Nonsmooth automatic differentiation: a cheap gradient principle and other complexity results

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Abstract

We provide a simple model to estimate the computational costs of the backward and forward modes of algorithmic differentiation for a wide class of nonsmooth programs. Prominent examples are the famous relu and convolutional neural networks together with their standard loss functions. Using the recent notion of conservative gradients, we then establish a “nonsmooth cheap gradient principle” for backpropagation encompassing most concrete applications. Nonsmooth backpropagation’s cheapness contrasts with concurrent forward approaches which have, at this day, dimensional-dependent worst case estimates. In order to understand this class of methods, we relate the complexity of computing a large number of directional derivatives to that of matrix multiplication. This shows a fundamental limitation for improving forward AD for that task. Finally, while the fastest algorithms for computing a Clarke subgradient are linear in the dimension, it appears that computing two distinct Clarke (resp. lexicographic) subgradients for simple neural networks is NP-Hard.

1 Introduction

Automatic evaluation of derivatives: Algorithmic differentiation (AD) appeared around 60 years ago [10,58], and has been since then constantly developed and used in many contexts, see [31,33] for a thorough discussion. Today it is at the core of modern learning architectures [51,40,9], to the point that training a neural network is ultimately a way to combine the outputs of AD. Many practical and theoretical developments are nowadays available: flexible and efficient numerical libraries [1,46,18], an implicit differentiation theory [32,33] and its extensions [2,6,15,13], the adjoint method [26,47,48] with application to neural ODEs [19], “piggyback” style differentiation of optimization algorithms [32,44,12,42], or differentiation of conjugate gradient algorithms [27].

Backward algorithmic differentiation, or backpropagation, plays a particular role when smooth optimization tasks are at stake as it evaluates the gradient of a function at the computational price of a few function evaluations. This property, called the cheap gradient principle [61,53], is at the root of the TensorFlow revolution. The key complexity theoretic version of this result is due to Baur and Strassen [8], it asserts that the arithmetic complexity of the evaluation of the derivative of a

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rational function is at most 5 times the complexity of function evaluation. These results are mainly for smooth differentiable functions \[8, 33\], little is known on the nonsmooth case.

The objective of this paper is precisely to present a simple, general, nonsmooth cheap conservative principle and to explore other complexity results for evaluating nonsmooth derivatives. Let us beforehand discuss the fundamental role of nonsmoothness.

**Nonsmooth AD & computational complexity:** Sorting values, pooling datas, thresholding functions, or determining closest points are some of the most essential numerical decision operations. They are ubiquitous in machine learning and modern optimization. All of them are nonsmooth, and most of them have a very desirable feature: they are cheap to compute, much cheaper than smoothed surrogates. For instance, the famous relu activation in deep learning, whose role is to threshold to zero negative values to allow for the inactivity of neurons, requires in theory only 2 bits encoding.

On the other hand, other nonlinear activations potentially require auxiliary algorithms for their evaluation incurring a higher computational cost. This simplicity of use also comes with the issue of finding an adequate way of training models and thus to differentiate objects.

The standard computational practice of AD consists in applying tools from the differentiable world directly on nonsmooth objects, replacing gradients by surrogate gradients, as for instance Clarke subgradients. This is how AD is performed within TensorFlow, PyTorch or Jax. This approach has shown tremendous success \[40\] and is massively used since the last 10 years. Yet, despite this empirical success, Barton et al. claimed in \[7\] that “there does not seem to exist [at this day] a true analogous reverse AD mode to compute generalized derivatives for nonsmooth functions”, illustrating the difficulty of nonsmooth AD. Conservative gradients were introduced as a faithful mathematical model to this approach by computer scientists \[16, 17, 15\]. Our study primarily aims at providing the conservative calculus with an adequate computational complexity theory, a theory which will therefore match the standard practical approach.

Among the other possible first-order options offered by nonsmooth calculus we also investigate properties of directional derivatives and those of the Clarke subdifferential. For directional derivatives our motivation comes from the fact that this nonsmooth operation has general calculus rules while the Clarke subdifferential is central in terms of variational interpretation.

**Contributions:** The main thesis of this work is that conservative gradients have computational properties similar to smooth derivatives, which are much more favorable than those of alternative nonsmooth oracles such as subgradients or directional derivatives.

- We provide a simple computational model for addressing the question of complexity theory of nonsmooth numerical programs.
- For the backward mode, we prove a cheap conservative gradient principle à la Baur-Strassen. It generalizes the state of the art and model most cases in neural network training. We establish that the cost of computing a conservative gradient is of the same order as the one of function evaluation, modulo constants.

Our results allow provide a theoretical validation of the fact that the cost of backpropagation does not depend on networks’ smoothness.

- For the forward mode, we relate the computational cost of computing $p$ directional derivatives to the cost of $p \times p$ matrix multiplication. We provide lower complexity bounds which illustrates the fact that this deficiency may be improved only to a limited extent. This applies to existing nonsmooth AD frameworks \[36, 37\].
- We establish that computing two distinct elements in the Clarke subdifferential of a given point is NP-hard for simple relu networks. This result also applies to lexicographic subdifferential. In contrast, we show that the problem can be solved in polynomial time for conservative gradients. This reflects the computational difficulty of dealing with the Clarke subdifferential.
- A consequence of independent interest is that deciding if a relu network is differentiable at one point is a NP hard problem.

**Relation with existing work:** Conservative gradients were introduced in \[16, 17\] to model “formal subdifferentiation” used by practitioners and in particular the famous nonsmooth “backpropagation”. They were further studied in \[41, 23, 15\] and empirically investigated in \[11\].
The quest for computationally cheap nonsmooth derivative has a long history in AD literature. Existing works of Griewank [43][30][23][29] are essentially based on piecewise smoothness structures [52]. A cheap subgradient principle was also given in [44], but it requires a very strong qualification condition. As illustrated in [28] such qualification conditions can be computationally hard to check in practice.

In another research line, based on chain rules for directional derivatives, Khan-Barton [36][37][38][71] studied the vector forward mode AD. In particular they investigated the forward AD framework to evaluate elements of the lexicographic subdifferential (see [45]), which is contained in the Clarke subdifferential. The computational ratio overhead they obtain is proportional to the ambient dimension. This contrasts with our cheap gradient principle whose constant is dimension-less.

While these contributions are most relevant to nonsmooth AD, their applicability to large scale learning models is limited. Indeed, they rely on forward AD, and suffer from worst case computational overhead scaling linearly in the dimension contrary to the dimension independent overhead of the “cheap gradient” principle.

Organization of the paper: Section 2 describes a general model of computation which allows to express computational cost and complexity of programs, functions and their derivatives. Section 3 presents elements of nonsmooth analysis and our extension of Baur-Strassen result with the cheap conservative gradient principle and its illustrations. In Section 4 we describe computational lower bounds for the evaluation of directional derivatives, and evaluation of distinct subgradients for simple neural networks.

2 Programs, complexity and Automatic Differentiation

2.1 Calculus model, programs, computational cost and complexity

A dictionary $\mathcal{D}$ is a finite set of real functions, each of them being paired with an elementary program implementing the corresponding function in real arithmetic. The set of elementary programs is denoted by $\mathcal{P}^0(\mathcal{D})$.

Let $\mathcal{D}$ be a dictionary and $k \in \mathbb{N}$. Starting from elementary programs, we define now inductively $\mathcal{P}^k(\mathcal{D})$ the set of numerical programs of level $k$ over $\mathcal{D}$. Let $p, q$ be the inputs and outputs sizes respectively and $m \geq p + q$.

A predecessor relation is a set valued map $\text{pr}: \{1, \ldots, m\} \to \{1, \ldots, m\}$ such that for $i = 1, \ldots, m$

- for $j \in \text{pr}(i)$, $j < i$.
- $\text{pr}(i)$ is empty if $i \leq p$ and nonempty otherwise.

An adapted program sequence $(g_i)_{i=p+1}^{m}$ in $\mathcal{P}^k(\mathcal{D})$, is a set of programs such that $g_i$ has $|\text{pr}(i)|$ input arguments and a single output, for all $i = p + 1, \ldots, m$.

Given $(p, q, m, \text{pr}, (g_i)_{i=p+1}^{m})$, the program given in Algorithm 1 is a program on $\mathcal{D}$.

This allows to define level $k+1$ programs on $\mathcal{D}$ which we denote by $\mathcal{P}^{k+1}(\mathcal{D})$. The set of programs with dictionary $\mathcal{D}$ is $\mathcal{P}(\mathcal{D}) = \bigcup_{k \geq 0} \mathcal{P}^k(\mathcal{D})$. We shall see however that $\mathcal{P}^k(\mathcal{D}) = \mathcal{P}^1(\mathcal{D})$ for all $k$ using modification of the computational graph.

A cost on a dictionary $\mathcal{D}$ is a nonnegative function on $\mathcal{D}$, it extends additively by induction on programs on $\mathcal{D}$ through the rule $\text{cost}(P) = \sum_{i=1}^{m} \text{cost}(g_i)$ where $P$ is a program on $\mathcal{D}$ as described in Algorithm 1.

A direct example is the dictionary of arithmetic functions $\{+, -, \times, /\}$, together addition or multiplication by a fixed constant, denoted by $+c$ and $\times c$ respectively. See also Section A.1. Throughout the paper, we assume that dictionaries contain at least operations $+$ and $\times$.

