# An Elementary Approach to Convergence Guarantees of Optimization Algorithms for Deep Networks

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#### Abstract

We present an approach to obtain convergence guarantees of optimization algorithms for deep networks based on elementary arguments and computations. The convergence analysis revolves around the analytical and computational structures of optimization oracles central to the implementation of deep networks in modern machine learning software. We provide a systematic way to compute estimates of the smoothness constants that govern the convergence behavior of first-order optimization algorithms used to train deep networks. Diverse examples related to modern deep networks are interspersed within the text to illustrate the approach.

## **1** Introduction

Deep networks have achieved remarkable performance in several application domains such as computer vision, natural language processing and genomics [15, 20, 7]. The input-output mapping implemented by a deep neural network is a chain of compositions of modules, where each module is typically a composition of a non-linear mapping, called an activation function, and an affine mapping. The last module in the chain is usually task-specific in that it relates to a performance accuracy for a specific task. This module can be expressed either explicitly in analytical form as in supervised classification or implicitly as a solution of an optimization problem as in dimension reduction or unsupervised clustering.

The optimization problem arising when training a deep network is often framed as a non-convex optimization problem, dismissing the structure of the objective yet central to the software implementation. Indeed optimization algorithms used to train deep networks proceed by making calls to first-order (or second-order) oracles relying on dynamic programming such as gradient back-propagation [25, 22, 16, 5, 2, 23, 9]. Gradient back-propagation is now part of modern machine learning software [1, 19]. We highlight here the elementary yet important fact that the chain-compositional structure of the objective naturally emerges through the smoothness constants governing the convergence guarantee of a gradient-based optimization algorithm. This provides a reference frame to relate the network architecture and the convergence rate through the smoothness constants. This also brings to light the benefit of specific modules popular among practitioners to improve the convergence.

In Sec. 2, we define the parameterized input-output map implemented by a deep network as a chain-composition of modules and write the corresponding optimization objective consisting in learning the parameters of this map. In Sec. 3, we detail the implementation of first-order and second-order oracles by dynamic programming; the classical gradient back-propagation algorithm is recovered as a canonical example. Gauss-Newton steps can also be simply stated in terms of calls to an automatic-differentiation oracle implemented in modern machine learning software libraries. In Sec. 4, we present the computation of the smoothness constants of a chain of computations given its components and the resulting convergence guarantees for gradient descent. Finally, in Sec. 5, we present the application of the approach to derive the smoothness constants for the VGG architecture and illustrate how our approach can be used to identify the benefits of batch-normalization [24, 13]. In the Appendix, we estimate the smoothness constants related to the VGG architecture and we investigate batch-normalization in the light of our approach [24, 13]. All the proofs and the notations are also provided in the Appendix.



Figure 1: Deep network architecture.

## **2 Problem formulation**

## 2.1 Deep network architecture

A feed-forward deep network of depth  $\tau$  can be described as a transformation of an input x into an output  $x_{\tau}$  through the composition of  $\tau$  blocks, called layers, illustrated in Fig. 1. Each layer is defined by a set of parameters. In general, (see Sec. 2.3 for a detailed decomposition), these parameters act on the input of the layer through an affine operation followed by a non-linear operation. Formally, the  $t^{\text{th}}$  layer can be described as a function of its parameters  $u_t$  and a given input  $x_{t-1}$  that outputs  $x_t$  as

$$x_t = \phi_t(x_{t-1}, u_t) = a_t(b_t(x_{t-1}, u_t)), \tag{1}$$

where  $b_t$  is generally linear in  $u_t$  and affine in  $x_{t-1}$  and  $a_t$  is non-linear.

Learning a deep network consists in minimizing w.r.t. its parameters an objective involving n inputs  $\bar{x}^{(1)}, \ldots, \bar{x}^{(n)} \in \mathbb{R}^{\delta}$ . Formally, the problem is written

$$\min_{\substack{(u_1,\dots,u_{\tau})\in\mathbb{R}^{p_1}\times\dots\times\mathbb{R}^{p_{\tau}}\\\text{subject to}}} h(x_{\tau}^{(1)},\dots,x_{\tau}^{(n)}) + r(u_1,\dots,u_{\tau}) \\ x_t^{(i)} = \phi_t(x_{t-1},u_t^{(i)}) \quad \text{for } t = 1,\dots,\tau, \quad i = 1,\dots,n, \\ x_0^{(i)} = \bar{x}^{(i)} \qquad \text{for } i = 1,\dots,n, \quad (2)$$

where  $u_t \in \mathbb{R}^{p_t}$  is the set of parameters at layer t whose dimension  $p_t$  can vary among layers and r is a regularization on the parameters of the network.

We are interested in the influence of the architecture on the optimization complexity of the problem. The architecture translates into a structure of the chain of computations involved in the optimization problem.

**Definition 2.1.** A chain of  $\tau$  computations  $\phi_t : \mathbb{R}^{d_{t-1}} \times \mathbb{R}^{p_t} \to \mathbb{R}^{d_t}$  is defined as  $f : \mathbb{R}^{d_0} \times \mathbb{R}^{\sum_{t=1}^{\tau} p_t} \to \mathbb{R}^{\sum_{t=1}^{\tau} d_t}$  such that for  $x_0 \in \mathbb{R}^{d_0}$  and  $u = (u_1; \ldots; u_{\tau}) \in \mathbb{R}^{\sum_{t=1}^{\tau} p_t}$  we have  $f(x_0, u) = (f_1(x_0, u); \ldots; f_{\tau}(x_0, u))$  with

$$f_t(x_0, u) = \phi_t(f_{t-1}(x_0, u), u_t) \quad \text{for } t = 1, \dots, \tau,$$
(3)

and  $f_0(x_0, u) = x_0$ . We denote  $f_{t,x_0}(u) = f_t(x_0, u)$  and  $f_{t,u}(x_0) = f_t(x_0, u)$ .

Denote then  $f^0$  the chain of computations associated to the layers of a deep network and consider the concatenation of the transformations of each input as a single transformation, i.e.,  $f_t(\bar{x}, u) = (f_t^0(\bar{x}^{(1)}, u); \ldots; f_t^0(\bar{x}^{(n)}, u))$  for  $t \in \{1, \ldots, \tau\}$ , and  $\bar{x} = (\bar{x}^{(1)}; \ldots; \bar{x}^{(n)})$ , the objective in (2) can be written as

$$\min_{\boldsymbol{\mu}\in\mathbb{R}^{\sum_{t=1}^{T}p_t}} h(f_{\tau}(\bar{x},u)) + r(u),\tag{4}$$

where  $f_{\tau} : \mathbb{R}^{nd_0} \times \mathbb{R}^{\sum_{t=1}^{\tau} p_t} \to \mathbb{R}^{nd_{\tau}}$  is the output of a chain of  $\tau$  computations with  $d_0 = \delta$ ,  $r : \mathbb{R}^{\sum_{t=1}^{\tau} p_t} \to \mathbb{R}$  is typically a decomposable differentiable function such as  $r(u) = \lambda \sum_{t=1}^{\tau} ||u_t||_2^2$  for  $\lambda \ge 0$ , and we present examples of learning objectives  $f : \mathbb{R}^{nd_{\tau}} \to \mathbb{R}$  below. Assumptions on differentiability and smoothness of the objective are detailed in Sec. 4.

### 2.2 Objectives

In the following, we consider the output of the chain of computations on n sample to be given as  $\hat{y} = (\hat{y}^{(1)}; \ldots; \hat{y}^{(n)}) = (f_{\tau}^0(\bar{x}^{(1)}, u); \ldots; f_{\tau}^0(\bar{x}^{(n)}, u)) = f_{\tau}(\bar{x}, u)$  for  $\bar{x} = (\bar{x}^{(1)}; \ldots; \bar{x}^{(n)})$ .

Supervised learning. For supervised learning, the objective can be decomposed as a finite sum

$$h(\hat{y}) = \frac{1}{n} \sum_{i=1}^{n} h^{(i)}(\hat{y}^{(i)}), \tag{5}$$

where  $h^{(i)}$  are losses on the labels predicted by the chain of computations, i.e.,  $h^{(i)}(\hat{y}^{(i)}) = \mathcal{L}(\hat{y}^{(i)}, y^{(i)})$  with  $y^{(i)}$  the label of  $\bar{x}_i$ , and  $\mathcal{L}$  is a given loss such as the squared loss or the logistic loss (see Appendix D.1).

**Unsupervised learning.** In unsupervised learning tasks the labels are unknown. The objective itself is defined through a minimization problem rather than through an explicit loss function. For example, a convex clustering objective [11] is written

$$h(\hat{y}) = \min_{y^{(1)}, \dots, y^{(n)} \in \mathbb{R}^q} \sum_{i=1}^n \frac{1}{2} \|y^{(i)} - \hat{y}^{(i)}\|_2^2 + \sum_{i < j} \|y^{(i)} - y^{(j)}\|_2.$$

We consider in Appendix D.2 different clustering objectives. Note that classical ones, such as the one of k-means or spectral clustering, are inherently non-smooth, i.e., non-continuously differentiable.

## 2.3 Layer decomposition

The  $t^{\text{th}}$  layer of a deep network can be described by the following components:

(i) a bi-affine operation such as a matrix multiplication or a convolution, denoted  $b_t : \mathbb{R}^{d_{t-1}} \times \mathbb{R}^{p_t} \to \mathbb{R}^{\eta_t}$  and decomposed as

$$b_t(x_{t-1}, u_t) = \beta_t(x_{t-1}, u_t) + \beta_t^u(u_t) + \beta_t^x(x_{t-1}) + \beta_t^0,$$
(6)

where  $\beta_t$  is bilinear,  $\beta_t^u$  and  $\beta_t^x$  are linear and  $\beta_t^0$  is a constant vector,

- (ii) an activation function, such as the element-wise application of a non-linear function, denoted  $\alpha_t : \mathbb{R}^{\eta_t} \to \mathbb{R}^{\eta_t}$ ,
- (iii) a reduction of dimension, such as a pooling operation, denoted  $\pi_t : \mathbb{R}^{\eta_t} \to \mathbb{R}^{d_t}$ ,
- (iv) a normalization of the output, such as batch-normalization, denoted  $\nu_t : \mathbb{R}^{d_t} \to \mathbb{R}^{d_t}$ .

By concatenating the non-affine operations, i.e., defining  $a_t = \nu_t \circ \pi_t \circ \alpha_t$ , a layer can be written as

$$\phi_t(x_{t-1}, u_t) = a_t(b_t(x_{t-1}, u_t)). \tag{7}$$

Note that some components may not be included, for example some layers do not include normalization. In the following, we consider the non-linear operation  $a_t$  to be an arbitrary composition of functions, i.e.,  $a_t = a_{t,k_t} \circ \ldots \circ a_{t,1}$ . We present common examples of the components of a deep network.

#### 2.3.1 Linear operations

In the following, we drop the dependency w.r.t. the layer t and denote by a tilde  $\tilde{\cdot}$  the quantities characterizing the output. We denote by semi-columns the concatenations of matrices by rows, i.e., for  $A \in \mathbb{R}^{d \times n}$ ,  $B \in \mathbb{R}^{q \times n}$ ,  $(A; B) = (A^{\top}, B^{\top})^{\top}$ .

