al., 2019; Mudrakarta et al., 2019; Zucchet et al., 2021) while keeping the weights of the neural network shared across tasks. Alternatively, the task-shared outer-parameters can be the weights of a neural network that acts as a feature extractor that will help a task-specific classifier or regressor parameterized by the inner-parameters to solve the task at hand (Raghu et al., 2020; Lee et al., 2019; Bertinetto et al., 2019).

### A.3 Generative adversarial networks

Generative adversarial networks (Goodfellow et al., 2014; Metz et al., 2017) consist in a generative and a discriminative network that are learned in an adversarial fashion. The discriminator, parametrized by \( \phi \) has to distinguish between samples generated by the generator and samples coming from the true data distribution \( p(x) \). On the other side, the objective of the generative model \( g_\theta \) is to generate samples that fool a perfect
discriminator $D_{\phi^*}$. The corresponding optimization bilevel optimization problem is:

$$\begin{align*}
\min_{\theta} & \quad -E_{z \sim \mathcal{N}(0,1)} \left[ \log D_{\phi^*}(g_{\theta}(z)) \right] \\
\text{s.t.} & \quad \phi^*_{\theta} \in \arg \min_{\phi} E_{x \sim p(x)} \left[ \log D_{\phi}(x) \right] + E_{z \sim \mathcal{N}(0,1)} \left[ \log (1 - D_{\phi}(g_{\theta}(z))) \right].
\end{align*}$$

(22)

### A.4 Actor-critic

Some reinforcement learning problems can be formulated as bilevel optimization, such as actor-critics (Konda and Tsitsiklis, 2000). The objective there is to learn an actor, which is a policy that tries to maximize the expected reward received while interacting with an environment. It receives help from a critic, an action-value function, which gives better feedback to the actor than the reward only. Following (Pfau and Vinyals, 2016; Yang et al., 2019; Zhou et al., 2020; Hong et al., 2020), training an actor-critic can be formulated as

$$\begin{align*}
\max_{\theta} & \quad \mathbb{E}_{s \sim \rho, \ a \sim \pi_{\theta}(\cdot | s)} \left[ Q_{\phi^*_{\theta}}(s, a) \right] \\
\text{s.t.} & \quad \phi^*_{\theta} \in \arg \min_{\phi} \mathbb{E}_{s \sim \rho, \ a \sim \pi_{\theta}(\cdot | s)} \left[ (Q_{\phi}(s, a) - Q^{\pi_{\theta}}(s, a))^2 \right],
\end{align*}$$

(23)

where $\rho$ is the initial state distribution, $\pi_{\theta}(\cdot | s)$ is the policy distribution parametrized by $\theta$ (the actor), $Q^{\pi_{\theta}}$ its corresponding Q-function and $Q_{\phi}$ the approximate Q network (the critic). Similar formulation exist in model-based reinforcement learning where the critic is replaced by a model which tries to predict the feature (Rajeswaran et al., 2020).

### A.5 Stackelberg games

Interestingly the last two examples can be given a game-theoretic interpretation through the notion of Stackelberg games. Stackelberg games (von Stackelberg, 1934) are a class of games where two players, a leader and a follower, play with a hierarchical order. The leader $\theta$ has a strategic advantage: it plays first and knows what will be the perfect answer of the follower $\phi$. In the bilevel optimization framework, the follower best response minimizes the inner-loss and the leader optimizes the outer-loss knowing the perfect answer of the follower $\phi^*_{\theta}$.

For generative adversarial networks, the generator is the leader and the discriminator the follower in the Stackelberg game terminology (Fiez et al., 2020). For actor-critic methods, the actor is the leader, as we ultimately want to get a good working policy, and the critic the follower (Zheng et al., 2021).

### B Pseudo-code for the conjugate gradient method

The pseudo-code of the conjugate gradients algorithm that estimates the quantity $\hat{\pi}$, as needed by Algorithm 1, is presented in Algorithm 2.
Algorithm 2: Conjugate gradient method

Input: number of steps $k$, estimate $\hat{\phi}$ of $\phi^*$

Result: $\hat{\pi}$

Note $A := \partial^2 L_{\text{in}}(\hat{\phi}, \theta)$ and $b := \partial_{\phi} L_{\text{out}}(\hat{\phi}, \theta)$;

Introduce $\hat{\pi}_0 := 0$, $r := b$, $p := r$;

for $i < k$ do
  $\alpha = (rr^\top)/(pAp^\top)$;
  $\hat{\pi}_{i+1} = \hat{\pi}_i + \alpha p$;
  $r' = r - \alpha p$;
  $\beta = r'r'^\top/rr^\top$;
  $p = r' + \beta p$;
  $r = r'$;

Return $\hat{\pi}$;

---

C Theoretical analysis for implicit differentiation methods

C.1 Proof of Theorem 3.1.2

We here prove Theorem 3.1.2. The proof is inspired from Pedregosa (2016), which proves a very similar result under local assumptions, and Rajeswaran et al. (2019) which uses global assumptions and study the regularized inner loss we studied in Section 1.3. The proof we here present uses the general formulation of the former with the stronger assumptions of the latter, in the goal of making the proof as insightful as possible to the reader.