Algorithm 1:

| Program data: |
|---------------|
| $(p, q, m, \text{pr}, (g_i)_{i=p+1}^{m})$. |

| Input: $x = (x_1, \ldots, x_p)$ |
|-------------------------------|
| 1: for $k = p + 1, p + 2, \ldots, m$ do |
| 2: $x_k = g_k(x_{\text{pr}(k)})$ where $x_{\text{pr}(k)} = (x_i)_{i \in \text{pr}(k)}$. |
| 3: end for |

| Return: $y := (x_j)_{j=m-q+1}^{m}$. |

1Constants need to be distinguished from variables (for instance to define a polynomial).
All program on \( D \) may be represented by a program in \( P_1(D) \) with the same cost, by expanding all \( g_i \) until they reduce to an elementary program. Cost evaluation is therefore done without loss of generality on such a program.

**Programs vs functions:** A program defines a unique input-output function: we say that such a program “computes” or “implements” the corresponding function and use the equivalence relation \( \sim \) for programs computing the same function. The equivalence classes correspond to functions expressible by programs with a given dictionary \( D \). Given a function \( f : \mathbb{R}^p \to \mathbb{R}^q \) and a program \( P \) on dictionary \( D \), with \( p \) inputs and \( q \) outputs, we write \( f = [P]_D \) to denote the fact that \( P \) is in the equivalence class of programs computing \( f \), that is \( P \) implements \( f \).

**Complexity of a function:** The complexity of a given function \( f \) on dictionary \( D \) is the quantity 

\[
\text{comp}(f, D) = \inf_{P = [f]_D} \text{cost}(P)
\]

where the infimum is over all programs implementing \( f \) on the dictionary \( D \). Note that this could be infinite and, if it is finite, then there exists a program which attains the minimum.

**Remark 1 (Programs as directed graphs)** A predecessor relation trivially describes a directed acyclic graph (DAG). Therefore a program \( P \) can equivalently be represented as a DAG whose nodes correspond either to input variables (empty predecessor) or computation nodes (nonempty predecessor). Directed edges connect predecessor nodes to their successors. Each computation node of \( P \) contains a program of lower level (with a single output node), number of input edges being coherent with number of arguments. The cost of a node is the cost of the underlying lower level program and the cost of \( P \) is the sum of the costs of its nodes. Nodes without outer edges are output nodes. Examples are given in Section 2.1.

### 2.2 Automatic differentiation and the “AD complexity lemma”

We pertain to programs implementing functions, that is Algorithm 1 with single outputs \( q = 1 \).

**Definition 1 (Algorithmic differentiation programs)** Let \( P \) be a program as in Section 2.1 with dictionary \( D \). Let \( D' \supset D \) be a derived dictionary where we add the operations required to express generalized derivatives. For each \( i = p + 1, \ldots, m \), we define \( d_i \) a derived program who returns a “vectorial first-order information” for \( d_i \) where \( [d_i]_{D'} : \mathbb{R}^{\text{pr}(i)} \to \mathbb{R}^{\text{pr}(i)} \).

The backward (resp. forward) AD program \( \text{backprop}(P) \) (resp. \( \text{forprop}(P) \)) are given as follows.

**Algorithm 2: Algorithmic differentiation**

**Program data:** \( (p, q, m, \text{pr}, (g_i)_{i=p+1}^m, (d_i)_{i=p+1}^m) \) with \( q = 1 \) in Algorithm 1

**Input:** variables \( (x_1, \ldots, x_m) \) computed by Algorithm 1

1: **Forward mode:** \( \text{forprop}(P) \)
2: Initialize: \( \hat{e}_{kx} = e_k \), \( k = 1, \ldots, p \).
3: for \( k = p + 1, \ldots, m \) do
4: \[ \hat{e}_{xk} = \sum_{j \in \text{pr}(k)} \hat{e}_{xj} d_k[j] \]
5: end for

Return: \( \hat{e}_{xm} \).

1: **Backward mode:** \( \text{backprop}(P) \)
2: Initialize: \( v = e_m \)
3: for \( t = m, \ldots, p + 1 \) do
4: for \( j \in \text{pr}(t) \) do
5: Update coordinate \( j \) of \( v \):
\[ v[j] := v[j] + v[t] d_i[j] \]
6: end for
7: end for

Return: \( (v[1], v[2], \ldots, v[p]) \).

The following is our first main complexity result and the proof is given in Section B.

**Lemma 1 (AD complexity Lemma)** Let \( P \) be a program with a single output node over a dictionary \( D \), given in compositional form as in Section 2.7. Let \( \text{backprop}(P) \) (resp. \( \text{forprop}(P) \)) be as

\[ 2^{\text{Typical example: a selection in Clarke subdifferential, this reduces to the gradient in the } C^1 \text{ case.} \]
in Definition[1] Then, setting:

$$
\omega_b = \max_{i=p+1,m} \left\{ \left( \text{cost}(d_i, g_i) + 2 \max(\text{cost}(+), \text{cost}(\times))p r(i) \right) / \text{cost}(g_i) \right\}, \tag{1}
$$

$$
\omega_f = \max_{i=p+1,m} \left\{ \left( \text{cost}(d_i, g_i) + p|pr(i)|\text{cost}(\times) + p|pr(i)| - 1\text{cost}(+) \right) / \text{cost}(g_i) \right\}
$$

we have cost(backprop($P$, $P$) $\leq \omega_b \times \text{cost}(P)$, and cost(forprop($P$, $P$) $\leq \omega_f \times \text{cost}(P)$.

Denote by $F$ a function implemented by a program $P$ in compositional form (Section [2.1]). If each $d_i$ used in Algorithm [2] is the gradient of a $C^1$ function, then backprop($P$) computes $\nabla F$ [33]. However, in general, without continuous differentiability, as observed in [33] [34] [16] [17], backprop($P$) does not necessarily compute an element of the subdifferential $\partial c F$, even if $d_i$ are selections in the Clarke subdifferential.

3 Computational complexity of conservative gradients

3.1 Nonsmooth generalized gradient

Given a locally Lipschitz continuous function $F : \mathbb{R}^p \to \mathbb{R}$, the Clarke subdifferential of $F$ is defined as

$$
\partial c F(x) = \text{conv} \left\{ \lim_{k \to +\infty} \nabla F(x_k) : x_k \in \text{diff}_F, x_k \to +\infty \right\}
$$

(2)

where diff$F$ is the full measure subset where $F$ is differentiable and $\nabla F$ is the standard gradient [20]. The subdifferential is set-valued, it takes values in subsets of $\mathbb{R}^p$, which we write $\partial c F : \mathbb{R}^p \rightharpoonup \mathbb{R}^p$. For each $x \in \mathbb{R}^p$, elements of $\partial c F(x)$ are called Clarke subgradients of $F$. A selection $d$ in the subdifferential $\partial c F$, is a function $d : \mathbb{R}^p \to \mathbb{R}^p$ such that for all $x \in \mathbb{R}^p$, $d(x) \in \partial c F(x)$. If $F$ is $C^1$ then $\partial c F = \{ \nabla F \}$ everywhere so the only possible selection is $d = \nabla F$. We will manipulate derived dictionaries, which typically choose a selection in the Clarke subdifferential, or more general set-valued maps.

Example 1 For relu: $t \to \max(0, t)$, we have $\partial c \text{relu}(t) = \{0\}$ if $t < 0$, $\{1\}$ if $t > 0$ and $[0, 1]$ if $t = 0$. We may define the function relu$'$ as a selection in $\partial c \text{relu}$:

$$
\text{relu}'(t) = 1, \text{ if } t > 0, \quad \text{relu}'(t) = 0, \text{ otherwise}.
$$

The chain-rule, essential to AD, generally fails for Clarke subgradients. This is why we consider now the more flexible notion of conservative gradients.

Definition 2 (Conservative gradient) Let $F : \mathbb{R}^p \to \mathbb{R}$ be a locally Lipschitz continuous function and $D_F : \mathbb{R}^p \rightharpoonup \mathbb{R}^p$ a locally bounded, nonempty and graph closed set-valued map. Then $D_F$ is a conservative gradient for $F$, if for any absolutely continuous curve $\gamma : [0, 1] \to \mathbb{R}^p$,

$$
\frac{d}{dt} F(\gamma(t)) = \langle v, \dot{\gamma}(t) \rangle \quad \forall v \in D_F(\gamma(t)), \text{ for almost all } t \in [0, 1].
$$

(3)

In this case, $F$ is called path differentiable. Conservative Jacobians are defined similarly. As in Section [5.1] $d : \mathbb{R}^p \to \mathbb{R}^p$ is a selection of $D_F$ if $d(x) \in D_F(x)$ for all $x \in \mathbb{R}^p$.

A rich class of path differentiable functions is given by locally Lipschitz continuous semi-algebraic functions with the Clarke subdifferential as a conservative gradient. Actually, virtually all functions used in machine learning are path differentiable [16] [17].

The most salient facts on path differentiable functions and their conservative gradients are:

* (Clarke subgradient), for all $x \in \mathbb{R}^p$, $\partial c F(x) \subset \text{conv}(D_F(x))$.

* (Gradient almost everywhere) Conservative gradients are gradients a.e [16].

* (First-order oracle) Selection in conservative gradients can be used as surrogate gradients, while preserving convergence guarantees. [16] [17] [15].

Conservative Jacobians can be composited while preserving conservativity [16], a feature which do not enjoy Clarke Jacobians: let $F : \mathbb{R}^p \to \mathbb{R}^m$ $G : \mathbb{R}^m \to \mathbb{R}^l$ be locally Lipschitz continuous mapping, $d_F : \mathbb{R}^p \to \mathbb{R}^{m \times p}$ and $d_G : \mathbb{R}^m \to \mathbb{R}^{l \times m}$ be selections in conservative Jacobians for $F$ and $G$ respectively. Then the product mapping $x \mapsto d_G(F(x)) \times d_F(x)$ is a selection in a conservative Jacobian for $G \circ F$. The use of conservative Jacobians provides a very convenient framework to model AD in the nonsmooth case, see [16] [17].
3.2 Cheap conservative principle and consequences

Theorem 1 (Cheap conservative principle) Let $P$ be a program over the dictionary $\mathcal{D}$ with $p$ inputs, and backprop($P$) its backpropagation program (see Definition 1). Assume that each derived program $d_i$ in $\mathcal{D}'$ outputs a selection in a conservative gradient for the function $[g_i]_{\mathcal{D}}$. Then, $[P]_{\mathcal{D}}$ is path differentiable and backprop($P$) computes a selection in a conservative gradient of $[P]_{\mathcal{D}}$, such that

$$\text{cost}(\text{backprop}(P), P) \leq \omega_p \text{ cost}(P),$$

where $\omega_p$ is given in (1) and is independent of the dimension $p$.