**Fully connected layer.** A *fully connected* layer taking an input of dimension  $\delta$  is written

$$\tilde{z} = W^{\top} z + w^0, \tag{8}$$

where  $z \in \mathbb{R}^{\delta}$  is the input,  $W \in \mathbb{R}^{\delta \times \tilde{\delta}}$  are the weights of the layer and  $w^0 \in \mathbb{R}^{\tilde{\delta}}$  define the intercepts. By vectorizing the parameters and the inputs, a fully connected layer can be written as

$$\begin{split} \tilde{x} &= \beta(x, u) + \beta^u(u), \\ \text{where} \qquad \beta(x, u) &= W^\top z \in \mathbb{R}^{\tilde{\delta}}, \ \beta^u(u) = w^0, \\ x &= z \in \mathbb{R}^{\delta}, \ u = \operatorname{Vec}(W; w^0) \in \mathbb{R}^{\tilde{\delta}(\delta+1)}. \end{split}$$

**Convolutional layer.** A convolutional layer convolves an input (images or signals) of dimension  $\delta$  denoted  $z \in \mathbb{R}^{\delta}$  with  $n^{f}$  affine filters of size  $s^{f}$  defined by weights  $W = (w_{1}, \ldots, w_{nf}) \in \mathbb{R}^{s^{f} \times n^{f}}$  and intercepts  $w^{0} = (w_{1}^{0}, \ldots, w_{nf}^{0}) \in \mathbb{R}^{n^{f}}$  through  $n^{p}$  patches. The  $k^{\text{th}}$  output of the convolution of the input by the  $j^{\text{th}}$  filter reads

$$\Xi_{j,k} = w_j^\top \Pi_k z + w_j^0, \tag{9}$$

where  $\Pi_k \in \mathbb{R}^{s^f \times \delta}$  extracts a patch of size  $s^f$  at a given position of the input z. The output  $\tilde{z}$  is then given by the concatenation  $\tilde{z}_{k+n^p(j-1)} = \Xi_{j,k}$ . By vectorizing the inputs and the outputs, the convolution operation is defined by a set of matrices  $(\Pi_k)_{k=1}^{n^p}$  such that

$$\begin{split} \tilde{x} &= \beta(x, u) + \beta^u(u), \\ \text{where} \qquad \beta(x, u) &= (w_j^\top \Pi_k z)_{j=1, \dots, n^f; k=1, \dots, n^p} \in \mathbb{R}^{n^f n^p}, \ \beta^u(u) = w^0 \otimes \mathbf{1}_{n^p} \\ x &= z \in \mathbb{R}^{\delta}, \ u = \operatorname{Vec}(W; w^0) \in \mathbb{R}^{(s^f+1)n^f}, \ W = (w_1, \dots, w_{n^f}). \end{split}$$

#### 2.3.2 Activation functions

We consider element-wise activation functions  $\alpha : \mathbb{R}^{\eta} \to \mathbb{R}^{\eta}$  such that for a given  $x = (x_1, \dots, x_{\eta}) \in \mathbb{R}^{\eta}$ ,

$$\alpha(x) = (\bar{\alpha}(x_1), \dots, \bar{\alpha}(x_\eta)), \tag{10}$$

for a given scalar function  $\bar{\alpha}$  such as  $\bar{\alpha}(x) = \max(x, 0)$  for the Rectified Linear Unit (ReLU) or  $\bar{\alpha}(x) = (1 + \exp(-x))^{-1}$  for the sigmoid function.

#### 2.3.3 Pooling functions

A pooling layer reduces the dimension of the output. For example, an average pooling convolves an input image with a mean filter. Formally, for an input  $z \in \mathbb{R}^{\delta}$ , the average pooling with a patch size  $s^{f}$  for inputs with  $n^{f}$  channels and  $n^{p}$  coordinates such that  $\delta = n^{f}n^{p}$  convolves the input with a filter  $P = \mathbf{1}_{sf} \mathbf{1}_{n^{f}}^{\top} / s^{f}$ . The output dimension for each input is  $\tilde{\delta} = n^{f}\tilde{n^{p}}$  and the patches, represented by some  $(\Pi_{k})_{k=1}^{\tilde{n^{p}}}$  acting in Eq. (9), are chosen such that it induces a reduction of dimension, i.e.,  $\tilde{n^{p}} \leq n^{p}$ .

### 2.3.4 Normalization functions

Given a batch of input  $Z \in \mathbb{R}^{\delta \times m}$  the batch-normalization outputs  $\tilde{Z}$  defined by

$$(\tilde{Z})_{ij} = \frac{Z_{ij} - \mu_i}{\sqrt{\epsilon + \sigma_i^2}},$$
(11)  
where  $\mu_i = \frac{1}{m} \sum_{j=1}^m Z_{ij}, \quad \sigma_i^2 = \frac{1}{m} \sum_{j=1}^m (Z_{ij} - \mu_i)^2,$ 

with  $\epsilon > 0$ , such that the vectorized formulation of the batch-normalization reads  $\nu(x) = \operatorname{Vec}(\tilde{Z})$  for  $x = \operatorname{Vec}(Z)$ .

## 2.4 Specific structures

#### 2.4.1 Auto-encoders

An auto-encoder seeks to learn a compact representation of some data  $\bar{x} \in \mathbb{R}^d$  by passing it through an encoder network with output dimension  $\hat{d} \ll d$  then a decoder network with output dimension d with the objective that the final output is close to the original input. Each network can be represented by a chain of computations. Given n data points  $\bar{x} = (\bar{x}^{(1)} : \ldots; \bar{x}^{(n)})$ , denoting  $f^e$  the encoder with parameters  $u_e$  such that  $f_{u_e}^e : \mathbb{R}^d \to \mathbb{R}^d$  and  $f^d$  the decoder with parameters  $u_d$  such that  $f_{u_d}^d : \mathbb{R}^d \to \mathbb{R}^d$ , the objective is

$$\min_{u^e, u^d} \frac{1}{n} \sum_{i=1}^n \|\bar{x}^{(i)} - f^d(f^e(\bar{x}^{(i)}, u_e), u_d)\|_2^2.$$

The composition of the encoder and the decoder form a chain of computations such that the overall objective can be written as in (4) as detailed in Appendix 2.3. Formally, denoting  $f^0: x_0, u \to f^d(f^e(x_0, u_e), u_d)$  for  $u = (u_d; u_e)$  the resulting chain of computations on a single input and  $f(\bar{x}, u) = (f^0(\bar{x}^{(1)}, u); \ldots; f^0(\bar{x}^{(n)}, u))$  the concatenation of the outputs applied to the set of inputs, the objective of an auto-encoder has the form  $h(f(\bar{x}, u))$  with  $h(\hat{x}) = \frac{1}{n} \sum_{i=1}^{n} ||\bar{x}_i - \hat{x}_i||_2^2$ .

#### 2.4.2 Dense, highway or residual networks

Dense networks use not only the last input but all previous ones. The output of such networks can be described as

$$f_{\tau}(x_0, v) = x_{\tau} \quad \text{with} \qquad x_t = \phi_t(x_{0:t-1}, v_t), \quad x_{0:t-1} = (x_0; \dots; x_{t-1}) \quad \text{for } t = 1, \dots, \tau, \tag{12}$$

where  $v_t = (u_{t,0}; \dots u_{t,t-1})$  are the parameters of the layer dispatched with one set of parameters per previous state and  $v = (v_1; \dots; v_{\tau})$ . The dynamics can be described as previously as  $\phi_t(x_{0:t-1}, v_t) = a_t(b_t(x_{0:t-1}, v_t))$ . The bilinear operation  $b_t$  is still a matrix multiplication or a convolution as previously presented except that it incorporates more variables. The non-linear operation  $a_t$  is also the same, i.e., it incorporates an activation function and, potentially, a pooling operation and a normalization operation.

Dense networks can naturally be translated as a single input-output transformation by defining layers of the form

$$x_{0:t} = \psi_t(x_{0:t-1}, v_t) = (x_0; \dots; x_{t-1}; \phi_t(x_{0:t-1}, v_t)) = (x_{0:t-1}; \phi_t(x_{0:t-1}, v_t)) \quad \text{for } t = 1, \dots, \tau,$$

and  $f_{\tau}(x_0, v) = E_{\tau} x_{0:\tau} = x_{\tau}$  where  $E_{\tau}$  is a linear projector that extracts  $x_{\tau}$  from  $x_{0:\tau}$ .

Highway networks are dense networks that consider only the last input and the penultimate one, i.e., they are of the form (12) except that they propagate only  $x_{t-1:t} = (x_{t-1}, x_t)$ . Namely they are defined by

$$x_{t-1:t} = \psi_t(x_{t-2:t-1}, v_t) = (x_{t-1}; \phi_t(x_{t-2:t-1}, v_t))$$
 for  $t = 1, \dots, \tau_t$ 

with  $v_t = (u_{t,t-2}; u_{t,t-1})$ . Finally, residual networks are highway networks with fixed parameters acting on the penultimate input. In the simple case where the current and penultimate inputs have the same dimension, they read

$$x_t = a_t(b_t(x_{t-1}, u_t) + x_{t-2}) = a_t(\hat{b}_t(x_{t-2:t-1}, u_t)) \quad \text{for } t = 1, \dots, \tau,$$
(13)

with  $x_{-1} = 0$ , where  $b_t$  and  $a_t$  are of the forms described above. This amounts to define layers  $\psi_t$  on  $x_{t-2:t-1}$  whose bi-affine operation  $\tilde{b}_t(x_{t-2:t-1}, u_t)$  has a non-zero affine term  $\tilde{\beta}_t^x$  on  $x_{t-2:t-1} = (x_{t-2}; x_{t-1})$ , see Appendix D.8.

#### 2.4.3 Implicit functions

We consider implicit functions that take the form

$$g(\alpha) = \operatorname*{arg\,min}_{\beta \in \mathbb{R}^b} \zeta(\alpha, \beta)$$

where  $\zeta$  is twice differentiable and  $\zeta(\alpha, \cdot)$  is strongly convex for any  $\alpha$  such that  $g(\alpha)$  is uniquely defined. These can be used either in the objective as seen before with clustering tasks, in that case  $\alpha = x_{\tau}$ . These can also be used in the layers such that  $\alpha = (x, u)$  and  $\phi(x, u) = \arg \min_{\beta \in \mathbb{R}^b} \zeta(x, u, \beta)$ .

If the minimizer is computed exactly, we can compute the gradient by invoking the implicit function theorem. Formally, denoting  $\xi(\alpha, \beta) = \nabla_{\beta} \zeta(\alpha, \beta)$ , the function  $g(\alpha)$  is defined by the implicit equation  $\xi(\alpha, g(\alpha)) = 0$  and its gradient is given by

 $\nabla g(\alpha) = -\nabla_{\alpha}\xi(\alpha, g(\alpha))\nabla_{\beta}\xi(\alpha, g(\alpha))^{-1} = -\nabla^{2}_{\alpha,\beta}\zeta(\alpha, g(\alpha))\nabla^{2}_{\beta,\beta}\zeta(\alpha, g(\alpha))^{-1}$ 

The smoothness constants of this layer for exact minimizations are provided in Appendix D.9.

If the minimizer is computed approximately through an algorithm, its derivative can be computed by using automatic differentiation through the chain of computations defining the algorithm (see Subsection 3.2 for a detailed explanation of automatic differentiation). Alternatively, an approximate gradient can be computed by using the above formula. The resulting approximation error of the gradient is given by the following lemma.