Let us first rewrite the assumptions and the statement of the theorem.

Assumption 3.1.1. Suppose that there exists positive real numbers $(\mu, \rho, B, L, M)$ such that:

i. $L_{\text{in}}$ is twice continuously differentiable and $L_{\text{out}}$ is continuously differentiable.

ii. $L_{\text{in}}$ is $\mu$-strongly convex as a function of $\phi$.

iii. The second-order derivatives (Hessian and cross derivatives) of $L_{\text{in}}$ are $\rho$-Lipschitz as functions of $\phi$.

iv. As functions of $\phi$, $L_{\text{out}}$ is $B$-Lipschitz, $L$-smooth and $\partial_{\theta} L_{\text{out}}$ is $M$-Lipschitz,

Theorem 3.1.2. Let $\phi^*_\theta$ be a minimizer of $L_{\text{in}}$ and $\hat{\phi}$ be its approximated value. Let $\hat{\pi}$ be an approximation of $\pi^*$ computed by one of the implicit differentiation methods. Let $\delta \in ]0, \frac{\mu}{4\rho}[\ be such that

$$\|\phi^*_\theta - \hat{\phi}\| \leq \delta$$

and $\delta' > 0$ such that

$$\|\hat{\pi} - \partial_{\phi} L_{\text{out}}(\hat{\phi}, \theta) \partial^2_{\phi} L_{\text{in}}(\hat{\phi}, \theta)^{-1}\| \leq \delta'.$$
Then, under Assumption 3.1.1, there exists a constant $C$ such that

$$||\nabla_\theta - \hat{\nabla}_\theta|| \leq C(\delta + \delta').$$

The main idea of the proof is to show that the outer-gradient estimation error introduced by the implicit differentiation algorithm comes from two different sources: the fixed-point approximation error and the finite number of steps in the estimation of $\hat{\pi}$. Bounding the impact of the first source will be straightforward but the second one requires more work. This stems in the fact that implicit differentiation methods do not directly approximate $\pi^*$ in their second phase but only the proxy $\partial_\phi L^{\text{out}}(\hat{\phi}, \theta) \partial_\phi^2 L^{\text{in}}(\hat{\phi}, \theta)^{-1}$. We therefore need to quantify how far is the proxy from $\pi^*$. This can be done by remarking that the two are solutions of two similar linear systems. Lemma C.1.1 is a result from perturbed linear systems theory that will allow us to upper bound the distance between the two.

**Lemma C.1.1** (Theorem 7.2 (Higham, 2002)). Let $Ax = b$ and $A'x' = b'$ two linear systems with $\|A - A'\| \leq \varepsilon_A$ and $\|b - b'\| \leq \varepsilon_b$. If $\varepsilon_A \|A^{-1}\| < 1$, then

$$\|x - x'\| \leq \frac{\|A^{-1}\|}{1 - \varepsilon_A \|A^{-1}\|} (\varepsilon_b + \varepsilon_A \|A^{-1}b\|\varepsilon_A).$$

**Proof.** Consider the quantity $A(x' - x)$. It is equal to

$$A(x' - x) = A'x' + (A - A')x' - Ax$$
$$= b' + (A - A')x' - b$$
$$= b' - b + (A - A')x + (A - A')(x' - x).$$

Then,

$$x' - x = A^{-1} (b' - b + (A - A')A^{-1}b + (A - A')(x' - x))$$

so

$$\|x' - x\| \leq \|A^{-1}\| (\varepsilon_b + \varepsilon_A \|A^{-1}b\| + \varepsilon_A \|x' - x\|),$$

which yields the required result after subtracting $\varepsilon_A \|A^{-1}\||x' - x||$ to both sides. $\square$

With this result, we can now prove Theorem 3.1.2.