We now explore the computational cost of AD for different dictionaries. We derive simple bounds by giving unit cost to elementary operations.

The class of relu programs Let $\mathcal{D}_{\text{relu}}$ be the dictionary composed of elementary arithmetic operations, logarithm, exponential and the relu function:

$$\mathcal{D}_{\text{relu}} := \{+, \times, +c, \times c, \text{inv}, \exp, \text{log}, \text{relu}\}.$$ 

A relu program $P$ is a program with dictionary $\mathcal{D}_{\text{relu}}$, it can be expressed in a compositional form (Section 2.1) with program sequences in $\mathcal{D}_{\text{relu}}$.

Assumption 1 (Computational Cost) In Algorithms 2, define the dictionary $\mathcal{D}_{\text{relu}}' := \mathcal{D}_{\text{relu}} \cup \{\text{relu}'\}$ with relu' given in Example 1; then, all operations from $\mathcal{D}_{\text{relu}}'$ have unit cost (see Remark 2).

Corollary 1 (Backprop complexity of relu programs) Let $P$ be a relu program, under Assumption 1, we have:

$$\text{cost}(\text{backprop}(P), P) \leq 5\text{cost}(P).$$

Table 1: We can compute the complexity constant of Lemma 1 for $\mathcal{D}_{\text{relu}}$ in the following Table to prove Corollary 1 (more details in appendix B.1). From Assumption 1, cost($+$) = cost($\times$) = 1. For $g \in \mathcal{D}_{\text{relu}}$, $d$ denotes its derived program with dictionary $\mathcal{D}_{\text{relu}}'$.

| $g$ | $+$, $\times$ | $+$, $\times c$ | log | exp | inv | relu |
|-----|--------------|----------------|-----|-----|-----|------|
| $\text{cost}(d, g)$ | 2 | 1 | 1 | 1 | 1 |
| $\text{cost}(d, g) + 2\text{cost}(\times)\text{pr}$ | 5 | 3 | 4 | 3 | 5 | 3 |

Remark 2 (On refined cost systems) The unit cost in Assumption 1 provides a simple interpretation of Corollary 1; the cost of a program represents the total number of numerical operations. This is a rough estimate of computational complexity, which could be refined with different weighting schemes. Despite this simplification, the obtained constant is robust to many different weighting choices. We detail an example in the Appendix B.2 for which the cost of all smooth nonlinear operations different from $+$ or $\times$ is $c_{\text{nonlin}} \geq 1$ and we model the cost of sign branching in computation of relu and relu' with constant $c_{\text{relu}} \geq 0$. This yields the same constant as in Corollary 1.

Chaining backpropagation derived programs Our proposed analysis is flexible enough to describe “programs of programs”.

To illustrate this, let $P$ be a program in compositional form (Section 2.1) with an adapted sequence of programs $(g_i)_{i=p+1}^m$. For any $i = p + 1, \ldots, m$, $g_i$ is a relu program with dictionary $\mathcal{D}_{\text{relu}}$ and such that $\text{cost}(g_i) = l_i$ (number of operations from $\mathcal{D}_{\text{relu}}$). For $l_i \gg p_i$, $g_i$ is a “long program” (with many operations compared to input size). Such programs are programs of relu programs.

We define derived programs as follows $d_i = \text{backprop}(g_i)$ (as in Definition 1) for all $i = p + 1, \ldots, m$. From Corollary 1, we have $\text{cost}(d_i, g_i)/\text{cost}(g_i) \leq 5$. Furthermore, we have $(2\max(\text{cost}(+), \text{cost}(\times))\text{pr}(i))/\text{cost}(g_i) = 2p_i/l_i$. We can estimate $\omega_p = 5 + 2\max(p_i/l_i)$ in Lemma 1. For long programs ($l_i \gg p_i$) this constant is close to 5, which is the constant obtained for the programs in Corollary 1. This illustrates the versatility of our approach as it allows to capture the complexity of chaining backprop operations, the resulting estimate being quite sharp in the regime of long programs.
**Beyond backpropagation** Programs may be differentiated by other means than backpropagation. Possible alternatives include, forward propagation, with applications in optimization and algorithmic unrolling \([44,42,43]\), implicit differentiation \([3,60,6,15]\) with application in optimization and hyperparameter optimization \([12]\), adjoint differentiation \([48]\) in programs with components involving ordinary differential equations \([23,19]\), or differentiation by other means, for example differentiation of conjugate gradient \([27]\) or cholesky algorithm \([55]\) or approximation of Jacobian matrices involving a non-uniform fast Fourier transform \([57]\).

Let \(P\) be a program in compositional form as in Section 2.1. For \(i = p + 1, \ldots, m\), we consider a program \(g_i\) associated to the derived program \(d_i\), which could be obtained by any means, including the techniques discussed above. Lemma 1 relates complexity of combining derived programs in Algorithm 2 to the following quantities.

- \(\text{cost}(g_i, d_i)/\text{cost}(g_i)\): the ratio “derivative’s cost vs evaluation’s cost” (the “computational overhead ratio” as defined in the next section).
- \(|\partial(i)| \text{cost}(\times)/\text{cost}(g_i)\): the ratio between multiplication cost and average cost per input argument.

The first quantity depends on the technique used to obtain \(d_i\) (forward propagation, adjoint method, implicit differentiation \(\ldots\)). The second quantity may be assumed to be smaller than 2 as a program applies one arithmetic operation to each input argument. As in the previous section, it becomes negligible for long programs (i.e., programs which perform many operations per input, on average). If the program sequence contains elementary operations (for example from \(D_{\text{relu}}\), together with long programs, then the first quantity may become the leading term in the complexity estimate of Lemma 1.

For example in an optimization context \([44,42,43]\), elements of the program sequence are optimization algorithms differentiated using forward propagation in Algorithm 2. The leading factor in \(w_0\) in Lemma 1 is \(\max(3p, 5)\), which has a linear dimension dependency, contrary to the estimate in Section 3.2. This illustrates the versatility of the proposed analysis as it allows to obtain estimates of the computational cost of automatic differentiation based on mixed techniques (here forward propagation combined with backpropagation).

### 4 On the computational hardness of generalized gradients

Throughout this section, the (computational) overhead ratio is the multiplicative factor required to evaluate both a function and its derivatives compared to mere function evaluation. We have shown that, for the reverse mode of AD, the overhead ratio is independent of the dimension \(p\) for conservative gradients. We discuss now this quantity for various nonsmooth oracles: lexicographic derivatives, for which forward AD has an overhead ratio of the order of \(p\) \([4]\); directional derivatives, for which we relate worst case complexity to the complexity of matrix multiplication. As for Clarke subgradient, we prove a hardness result related to enumeration.

#### 4.1 The computational overhead ratio for evaluating \(p\) directional derivatives

Given \(F : \mathbb{R}^p \rightarrow \mathbb{R}\) be locally Lipschitz and \(x, d \in \mathbb{R}^p\), the directional derivative of \(F\) at \(x\) in direction \(d\) is given by \(\lim_{t \to 0} (F(x + td) - F(x))/t\) when the limit exists. Directional derivatives admit a chain rule \([54]\) Proposition 3.6], therefore, directional derivatives (whose input is one-dimensional) can be computed using techniques of forward automatic differentiation at a computational cost similar to function evaluation \([36,37,38]\).

**Complexity of matrix multiplication**: Throughout this section, we set \(D = \{+, \times, +c, \times c\}\) and assume that elementary operations have unit cost. Denote by \(c(p)\) the minimal number of additions and multiplications required to multiply square matrices of size \(p \times p\). More precisely, if \(f : \mathbb{R}^{p \times p} \times \mathbb{R}^{p \times p} \rightarrow \mathbb{R}^{p \times p}\) is such that \(f(A, B) = AB\) for all, square matrices \(A, B \in \mathbb{R}^{p \times p}\), we have \(c(p) = \text{comp}(f, D)\).

Note that \(c(p) \geq p^2\) as one needs to apply at least one operation to each of the \(2p^2\) entries. Since the seminal work of Strassen \([56]\), it is known that \(c(p) = O(p^{\log_2(7)}).\) Determining the precise exponent has been an object of intense research \([50]\). Asymptotically, one has \(2 \leq \log(c(p))/\log(p) < 2.373\), see \([59,59]\), the best known bound being given in \([4]\). Roughly stated, the “fastest” algorithm
for performing $p \times p$ matrix multiplication runs with $O(p^{2.373})$ operations. These estimates are of a theoretical nature, existence proofs may be non constructive, and the resulting algorithms may suffer from the curse of recursion: efficiency becomes sensible only for inaccessible matrix sizes. According to [25], for values $p \leq 10^6$ the most efficient methods resulting in practical algorithms have complexity of the order $p^{2.774}$.

**Directional derivatives:** Given a function $F : \mathbb{R}^p \times \mathbb{R}^q \to \mathbb{R}$, we denote by $F_1^p : \mathbb{R}^p \times \mathbb{R}^q \times \mathbb{R}^{p \times p} \to \mathbb{R}^p$ the function which associates to $x \in \mathbb{R}^p$, $y \in \mathbb{R}^q$ and a matrix $A \in \mathbb{R}^{p \times p}$ the $p$ directional derivatives with respect to $x$ variable, for fixed $y$, in directions given by the columns of $A$.