**Lemma 2.2.** Let  $\zeta : (\alpha, \beta) \to \zeta(\alpha, \beta) \in \mathbb{R}$  for  $\alpha \in \mathbb{R}^a, \beta \in \mathbb{R}^b$  be s.t.  $\zeta(\alpha, \cdot)$  is  $\mu_{\zeta}$ -strongly convex for any  $\alpha$  and denote  $\xi(\alpha, \beta) = \nabla_{\beta}\zeta(\alpha, \beta)$ . Denote  $g(\alpha) = \arg\min_{\beta \in \mathbb{R}^b} \zeta(\alpha, \beta)$  and  $\hat{g}(\alpha) \approx \arg\min_{\beta \in \mathbb{R}^b} \zeta(\alpha, \beta)$  be an approximate minimizer. Provided that  $\zeta$  has a  $L_{\zeta}$ -Lipschitz gradient and a  $H_{\zeta}$ -Lipschitz Hessian, the approximation error of using

$$\widehat{\nabla}\widehat{g}(\alpha) = -\nabla_{\alpha}\xi(\alpha,\widehat{g}(\alpha))\nabla_{\beta}\xi(\alpha,\widehat{g}(\alpha))^{-1}$$

instead of  $\nabla g(\alpha)$  is bounded as

$$\|\widehat{\nabla}\widehat{g}(\alpha) - \nabla g(\alpha)\|_2 \le H_{\zeta}\mu_{\zeta}^{-1}(1 + L_{\zeta}\mu_{\zeta}^{-1})\|\widehat{g}(\alpha) - g(\alpha)\|_2.$$

## **3** Oracle arithmetic complexity

For each class of optimization algorithm considered (gradient descent, Gauss-Newton, Newton), we define the appropriate optimization oracle called at each step of the optimization algorithm which can be efficiently computed through a dynamic programming procedure. For a gradient step, we retrieve the gradient back-propagation algorithm. The gradient back-propagation algorithm forms then the basis of automatic-differentiation procedures.

#### 3.1 Oracle reformulations

In the following, we use the notations presented in Sec. A for gradients, Hessians and tensors. Briefly,  $\nabla f(x)$  is used to denote the gradient of a function f at x, which, if  $f : \mathbb{R}^p \to \mathbb{R}^d$  is multivariate, is the transpose of the Jacobian, i.e.,  $\nabla f(x) \in \mathbb{R}^{p \times d}$ . For a multivariate function  $f : \mathbb{R}^p \to \mathbb{R}^d$ , its second order information at x is represented by a tensor  $\nabla^2 f(x) \in \mathbb{R}^{p \times p \times d}$ , and we denote for example  $\nabla^2 f(x)[y, y, \cdot] = (y^\top \nabla^2 f^{(1)}(x))y; \ldots; y^\top \nabla^2 f^{(n)}(x)y) \in \mathbb{R}^d$ . For a function  $f : \mathbb{R}^p \to \mathbb{R}^d$ , we define, provided that  $\nabla f(x), \nabla f^2(x)$  are defined,

$$\ell_f^x(y) = \nabla f(x)^\top y, \qquad q_f^x(y) = \nabla f(x)^\top y + \frac{1}{2} \nabla^2 f(x)[y, y, \cdot],$$
(14)

such that the linear and quadratic approximations of f around x are  $f(x + y) \approx f(x) + \ell_f^x(y)$  and  $f(x + y) \approx f(x) + q_f^x(y)$  respectively.

We consider optimization oracles as procedures that compute either the next step of an optimization method or a decent direction along which the next step of an optimization method is taken. Formally, the optimization oracles for an objective f are defined by a model  $m_f^u$  that approximates the objective around the current point u as  $f(u + v) \approx f(u) + m_f^u(v)$ . The models can be minimized with an additional proximal term that ensures that the minimizer lies in a region where the model approximates well the objective as

$$v_{\gamma}^{*} = \operatorname*{arg\,min}_{v \in \mathbb{R}^{p}} m_{f}^{u}(v) + \frac{1}{2\gamma} \|v\|_{2}^{2}, \qquad u_{\mathrm{new}} = u + v_{\gamma}^{*}.$$

The parameter  $\gamma$  acts as a stepsize that controls how large should be the step (the smaller the  $\gamma$ , the smaller the  $v_{\gamma}^*$ ). Alternatively the model can be minimized directly providing a descent direction along which the next iterate is taken as

$$v^* = \mathop{\arg\min}_{v \in \mathbb{R}^p} m^u_f(v) \qquad u_{\mathrm{new}} = u + \gamma v^*,$$

where  $\gamma$  is found by a line-search using e.g. an Armijo condition [18].

On a point  $u \in \mathbb{R}^p$ , given a regularization  $\kappa$ , for an objective of the form  $h \circ \psi + r : \mathbb{R}^p \to \mathbb{R}$ , (i) a *gradient* oracle is defined as

$$v^* = \underset{v \in \mathbb{R}^p}{\arg\min} \ell^u_{h \circ \psi}(v) + \ell^u_r(v) + \frac{\kappa}{2} \|v\|_2^2,$$
(15)

(ii) a (regularized) Gauss-Newton oracle is defined as

$$v^* = \underset{v \in \mathbb{R}^p}{\arg\min} q_h^{\psi(u)}(\ell_{\psi}^u(v)) + q_r^u(v) + \frac{\kappa}{2} \|v\|_2^2,$$
(16)

(iii) a (regularized) Newton oracle is defined as

$$v^* = \underset{v \in \mathbb{R}^p}{\arg\min} q_{h \circ \psi}^u(v) + q_r^u(v) + \frac{\kappa}{2} \|v\|_2^2.$$
(17)

**Proposition 3.1.** Let f be a chain of  $\tau$  computations  $\phi_t : \mathbb{R}^{d_{t-1}} \times \mathbb{R}^{p_t} \to \mathbb{R}^{d_t}$ ,  $u = (u_1; \ldots; u_{\tau})$  and  $x_0 \in \mathbb{R}^{d_0}$ . Denote  $\psi = f_{x_0,\tau}$  and  $f(x_0, u) = (x_1; \ldots; x_{\tau})$ . Assume r to be decomposable as  $r(u) = \sum_{t=1}^{\tau} r_t(u_t)$ . Gradient (15), Gauss-Newton (16) and Newton (17) oracles on  $h \circ \psi + r$  are the solutions  $v^* = (v_1^*; \ldots; v_{\tau}^*)$  of problems of the form

$$\min_{\substack{v_1, \dots, v_\tau \in \mathbb{R}^{p_1} \times \dots \times \mathbb{R}^{q_\tau} \\ y_0, \dots, y_\tau \in \mathbb{R}^{d_0} \times \dots \times \mathbb{R}^{d_\tau}}}_{subject to} \quad \sum_{t=1}^{\tau} \frac{1}{2} y_t^\top P_t y_t + p_t^\top y_t + y_{t-1}^\top R_t v_t + \frac{1}{2} v_t^\top Q_t v_t + q_t^\top v_t + \frac{\kappa}{2} \|v_t\|_2^2 \tag{18}$$

$$subject to \quad y_t = A_t y_{t-1} + B_t v_t \quad \text{for} \quad t \in \{1, \dots, \tau\}, \\ y_0 = 0,$$

where

$$A_t = \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t)^{\top}, \quad B_t = \nabla_{u_t} \phi_t(x_{t-1}, u_t)^{\top},$$
$$p_\tau = \nabla h(\psi(u)), \quad p_t = 0 \quad \text{for } t \neq \tau,$$
$$q_t = \nabla r_t(u_t),$$

1. for gradient oracles (15),

$$P_t = 0, \quad R_t = 0, \quad Q_t = 0,$$

2. for Gauss-Newton oracles (16),

$$P_{\tau} = \nabla^2 h(\psi(u)), \quad P_t = 0 \quad \text{for } t \neq \tau, \quad R_t = 0, \quad Q_t = \nabla^2 r_t(u_t),$$

3. for Newton oracles (17), defining

$$\lambda_{\tau} = \nabla h(\psi(u)), \quad \lambda_{t-1} = \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t) \lambda_t \quad \text{for } t \in \{1, \dots, \tau\},$$

we have

$$P_{\tau} = \nabla^2 h(\psi(u)), \quad P_{t-1} = \nabla^2_{x_{t-1}x_{t-1}} \phi_t(x_{t-1}, u_t)[\cdot, \cdot, \lambda_t] \quad \text{for } t \in \{1, \dots, \tau\},$$
  
$$R_t = \nabla^2_{x_{t-1}u_t} \phi_t(x_{t-1}, u_t)[\cdot, \cdot, \lambda_t], \quad Q_t = \nabla^2 r_t(u_t) + \nabla^2_{u_tu_t} \phi_t(x_{t-1}, u_t)[\cdot, \cdot, \lambda_t].$$

Problems of the form

$$\min_{\substack{u_1,\dots,u_\tau \in \mathbb{R}^{p_1} \times \dots \times \mathbb{R}^{p_\tau} \\ x_0,\dots,x_\tau \in \mathbb{R}^{d_0} \times \dots \times \mathbb{R}^{d_\tau}}} \sum_{t=1}^{\tau} h_t(x_t) + \sum_{t=1}^{\tau} g_t(u_t)$$
subject to
$$x_t = \phi_t(x_{t-1}, u_t) \quad \text{for } t \in \{1,\dots,\tau\},$$

$$x_0 = \hat{x}_0$$
(19)

can be decomposed into nested subproblems defined as the cost-to-go from  $\hat{x}_t$  at time t by

$$\cot_{t}(\hat{x}_{t}) = \min_{\substack{u_{t+1}, \dots, u_{\tau} \in \mathbb{R}^{p_{t+1}} \times \dots \times \mathbb{R}^{p_{\tau}} \\ x_{t}, \dots, x_{\tau} \in \mathbb{R}^{d_{t}} \times \dots \times \mathbb{R}^{d_{\tau}}}} \sum_{t'=t}^{\tau} h_{t'}(x_{t'}) + \sum_{t'=t+1}^{\tau} g_{t'}(u_{t'}) \\ \text{subject to} \quad x_{t'} = \phi_{t'}(x_{t'-1}, u_{t'}) \quad \text{for } t' \in \{t+1, \dots, \tau\}, \\ x_{t} = \hat{x}_{t},$$

such that they follow the recursive relation

$$\operatorname{cost}_{t}(\hat{x}_{t}) = \min_{u_{t+1} \in \mathbb{R}^{p_{t+1}}} \{ h_{t}(\hat{x}_{t}) + g_{t+1}(u_{t+1}) + \operatorname{cost}_{t+1}(\phi_{t+1}(x_{t}, u_{t+1})) \}.$$
(20)

This principle cannot be used directly on the original problem, since Eq. (20) cannot be solved analytically for generic problems of the form (19). However, for quadratic problems with linear compositions of the form (18), this principle can be used to solve problems (18) by dynamic programming [4]. Therefore as a corollary of Prop. 3.1, the complexity of all optimization steps given in (15), (16), (17) is linear w.r.t. to the length  $\tau$  of the chain. Precisely, Prop. 3.1 shows that each optimization step amounts to reducing the complexity of the recursive relation (20) to an analytic problem.

In particular, while the Hessian of the objective scales as  $\sum_{t=1}^{\tau} p_t$ , a Newton step has a linear and not cubic complexity with respect to  $\tau$ . We present in Appendix B the detailed computation of a Newton step, alternative derivations were first proposed in the control literature [6]. This involves the inversion of intermediate quadratic costs at each layer. Gauss-Newton steps can also be solved by dynamic programming and can be more efficiently implemented using an automatic-differentiation oracles as we explain below.