**Proof of Theorem 3.1.2.** Recall that

$$\nabla_\theta^\top = \frac{\partial L^{\text{out}}}{\partial \theta}(\phi^*_\theta, \theta) - \pi^* \frac{\partial^2 L^{\text{in}}}{\partial \theta \partial \phi}(\phi^*_\theta, \theta)$$

for

$$\pi^* = \frac{\partial L^{\text{out}}}{\partial \phi}(\phi^*_\theta, \theta) \left(\frac{\partial^2 L^{\text{in}}}{\partial \phi^2}(\phi^*_\theta, \theta)\right)^{-1}.$$
is estimated with
\[ \hat{\nabla}_\theta^\top = \frac{\partial L_{\text{out}}}{\partial \theta}(\hat{\phi}, \theta) - \hat{\pi} \frac{\partial^2 L_{\text{in}}}{\partial \theta \partial \phi}(\hat{\phi}, \theta). \]

We introduce the shorthand \( \chi^* := \partial_\theta \partial_\phi L_{\text{in}}(\phi^*_\theta, \theta) \) and \( \hat{\chi} \) its estimated counterpart. We then have
\[
\| \nabla_\theta - \hat{\nabla}_\theta \| \leq \left\| \partial_\theta L_{\text{out}}(\phi^*_\theta, \theta) - \partial_\theta L_{\text{out}}(\hat{\phi}, \theta) \right\| + \| \pi^* - \hat{\pi} \| \|
\leq \left\| \left[ \partial_\theta L_{\text{out}}(\phi^*_\theta, \theta) - \partial_\theta L_{\text{out}}(\hat{\phi}, \theta) \right] + \left[ \pi^*(\chi^* - \hat{\chi}) \right] + \left[ (\pi^* - \hat{\pi})\hat{\chi} \right] \right\|
\]

We bound each term.

a) From the Lipschitz continuity of \( \partial_\theta L_{\text{out}} \) comes
\[
\| \partial_\theta L_{\text{out}}(\phi^*_\theta, \theta) - \partial_\theta L_{\text{out}}(\hat{\phi}, \theta) \| \leq M \| \phi^*_\theta - \hat{\phi} \| \leq M \delta.
\]

b) The \( \mu \)-strong convexity of \( L_{\text{in}} \) and the \( B \)-Lipschitz continuity of \( L_{\text{out}} \) implies that
\[
\| \pi^* \| \leq \| \partial_\phi L_{\text{out}}(\phi^*_\theta, \theta) \| \| \partial^2_\phi L_{\text{in}}(\phi^*_\theta, \theta)^{-1} \| \leq \frac{1}{\mu} B.
\]

Using the Lipschitz continuity of the cross derivatives of \( L_{\text{in}} \) we have
\[
\| \hat{\chi} - \chi^* \| \leq \rho \delta
\]
so
\[
\| (\chi^* - \hat{\chi})\pi^* \| \leq \rho \delta\| \pi^* \| \leq \rho \delta \frac{B}{\mu}.
\]

c) Lipschitz continuity of \( \partial_\theta L_{\text{in}} \) yields \( \| \partial_\theta \partial_\phi L_{\text{in}}(\hat{\phi}, \theta) \| \leq M \). With the symmetry of the cross derivatives and the fact that the norm of a matrix equals the norm of its transpose, we have \( \| \hat{\chi} \| \leq M \) and
\[
\| \hat{\chi}(\pi^* - \hat{\pi}) \| \leq M \| \pi^* - \hat{\pi} \|
\]

In the term \( \| \hat{\pi} - \pi^* \| \), we still take into account the error made in the fixed point approximation. We can separate it with
\[
\| \hat{\pi} - \pi^* \| \leq \| \hat{\pi} - \partial_\phi L_{\text{out}}(\hat{\phi}, \theta) \partial^2_\phi L_{\text{in}}(\hat{\phi}, \theta)^{-1} \|
\]
\[
+ \| \partial_\phi L_{\text{out}}(\hat{\phi}, \theta) \partial^2_\phi L_{\text{in}}(\hat{\phi}, \theta)^{-1} - \pi^* \|
\]
\[
\leq \delta' + \| \partial_\phi L_{\text{out}}(\hat{\phi}, \theta) \partial^2_\phi L_{\text{in}}(\hat{\phi}, \theta)^{-1} - \pi^* \|.
\]

The second term now only depends on the fixed point approximation error and can be bounded using Lemma C.1.1. Due to the \( \rho \)-Hessian Lipschitz property of \( L_{\text{in}} \),
\[
\varepsilon_A := \| \partial^2_\phi L_{\text{in}}(\phi^*_\theta, \theta) - \partial^2_\phi L_{\text{in}}(\hat{\phi}, \theta) \| \leq \rho \delta.
\]