The proof of the following theorem is given in Section C.

**Theorem 2 (Computational ratio for directional derivatives)** There exists a function $F : \mathbb{R}^p \times \mathbb{R}^q \to \mathbb{R}$ and a program $P_F$ implementing $F$ with dictionary $\mathcal{D} \cup \{\cdot \mid \cdot\}$ (all operations have unit cost), such that for any program $P'$ implementing the function $(y, A) \mapsto F_1^p(0, y, A)$ with derived dictionary $\mathcal{D} \cup \{\cdot \mid \cdot\},$ $\text{sign}()$, $\text{cost}(P')/\text{cost}(P_F) \geq (c(p) - 5p)/(30p^2).$ (4)

Note that there exist programs $P'$ as in Theorem 2, these can be obtained for example using a dedicated forward mode of automatic differentiation on $F$ [36, 37], noting that for $f = |\cdot|$, $f'(x, d) = \text{sign}(x) \times d + |d| \times (1 - \text{sign}(x))$, for all $x, d \in \mathbb{R}$, with the convention that $\text{sign}(0) = 0$. The computational overhead is of the order of $p$ which is greater than $c(p)/p^2$. The bound in Theorem 2 is sharp up to multiplicative constants for linear relu networks, see Remark 3 in Appendix A.2.

The main message of this section is that $c(p)/p^2$ is a measure of the multiplicative computational overhead ratio for evaluating $p$ directional derivatives. This illustrates a potential bottleneck of the forward directional derivative propagation in a nonsmooth context: if there was a “cheap $p$ directional derivatives principle” this would mean that matrix multiplication is easy to the point that $c(p) = O(p^2)$. Indeed the best known upper bounds entails an overhead of the order $p^{0.373}$ asymptotically, and the best known upper bound related to a practical algorithm for moderate matrix size results in an overhead of the order $p^{0.774}$. In practice, for moderate values of $p$, $c(p)$ is quite large compared to $p^2$. This is to be compared with a constant overhead incurred by backpropagation which computes selection in conservative gradients. This is discussed further in Appendix A.2.

The proposed bound applies to algorithms described in [36, 37] which require $p$ directional derivatives evaluation.

### 4.2 Computing Clarke subgradients using forward automatic differentiation

In [36, 37, 38], several automatic differentiation strategies are proposed to evaluate elements of the Clarke subdifferential. These approaches are based on directional and lexicographic derivatives [45] for which there exists a chain rule under specific structural assumptions. As explained in [7], these methods are based on vector forward mode of automatic differentiation and therefore suffer from computational ratio overhead which scales linearly in $p$ contrary to the reverse AD mode in Theorem 1. Reducing this factor to a constant is an open question even for compositional functions involving only univariate nonsmoothness such as absolute value [55]. More details on these approaches is given in Appendix A.2.1.

#### 4.3 Computational hardness of subgradient enumeration

##### 4.3.1 Linear relu network and gradient enumeration

By abuse of notation, for $v \in \mathbb{R}^p$, we set relu($v$) to be the coordinatewise application of the relu function. Given a set of matrices $M_1 \in \mathbb{R}^{p_1 \times p}$, $M_2 \in \mathbb{R}^{p_2 \times p_1}$, ..., $M_{L-1} \in \mathbb{R}^{p_{L-1} \times p_{L-2}}$, $M_L \in \mathbb{R}^{1 \times p_{L-1}}$ we consider the associated relu network $F : \mathbb{R}^p \to \mathbb{R}$, $F : x \mapsto M_L \text{relu}(M_{L-1} \text{relu}(...M_1 x))$. (5)

This function is positively homogeneous, it satisfies $F(0) = 0$. The input output relation is piecewise linear with finitely many pieces (see e.g. [5, 49]), therefore, its Clarke subgradient is a polyhedron.
We consider the following problem.

The decision version of Problem 1, under the same assumptions, is to decide if there exists two distinct elements in \( D_F \) or one element if it is a singleton.

This problem enters the field of computational complexity as one can associate to it an obvious notion of representation size provided that we associate to each matrix entry a representation size.

In what follows we will consider integral or rational entries with the common notion of bit size [53].

4.3.2 Clarke enumeration is NP-hard for relu networks at one point

The decision version of Problem 1 under the same assumptions, is to decide if there exists two distinct elements in \( D_F(x) \), that is, decide if \( D_F(x) \) is not reduced to a singleton. The following is proved by reduction to 3-SAT. The proof consists in representing a 3-SAT boolean formula using a linear relu network, it is described in details in appendix D.1.

Theorem 3 (Finding two Clarke subgradients is NP-Hard) Decision version of problem (1) with matrix and vector entries in \( \{-1, 0, 1\} \) and \( D_F = \partial^c F \) is NP-hard.

Corollary 2 (Deciding differentiability of a NN is NP-Hard) Given a linear relu network as in (5), \( x \in \mathbb{R}^p \) and \( D_F : \mathbb{R}^p \to \mathbb{R}^p \) a conservative gradient for \( F \). Compute two distinct elements in \( D_F(x) \) or one element if it is a singleton.

It follows from [45, Proposition 2.7] that, for linear relu network \( F \) as in (5), the lexicographic subdifferential [45] is the set of neighboring gradients and is contained in Clarke subdifferential.

Corollary 3 (Finding two lexicographic subgradients is NP-Hard) Theorem 3 remains true if \( D_F \) is the lexicographic subdifferential.

4.3.3 Tractability for autodiff conservative gradient

The counterpart of Problem 1 for the autodiff conservative gradient in Definition 3 is tractable. This illustrates a major difference between Clarke subgradient and automatic differentiation conservative gradient from a computational complexity perspective. The proof is in Section D.2 by reduction to a graph shortest path problem.

Proposition 1 Problem (1) with matrix entries in \( \mathbb{Q} \) and \( D_F = D_F^c \) can be solved in polynomial time.

5 Conclusion

We have extended the “cheap gradient” principle to nonsmooth automatic differentiation with a flexible extension of Baur-Strassen result: the overhead of computing conservative gradients is independent of the dimension. This illustrates the favorable computational properties of conservative
gradients. On the other hand, we have shown that efficiency of forward AD for computing multiple directional derivatives can be improved only to a limited extent due to its intrinsic connection with matrix multiplication. Finally, we have shown that for simple relu networks, enumeration of Clarke subgradients is computationally hard, contrary to enumeration of conservative gradients.

The global picture is significantly different from the smooth case for which the “cheap gradient” principle is well understood, illustrating the relevance of explicitly consider nonsmoothness. The present results confirm the centrality of the notion of conservative gradients in nonsmooth AD and machine learning: it is a nonsmooth generalization of gradients with a “cheap” principle, contrary to concurrent notions. The most important open question in this context is that of the complexity of subgradient computation, or in other words the existence of a “cheap subgradient principle”, for which we conjecture that the answer is negative in general.

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This is the appendix for “Nonsmooth automatic differentiation: a cheap gradient principle and other complexity results”.

Contents

A  Further comments, discussion and technical elements 14
B  Proofs related to Section 2 15
C  Proofs of Section 4 18
D  Proofs of Section 4.3 19

A  Further comments, discussion and technical elements

A.1  Comments on Section 2

A.1.1  Computational model in Section 2.1

Illustration of Sections 2.1 We represent programs using the DAG representation as in Remark 1. Let us define a simple dictionary $D := \{+ \times\}$ and introduce a level 0 elementary program $P_0$ such that $P_0(a, b) = a + b$ meaning that $P_0$ computes the quantity $a + b$. $P_0$ is identified with $+$ from the dictionary. We also introduce a level 1 program $P_1$ such that $P_1(a, b, c) = a \times (b + c)$. We can construct an equivalent level 1 program, $Q_1$ such that $Q_1(a, b, c) = a \times b + a \times c$. In this case, we have $P_1 \sim Q_1$, or $[P_1]_D = [Q_1]_D$ since they compute the same quantity. The level 2 program $P_2$ is such that $P_2(a, b, c, d) = (a + b) \times (c + d) = Q_1(a, c, d) + P_1(b, c, d)$ and uses level 1 programs $Q_1$ and $P_1$ in its computation nodes. The Directed Acyclic Graphs (DAGs) representing these programs are given in Figure 1. Assuming $\text{cost}(+) = \text{cost}(\times) = 1$, we have $\text{cost}(P_0) = 1$, $\text{cost}(P_1) = 2$, $\text{cost}(Q_1) = 3$ and $\text{cost}(P_2) = \text{cost}(Q_1) + \text{cost}(P_1) + \text{cost}(\times) = 6$.

![Figure 1: DAG illustrating different programs with dictionary $D := \{+ \times\}$. (a) $P_0(a, b) = a + b$, of level 0 which is identified with $+$ from the dictionary, (b) $P_1(a, b, c) = a(b + c)$, of level 1, (c) $Q_1(a, b, c) = ab + ac$, of level 1 and equivalent to $P_1$, (d) $P_2(a, b, c, d) = (a + b)(c + d) = Q_1(a, c, d) + P_1(b, c, d)$, of level 2.](image)

A.2  Comments on Section 4

A.2.1  Forward AD and Clarke subgradients

Nesterov introduced in [45] the notion of lexicographic subdifferential, denoted here $\partial_L F$ for a Lipschitz function $F: \mathbb{R}^p \rightarrow \mathbb{R}$. The construction of $\partial_L F$ is based on successive local approximations of $F$ with directional derivatives, and one has $\partial_L F(x) \subset \partial^c F(x)$ for all $x$ such that the first term is well defined.