### 3.2 Automatic differentiation

#### 3.2.1 Algorithm

As explained in last subsection and shown in Appendix B, a gradient step can naturally be derived as a dynamic programming procedure applied to the subproblem (18). However, the implementation of the gradient step provides itself a different kind of oracle on the chain of computations as defined below.

**Definition 3.2.** Given a chain of computations  $f : \mathbb{R}^{\sum_{t=1}^{\tau} p_t} \times \mathbb{R}^{d_0} \to \mathbb{R}^{\sum_{t=1}^{\tau} d_t}$  as defined in Def. 2.1,  $u \in \mathbb{R}^{\sum_{t=1}^{\tau} p_t}$  and  $x_0 \in \mathbb{R}^{d_0}$ , an automatic differentiation oracle is a procedure that gives access to

$$\mu \to \nabla f_{x_0,\tau}(u)\mu$$
 for any  $\mu \in \mathbb{R}^{d_{\tau}}$ 

The subtle difference is that we have access to  $\nabla f_{x_0,\tau}(u)$  not as a matrix but as a linear operator. The matrix  $\nabla f_{x_0,\tau}(u)$  can also be computed and stored to perform gradient vector products. Yet, this requires a surplus of storage and of computations that are generally not necessary for our purposes. The only quantities that need to be stored are given by the forward pass. Then, these quantities can be used to compute any gradient vector product directly.

The definition of an automatic differentiation oracle is composed of two steps:

- 1. a forward pass that computes  $f_{x_0,\tau}(u)$  and stores the information necessary to compute gradient-vector products.
- 2. the compilation of a *backward* pass that computes  $\mu \to \nabla f_{x_0,\tau}(u)\mu$  for any  $\mu \in \mathbb{R}^{d_{\tau}}$  given the information collected in the forward pass.

Note that the two aforementioned passes are decorrelated in the sense that the forward pass does not require the knowledge of the slope  $\mu$  for which  $\nabla f_{x_0,\tau}(u)\mu$  is computed.

We present in Algo. 1 and Algo. 2 the classical forward-backward passes used in modern automatic-differentiation libraries. The implementation of the automatic differentiation oracle as a procedure that computes both the value of the chain  $f_{x_0,\tau}(u)$  and the linear operator  $\mu \to f_{x_0,\tau}(u)\mu$  is then presented in Algo. 3 and illustrated in Fig. 2.

Computing the gradient  $g = \nabla (h \circ f_{x_0,\tau})(u)$  on  $u \in \mathbb{R}^p$  amounts then to

- 1. computing with Algo. 3,  $f_{x_0,\tau}(u), \mu \to \nabla f_{x_0,\tau}(u)\mu = \text{Autodiff}(f, u),$
- 2. computing  $\mu = \nabla h(f_{x_0,\tau}(u))$  then  $g = \nabla f_{x_0,\tau}(u)\mu$ .

## Algorithm 1 Forward pass

Inputs: Chain of computations f defined by (φ<sub>t</sub>)<sub>t=1,...,τ</sub>, input x as in Def. 2.1, variable u = (u<sub>1</sub>;...; u<sub>τ</sub>)
 Initialize x<sub>0</sub> = x
 for t = 1,...,τ do

- 4: Compute  $x_t = \phi_t(x_{t-1}, u_t)$
- 5: Store  $\nabla \phi_t(x_{t-1}, u_t)$
- 6: **end for**
- 7: **Output:**  $x_{\tau}, \nabla \phi_t(x_{t-1}, u_t)$  for  $t \in \{1, ..., \tau\}$ .

#### Algorithm 2 Backward pass

1: Inputs: Slope  $\mu$ , intermediate gradients  $\nabla \phi_t(x_{t-1}, u_t)$  for  $t \in \{1, ..., \tau\}$ 2: Initialize  $\lambda_{\tau} = \mu$ 3: for  $t = \tau, ..., 1$  do 4: Compute  $\lambda_{t-1} = \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t) \lambda_t$ 5: Store  $g_t = \nabla_{u_t} \phi_t(x_{t-1}, u_t) \lambda_t$ 6: end for 7: Output:  $(g_1, ..., g_{\tau}) = \nabla f_{x_0, \tau}(u) \mu$ 

Algorithm 3 Chain of computations with automatic-differentiation oracle (Autodiff)

- 1: Inputs: Chain of computations f defined by  $(\phi_t)_{t=1,...,\tau}$ , input x as in Def. 2.1, variable  $u = (u_1; ...; u_{\tau})$
- 2: Compute using Algo. 1  $(x_{\tau}, (\nabla \phi_t(x_{t-1}, u_t)_{t=1}^{\tau}) = \text{Forward}(f, u)$  which gives  $f_{x_0, \tau}(u) = x_{\tau}$
- 3: Define  $\mu \to \nabla f_{x_0,\tau}(u)\mu$  as  $\mu \to \text{Backward}(\mu, (\nabla \phi_t(x_{t-1}, u_t))_{t=1}^{\tau})$  according to Algo. 2.
- 4: **Output:**  $f_{x_0,\tau}(u), \mu \to \nabla f_{x_0,\tau}(u)\mu$



Figure 2: Automatic differentiation of a chain of computations.

#### 3.2.2 Complexity

Without additional information on the structure of the layers, the space and time complexities of the forward-backward algorithm is of the order of

$$\mathcal{S}_{\text{FB}} \leq \sum_{t=1}^{\tau} (p_t + d_{t-1}) d_t,$$
  
$$\mathcal{T}_{\text{FB}} \leq \sum_{t=1}^{\tau} \mathcal{T}(\phi_t, \nabla \phi_t) + 2 \sum_{t=1}^{\tau} (d_{t-1} d_t + p_t d_t)$$

respectively, where  $\mathcal{T}(\phi_t, \nabla \phi_t)$  is the time complexity of computing  $\phi_t, \nabla \phi_t$  during the backward pass. The units chosen are for the space complexity the cost of storing one digit and for the time complexity the cost of performing an addition or a multiplication.

Provided that for all  $t \in \{1, \ldots, \tau\}$ ,

$$\mathcal{T}(\phi_t, \nabla \phi_t) + 2(d_{t-1}d_t + p_t d_t) \le Q \mathcal{T}(\phi_t), \tag{21}$$

where  $\mathcal{T}(\phi_t)$  is the time complexity of computing  $\phi_t$  and  $Q \ge 0$  is a constant, we get that

$$\mathcal{T}_{\mathrm{FB}} \leq Q\mathcal{T}(f),$$

where  $\mathcal{T}(f)$  is the complexity of computing the chain of computations [14]. We retrieve Baur-Strassen's theorem which states that the complexity of computing the derivative of a function formulated as a chain of computations is of the order of the complexity of computing the function itself [3, 10].

For chain of computations of the form (7), this cost can be refined as shown in Appendix B. Specifically, for a chain of fully-connected layers with element-wise activation function, no normalization or pooling, the cost of the backward pass is then of the order of  $\mathcal{O}\left(\sum_{t=1}^{\tau} 2m\delta_t(\delta_{t-1}+1)\right)$  elementary operations. For a chain of convolutional layers with element-wise activation function, no normalization or pooling, the cost of the backward pass is of the order of  $\mathcal{O}\left(\sum_{t=1}^{\tau} 2m\delta_t(\delta_{t-1}+1)\right)$  elementary operations. For a chain of convolutional layers with element-wise activation function, no normalization or pooling, the cost of the backward pass is of the order of  $\mathcal{O}\left(\sum_{t=1}^{\tau} (2n_t^p n_t^f s_t^f + n_t^p n_t^f + \delta_t)m\right)$  elementary operations.

## 3.3 Gauss-Newton by automatic differentiation

The Gauss-Newton step can also be solved by making calls to an automatic differentiation oracle.

**Proposition 3.3.** Consider the Gauss-Newton oracle (16) on  $u = (u_1; ...; u_\tau)$  for a convex objective h, a convex decomposable regularization  $r(u) = \sum_{t=1}^{\tau} r_t(u_t)$  and a differentiable chain of computations f with output  $\psi = f_{x_0,\tau}$  on some input  $x_0$ . We have that

1. the Gauss-Newton oracle amounts to solving

$$\min_{\mu \in \mathbb{R}^{d_{\tau}}} \left( q_h^{\psi(u)} \right)^{\star}(\mu) + \left( q_r^u + \kappa \| \cdot \|_2^2 / 2 \right)^{\star} (-\nabla \psi(u)\mu), \tag{22}$$

where for a function f we denote by  $f^*$  its convex conjugate,

- 2. the Gauss-Newton oracle is  $v^* = \nabla \left(q_r^u + \kappa \|\cdot\|_2^2/2\right)^* \left(-\nabla \psi(u)\mu^*\right)$  where  $\mu^*$  is the solution of (22),
- *3.* the dual problem (22) can be solved by  $2d_{\tau} + 1$  calls to an automatic differentiation procedure.

Proposition 3.3 shows that a Gauss-Newton step is only  $2d_{\tau} + 1$  times more expansive than a gradient-step. Precisely, for a deep network with a supervised objective, we have  $d_{\tau} = nk$  where n is the number of samples and k is the number of classes. A gradient step makes then one call to an automatic differentiation procedure to get the gradient of the batch and the Gauss-Newton method will then make 2nk + 1 more calls. If mini-batch Gauss-Newton steps are considered then the cost reduces to 2mk + 1 calls to an automatic differentiation oracle, where m is the size of the mini-batch.

## 4 Optimization complexity

We present smoothness properties with respect to the Euclidean norm  $\|\cdot\|_2$ , whose operator norm is denoted  $\|\cdot\|_{2,2}$ . In the following, for a function  $f : \mathbb{R}^d \to \mathbb{R}^n$  and a set  $C \subset \text{dom } f \subset \mathbb{R}^d$ , we denote by

$$m_f^C = \sup_{x \in C} \|f(x)\|_2, \quad \ell_f^C = \sup_{\substack{x,y \in C \\ x \neq y}} \frac{\|f(x) - f(y)\|_2}{\|x - y\|_2}, \quad L_f^C = \sup_{\substack{x,y \in C \\ x \neq y}} \frac{\|\nabla f(x) - \nabla f(y)\|_{2,2}}{\|x - y\|_2},$$

a bound of h on C, the Lipschitz-continuity parameter of h on C, and the smoothness parameter of h on C (i.e., the Lipschitz-continuity parameter of its gradient if it exists), all with respect to  $\|\cdot\|_2$ . Note that if  $x = \operatorname{Vec}(X)$  for a given matrix X,  $\|x\|_2 = \|X\|_F$ . We denote by  $m_f, \ell_f, L_f$  the same quantities defined on the domain of f, e.g.,  $m_f = m_f^{\operatorname{dom} f}$ . We denote by  $\mathcal{C}_{m,\ell,L}$  the class of functions f such that  $m_f = m, \ell_f = \ell, L_f = L$ . In the following, we allow the quantities mf,  $\ell_f, L_f$  to be infinite if for example the function is unbounded or the smoothness constant is not defined. The procedures presented below output infinite estimates if the combinations of the smoothness properties do not allow for finite estimates. On the other hand, they provide finite estimates automatically if they are available. In the following we denote  $\bigotimes_{t=1}^{\tau} B_{R_t}(\mathbb{R}^{p_t}) = \{u = (u_1; \ldots; u_\tau) \in \mathbb{R}^{\sum_{t=1}^{\tau} p_t} : u_t \in \mathbb{R}^{p_t}, \|u_t\|_2 \le R_t\}.$ 

### 4.1 Convergence rate to a stationary point

We recall the convergence rate to a stationary point of a gradient descent and a stochastic gradient descent on constrained problems.