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The use of the lemma is then justified by the upper bound assumption on $\delta$:

$$\varepsilon_A \|\partial^2 \phi^* \| \leq \rho \delta / \mu \leq 1/2 < 1.$$ 

The smoothness of $L^\text{in}$ implies

$$\varepsilon_b := \|\partial \phi^* \| \leq L \delta.$$ 

We can now apply the lemma, which yields

$$\|\partial \phi \| \leq \frac{\mu^{-1}}{1 - 1/2} (L \delta + \|\pi^*\| \rho \delta) \leq \frac{2 \delta}{\mu} \left( L + \frac{B \rho}{\mu} \right).$$

We have therefore proved

$$\|\hat{\chi} (\hat{\pi} - \pi^*)\| \leq M \left( \delta + \frac{2 \delta}{\mu} \left( L + \frac{B \rho}{\mu} \right) \right).$$

Gathering the three bounds gives

$$\|\nabla \theta - \hat{\nabla} \theta\| \leq M \delta + \frac{B \rho}{\mu} \delta + M \left( \delta + \frac{2 \delta}{\mu} \left( L + \frac{B \rho}{\mu} \right) \right).$$

Choosing

$$C := M + \frac{B \rho + 2ML}{\mu} + \frac{2MB \rho}{\mu^2}$$

finishes the proof.

\[\square\]

### C.2 Extension to local assumptions

In Theorem 3.1.2 we assumed the strong convexity of $L^\text{in}$ to get a bound on the outer-gradient estimation error. We can get a more local version of it if we only assume that the Hessian at a minimum $\phi^*$ of $L^\text{in}$ is positive definite, i.e., that the minimum is not flat. The idea is to show that when the Hessian is continuous and it is positive definite at $\phi^*_0$, $L^\text{in}$ will be strongly convex in a neighborhood of $\phi^*_0$, which allows to go back to the assumptions of Theorem 3.1.2. This is formalized in Fact C.2.1.

**Fact C.2.1.** Let $\phi^*$ be a local minimum of $L^\text{in}$ such that $\partial^2 \phi^* \theta$ is positive definite. Note $\mu$ its smallest (strictly positive) eigenvalue. If $L^\text{in}$ is $\rho$-Lipschitz Hessian, then $L^\text{in}$ is $\mu/2$-strongly convex on the ball of radius $\mu/2\rho$ centered on $\phi^*$.

Interestingly, the Hessian of $L^\text{in}$ at $\hat{\phi}$ is not necessarily positive semi-definite when $\hat{\phi}$ outside the ball centered in $\hat{\phi}$ with radius $\mu/\rho$ (with the notations of Assumption 3.1.1 and Fact C.2.1). In this case, the quadratic form (10) is not bounded from below and procedures that try to minimize it will diverge.
D Theoretical considerations for equilibrium propagation

D.1 Proof idea for Theorem 3.2.3

We here provide the main elements of the proof of the robustness analysis of Theorem 3.2.3, following the same scheme as in Zucchet et al. (2021). Let us first restate the assumptions and the theorem.

**Assumption 3.2.2.** Assume that \( L^{in} \) and \( L^{out} \) are three-times continuously differentiable. Additionally, suppose that there exists positive real numbers \((B^{in}, B^{out}, L, \mu, \rho, \sigma)\) such that \( L^{in} \) and \( L^{out} \), as functions of \( \phi \), verify the following properties:

i. \( \partial_\theta L^{in} \) is \( B^{in} \)-Lipschitz and \( \partial_\theta L^{out} \) is \( B^{out} \)-Lipschitz.

ii. \( L^{in} \) and \( L^{out} \) are \( L \)-smooth and \( \mu \)-strongly convex.

iii. their Hessians are \( \rho \)-Lipschitz.

iv. \( \partial_\phi \partial_\theta L^{in} \) and \( \partial_\phi \partial_\theta L^{out} \) are \( \sigma \)-Lipschitz.

**Theorem 3.2.3** (Equilibrium propagation error bound (Zucchet et al., 2021)). Let \( \beta > 0 \) and \((\delta, \delta')\) be such that

\[
\|\hat{\phi}_0 - \phi_{\theta,0}^*\| \leq \delta
\]

and

\[
\|\hat{\phi}_\beta - \phi_{\theta,\beta}^*\| \leq \delta'.
\]

Then, under Assumption 3.2.2, there exists a \( \theta \)-dependent constant \( C \) such that

\[
\|\hat{\nabla}_\theta - \nabla_\theta\| \leq \frac{B^{in}(\delta + \delta')}{\beta} + B^{out} \delta' + C \frac{\beta}{1 + \beta} =: \mathcal{B}(\delta, \delta', \beta).
\]

We first introduce without proof several technical lemmas and show how they can be used to prove the desired result. To keep notations concise, we now omit the \( \theta \) dependencies as soon as we consider it fixed.