It is known that automatic differentiation can be used to compute directional derivatives, particularly the forward mode of automatic differentiation [33]. Based on this observation, Khan and Barton developed several algorithms to evaluate elements of $\partial^c F$, based on directional derivatives [36, 37, 38].
They concentrate on piecewise $C^1$ functions, see for example [52], and propose to handle compositional structures with different restrictions on the function class considered, such as functions in abs-normal forms [36], or broader classes [37][7].

All these procedures either require to evaluate $p$ directional derivatives [36, 37], or rely on forward chain rule propagation for lexicographic derivatives [38][7], which also require to maintain $p$ directional derivatives. For this reason, all these methods suffer from a multiplicative computational overhead ratio of the order of $p$ in the worst case, and it is not known if this could be improved [7], although efforts have been made in this direction [35].

### A.2.2 Matrix multiplications

**Remark 3** The lower bound described in Theorem 2 is sharp for a linear relu network $F$ as in (5) involving only square $p \times p$ matrices. Indeed, $p$ directional derivatives of $F$ in directions $a_1, \ldots, a_p$, can be computed with roughly $Lc^p p^q$ operations, using a matrix multiplication algorithm realizing the $c(p)$ bound, for example using the forward mode of AD [36][37]. The naive $P_F$ algorithm for forward evaluation performs roughly $2Lp^2$ operations which results in the bound (neglecting terms of order one in numerator and denominator),

$$\text{comp}(F_{d}, D \cup \{|\cdot|, \text{sign}(\cdot)|}) \leq \frac{c(p)}{2p^2},$$

for this class of networks, to be compared with (4). Finally, we remark that in the smooth case such complexity estimates reduce to gradient computation which can be done using backward algorithmic differentiation with a constant multiplicative overhead ratio.

We denote by $F_d$, the function $F_d: (y, A) \mapsto F'_1(0, y, A)$ which computes $p$ directional derivatives at a given point. Setting $\omega = \limsup_{p \to \infty} \log(c(p))/\log(p)$, since $P'$ is an arbitrary program implementing $F_d$, we have shown that asymptotically, for any $\epsilon > 0$

$$\sup_{p, F=[P_F]} \frac{\text{comp}(F_d, D \cup \{|\cdot|, \text{sign}(\cdot)|})}{\text{cost}(P_F)} \times p^{2-\omega-\epsilon} = +\infty,$$

where the supremum is over all $p$ and all functions $F: \mathbb{R}^{p \times q} \to \mathbb{R}$ implemented by a program $P_F$ with dictionary $D \cup \{|\cdot|\}$. It is not known whether $\omega > 2$.

### B Proofs related to Section 2

**Proof of Lemma 1** Given a program $P$ as in Section 2.1, we have the following costs estimates which can be deduced from the definition of the cost of a program in Section 2.1.

- **Algorithm 1** forward evaluation:

  $$\text{cost}(P) = \sum_{i=p+1}^{m} \text{cost}(g_i) \tag{7}$$

- **Algorithm 2** backward AD cost:

  $$\text{cost}(\text{backprop}(P), P) = \sum_{i=p+1}^{m} \text{cost}(d_i, g_i) + |p|\text{pr}(i)|\text{cost}(\cdot) + \text{cost}(\times)). \tag{8}$$

- **Algorithm 2** forward AD cost:

  $$\text{cost}(\text{forprop}(P), P) = \sum_{i=p+1}^{m} \text{cost}(d_i, g_i) + p|\text{pr}(i)|\text{cost}(\times) + p(|\text{pr}(i)| - 1)\text{cost}(\cdot). \tag{9}$$

Let us derive the complexity bound of Algorithm 1 according to Algorithm 2.
where

\[ \omega \]

The proof of Corollary 1 follows from Lemma 1 by computing the relevant constants. They are

where the inequality is due to factorization by the maximal value. Using (7), we obtain

\[ \omega \]

\[ \text{cost}(\text{backprop}(P), P) \leq \omega_b \times \text{cost}(P) \]

where \( \omega_b \) is given in (1).

Forward AD complexity result: Using (9) and the fact that cost has value in \( \mathbb{R}^*_+ \), we have

\[
\text{cost}(\text{forprop}(P), P) = \sum_{i=p+1}^{m} \text{cost}(d_i, g_i) + p |pr(i)| (\text{cost}(+) + \text{cost}(\times)) \\
= \sum_{i=p+1}^{m} \text{cost}(g_i) \times \frac{\text{cost}(d_i, g_i) + p |pr(i)| (\text{cost}(+) + \text{cost}(\times))}{\text{cost}(g_i)} \\
\leq \max_{i=p+1,m} \left( \frac{\text{cost}(d_i, g_i) + p |pr(i)| (\text{cost}(+) + \text{cost}(\times))}{\text{cost}(g_i)} \right) \sum_{i=p+1}^{m} \text{cost}(g_i),
\]

where the inequality is due to factorization by the maximal value. Using (7), we obtain

\[
\text{cost}(\text{forprop}(P), P) \leq \omega_f \times \text{cost}(P)
\]

where \( \omega_f \) is given in (1).

Proof of Theorem 1: According to the statement of the theorem, \( d_i \) is a differentiated program that computes a selection in a conservative gradient for each \( g_i \). As consequence, \( g_i \) is path differentiable. Let \( x = (x_1, \ldots, x_p) \) be the input of \( P \). By definition, we have \( [P]_D = [g_m \circ g_{m-1} \circ \ldots \circ g_{p+1}(x)]_D \). From section 3.1, it follows that \( [P]_D \) is path differentiable as a composition of path differentiable functions and \( \text{backprop}(P) \) computes a selection in a conservative gradient of \( [P]_D \). Finally, using Lemma 1 we derive the complexity result who is independent of number of inputs of \( f \) in the backward mode case.

\[ \square \]

B.1 Justification of the complexity Table 1 of the \( D_{\text{relu}} \)-Dictionary.

The proof of Corollary 1 follows from Lemma 1 by computing the relevant constants. They are shown in Table 1. Let us justify the proposed numbers.

Case 1 (cost(\times), cost(+)) Let us define \( [g]_{D_{\text{relu}}} (a, b) = a \times b \). To evaluate \( g \), we need one operation from \( D_{\text{relu}} \). For the derived program related to \( g \), we do not need additional operation from \( D'_{\text{relu}} \). Finally, from Assumption 1, we can deduce that cost(\( g \)) = 1 and cost(\( d, g \)) = 1. We get the same result for cost(+) by applying identical reasoning.

Case 2 (cost(\times c), cost(+ c)) Let us define \( [g]_{D_{\text{relu}}} (a) = c \times a \). To evaluate \( g \), we need one operation from \( D_{\text{relu}} \). For the derived program related to \( g \), we do not need additional operation from \( D'_{\text{relu}} \). Finally, from Assumption 1, we can deduce that cost(\( g \)) = 1 and cost(\( d, g \)) = 1. We get the same result for cost(+ c) by applying identical reasoning.
Case 3 (cost(log)) Let us define \([g]_{D_{\text{relu}}} (a) = \log(a)\). To evaluate \(g\), we need one operation from \(D_{\text{relu}}\). For the derived program related to \(g\), we need one inverse \((\frac{1}{g})\) operation from \(D'_{\text{relu}}\). Finally, from Assumption 7, we can deduce that cost\((g) = 1 \text{ and cost}(d, g) = 2\). 

Case 4 (cost(exp)) Let us define \([g]_{D_{\text{relu}}} (a) = \exp(a)\). To evaluate \(g\), we need one operation from \(D_{\text{relu}}\). For the derived program related to \(g\), we do not need additional operation from \(D'_{\text{relu}}\). Finally, from Assumption 7, we can deduce that cost\((g) = 1 \text{ and cost}(d, g) = 1\).

Case 5 (cost(inv)) Let us define \([g]_{D_{\text{relu}}} (a) = \frac{1}{a}\). To evaluate \(g\), we need one operation from \(D_{\text{relu}}\). For the derived program related to \(g\), we need two multiplications and one \((-1)\) multiplication operation from \(D'_{\text{relu}}\). Finally, from Assumption 7, we can deduce that cost\((g) = 1 \text{ and cost}(d, g) = 3\).

Case 6 (cost(relu)) Let us define \([g]_{D_{\text{relu}}} (x) = \text{relu}(x) = \max(x, 0)\). To evaluate \(g\), we need to evaluate the sign of \(x\). The derived program relu’ can be computed also from the sign of \(x\) without further operation. We have cost\((g) = 1\) by hypothesis, but it is also reasonable to consider cost\((d, g) = 1\) as both operations only require sign evaluation of the same object.

Remark 4 Since \(D_{\text{relu}}\) dictionary contains the relu function, we can build other non-smooth functions such as the maximum and the absolute value. For example, \(\max\{x, y\} = \text{relu}(x - y) + \text{relu}(y) - \text{relu}(-y)\).

B.2 An extension of Table 1

The justifications of the following is similar to Section B.1, simply taking into consideration different types of operations. Taking \(c_{\text{nonlin}} = c_{\text{relu}} = 1\), we recover Table 1. We replace relu by \(\times_{\text{relu}}\) which correspond to its usage in practice and allow to balance the cost of relu operations and that of multiplications.