Theorem 4.1 (8, Theorems 1 and 2). Consider problems of the form

(i) 
$$\min_{u \in \mathbb{R}^p} \{F(u) := h(\psi(u)) + r(u)\}, \quad or \quad (ii) \quad \min_{u \in \mathbb{R}^p} \{F(u) := \frac{1}{n} \sum_{i=1}^n h_i(\psi_i(u)) + r(u)\}$$
  
subject to  $u \in C$ ,  $u \in C$ ,

where C is a closed convex set and F is  $L_F^C$  smooth on C. For problem (ii), consider that we have access to an unbiased estimate  $\widehat{\nabla}F(u)$  of  $\nabla F(u)$  with a variance bounded as  $\mathbb{E}(\|\widehat{\nabla}F(u) - \nabla F(u)\|_2^2) \leq \sigma^2$ .

A projected gradient descent applied on problem (i) with step-size  $\gamma = (L_F^C)^{-1}$  converges to an  $\varepsilon$ -stationary point in at most

$$\mathcal{O}\left(\frac{L_F^C(F(u_0) - F^*)}{\epsilon^2}\right)$$

iterations, where  $u_0$  is the initial point and  $F^* = \min_{u \in C} F(u)$ .

A stochastic projected gradient descent applied on problem (ii) with step-size  $\gamma = (2L_F^C)^{-1}$  converges in expectation to an  $(\varepsilon + \sigma)$ -stationary point in at most

$$\mathcal{O}\left(\frac{L_F^C(F(u_0) - F^*)}{\epsilon^2}\right)$$

iterations, where  $u_0$  is the initial point and  $F^* = \min_{u \in C} F(u)$ .

#### Remarks.

1. Since a gradient descent is monotonically decreasing, a gradient descent applied to the unconstrained problem converges to an  $\varepsilon$ -stationary point in at most

$$\mathcal{O}\left(\frac{L_F^{S_0}(F(u_0) - F^*)}{\epsilon^2}\right)$$

iterations, where  $S_0 = \{u \in \mathbb{R}^p : F(u) \le F(u_0)\}$  is the initial sub-level set.

2. Tighter rates of convergence can be obtained for the finite-sum problem (ii) by using variance reduction methods and by varying mini-batch sizes [17]. They would then depend on the smoothness constants of the objective or the maximal smoothness of the components on C, i.e.,  $\max_{i=1,...,n} L_{h_i \circ \psi_i + r}^C$ . The smoothness of the objectives F defined in Theorem 4.1 can be derived from the smoothness properties of their components.

**Proposition 4.2.** Consider a closed convex set  $C \subset \mathbb{R}^p$ ,  $\psi \in \mathcal{C}_{m_{\psi}^C, \ell_{\psi}^C, L_{\psi}^C}^C$ ,  $r \in \mathcal{C}_{L_r}$  and  $h \in \mathcal{C}_{\ell_h, L_h}$  with  $\ell_h = +\infty$  if h is not Lipschitz-continuous. The smoothness of  $F = h \circ \psi + r$  on C is bounded as

$$L_F^C \le L_{\psi}^C \tilde{\ell}_h^C + \left(\ell_{\psi}^C\right)^2 L_h + L_r$$

where  $\tilde{\ell}_{h}^{C} = \min\{\ell_{h}, \min_{z \in \psi(C)} \|\nabla h(z)\|_{2} + L_{h}\ell_{\psi}^{C}D^{C}\}$ , where  $D^{C} = \sup_{x,y \in C} \|x-y\|_{2}$ .

What remain to characterize are the smoothness properties of a chain of computations.

#### 4.2 Smoothness estimates

We present the smoothness computations for a deep network. Generic estimations of the smoothness properties of a chain of computation are presented in Appendix C. The propositions below give *upper bounds* on the smoothness constants of the function achieved through chain-composition. For a trivial composition such as  $f \circ f^{-1}$ , the upper bound is clearly loose. The upper bounds we present here are informative for non-trivial architectures.

The estimation is done by a forward pass on the network, as illustrated in Fig. 3. The reasoning is based on the following lemma.

**Lemma 4.3.** Consider a chain f of  $\tau$  computations  $\phi_t \in C_{\ell_{\phi_t}, L_{\phi_t}}$  initialized at some  $x_0 \in \mathbb{R}^{d_0}$ . (i) We have  $\ell_{f_{\tau, x_0}} \leq \ell_{\tau}$ , where

$$\ell_0 = 0, \ \ell_t = \ell_{\phi_t} + \ell_{t-1}\ell_{\phi_t}, \ for \ t \in \{1, \dots, \tau\}.$$

(ii) We have  $L_{f_{\tau,x_0}} \leq L_{\tau}$ , where

$$L_0 = 0, \ L_t = L_{t-1}\ell_{\phi_t} + L_{\phi_t}(1+\ell_{t-1})^2, \ for \ t \in \{1,\ldots,\tau\}.$$

In the case of deep networks, the computations are not Lipschitz continuous due to the presence of bi-affine functions. Yet, provided that inputs of computations are bounded and that we have access to the smoothness of the computations, we can have an estimate of the Lipschitz-continuity of the computations restricted to these bounded sets.

**Corollary 4.4.** Consider a chain f of  $\tau$  of computations  $\phi_t \in C_{m_{\phi_t},\ell_{\phi_t},L_{\phi_t}}$  initialized at some  $x_0 \in \mathbb{R}^{d_0}$  and consider  $C = \bigotimes_{t=1}^{\tau} B_{R_t}(\mathbb{R}^{p_t})$ . Then the smoothness of the output of the chain  $f_{\tau,x_0}$  on C, can be estimated as in Lemma 4.3 by replacing  $\ell_{\phi_t}$  with  $\tilde{\ell}_{\phi_t}$  defined by

$$\ell_{\phi_t} = \min\{\ell_{\phi_t}, L_{\phi_t}(m_{t-1} + R_t) + \|\nabla\phi_t(0, 0)\|_{2,2}\},\$$
  
$$m_t = \min\{m_{\phi_t}, \tilde{\ell}_{\phi_t}(m_{t-1} + R_t) + \|\phi_t(0, 0)\|_{2}\},\$$

for  $t \in \{1, \ldots, \tau\}$ , with  $m_0 = ||x_0||_2$ .

We specialize the result to deep networks. We denote by  $\mathcal{B}_{L,l^u,l^x}$  the set of *L*-smooth bi-affine functions *b* such that  $\|\nabla_u b(0,0)\|_{2,2} = l^u$ ,  $\|\nabla_x b(0,0)\|_{2,2} = l^x$ , i.e., functions of the form

$$b(x, u) = \beta(x, u) + \beta^u(u) + \beta^x(x) + \beta^0,$$

with  $\beta$  bilinear and L-smooth,  $\beta^u$ ,  $\beta^x$  linear and  $l^u$ ,  $l^x$  Lipschitz continuous respectively and  $\beta^0$  a constant vector.

**Proposition 4.5.** Consider a chain f of  $\tau$  computations whose layers  $\phi_t$  are defined by

$$\phi_t(x_{t-1}, u_t) = a_t(b_t(x_{t-1}, u_t)),$$

for  $t \in \{1, \ldots, \tau\}$ , where  $b_t \in \mathcal{B}_{L_{b_t}, l_{b_s}^u}$ ,  $l_{b_s}^u$ ,  $l_{b_s}^u$ , and  $a_t$  is decomposed as

$$a_t = a_{t,k_t} \circ \ldots \circ a_{t,1},$$

with  $a_{t,i} \in \mathcal{C}_{m_{a_{t,i}},\ell_{a_{t,i}},L_{a_{t,i}}}$ . Consider  $C = \bigotimes_{t=1}^{\tau} B_{R_t}(\mathbb{R}^{p_t})$ . The outputs  $m_{\tau}$ ,  $\ell_{\tau}$  and  $L_{\tau}$  of Algo. 4 satisfy  $m_{f_{\tau,x_0}}^C \leq m_{\tau}$ ,  $\ell_{f_{\tau,x_0}}^C \leq \ell_{\tau}$ ,  $L_{f_{\tau,x_0}}^C \leq L_{\tau}$ .



Figure 3: Smoothness estimates computations.

#### Algorithm 4 Automatic smoothness computations

## 1: Inputs:

- 1. Chain of computations f defined by  $\phi_t = a_t \circ b_t$  for  $t \in \{1, \ldots, \tau\}$  with  $a_t = a_{t,k_t} \circ \ldots \circ a_{t,1}$
- 2. Smoothness properties  $L_{b_t}, l_{b_t}^u, l_{b_t}^x$  of the biaffine function  $b_t \in \mathcal{B}_{L_{b_t}, l_{b_t}^u}, l_{b_t}^x$
- 3. Smoothness properties  $m_{a_{t,i}}, \ell_{a_{t,i}}, L_{a_{t,i}}$  of the nonlinear functions  $a_{t,i} \in \mathcal{C}_{m_{a_{t,i}}, \ell_{a_{t,i}}, L_{a_{t,i}}}$
- 4. Initial point  $x_0$
- 5. Bounds  $R_t$  on the parameters

2: Initialize  $m_0 = ||x_0||_2, \ell_0 = 0, L_0 = 0$ 3: for  $t = 1, ..., \tau$  do  $\ell_{t,0}^x = L_{b_t} R_t + l_{b_t}^x, \quad \ell_{t,0}^u = L_{b_t} m_{t-1} + l_{b_t}^u, \quad \ell_{t,0}^0 = 1$  $m_{t,0} = \ell_{t,0}^x m_{t-1} + \ell_{t,0}^u R_t + \|b_t(0,0)\|_2$ 4: 5: 6:  $L_{t,0} = 0$ 7: for  $j = 1, ..., k_t$  do  $\tilde{\ell}_{a_{t,j}} = \min\{\ell_{a_{t,j}}, \|\nabla a_{t,j}(0)\|_2 + L_{a_{t,j}}m_{t,j-1}\}$ 8:  $m_{t,j} = \min\{m_{a_{t,j}}, \|a_{t,j}(0)\|_2 + \tilde{\ell}_{a_{t,j}}m_{t,j-1}\}$ 9: 
$$\begin{split} \boldsymbol{\ell}_{t,j}^0 &= \tilde{\ell}_{a_{t,j}} \ell_{t,j-1}^0 \\ \boldsymbol{L}_{t,j} &= \boldsymbol{L}_{t,j-1} \ell_{a_{t,j}} + \boldsymbol{L}_{a_{t,j}} (\ell_{t,j-1}^0)^2 \end{split}$$
10: 11: end for 12: 
$$\begin{split} m_t &= m_{t,k_t} \\ \ell_t &= \ell_{t,0}^x \ell_{t,k_t}^0 \ell_{t-1} + \ell_{t,0}^u \ell_{t,k_t}^0 \\ L_t &= L_{t-1} \ell_{t,0}^x \ell_{t,k_t}^0 + (L_{b_t} R_t + l_{b_t})^2 L_{t,k_t} \ell_{t-1}^2 \end{split}$$
13: 14: 15:  $+2\left((L_{b_t}m_{t-1}+l_{b_t}^u)(L_{b_t}R_t+l_{b_t}^x)L_{t,k_t}+L_{b_t}\ell_{t,k_t}^0\right)\ell_{t-1}$  $+(L_{b_t}^{\check{}}m_{t-1}+l_{b_t}^u)^2L_{t,k_t}$ 16: end for 17: **Output:**  $m_{\tau}, \ell_{\tau}, L_{\tau}$ 

The proof of the above lemma is the consequence of simple technical lemmas provided in Appendix C. Note that the smoothness of the chain with respect to its input given a fixed set of parameters can also easily be estimated by a similar method; see Corollary C.5 in Appendix C.