**Lemma D.1.1.** Under Assumption 3.2.2.ii, there exists a \( \theta \)-dependent constant \( R \) such that, for every positive \( \beta \),

\[
\left\| \frac{d\phi_{\beta}^*}{d\beta} \right\| \leq \frac{LR}{(1 + \beta)^2 \mu}.
\]

**Lemma D.1.2.** Under Assumptions 3.2.2.ii and 3.2.2.iii,

\[
\left\| \frac{d^2\phi_{\beta}^*}{d\beta^2} \right\| \leq \frac{\rho}{\mu} \left\| \frac{d\phi_{\beta}^*}{d\beta} \right\|^2 + \frac{2L}{(1 + \beta)\mu} \left\| \frac{d\phi_{\beta}^*}{d\beta} \right\|.
\]

When Lemma D.1.2 is combined with Lemma D.1.1,

\[
\left\| \frac{d^2\phi_{\beta}^*}{d\beta^2} \right\| \leq \frac{1}{(1 + \beta)^3}.
\]
up to some constant factor.

**Lemma D.1.3.** Under Assumptions 3.2.2.ii, 3.2.2.iii and 3.2.2.iv, there exists a \( \theta \)-dependent constant \( M \) such that

\[
\left\| \frac{d^2}{d\beta^2} \frac{\partial L}{\partial \theta}(\phi^*_\beta, \beta) \right\| \leq M \left( \left\| \frac{d\phi^*_\beta}{d\beta} \right\| + (1 + \beta) \left( \left\| \frac{d\phi^*_\beta}{d\beta} \right\|^2 + \left\| \frac{d^2\phi^*_\beta}{d\beta^2} \right\| \right) \right).
\]

We now have all the necessary tools to prove Theorem 3.2.3.

**Proof of Theorem 3.2.3.** Let us first introduce the outer-gradient estimate at fixed-point:

\[
\left( \tilde{\nabla}_\theta \right)^\top := \frac{1}{\beta} \left( \frac{\partial L}{\partial \theta}(\hat{\phi}_{\theta, \beta}^*, \theta, \beta) - \frac{\partial L}{\partial \theta}(\hat{\phi}_{\theta, 0}^*, \theta, 0) \right).
\]

Note that the difference with the outer-gradient estimate \( \hat{\nabla}_\theta \) is that we here evaluate \( \frac{\partial L}{\partial \theta} \) at the true fixed-points when use the estimated values in \( \tilde{\nabla}_\theta \).

The idea behind the proof is the following: we first separate the outer-gradient approximation error \( \| \nabla_\theta - \tilde{\nabla}_\theta \| \) into the fixed point approximation induced error \( \| \hat{\nabla}_\theta - \tilde{\nabla}_\theta \| \) and the finite difference error \( \| \nabla_\theta - \hat{\nabla}_\theta \| \), and then individually bound those two errors:

a) Bounding the first term directly results from the Lipschitz continuity property of the partial derivatives (Assumption 3.2.2.i). It yields the \( B_{\text{in}}(\delta + \delta')/\beta + B_{\text{out}} \delta' \) part of the bound.

b) The second term requires more work. We use Taylor’s Theorem to show that \( \hat{\nabla}_\theta^* - \nabla_\theta \) is equal to some integral remainder. It then remains to bound what is inside the integral remainder, that is the second-order derivative \( \frac{d^2}{d\beta^2} \frac{\partial L}{\partial \theta}(\phi^*_\beta, \beta) \).

This is exactly what the lemmas we have introduced above do: Lemmas D.1.1 and D.1.2 bound the first and second-order derivatives of \( \beta \mapsto \phi^*_\beta \) and Lemma D.1.3 bounds \( \frac{d^2}{d\beta^2} \frac{\partial L}{\partial \theta}(\phi^*_\beta, \beta) \) with the norm of the two derivatives we have just bounded. We only need to manipulate the exact (and not the approximate) fixed points to this term.