Table 2: Extension of cost table. \(c_{\text{nonlin}} \geq 1\) is the cost of nonlinear operations and \(c_{\text{relu}} \geq 0\) is the cost of sign valuation for relu or relu’.

| \(g\) | \((+, \times)\) | \((+c, \times c)\) | \(\log\) | \(\exp\) | \(\text{inv}\) | \(\times_{\text{relu}}\) |
|------|----------------|----------------|-------|------|------|----------------|
| \(\text{cost}(g)\) | 1 | 1 | 1 \(c_{\text{nonlin}}\) | 1 \(c_{\text{nonlin}}\) | 1 \(c_{\text{nonlin}}\) | 1 + \(c_{\text{relu}}\) |
| \(\text{cost}(d, g)\) | 2 | 1 | 1 | 1 | 1 | 2 |
| \(\text{cost}(d, g)\) | 1 | 1 | 2 \(c_{\text{nonlin}}\) | 1 \(c_{\text{nonlin}}\) | 1 + \(c_{\text{relu}}\) |
| \(\text{cost}(g)\) | 1 | 1 | 2 | 1 | \(\frac{c_{\text{nonlin}} + 2}{c_{\text{nonlin}}}\) | 1 |
| \(\text{cost}(\times\text{pr})\) | 4 | 2 | \(\frac{1}{c_{\text{nonlin}}}\) | \(\frac{1}{c_{\text{nonlin}}}\) | \(\frac{1}{c_{\text{nonlin}}}\) | 2 + \(c_{\text{relu}}\) |
| \(\text{cost}(\text{pr})\) | 5 | 3 | \(\leq 4\) | \(\leq 3\) | \(\leq 5\) | \(\leq 5\) |

The justification is the same as in Section B.1 taking into consideration different types of operations. For the \(\times_{\text{relu}}\) operation, the justification is as follows.

Case 7 (\(\times\text{cost(relu)}\)) The operation has two argument and requires one sign evaluation and one multiplication in the worst case, so we assign it the cost \(1 + c_{\text{relu}}\). The differentiated program \(d\) should compute the function \((a, b) \rightarrow (\text{relu}(b), a \times \text{relu}'(b))\). One can write a program to compute jointly \(g\) and \(d\) as follows: return \((a \times b, b, a)\) if \(b \geq 0\) and \((0, 0, 0)\) if \(b < 0\). This only requires a bit sign check which cost is \(c_{\text{relu}}\) and a multiplication. We therefore model this operation such that \(\text{cost}(g) = 1\) and \(\text{cost}(d, g) = \text{cost}(g) = 1 + c_{\text{relu}}\).

Further refinements could be considered including various type of computational operations, such as memory moves, these are beyond the scope of the present paper.
C Proofs of Section 4

C.1 Proof of the main result

Proof of Theorem 2. Let \( U \in \mathbb{R}^{p \times p} \) be an orthogonal matrix with entries in \( \{-1, 1\} \) which columns are denoted by \( u_1, \ldots, u_p \) (with squared norm \( p \)). Assume that we have as variables a matrix \( M \in \mathbb{R}^{p \times p} \) and two matrices \( A, B \in \mathbb{R}^{p \times p} \) with columns \( a_1, \ldots, a_p \) and \( b_1, \ldots, b_p \) respectively.

Consider the function

\[
F: (x, B, M) \mapsto \frac{1}{p} \sum_{i=1}^{p} |[UB^T M x]|_i.
\]

The pair \((M, B)\) will be identified as \( y \) in the statement of the theorem. Considering the dictionary of elementary functions \( \mathcal{D} \cup \{ | \cdot | \} \), \( F \) has a direct representation as a program \( P_F \). We have \( \text{cost}(P_F) = 6p^2 - 3p + 2p \leq 6p^2 \) where we count \( 2p^2 - p \) operation for each matrix vector multiplication (there are three of them), \( p \) operations for the coordinatewise absolute value and \( p - 1 \) for the outer sum and 1 for the division. Now consider the constraints

\[
\text{sign}(UB^T M a_i) = u_i, \quad i = 1, \ldots, p.
\]

The set of matrices \( A, B, M \) satisfying this constraint is an open set, call it \( S \). We now restrict our attention to this open set and argue that \( \text{cost}(P') \) does not change if the input variables are constrained to be in \( S \).

We have for all \( i = 1, \ldots, p \) and \((A, B, M) \in S\), the following directional derivatives with respect to variable \( x \)

\[
F'_i((0, B, M, a_i) = \frac{1}{p} \text{sign}(UB^T M a_i) U B^T M a_i = \frac{1}{p} u_i U B^T M a_i = b_i^T M a_i.
\]

Setting the function \( G: (A, B, M) \mapsto \sum_{i=1}^{p} F'_i((0, B, M, a_i) = \text{Tr}(M A B^T) \), we have that \( G \) is a polynomial and \( \nabla_M G(A, B, M) = \sum_{i=1}^{p} b_i a_i^T = B A^T \). Note that this does not depend on \( M \).

Fix \( P' \) as in the statement of the theorem.

Claim 1 There is a program \( P_2 \) on dictionary \( \mathcal{D} \) such that \( G = [P_2]_\mathcal{D} \) (on the whole space) and \( \text{cost}(P_2) \leq \text{cost}(P') + p \).

We use the DAG representation of programs as in Remark 1. Therefore \( P' \) is described by a DAG which node are either input nodes or computation nodes implementing functions from \( \mathcal{D} \cup \{|\cdot|, \text{sign}\} \).

We will modify the program by simple modifications of the computation nodes. We may obtain a program \( P_0 \) implementing \( G \) on \( S \) with dictionary \( \mathcal{D} \cup \{|\cdot|, \text{sign}()\} \) with \( \text{cost}(P_0) \leq \text{cost}(P') + p \) by summing the outputs of \( P' \). The sign nodes in \( P_0 \) represent a semialgebraic function \([21, 22]\). Reducing \( S \) if necessary, we obtain a program \( P_1 \) on dictionary \( \mathcal{D} \cup \{|\cdot|\} \) such that \( P_1 \sim P_0 \) on \( S \) by replacing each sign node in \( P_0 \) by the corresponding constants. We have \( \text{cost}(P_1) \leq \text{cost}(P_0) \) (we replace computing nodes by constants). By Lemma 2 there is a program \( P_2 \) on \( \mathcal{D} \) such that \( \text{cost}(P_2) = \text{cost}(P_1) \leq \text{cost}(P_0) \leq \text{cost}(P') + p \) and \( G = [P_2]_\mathcal{D} \) (on the whole space). This proves the claim.

We may obtain a program \( D_2 \) implementing \( \nabla_M G \) with dictionary \( \mathcal{D} \) by backward algorithmic differentiation on \( P_2 \), that is \( D_2 = \text{backprop}(P_2) \). we have therefore

\[
\text{comp}(BA^T, \mathcal{D}) \leq \text{cost}(D_2) \\
\leq \text{cost}(P_2, D_2) \\
\leq 5\text{cost}(P_2) \\
\leq 5p + 5\text{cost}(P'),
\]

where the first inequality is because \( D_2 \) is a program computing \( B A^T \) for all \( A, B \) on dictionary \( \mathcal{D} \), the second is because adding computation increases the cost, the third is a property of backward algorithmic differentiation on \( \mathcal{D} \) and the last one is by construction of \( P_2 \). Note that \( \text{comp}(BA^T, \mathcal{D}) = c(p) \) by definition, therefore we have the claimed lower bound

\[
\frac{\text{cost}(P')}{\text{cost}(P_F)} \geq \frac{c(p) - 5p}{5\text{cost}(P_F)} = \frac{c(p) - 5p}{30p^2}.
\]

\[\square\]
C.2 An additional Lemma

Lemma 2 Let $Q : \mathbb{R}^p \rightarrow \mathbb{R}$ be a polynomial and $P_1$ be a program (without loss of generality of level 1) on the dictionary $\mathcal{D}_1 = \{+, \times, |, +c, \times c\}$, such that $Q = [P_1]_{\mathcal{D}_1}$ for all inputs restricted to an open set $S \subset \mathbb{R}^p$. Then there is a level 1 program $P_2$ on the dictionary $\mathcal{D}_2 = \mathcal{D}_1 \setminus \{|\cdot|\}$ such that $Q = [P_2]_{\mathcal{D}_2}$ (for all inputs in $\mathbb{R}^p$). Furthermore, if $\cost(|\cdot|) = \cost(x \cdot c)$, then, $\cost(P_2) = \cost(P_1)$.

Proof: We use the DAG representation of programs as in Remark 1. Therefore $P_1$ is described by a DAG which node are either input nodes or computation nodes implementing functions from $\mathcal{D}_1$. The function computed by $P_1$ as well as each of its nodes are semi-algebraic [14, 21, 22]. For each $|\cdot|$ node in the graph representing $P_1$ (assume that there are $N$ of them) we associate a number: the sign of its input (with the convention that $\text{sign}(0) = 0$). This defines a semi-algebraic function $G : \mathbb{R}^p \rightarrow \{-1, 0, 1\}^N$. As it has values in a finite set, by semi-algebraicity, there is an open subset of $S' \subset S$ such that $G$ is constant on $S'$. Consider $P_2$ which computation graph is the same as that of $P_1$ except that each absolute value node is replaced by multiplication by the corresponding sign (which is constant on $S'$). Then $Q = [P_1]_{\mathcal{D}_1} = [P_2]_{\mathcal{D}_2}$ for all inputs in the open set $S'$. All computation nodes of programs on $\mathcal{D}_2$ are multivariate polynomials and two polynomials which agree on an open set are equal globally. This concludes the proof.

D Proofs of Section 4.3

D.1 Proof of the main hardness result

Preliminary on 3-SAT We will use reduction to 3-SAT problem which is among the most well known NP-complete problems. Recall that a boolean formula is built from boolean variables, and operators: AND (conjunction, denoted $\land$) OR (disjunction, $\lor$) and NOT (negation, $\neg$). A literal, is either a variable or the negation of a variable. A clause is a disjunction of literals (or a single literal). A formula is in conjunctive normal form (CNF), if it is a conjunction of clauses or a clause. 3-SAT is the decidability problem associated to CNF formulas with clauses containing 3 literals, such formulas are called 3-CNF formulas.