The smoothness properties of a chain of composition around a given point follows then directly as stated in the following corollary.

**Corollary 4.6.** Consider a chain f of  $\tau$  computations as defined in Prop. 4.5 and  $u^* = (u_1^*; \ldots, u_{\tau}^*) \in \mathbb{R}^p$ . The smoothness properties of f on  $C' = \{u = (u_1; \ldots; u_{\tau}) \in \mathbb{R}^p : \forall t \in \{1, \ldots, \tau\}, \|u_t - u_t^*\| \leq R_t'\}$  are given as in Prop. 4.5 by considering

$$\begin{aligned} R'_t & \text{ in place of } \quad R_t, \\ l_{\beta_t^x} + L_{\beta_t} \| u_t^* \|_2 & \text{ in place of } \quad l_{\beta_t^x}, \\ \| \beta_t^0 \|_2 + l_{\beta_t^u} \| u_t^* \|_2 & \text{ in place of } \quad \| \beta_t^0 \|_2. \end{aligned}$$

## 5 Application

We apply our framework to assess the smoothness properties of the Visual Geometry Group (VGG) deep network used for image classification [24].

## 5.1 VGG network

The VGG Network is a benchmark network for image classification with deep networks. The objective is to classify images among 1000 classes. Its architecture is composed of 16 layers described in Appendix F. We consider in the following smoothness properties for mini-batches with size m = 128, i.e., by concatenating m chains of computations  $f^{(i)}$  each defined by a different input. This highlights the impact of the size of the mini-batch for batch-normalization.

**Smoothness computations.** To compute the Lipschitz-continuity and smoothness parameters, we recall the list of Lipschitz continuity and smoothness constants of each layer of interest. For the bilinear and linear operations we denote by L the smoothness of the bilinear operation  $\beta$  and by  $\ell$  the Lipschitz-continuity of the linear operation  $\beta^u$ . The smoothness constants of interest are

- 1.  $\ell_{\text{conv}} = \sqrt{m} \left[\frac{k}{s}\right], L_{\text{conv}} = \left[\frac{k}{s}\right]$ , where the patch is of size  $k \times k$  and the stride is s,
- 2.  $\ell_{\text{full}} = \sqrt{m}, L_{\text{full}} = 1,$
- 3.  $\ell_{\text{ReLu}} = 1$ ,  $L_{\text{ReLu}}$  not defined,
- 4.  $\ell_{\text{softmax}} = 2$ ,  $L_{\text{softmax}} = 4$ ,
- 5.  $\ell_{\text{maxpool}} = 1, L_{\text{maxpool}}$  not defined,
- 6.  $\ell_{\log} = 2, L_{\log} = 2.$

A Lipschitz-continuity estimate of this architecture can then be computed using Prop. 4.5 on a Cartesian product of balls  $C = \{w = (u_1; \ldots; u_{16}) : ||u_t||_2 \le R\}$  for R = 1 for example.

#### 5.2 Variations of VGG

**Smooth VGG.** First, the VGG architecture can be made continuously differentiable by considering the soft-plus activation instead of the ReLU activation and average pooling instead of the max-pooling operation. As shown in Appendix D, we have

ℓ<sub>avgpool</sub> = 1, L<sub>avgpool</sub> = 0,
 ℓ<sub>softplus</sub> = 1, L<sub>softplus</sub> = 1/4.

Denoting  $\ell_{\text{VGG}}$  and  $\ell_{\text{VGG-smooth}}$  the Lipschitz-continuity estimates of the original VGG network and the modified original network on a Cartesian product of balls  $C = \{u = (u_1; \ldots; u_{16}) : ||u_t||_2 \le 1\}$  with  $||x||_2 = 1$ , we get using Prop. 4.5,  $\frac{|\ell_{\text{VGG}} - \ell_{\text{VGG-smooth}}|}{\ell_{\text{VGG}}} \le 10^{-4}$ .

**Batch-normalization effect.** We can also compare the smoothness properties of the smoothed network with the same network modified by adding the batch-normalization layer for m inputs and  $\epsilon$  normalization parameter at each convolutional layer. As shown in Appendix D, the batch-normalization satisfies

1. 
$$m_{\text{batch}} = \delta m, \ell_{\text{batch}} = 2\epsilon^{-1/2}, L_{\text{batch}} = 2m^{-1/2}\epsilon^{-1}$$

Denoting  $\ell_{\text{VGG-smooth}}$ ,  $L_{\text{VGG-smooth}}$  and  $\ell_{\text{VGG-batch}}$ ,  $L_{\text{VGG-batch}}$  the Lipschitz-continuity and smoothness estimates of the smoothed VGG network with and without batch-normalization respectively on a Cartesian product of balls  $C = \{u = (u_1; \ldots; u_{16}) : ||u_t||_2 \le 1\}$  with  $||x||_2 = 1$ , we get using Prop. 4.5,

for $\epsilon = 10^{-2}$ ,	$\ell_{ m VGG-smooth}$ $L_{ m VGG-smooth}$	$\leq \ell_{ m VGG-batch}$ $\leq L_{ m VGG-batch}$
for $\epsilon = 10^2$ ,	$\ell_{ m VGG-smooth}$ $L_{ m VGG-smooth}$	$\geq \ell_{\text{VGG-batch}}$ $\geq L_{\text{VGG-batch}}$

Intuitively, the batch-norm bounds the output of each layer, mitigating the increase of  $m_t$  in the computations of the estimates of the smoothness in lines 8 and 9 of Algo. 4. Yet, for a small  $\epsilon$ , this effect is balanced by the non-smoothness of the batch-norm layer (which for  $\epsilon \to 0$  tends to have an infinite slope around 0).

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## **A** Notations

## A.1 Matrices

For a matrix  $M \in \mathbb{R}^{d \times n}$ , we denote by  $\operatorname{Vec}(M)$  the concatenation of the columns of M. We denote  $||M||_{2,2} = \sup_{x \neq 0, y \neq 0} \frac{x^\top M y}{||x||_2 ||y||_2}$  its norm induced by the Euclidean norm and  $||M||_F = \sqrt{\sum_{ij} M_{ij}^2}$  its Frobenius norm.

## A.2 Tensors

A tensor  $\mathcal{A} = (a_{ijk})_{i \in \{1,\dots,d\}, j \in \{1,\dots,n\}, k \in \{1,\dots,p\}} \in \mathbb{R}^{d \times n \times p}$  is represented as a list of matrices  $\mathcal{A} = (A_1,\dots,A_p)$  where  $A_k = (a_{ijk})_{i \in \{1,\dots,d\}, j \in \{1,\dots,n\}} \in \mathbb{R}^{d \times n}$  for  $k \in \{1,\dots,p\}$ .

**Tensor-matrix product.** Given matrices  $P \in \mathbb{R}^{d \times d'}, Q \in \mathbb{R}^{n \times n'}, R \in \mathbb{R}^{p \times p'}$ , we denote

$$\mathcal{A}[P,Q,R] = \left(\sum_{k=1}^{p} R_{k,1} P^{\top} A_k Q, \dots, \sum_{k=1}^{p} R_{k,p'} P^{\top} A_k Q\right) \in \mathbb{R}^{d' \times n' \times p}$$

If P, Q or R are identity matrices, we use the symbol " $\cdot$ " in place of the identity matrix. For example, we denote  $\mathcal{A}[P, Q, \mathbf{I}_p] = \mathcal{A}[P, Q, \cdot] = (P^\top A_1 Q, \dots, P^\top A_p Q).$ 

**Fact A.1.** Let  $\mathcal{A} \in \mathbb{R}^{d \times p \times n}$ ,  $P \in \mathbb{R}^{d \times d'}$ ,  $Q \in \mathbb{R}^{p \times p'}$ ,  $R \in \mathbb{R}^{n \times n'}$  and  $S \in \mathbb{R}^{d' \times d''}$ ,  $T \in \mathbb{R}^{p' \times p''}$ ,  $U \in \mathbb{R}^{n' \times n''}$ . Denote  $\mathcal{A}' = \mathcal{A}[P, Q, R] \in \mathbb{R}^{d' \times p' \times n'}$ . Then

$$\mathcal{A}'[S,T,U] = \mathcal{A}[PS,QT,RU] \in \mathbb{R}^{d'' \times p'' \times n''}.$$

**Flat tensors.** If P, Q or R are vectors we consider the flatten object. In particular, for  $x \in \mathbb{R}^d$ ,  $y \in \mathbb{R}^n$ , we denote

$$\mathcal{A}[x, y, \cdot] = \begin{pmatrix} x^{\top} A_1 y \\ \vdots \\ x^{\top} A_p y \end{pmatrix} \in \mathbb{R}^p,$$

rather than having  $\mathcal{A}[x, y, \cdot] \in \mathbb{R}^{1 \times 1 \times p}$ . Similarly, for  $z \in \mathbb{R}^p$ , we have

$$\mathcal{A}[\cdot,\cdot,z] = \sum_{k=1}^{p} z_k A_k \in \mathbb{R}^{d \times n}.$$

**Transpose.** For a tensor  $\mathcal{A} = (A_1, \dots, A_p) \in \mathbb{R}^{d,n,p}$  we denote  $\mathcal{A}^t = (A_1^\top, \dots, A_p^\top) \in \mathbb{R}^{n,d,p}$ .

**Outer product.** We denote the outer product of three vectors  $x \in \mathbb{R}^d$ ,  $y \in \mathbb{R}^n$ ,  $z \in \mathbb{R}^p$  as  $x \boxtimes y \boxtimes z \in \mathbb{R}^{d \times n \times p}$  such that

$$(x \boxtimes y \boxtimes z)_{ijk} = x_i y_j z_k$$

**Tensor norm.** We define the norm of a tensor A induced by the Euclidean norm as follows.

**Definition A.2.** The norm of a tensor  $\mathcal{A}$  induced by the Euclidean norm is defined as

$$\|\mathcal{A}\|_{2,2,2} = \sup_{x \neq 0, y \neq 0, z \neq 0} \frac{\mathcal{A}[x, y, z]}{\|x\|_2 \|y\|_2 \|z\|_2}.$$
(23)

**Fact A.3.** The tensor norm satisfies the following properties, for a given tensor  $\mathcal{A} \in \mathbb{R}^{d \times n \times p}$ ,

1.  $\|\mathcal{A}\|_{2,2,2} = \|\mathcal{A}^t\|_{2,2,2}$ , 2.  $\|\mathcal{A}[P,Q,R]\|_{2,2,2} \le \|\mathcal{A}\|_{2,2,2} \|P\|_{2,2} \|Q\|_{2,2} \|R\|_{2,2}$  for P,Q,R with appropriate sizes, 3.  $\|\mathcal{A}\|_{2,2,2} = \sup_{z\neq 0} \frac{\|\sum_{k=1}^p z_k A_k\|_{2,2}}{\|z\|_2}$ .