We can now do the proof. We first separate the sources of error from the outer-gradient estimation error using the triangle inequality:

\[
\| \hat{\nabla}_\theta - \nabla_\theta \| \leq \underbrace{\| \hat{\nabla}_\theta - \tilde{\nabla}_\theta \| \}_{\text{a)}} + \underbrace{\| \tilde{\nabla}_\theta - \nabla_\theta \| \}_{\text{b)}}
\]

We bound each of the error terms individually:

a) Recall that

\[
\hat{\nabla}_\theta^\top = \frac{1}{\beta} \left( \frac{\partial L}{\partial \theta}(\phi^*_\beta, \beta) - \frac{\partial L}{\partial \theta}(\hat{\phi}_{\theta, 0}^*, 0) \right)
\]
and that a similar formula holds for $\hat{\nabla}_\theta^*$ (evaluated at the fixed points instead of the approximations). It follows that

$$
\|\hat{\nabla}_\theta - \hat{\nabla}_\theta^*\| \leq \frac{1}{\beta} \left( \left\| \frac{\partial \mathcal{L}}{\partial \theta}(\phi_\beta, \beta) - \frac{\partial \mathcal{L}}{\partial \theta}(\phi_\beta^*, \beta) \right\| + \left\| \frac{\partial \mathcal{L}}{\partial \theta}(\phi_0, 0) - \frac{\partial \mathcal{L}}{\partial \theta}(\phi_0^*, 0) \right\| \right).
$$

Since $\phi \mapsto \frac{\partial \mathcal{L}}{\partial \theta}(\phi, \beta)$ is a $(B^{in} + \beta B^{out})$-Lipschitz function as a sum of $\frac{\partial \mathcal{L}}{\partial \theta}$ and $\beta \frac{\partial \mathcal{L}}{\partial \theta}$, two Lipschitz continuous functions with constants $B^{in}$ and $\beta B^{out}$, two Lipschitz continuous functions with constants $B^{in}$ and $\beta B^{out}$,

$$
\|\hat{\nabla}_\theta - \hat{\nabla}_\theta^*\| \leq \frac{B^{in} + \beta B^{out}}{\beta} \|\hat{\phi}_\beta - \phi_\beta^*\| + \frac{B^{in}}{\beta} \|\hat{\phi}_0 - \phi_0^*\|
$$

$$
\leq \frac{B^{in} + \beta B^{out}}{\beta} \delta' + \frac{B^{in}}{\beta} \delta.
$$

b) Taylor’s Theorem applied to $\beta \mapsto \frac{\partial \mathcal{L}}{\partial \theta}(\phi_\beta^*, \beta)$ up to the first order of differentiation yields

$$
\frac{\partial \mathcal{L}}{\partial \theta}(\phi_\beta^*, \beta) = \frac{\partial \mathcal{L}}{\partial \theta}(\phi_0^*, 0) + \beta \frac{d}{d\beta} \frac{\partial \mathcal{L}}{\partial \theta}(\phi_0^*, 0) + \int_0^\beta (\beta - t) \frac{d^2}{d\beta^2} \frac{\partial \mathcal{L}}{\partial \theta}(\phi_t^*, t) dt.
$$

The equilibrium propagation theorem, which is applicable thanks to Assumption 3.2.2.ii, gives

$$
\nabla_\theta = \left. \frac{d}{d\beta} \frac{\partial \mathcal{L}}{\partial \theta}(\phi_\beta^*, \beta) \right|_{\beta=0},
$$

hence

$$
\|\hat{\nabla}_\theta^* - \nabla_\theta\| = \frac{1}{\beta} \left\| \int_0^\beta (\beta - t) \frac{d^2}{d\beta^2} \frac{\partial \mathcal{L}}{\partial \theta}(\phi_t^*, t) dt \right\|.
$$

Using the integral version of Cauchy-Schwartz inequality, we have

$$
\|\hat{\nabla}_\theta^* - \nabla_\theta\| \leq \frac{1}{\beta} \int_0^\beta (\beta - t) \left\| \frac{d^2}{d\beta^2} \frac{\partial \mathcal{L}}{\partial \theta}(\phi_t^*, t) \right\| dt.
$$

We now use Lemma D.1.3 combined with Lemmas D.1.1 and D.1.2 to bound $d^2_\beta \frac{\partial \mathcal{L}}{\partial \theta}(\phi_t^*, t)$. We focus on the $\beta$ dependencies and don’t write any of the constant factors:

$$
\left\| \frac{d^2}{d\beta^2} \frac{\partial \mathcal{L}}{\partial \theta}(\phi_t^*, t) \right\| \leq \left\| \frac{d\phi_t^*}{d\beta} \right\| + (1 + t) \left( \left\| \frac{d\phi_t^*}{d\beta} \right\|^2 + \left\| \frac{d^2\phi_t^*}{d\beta^2} \right\| \right)
$$

$$
\leq \frac{1}{(1 + t)^2} + (1 + t) \left( \frac{1}{(1 + t)^4} + \frac{1}{(1 + t)^3} \right)
$$