Example 2 The formula $(b_1 \lor b_2 \lor \neg b_3) \land (b_1 \lor b_4 \lor \neg b_5) \land (\neg b_2 \lor \neg b_3 \lor b_6)$ is 3-CNF with 6 boolean variables $b_1, \ldots, b_6$ and 3 clauses.

Problem 2 (3-SAT) Given $p, n \in \mathbb{N}$ and a boolean function $\pi$ with $p$ boolean arguments $b_1, \ldots, b_p$ represented by a 3-CNF formula with $n$ clauses, decide if there exists an assignment $(b_1, \ldots, b_p) \in \{0, 1\}^p$ such that $\pi(b_1, \ldots, b_p) = 1$.

Proof of Theorem 3

The reduction is to 3-SAT.

Consider a 3-CNF function $\pi$ in $p$ variables $b_1, \ldots, b_p$, with $n$ clauses of size 3. We may assume without loss of generality that $n$ is of the form $2^k$ for $k \in \mathbb{N}$ by adding clauses which are always true and increasing the number of clauses by a factor at most 2. We will consider $p$ real variables $x_1, \ldots, x_p$. Consider the first clause of $\pi$, say for example $(b_1 \lor b_2 \lor \neg b_3)$. We associate to each literal the corresponding variable $x$ if the literal is equal to a variable, and $-x$ if it is the negation of the corresponding variable, for example $x_1, x_2, -x_3$. These are combined using relu $\circ$ max resulting in the expression $\text{relu}(\text{max}\{x_1, x_2, -x_3\})$.

We proceed similarly for each clause, we obtain $n = 2^k$ expressions involving relu $\circ$ max where the max is over three numbers. The max of 3 numbers is the same as the max of 4 numbers (by copying one of the inputs) and, according to Lemma 4, can be represented by a relu network with 2 relu layers of size at most $3 \times 2 = 6$ with weight matrices in $\{-1, 0, 1\}$.

We may therefore represent the $n$ relu $\circ$ max expressions with a network with $p$ inputs and $n$ outputs, with 3 relu layers (2 for each max and one for the outer relu) of size at most $6n$ (6 nodes for each max) involving matrices with entries in $\{-1, 0, 1\}$. These expressions are combined using the operator min applied to the $n = 2^k$ clause. Thanks to Lemma 4 again, using $\min\{a, b\} =$
We call the resulting network $F$. It has a representation as in (5), with matrices with entries in $Z_3 = \{-1, 0, 1\}$ as in Problem 1. It contains $\log_2(n) + 3$ relu layers of size at most $6n$ and it has therefore a description which size is polynomially bounded in $n$ which is proportional to the bit size representation of the 3-CNF formula $\pi$.

**Example 3** If the 3-CNF formula is given by $(b_1 \lor b_2 \lor \neg b_3) \land (b_1 \lor b_4 \lor \neg b_5) \land (\neg b_2 \lor \neg b_3 \lor b_6) \land (b_2 \lor \neg b_3 \lor b_6)$ with $p = 6$ boolean variables and $n = 4$ clauses, we will obtain a network computing the following expression in 6 real variables $x_1, \ldots, x_6$:

$$
\begin{align*}
F(x_1, \ldots, x_6) &= \min(\text{relu}(\max(x_1, x_2, -x_3)), \text{relu}(\max(x_1, x_4, -x_5)), \\
& \quad \text{relu}(\max(-x_2, -x_3, x_6)), \text{relu}(\max(x_2, -x_2, x_6))).
\end{align*}
$$

We have the following rules for min and max over real numbers $a, b, c$ (we use the convention $\text{sign}(0) = 0$).

- $\max(a, b, c) > 0 \iff (a > 0) \lor (b > 0) \lor (c > 0)$.
- $\max(a, b, c) > 0 \iff \max(\text{sign}(a), \text{sign}(b), \text{sign}(c)) > 0$.
- $\min(a, b, c) > 0 \iff (a > 0) \land (b > 0) \land (c > 0)$.
- $\min(a, b, c) > 0 \iff \min(\text{sign}(a), \text{sign}(b), \text{sign}(c)) > 0$.
- $a > 0 \iff (-a < 0) \iff \text{sign}(a) > 0$.
- $\text{relu}(\max(\text{sign}(a), \text{sign}(b), \text{sign}(c))) \in \{0, 1\}$.

Because of the min $\circ \text{relu}$ structure, we have $F(x) \geq 0$ for all $x$, furthermore, $F(0) = 0$, so that 0 is a global minimum of $F$ and $0 \in \partial^c F(0)$. For any $x$, we have $F(x) > 0$ if and only if the output of each max is positive, if and only if each max clause contains a positive argument. We therefore have that $F(x) > 0$ if and only if $F(\text{sign}(x)) > 0$ where sign is the coordinatewise application of the sign, taking value 0 at 0.

We have the following chain of equivalence

$$
\begin{align*}
\partial^c F(0) &\neq \{0\} \\
\iff &\exists x \in \mathbb{R}^p, \ F(x) \neq 0 \\
\iff &\exists x \in \mathbb{R}^p, \ F(x) > 0 \\
\iff &\exists x \in \mathbb{R}^p, \ x_i \neq 0 (\forall i = 1, \ldots, p) \ F(x) > 0 \\
\iff &\exists x \in \mathbb{R}^p, \ x_i \neq 0 (\forall i = 1, \ldots, p) \ F(\text{sign}(x)) > 0 \\
\iff &\exists x \in \{-1, 1\}^p, \ F(x) > 0 \\
\iff &\exists x \in \{-1, 1\}^p, \ b_i = \mathbb{I}(x_i = 1) (i = 1 \ldots p),
\end{align*}
$$

where $\mathbb{I}$ outputs 1 if the boolean argument is true, and 0 otherwise. The first equivalence is by Lemma 3, the second is because $F \geq 0$, the third is because $F$ is continuous, the fourth is by the discussion above and the fifth is obvious because all possible $\{-1, 1\}$ patterns can be described as coordinatewise sign applied vectors in $\mathbb{R}^p$ with nonzero entries. For the last equivalence, for $x_i \in \{-1, 1\}$ we set $b_i = 0$ if $x_i = -1$ and $b_i = 1$ if $x_i = 1$. Each relu $\circ$ max applied to the sign vector corresponds to a clause and its output is in $\{0, 1\}$. The output of each relu $\circ$ max clause is 1 if and only if at least one of its argument is 1, if and only if one of the literal of the corresponding disjunction is 1 if and only if the disjunction applied to the corresponding boolean variables is true. Otherwise, it is 0. Similarly, the min combination has positive output if and only if all max outputs are 1 and if only if all the disjunctions applied to variables $b_i$ are true.

This shows that Problem 1 is NP-hard, because $0 \in \partial^c F(0)$ and $\partial^c F(0) \neq \{0\}$ if and only if there exists two distinct elements in $\partial^c F(0)$.

### D.2 Proof of feasibility for autodiff conservative gradient

**Proof of Proposition 1:** Consider the following polynomial expression:

$$
M_1^T(Q_1 + Q_1) \cdots M_{L-1}^T(Q_{L-1} + Q_{L-1})M_L^T, \quad (11)
$$

where we decomposed \( D_i = \bar{Q}_i + Q_i \) in Definition\(^3\) such that \( \bar{Q}_i \) is constant, diagonal, with zero entries except for the 1 entries which are enforced by the network sign pattern: strictly positive activation before application of \( \text{relu} \) when network is evaluated at \( x \). Furthermore, \( Q_i \) contains \( q_i \leq p_i \) diagonal variables to be chosen in \([0,1]\) corresponding to the zero activation pattern before application of \( \text{relu} \), for \( i = 1, \ldots, L - 1 \). The strictly negative values before application of \( \text{relu} \) do not play an additional role, they correspond diagonal entries constrained to 0 in both \( \bar{Q}_i \) and \( Q_i \), \( i = 1, \ldots, L - 1 \). Note that a polynomial is constant on a box if and only if it is constant so the polynomial expression in (11) is constant when diagonal entries are constrained in \([0,1]\), if and only if it is constant. So the problem reduces to decide if the polynomial expression in (11) is non constant, with respect to variables \( Q_1, \ldots, Q_{L-1} \). We show that this reduces to a graph connectivity problem over \( 2 + \sum_{i=1}^{l-1} q_i \) vertices and edge weight given by partial products in (11).

First, the problem can be reduced to finding a non-zero value in the expression in (11). Indeed, one can subtract the value obtained choosing \( Q_i = 0 \), \( i = 1, \ldots, L - 1 \) and use the following block representation:

\[
\begin{pmatrix}
M_1^T & -M_1^T \\

\end{pmatrix}
\begin{pmatrix}
\bar{Q}_1 + Q_1 & 0 \\
0 & \bar{Q}_1 \\

\end{pmatrix}
\cdots
\begin{pmatrix}
M_{L-1}^T & 0 \\
0 & M_{L-1}^T \\

\end{pmatrix}
\begin{pmatrix}
\bar{Q}_{L-1} + Q_{L-1} & 0 \\
0 & \bar{Q}_{L-1} \\

\end{pmatrix}
\begin{pmatrix}
M_L^T \\
M_L^T \\

\end{pmatrix}
\]

\[
= M_1^T (\bar{Q}_1 + Q_1) \cdots M_{L-1}^T (\bar{Q}_{L-1} + Q_{L-1}) M_L^T - M_1^T \bar{Q}_1 \cdots M_{L-1}^T \bar{Q}_{L-1} M_L^T. \tag{12}
\]

Therefore, expression (11) is nonconstant if and only if expression in (12) takes a nonzero value for some assignment of \( Q_1, \ldots, Q_{L-1} \). The number of variables in (11) and (12) is the same and they have exactly the same form. Therefore we assume without loss of generality that the problem is to decide if the polynomial expression in (11) is not equal to the null polynomial.