#### A.3 Gradients

For a multivariate function  $f : \mathbb{R}^d \to \mathbb{R}^n$ , composed of n real functions  $f^{(j)}$  for  $j \in \{1, \ldots, n\}$ , we denote  $\nabla f(x) = (\nabla f^{(1)}(x), \ldots, \nabla f^{(n)}(x)) \in \mathbb{R}^{d \times n}$ , that is the transpose of its Jacobian on  $x, \nabla f(x) = (\frac{\partial f^{(j)}}{\partial x_i}(x))_{i \in \{1, \ldots, d\}, j \in \{1, \ldots, n\}} \in \mathbb{R}^{d \times n}$ . We represent its 2nd order information by a tensor  $\nabla^2 f(x) = (\nabla^2 f^{(1)}(x), \ldots, \nabla^2 f^{(n)}(x)) \in \mathbb{R}^{d \times d \times n}$ .

**Fact A.4.** We have for  $f : \mathbb{R}^d \to \mathbb{R}^n$ , twice differentiable, and  $C \subset \text{dom } f$  convex,

$$\ell_f^C = \sup_{\substack{x,y \in C \\ x \neq y}} \frac{\|f(x) - f(y)\|_2}{\|x - y\|_2} = \sup_{x \in C} \|\nabla f(x)\|_{2,2}, \quad L_f^C = \sup_{\substack{x,y \in C \\ x \neq y}} \frac{\|\nabla f(x) - \nabla f(y)\|_{2,2}}{\|x - y\|_2} = \sup_{x \in C} \|\nabla^2 f(x)\|_{2,2,2}.$$

where  $\|\nabla f(x)\|_{2,2}$  denotes the operator norm of  $\nabla f(x)$  and  $\|\nabla^2 f(x)\|_{2,2,2}$  denotes the tensor norm of  $\nabla^2 f(x)$  both with respect to the Euclidean norm.

*Proof.* We have for  $x, y \in C$ ,

$$\|f(x) - f(y)\|_{2} = \|\int_{0}^{1} \nabla f(x + t(y - x))^{\top} (y - x) dt\|_{2} \le \sup_{x \in C} \|\nabla f(x)\|_{2,2} \|x - y\|_{2},$$
$$\|\nabla f(x) - \nabla f(y)\|_{2,2} = \|\int_{0}^{1} \nabla^{2} f(x + t(y - x))[y - x, \cdot, \cdot] dt\|_{2,2} \le \sup_{x \in C} \|\nabla^{2} f(x)\|_{2,2,2} \|x - y\|_{2},$$

which gives  $\ell_f^C \leq \sup_{x \in C} \|\nabla f(x)\|_{2,2}$  and  $L_f^C \leq \sup_{x \in C} \|\nabla^2 f(x)\|_{2,2,2}$ . The equalities come from the definitions of the gradient and the Hessian.

For a real function,  $f : \mathbb{R}^d \times \mathbb{R}^p \mapsto \mathbb{R}$ , whose value is denoted f(x, y), we decompose its gradient  $\nabla f(x, y) \in \mathbb{R}^{d+p}$ on  $(x, y) \in \mathbb{R}^d \times \mathbb{R}^p$  as

$$\nabla f(x,y) = \begin{pmatrix} \nabla_x f(x,y) \\ \nabla_y f(x,y) \end{pmatrix} \quad \text{with} \quad \nabla_x f(x,y) \in \mathbb{R}^d, \quad \nabla_y f(x,y) \in \mathbb{R}^p.$$

Similarly we decompose its Hessian  $\nabla f(x,y) \in \mathbb{R}^{(d+p) \times (d+p)}$  on blocks that correspond to the variables (x,y) as follows

$$\nabla^2 f(x,y) = \begin{pmatrix} \nabla_{xx} f(x,y) & \nabla_{xy} f(x,y) \\ \nabla_{yx} f(x,y) & \nabla_{yy} f(x,y) \end{pmatrix}$$
  
with  $\nabla_{xx} f(x,y) \in \mathbb{R}^{d \times d}, \quad \nabla_{yy} f(x,y) \in \mathbb{R}^{p \times p}, \quad \nabla_{xy} f(x,y) = \nabla_{yx} f(x,y)^\top \in \mathbb{R}^{d \times p}.$ 

Given a function  $f : \mathbb{R}^{d+p} \mapsto \mathbb{R}^n$  and  $(x, y) \in \mathbb{R}^d \times \mathbb{R}^p$ , we denote  $\nabla_x f(x, y) = (\nabla_x f^{(1)}(x, y), \dots, \nabla_x f^{(n)}(x, y)) \in \mathbb{R}^{d \times n}$  and we define similarly  $\nabla_y f(x, y) \in \mathbb{R}^{p \times n}$ .

For its second order information we define  $\nabla_{xx}f(x,y) = (\nabla_{xx}f^{(1)}(x,y), \dots, \nabla_{xx}f^{(n)}(x,y))$ , similarly for  $\nabla_{xx}f(x,y)$ . Dimension of these definitions are

$$\nabla_x f(x,y) \in \mathbb{R}^{d \times n}, \quad \nabla_y f(x,y) \in \mathbb{R}^{p \times n},$$
$$\nabla_{xx} f(x,y) \in \mathbb{R}^{d \times d \times n}, \quad \nabla_{yy} f(x,y) \in \mathbb{R}^{p \times p \times n},$$
$$\nabla_{xy} f(x,y) \in \mathbb{R}^{d \times p \times n}, \quad \nabla_{yx} f(x,y) \in \mathbb{R}^{p \times d \times n}.$$

## A.4 Matrix functions

For a differentiable matrix-valued multivariate function  $g : \mathbb{R}^d \to \mathbb{R}^{p \times n}$  such that  $g(x) = (g_{j,k}(x)_{1 \le j \le p, 1 \le k \le n})$ , we denote its first order information as a tensor

$$\nabla g(x) = \left(\frac{\partial g_{j,k}(x)}{\partial x_i}\right)_{1 \le i \le d, 1 \le j \le p, 1 \le k \le n} \in \mathbb{R}^{d \times p \times n}$$

This notation is consistent with previous ones, i.e., for  $f : \mathbb{R}^{d+p} \mapsto \mathbb{R}^n$  and  $g(y) = \nabla_y f(x, y) \in \mathbb{R}^{p \times n}$ , then  $\nabla g(y) = \nabla_{xy}^2 f(x, y) \in \mathbb{R}^{d \times p \times n}$ . From previous definitions, we have the following fact.

**Fact A.5.** For a differentiable matrix-valued multivariate function  $g : \mathbb{R}^d \to \mathbb{R}^{p \times n}$ ,  $A \in \mathbb{R}^{p' \times p}$ ,  $B \in \mathbb{R}^{n \times n'}$ , denoting  $h(x) = Ag(x)B \in \mathbb{R}^{p' \times n'}$ , we have

$$\nabla h(x) = \nabla g(x)[\cdot, A^{\top}, B] \in \mathbb{R}^{d \times p' \times n'}$$

### A.5 Bilinear functions

**Definition A.6.** A function  $\beta : \mathbb{R}^d \times \mathbb{R}^n \to \mathbb{R}^p$  is bilinear if it is represented by a tensor  $\mathcal{B} \in \mathbb{R}^{d \times n \times p}$  such that for any  $x \in \mathbb{R}^d$ ,  $y \in \mathbb{R}^n$ ,

$$\beta(x, y) = \mathcal{B}[x, y, \cdot].$$

The gradient of a bilinear function  $\beta$  represented by a tensor  $\mathcal{B} \in \mathbb{R}^{d \times n \times p}$  at a point x, y is given by

$$\nabla_x \beta(x, y) = \mathcal{B}[\cdot, y, \cdot] \in \mathbb{R}^{d \times p}, \qquad \nabla_y \beta(x, y) = \mathcal{B}[x, \cdot, \cdot] \in \mathbb{R}^{n \times p}.$$
(24)

The Hessian of the bilinear function is given

$$\nabla_{xx}^2 \beta(x,y) = 0, \quad \nabla_{yy}^2 \beta(x,y) = 0, \quad \nabla_{xy}^2 \beta(x,y) = \mathcal{B}, \quad \nabla_{yx}^2 \beta(x,y) = \mathcal{B}^t.$$
(25)

A bilinear function is not Lipschitz continuous as can be seen from Eq. (24). It is smooth w.r.t. the Euclidean norm with a smoothness constant given by the tensor norm of  $\mathcal{B}$  as shown in the following proposition.

**Lemma A.7.** The smoothness of a bilinear function  $\beta$  defined by a tensor  $\mathcal{B}$  is upper bounded as  $L_{\beta} \leq \|\mathcal{B}\|_{2,2,2}$ .

Proof. We have

$$\|\nabla^2 \beta(x,y)\|_{2,2,2} = \sup_{z \neq 0} \frac{\|\sum_{k=1}^p z_k \tilde{B}_k\|_{2,2}}{\|z\|_2}$$

where  $\nabla^2 \beta(x, y) = (\tilde{B}_1, \dots, \tilde{B}_p)$ . We have by Eq. (25) that  $\sum_{k=1}^p z_k \tilde{B}_k$  is of the form

$$\sum_{k=1}^{p} z_k \tilde{B}_k = \begin{pmatrix} 0 & \sum_{k=1}^{p} z_k B_k \\ \sum_{k=1}^{p} z_k B_k^\top & 0 \end{pmatrix}$$

where  $\mathcal{B} = (B_1, ..., B_p)$ . Therefore we get  $\|\sum_{k=1}^p z_k \tilde{B}_k\|_{2,2} = \|\sum_{k=1}^p z_k B_k\|_{2,2}$ , see [12, Theorem 7.3.3.]. Therefore

$$\|\nabla^2 \beta(x,y)\|_2 = \sup_{z \neq 0} \frac{\|\sum_{k=1}^p z_k \tilde{B}_k\|_{2,2}}{\|z\|_2} = \sup_{z \neq 0} \frac{\|\sum_{k=1}^p z_k B_k\|_{2,2}}{\|z\|_2} = \|\mathcal{B}\|_{2,2,2}.$$

## **B** Oracle arithmetic complexity proofs

#### **B.1** Feasibility of the optimization oracle steps

The gradient step (15) is always feasible for any  $\kappa > 0$ , the Gauss-Newton step (16) is feasible for any  $\kappa > 0$  if h, r are convex and the Newton step is feasible for any  $\kappa > 0$  if  $h \circ f$  and r are convex. A sufficient condition for the Newton step to be feasible if  $h \circ f$  is not convex but  $h \circ f$  and r are smooth is to choose  $\kappa < (L_{h \circ f} + L_r)^{-1}$ . In other words, the step-size must be chosen small enough such that the Newton step is a convex problem.

## **B.2** Optimization oracles as linear quadratic problems

**Lemma B.1.** Let f be a chain of  $\tau$  computations  $\phi_t$ . Let  $u = (u_1; \ldots; u_\tau) \in \mathbb{R}^{\sum_{t=1}^{\tau} p_t}$ ,  $x_0 \in \mathbb{R}^{d_0}$ , denote  $x_t = f_t(x_0, u)$  and  $E_t^{\top} = (0_{p_t d_0}, 0_{p_t p_1}, \ldots, I_{p_t p_t}, \ldots, 0_{p_t p_\tau}) \in \mathbb{R}^{p_t \times (d_0 + \sum_{t=1}^{\tau} p_t)}$  such that  $E_t^{\top}(x_0; u) = u_t$  for  $t \in \{1, \ldots, \tau\}$ .