$$
\leq (1 + t)^{-2}.
$$
It follows that
\[
\beta \| \hat{\nabla}_\beta - \nabla_\theta \| \leq \int_0^\beta \frac{(\beta - t)}{(1 + t)^2} dt \\
= (1 + \beta) \int_0^\beta \frac{1}{(1 + t)^2} dt - \int_0^\beta \frac{1}{(1 + t)} dt \\
= (1 + \beta) - \frac{1}{1 + \beta} - \ln(1 + \beta) \\
\leq \beta - \frac{1}{1 + \beta} \\
= \frac{\beta^2}{1 + \beta}.
\]

where the inequality comes from the \( \ln(x) \geq 1 - \frac{1}{x} \) inequality for positive \( x \) (applied to \( x = 1 + \beta \)). There hence exists a constant \( C \) such that
\[
\| \hat{\nabla}_\beta - \nabla_\theta \| \leq C \frac{\beta}{1 + \beta}.
\]

\[\Box\]

D.2 Proof of Corollary 3.2.4

**Corollary 3.2.4** (Corollary of Theorem 3.2.2 (Zucchet et al., 2021)). Under Assumption 3.2.2, if we suppose that for every \( \beta > 0 \) we approximate the two equilibrium points with precision \( \delta \) and \( \delta' \) and if \( (\delta + \delta') < C/B^{\text{in}} \), the best achievable bound in Theorem 3.2.3 is smaller than
\[
B^{\text{out}} \delta' + 2 \sqrt{C B^{\text{in}} (\delta + \delta')}.
\]

**Proof.** The derivative of the bound \( B \) obtained in Theorem 3.2.3 with respect to \( \beta \) is
\[
\frac{\partial B}{\partial \beta}(\delta, \delta', \beta) = -\frac{B^{\text{in}}(\delta + \delta')}{\beta^2} + \frac{C}{(1 + \beta)^2}
\]

and vanishes for \( \beta \) verifying
\[
\beta \left( \sqrt{C} - \sqrt{B^{\text{in}}(\delta + \delta')} \right) = \sqrt{B^{\text{in}}(\delta + \delta')}.
\]

As \( (\delta + \delta') < C/B^{\text{in}} \), the previous criterion is met when \( \beta \) is equal to
\[
\beta^* := \frac{\sqrt{B^{\text{in}}(\delta + \delta')}}{\sqrt{C} - \sqrt{B^{\text{in}}(\delta + \delta')}}
\]
The optimal bound is then

$$B(\delta, \delta', \beta^*) = B^{out}_{\delta'} + \sqrt{B^{in}(\delta + \delta')} \left( \sqrt{C} - \sqrt{B^{in}(\delta + \delta')} \right) + \sqrt{CB^{in}(\delta + \delta')}$$

$$\leq B^{out}_{\delta'} + 2\sqrt{CB^{in}(\delta + \delta')}.$$

### D.3 Multiple points estimator

In Section 3.2, we have presented a way to estimate the outer-gradient formula given by the equilibrium propagation theorem using 2 points. Recall that the equilibrium propagation allows to reformulate the outer-gradient $\nabla_\theta$ as

$$\nabla_\theta = \frac{d}{d\beta} \frac{\partial L}{\partial \theta}(\phi_{\theta,\beta}^*, \theta, \beta) \bigg|_{\beta = 0}.$$ 

The simplest finite different estimator is the two points estimator that we have presented in Section 3.2:

$$\hat{\nabla}_\theta = \frac{1}{\beta} \left( \frac{\partial L}{\partial \theta}(\phi_{0,\beta}^*, \theta, \beta) - \frac{\partial L}{\partial \theta}(\phi_{0,0}^*, \theta, 0) \right).$$

We now derive an estimator that uses several points to make a more accurate estimation of the derivative.

**Forward finite differences.** The objective of this paragraph is to derive the $p$-forward finite difference learning rule that uses $p$ points to get a finer approximation of the outer-gradient. Consider the values of the function $f : t \mapsto \frac{\partial L}{\partial \theta}(\phi_{\theta,t}^*, \theta, t)$ for $t \in \{0, \beta, \ldots, (p - 1)\beta\}$. We seek to find a linear combination of those measurements that approximates $\nabla_\theta = \frac{d}{d\beta} \frac{\partial L}{\partial \theta}(\phi_{\theta,\beta}^*, \theta, \beta) \bigg|_{\beta = 0} = f'(0)$, i.e., find a vector $\alpha \in \mathbb{R}^p$ such that

$$\sum_{i=0}^{p-1} \alpha_i f(i\beta) = \beta f'(0) + O(\beta^p). \quad (24)$$

Taylor series approximation (around $\beta = 0$) and an inversion of the summation indices yield