Expression (11) is a vector function each of its coordinates being a polynomial function. It is not uniformly null if and only if and only if there exists a coordinate which is not the null polynomial, so we may add a diagonal matrix \( Q_0 \) with \( p_0 = p \) diagonal entries in \([0,1]\) (and \( Q_0 = 0 \) for the sake of symmetry) and \( M_0 \in \mathbb{R}^{p \times 1} \) the vector of all ones and find a nonzero value for the product

\[
M_1^T (Q_0 + Q_1) M_1^T (Q_1 + Q_1) \cdots M_{L-1}^T (Q_{L-1} + Q_{L-1}) M_L^T. \tag{13}
\]

Expression (13) is now real valued and therefore defines a polynomial. For each \( 0 \leq l \leq L - 1 \), denote by \( d_l \in [0,1]^q \), the vector containing the diagonal entries of matrix \( Q_l \), this corresponds exactly to the variable diagonal elements of \( D_i \) in Definition\(^5\). Denote by \( P(d_0, \ldots, d_L) \) the obtained polynomial, \( P \) is multilinear in \( d_0, \ldots, d_{L-1} \), that is, it has an affine dependency for one block vector if the others are fixed. Therefore the hessian of \( P \) has zero diagonal blocks and the function is harmonic (hessian has zero trace), as a consequence, the maximum principle for harmonic functions entails that its maximum and minimum on any polytope are attained at vertices.

For \( i = 0, \ldots, L - 1 \) denote by \( \Delta_i \subset \mathbb{R}^q \), the convex hull of the origin and the canonical basis vectors, this is a \( q \), dimensional simplex with nonempty interior. The polynomial \( P \) in (13) is identically zero if and only if it vanishes on the product of simplices \( \Delta_0 \times \cdots \times \Delta_{L-1} \) (which has non empty interior), if and only if it vanishes on the product set of the edges of these simplices by the maximum principle. In other words, \( P \) is not identically zero, if and only if it contains a nonzero element when each \( d_l \) is restricted to be an element of the canonical basis (zero vector with exactly one nonzero entry) or the null vector.

Define a graph with a layer structure:

- The source layer \( V_{-1} \) contains a single source node, \( v_{-1,1} \).
- The zero-th layer \( V_0 \) contains \( q_0 = p \) nodes \( v_{0,1} \cdots v_{0,q_0} \).
- Recursively, the \( i \)-th layer \( V_i \) contains \( q_i \) nodes \( v_{i,1} \cdots v_{i,q_i} \), for \( i = 1 \ldots L - 1 \).
- The sink layer \( V_L \) contains a single node \( v_{L,1} \).

We connect nodes between consecutive layers, respecting the order induced by the layer structure. For \( i = -1, \ldots L - 1 \) and \( j = 0, \ldots, L \), with \( j > i \), we connect layers \( V_i \) and \( V_j \) as follows

- Compute the quantity

\[
R = \left( \prod_{m=i+1}^{j-1} M_m^T Q_m \right) \times M_j^T,
\]

where if \( j = i + 1 \) the product reduces to the identity \((R = M_j^T)\).
We know that the resulting graph has a number of nodes equal to the number of nodes plus the input matrices. Computation of edges can be done in polynomial time: it requires at most \(4(L+1)^2\) matrix products involving at most \(2L+1\) matrices. Indeed the product of \(m\) matrices has polynomial time complexity in the representation bit size of the \(m\) input matrices.

In this graph, a directed path from the source to the sink visits each layer at most once, and in that case it visits a single node. Each such path corresponds to a monomial with nonzero coefficient appearing in the polynomial \(P\) in \(L\) by construction of the graph structure. Conversely each nonzero coefficient of a given monomial in \(L\) is uniquely associated to a path in the graph which corresponds to the nodes associated to variables in the monomial. Therefore, the source is connected to the sink if and only if there is a nonzero monomial in \(L\), if and only if the corresponding polynomial is nonzero. Furthermore, each path corresponds to the evaluation of the program at an edge of the product \(\Delta_0 \times \ldots \times \Delta_{L-1}\). Therefore finding a path connecting the source to the sink allows to compute a nonzero element in the product and if no such path exists, we conclude that \(D_F(0) = \{0\}\). This shows that the problem is solvable in polynomial time and concludes the proof.

D.3 Additional lemmas

The following lemma provides a characterization of singleton subgradient for linear relu networks.

**Lemma 3** Let \(F\) be a linear relu network, then \(\partial^c F(0) = \{0\}\) if and only if \(F\) is constant.

**Proof:** If \(F\) is constant, the result is immediate because \(F \equiv 0\). Now, suppose that \(\partial^c F(0) = \{0\}\). We know that \(F\) is piecewise linear and there exists a finite set of polyhedra whose union is \(\mathbb{R}^p\), where \(F\) is affine linear over each polyhedron. Furthermore, \(F\) is positively homogeneous, therefore for each \(x \in \mathbb{R}^p\), \(\partial^c F(x) = \partial^c F(\lambda x)\) with \(\lambda > 0\). Setting \(R \subset \mathbb{R}^p\), the full measure set where \(F\) is differentiable, one has that for all \(x \in \mathbb{R}^p\) and

\[
\partial^c F(x) = \text{conv} \left\{ v \in \mathbb{R}^p, \exists y_k \to 0 \text{ with } y_k \in R, v_k = \nabla F(y_k) \to v \right\} = \{0\}.
\]

Therefore, the each affine part has zero derivative on each polyhedra and by continuity we conclude that \(F\) is constant.

The next lemma describes an explicit representation of maximum of finitely many numbers using a relu network with weights in \{-1, 0, 1\}.

**Lemma 4** Given \(k \in \mathbb{N}, k > 0\), there exists \(F\), a relu network with \(k\) relu layers of size at most \(3 \times 2^{k-1}\) and weight matrices with entries in \{-1, 0, 1\}, with \(p = 2^k\) inputs such that for any \(x \in \mathbb{R}^p\),

\[F(x) = \max_{i=1,\ldots,2^k} x_i.\]

**Proof:** We proceed by recursion on \(k\). Note that for any \(x_1, x_2 \in \mathbb{R}\)

\[
\max\{x_1, x_2\} = \text{relu}(x_1 - x_2) + x_2 = \text{relu}(x_1 - x_2) + \text{relu}(x_2) - \text{relu}(-x_2).
\]

Set the matrices

\[
A = \begin{pmatrix} 1 & -1 \\ 0 & 1 \\ 0 & -1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 1 & -1 \end{pmatrix}.
\]
The function \( F_1 : \mathbb{R}^2 \to \mathbb{R} \) given by
\[
F_1(x) = \text{Brelu}(Ax)
\]
satisfies \( F_1(x) = \max\{x_1, x_2\} \). This proves the result for \( k = 1 \).

Now assume that for \( k \geq 1 \), we have a network with \( k \) \text{relu} layers of size at most \( 3 \times 2^k \) represented by matrices \( M_1, \ldots, M_{k+1} \) with entries in \( \{-1, 0, 1\} \), such that the corresponding \text{relu} network, as in (5) \( F_k : \mathbb{R}^{2^k} \to \mathbb{R} \) satisfies for all \( x \in \mathbb{R}^{2^k} \),
\[
F_k(x) = \max_{i=1, \ldots, 2^k} x_i.
\]

Set \( \tilde{F}_k \) the concatenation of two copies of \( F_k \), that is \( \tilde{F}_k : \mathbb{R}^{2^{k+1}} \to \mathbb{R}^2 \), such that for all \( x, y \in \mathbb{R}^{2^k} \),
\[
\tilde{F}_k(x, y) = \left( \begin{array}{c}
\max_{i=1, \ldots, 2^k} x_i \\
\max_{i=1, \ldots, 2^k} y_i 
\end{array} \right).
\]

The matrices representing \( \tilde{F}_k \) can be described in block form
\[
\tilde{M}_i = \left( \begin{array}{cc}
M_i & 0 \\
0 & M_i
\end{array} \right) \in \mathbb{R}^{(2p_i) \times (2p_i - 1)}
\]
for \( i = 1, \ldots, k + 1 \), where \( p_0 = 2^k \) and \( p_k = 1 \). This network is made of \( k \) layers of size at most \( 3 \times 2^{k+1} \), it has \( 2^{k+1} \) inputs and two outputs and its weight matrices have elements in \( \{-1, 0, 1\} \).

The block representation of the last matrix of this network is of the form
\[
\left( \begin{array}{cc}
M_{k+1} & 0 \\
0 & M_{k+1}
\end{array} \right) \in \mathbb{R}^{2 \times l}
\]
where \( l \) is the size of the row vector \( M_{k+1} \). We have
\[
A \times M_{k+1} = \begin{pmatrix} 1 & -1 \\ 0 & 1 \\ 0 & -1 \end{pmatrix} \times \begin{pmatrix} M_{k+1} & 0 \\ 0 & M_{k+1} \end{pmatrix} = \begin{pmatrix} M_{k+1} & -M_{k+1} \\ 0 & M_{k+1} \\ 0 & -M_{k+1} \end{pmatrix} \in \mathbb{R}^{3 \times (2l)}.
\]

We set \( F_{k+1}(x, y) = F_1(F_k(x), F_k(y)) = F_1(\tilde{F}_k(x, y)) \) for all \( x, y \in \mathbb{R}^{2^k} \). In matrix notation we have
\[
F_{k+1}(x, y) = \text{Brelu}(A\tilde{F}_k(x, y)).
\]

The involved matrices are \( M_{k+2} = B, A \times \tilde{M}_{k+1} \) and \( \tilde{M}_1 \ldots \tilde{M}_1 \). They all have entries in \( \{-1, 0, 1\} \) and the corresponding network has layers of size at most \( 3 \times 2^{k+1} \). The result then holds by recursion. \( \square \)