$$\sum_{i=0}^{p-1} \alpha_i f(i\beta) = \sum_{i=0}^{p-1} \alpha_i \left( \sum_{k=0}^{p-1} f^{(k)}(0) \frac{(i\beta)^k}{k!} + O(\beta^p) \right)$$

$$= \sum_{k=0}^{p-1} \sum_{i=0}^{p-1} \alpha_i f^{(k)}(0) \frac{(i\beta)^k}{k!} + O(\beta^p) \quad (25)$$

$$= \sum_{k=0}^{p-1} f^{(k)}(0) \frac{\beta^k}{k!} \sum_{i=0}^{p-1} \alpha_i i^k + O(\beta^p).$$
In (24) and (25), we have two polynomials in $\beta$ that we want to be equal so all their coefficients have to be the same. We hence need to solve

$$
(\binom{i_k}{i,k} \alpha = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots 
\end{pmatrix},
$$

(26)

where $(\binom{i_k}{i,k})$ is a $p \times p$ invertible Vandermonde matrix. The resolution of such a system can easily be done numerically. The values of $\alpha$ for small $p$ are:

| $p$ | $\alpha_0$ | $\alpha_1$ | $\alpha_2$ | $\alpha_3$ | $\alpha_4$ |
|-----|-------------|-------------|-------------|-------------|-------------|
| 2   | -1          | 1           | 0           | 0           | 0           |
| 3   | -3/2        | 2           | -1/2        | 0           | 0           |
| 4   | -11/6       | 3           | -3/2        | 1/3         | 0           |
| 5   | -25/12      | 4           | -3          | 4/3         | -1/4        |

Note that the 2-forward finite difference learning rule is the same as the finite difference one. In the following, we assume that $\alpha$ satisfies (26). The resulting algorithm is presented in Algorithm 3.

**Algorithm 3: $p$-forward finite difference learning rule**

**Result:** Estimation of $\nabla_\theta$

For every $i \in \{0, \ldots, (p-1)\beta\}$, minimize $\phi \mapsto L(\phi, \theta, i\beta)$, starting from the solution of last step, and note $\hat{\phi}_{i\beta}$ the result;

Estimate $\nabla_\theta$, the derivative of $\theta \mapsto L^{\text{out}}(\phi^*_\theta, \theta)$, using

$$
(\hat{\nabla}_\theta^p)^\top = \frac{1}{\beta} \sum_{i=0}^{p-1} \alpha_i \frac{\partial L}{\partial \theta}(\hat{\phi}_{i\beta}, \theta, i\beta).
$$

Return $\hat{\nabla}_\theta^p$.

**Why forward finite differences?** There exists different kind of finite difference estimators that use multiple points. We chose to present the forward difference ones above as they are the ones that only use estimates for positive $\beta$ values. We illustrate why this may be important on an example.

When using $p = 3$ points, the bias reduction obtained with a forward estimate is similar to the obtained with the symmetric or central estimate

$$
\frac{1}{2\beta} \left( \frac{\partial L}{\partial \theta}(\phi^*_{\theta,\beta}, \theta, \beta) - \frac{\partial L}{\partial \theta}(\phi^*_{\theta,-\beta}, \theta, -\beta) \right)
$$

(27)

---

7See https://en.wikipedia.org/wiki/Finite_difference.
that is used in Laborieux et al. (2021). However, negative $\beta$ values can prove to be problematic. To illustrate that, consider $L^{\text{in}}$ and $L^{\text{out}}$, two $\mu$-strongly convex and $L$-smooth functions (e.g. $L^{\text{in}}(\phi) = L\|\phi\|^2/2$ and $L^{\text{out}}(\phi) = \mu\|\phi\|^2/2$). Then $L$ (here equal to $(L + \beta\mu)\|\phi\|^2/2$) is not bounded from below when $\beta < -L/\mu$ so $\phi^{*}_{\theta, -\beta}$ does not exist anymore and the estimate diverges. When using negative $\beta$ values one therefore as to be careful that all the phases converge.

**When are multiple points estimators worth it?** One can think that adding more points will always lead to a more precise estimation of the outer-gradient. If the approximations $\hat{\phi}_{i\beta}$ of the minimizers $\phi^{*}_{i\beta, \theta}$ are perfect, it will always be the case as the bias is a $O(\beta^p)$ with $p$ the number of points. Using the terminology used in the proof of Theorem 3.2.3, this means that the finite difference error decreases when the number of point increases. However, when we can only obtain approximate minimizers, adding more points aggregates the fixed-point approximation errors made in each phase thus potentially making the estimation error bigger. Whether more points would be useful or not is therefore a practical matter.