*1.* If  $\phi_t$  are differentiable, then

$$\nabla f_t(x_0, u) = \nabla f_{t-1}(x_0, u) \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t) + E_t \nabla_{u_t} \phi_t(x_{t-1}, u_t)$$
(26)

with  $\nabla f_0(x_0, u) = E_0$ , with  $E_0^{\top} = (I_{d_0 d_0}, 0_{d_0 p_1}, \dots, \dots, 0_{d_0 p_{\tau}}) \in \mathbb{R}^{d_0 \times (d_0 + \sum_{t=1}^{\tau} p_t)}$  such that  $E_0^{\top}(x_0; u) = x_0$ .

2. If  $\phi_t$  are twice differentiable,

$$\nabla^{2} f_{t}(x_{0}, u) = \nabla^{2} f_{t-1}(x_{0}, u) [\cdot, \cdot, \nabla_{x_{t-1}} \phi_{t}(x_{t-1}, u_{t})]$$

$$+ \nabla^{2}_{x_{t-1}x_{t-1}} \phi_{t}(x_{t-1}, u_{t}) [\nabla f_{t-1}(x_{0}, u)^{\top}, \nabla f_{t-1}(x_{0}, u)^{\top}, \cdot]$$

$$+ \nabla^{2}_{x_{t-1}u_{t}} \phi_{t}(x_{t-1}, u_{t}) [\nabla f_{t-1}(x_{0}, u)^{\top}, E_{t}^{\top}, \cdot]$$

$$+ \nabla^{2}_{u_{t}x_{t-1}} \phi_{t}(x_{t-1}, u_{t}) [E_{t}^{\top}, \nabla f_{t-1}(x_{0}, u)^{\top}, \cdot]$$

$$+ \nabla^{2}_{u_{t}u_{t}} \phi_{t}(x_{t-1}, u_{t}) [E_{t}^{\top}, E_{t}^{\top}, \cdot]$$

$$(27)$$

with  $\nabla^2 f_0(x_0, u) = 0.$ 

*Proof.* It follows from the definition of the chain of computations and the notations used for tensors. Precisely we have that

$$f_t(x_0, u) = \phi_t(f_{t-1}(x_0, u), E_t^{\top}(x_0; u)),$$

hence the first result that can be written

$$\nabla f_t(x_0, u) = \nabla f_{t-1}(x_0, u) \nabla_{x_{t-1}} \phi_t(f_{t-1}(x_0, u), E_t^{\top}(x_0; u)) + E_t \nabla_{u_t} \phi_t(f_{t-1}(x_0, u), E_t^{\top}(x_0; u)),$$

hence the second result using the tensor notations.

**Proposition 3.1.** Let f be a chain of  $\tau$  computations  $\phi_t : \mathbb{R}^{d_{t-1}} \times \mathbb{R}^{p_t} \to \mathbb{R}^{d_t}$ ,  $u = (u_1; \ldots; u_{\tau})$  and  $x_0 \in \mathbb{R}^{d_0}$ . Denote  $\psi = f_{x_0,\tau}$  and  $f(x_0, u) = (x_1; \ldots; x_{\tau})$ . Assume r to be decomposable as  $r(u) = \sum_{t=1}^{\tau} r_t(u_t)$ . Gradient (15), Gauss-Newton (16) and Newton (17) oracles on  $h \circ \psi + r$  are the solutions  $v^* = (v_1^*; \ldots; v_{\tau}^*)$  of problems of the form

$$\min_{\substack{v_1, \dots, v_\tau \in \mathbb{R}^{p_1} \times \dots \times \mathbb{R}^{p_\tau} \\ y_0, \dots, y_\tau \in \mathbb{R}^{d_0} \times \dots \times \mathbb{R}^{d_\tau}}} \sum_{t=1}^{\tau} \frac{1}{2} y_t^\top P_t y_t + p_t^\top y_t + y_{t-1}^\top R_t v_t + \frac{1}{2} v_t^\top Q_t v_t + q_t^\top v_t + \frac{\kappa}{2} \|v_t\|_2^2 \tag{18}$$

$$subject to \quad y_t = A_t y_{t-1} + B_t v_t \quad for \quad t \in \{1, \dots, \tau\}, \\ y_0 = 0,$$

where

$$\begin{aligned} A_t &= \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t)^\top, \quad B_t &= \nabla_{u_t} \phi_t(x_{t-1}, u_t)^\top, \\ p_\tau &= \nabla h(\psi(u)), \quad p_t = 0 \quad \text{for } t \neq \tau, \\ q_t &= \nabla r_t(u_t), \end{aligned}$$

1. for gradient oracles (15),

$$P_t = 0, \quad R_t = 0, \quad Q_t = 0,$$

2. for Gauss-Newton oracles (16),

$$P_{\tau} = \nabla^2 h(\psi(u)), \quad P_t = 0 \quad \text{for } t \neq \tau, \quad R_t = 0, \quad Q_t = \nabla^2 r_t(u_t)$$

3. for Newton oracles (17), defining

$$\lambda_{\tau} = \nabla h(\psi(u)), \quad \lambda_{t-1} = \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t) \lambda_t \quad \text{for } t \in \{1, \dots, \tau\}.$$

we have

$$P_{\tau} = \nabla^2 h(\psi(u)), \quad P_{t-1} = \nabla^2_{x_{t-1}x_{t-1}} \phi_t(x_{t-1}, u_t)[\cdot, \cdot, \lambda_t] \quad \text{for } t \in \{1, \dots, \tau\},$$
  
$$R_t = \nabla^2_{x_{t-1}u_t} \phi_t(x_{t-1}, u_t)[\cdot, \cdot, \lambda_t], \quad Q_t = \nabla^2 r_t(u_t) + \nabla^2_{u_tu_t} \phi_t(x_{t-1}, u_t)[\cdot, \cdot, \lambda_t].$$

*Proof.* To reformulate the optimization oracle problems as quadratic problems with linear dynamics we reformulate  $\nabla \psi(u)^{\top} v$  as a linear chain of compositions and  $\nabla^2 \psi(u)[v, v, \nabla h(\psi(u))]$  as a quadratic on the linear trajectory defined by the gradient and the parameters using Lemma B.1. Precisely, for  $u = (u_1, \ldots; u_{\tau})$  and  $v = (v_1; \ldots; v_{\tau})$ , denoting  $f_{x_0}(u) = (x_1; \ldots; x_{\tau})$  and  $\nabla f_{x_0}(u)^{\top} v = (y_1; \ldots; y_{\tau})$  with  $\nabla f_{x_0,t}(u)^{\top} v = y_t$ , we have from (26)

$$y_t = \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t)^\top y_{t-1} + \nabla_{u_t} \phi_t(x_{t-1}, u_t)^\top v_t, \quad \text{for} \quad t \in \{1, \dots, \tau\}$$

$$y_0 = 0,$$
(28)

and  $\nabla \psi(u)^{\top} v = \nabla f_{x_0,\tau}(u)^{\top} v = y_{\tau}$ . For the second order derivatives, from (27), we have for  $v = (v_1; \ldots; v_{\tau})$  and  $\lambda_t \in \mathbb{R}^{d_t}$ ,

$$\frac{1}{2}\nabla^2 f_{x_0,t}(u)[v,v,\lambda_t] = \nabla^2 f_{x_0,t-1}(u)[v,v,\nabla_{x_{t-1}}\phi_t(x_{t-1},u_t)\lambda_t] \\ + \frac{1}{2}\nabla^2_{x_{t-1}x_{t-1}}\phi_t(x_{t-1},u_t)[y_{t-1},y_{t-1},\lambda_t] \\ + \nabla^2_{x_{t-1}u_t}\phi_t(x_{t-1},u_t)[y_{t-1},v_t,\lambda_t] \\ + \frac{1}{2}\nabla^2_{u_tu_t}\phi_t(x_{t-1},u_t)[v_t,v_t,\lambda_t]$$

Hence we get

$$\frac{1}{2}\nabla^{2}\psi(u)[v,v,\nabla h(\psi(u))] = \sum_{t=1}^{\tau} \frac{1}{2}\nabla^{2}_{x_{t-1}x_{t-1}}\phi_{t}(x_{t-1},u_{t})[y_{t-1},y_{t-1},\lambda_{t}] + \nabla^{2}_{x_{t-1}u_{t}}\phi_{t}(x_{t-1},u_{t})[y_{t-1},v_{t},\lambda_{t}] + \frac{1}{2}\nabla^{2}_{u_{t}u_{t}}\phi_{t}(x_{t-1},u_{t})[v_{t},v_{t},\lambda_{t}]$$
(29)

where  $y_t$  are given in (28) and  $\lambda_t$  are defined by

$$\lambda_{\tau} = \nabla h(\psi(u)), \quad \lambda_{t-1} = \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t) \lambda_t \quad \text{for} \quad t \in \{1, \dots, \tau\}.$$

The results follow by using the decomposability of r and inserting (28) and (29).

We present the resolution of the Newton step by dynamic programming in Algo. 5 whose implementation is justified in Proposition B.2. Note that the gradient is computed during the first backward pass which can reduce the computations by factorizing those computations. For the Gauss-Newton steps the same dynamic programming approach can be applied, however it is less computationally expansive to use automatic differentiation procedures as presented in Sec. 3.

**Proposition B.2.** Consider problem (18) and assume it is bounded below, then the cost-to-go functions defined for  $t \in \{0, ..., \tau\}$  and  $x_t \in \mathbb{R}^{\delta_t}$  as

$$\begin{aligned}
\cot_{t}(x_{t}) &= \min_{\substack{v_{t+1}, \dots, v_{\tau} \\ y_{t}, \dots, y_{\tau}}} \quad \sum_{t'=t}^{\tau} \frac{1}{2} y_{t'}^{\top} P_{t'} y_{t'} + p_{t'}^{\top} y_{t'} + \sum_{t'=t+1}^{\tau} y_{t'-1}^{\top} R_{t'} v_{t'} + \frac{1}{2} v_{t'}^{\top} Q_{t'} v_{t'} + q_{t'}^{\top} v_{t'} + \frac{\kappa}{2} \|v_{t'}\|_{2}^{2} \quad (30) \\
subject to \quad y_{t'} &= A_{t'} y_{t'-1} + B_{t'} v_{t'} \quad for \quad t' \in \{t+1, \dots, \tau\}, \\
y_{t} &= x_{t},
\end{aligned}$$

where  $P_0 = 0$ ,  $p_0 = 0$ , are quadratics of the form

$$\operatorname{cost}_t(x_t) = \frac{1}{2} x_t^{\mathsf{T}} C_t x_t + c_t^{\mathsf{T}} x_t + \operatorname{cste}, \tag{31}$$

where  $C_t, c_t$  are defined recursively in line 20 Algo. 5 with  $C_t = C_t^{\top}$  and cste is a constant. The solution of (18) is given by, starting from  $y_0 = 0$ ,

$$v_t^* = K_t y_{t-1} + k_t$$
  $y_t = A_t y_{t-1} + B_t v_t^*$ 

where  $K_t$  and  $k_t$  are defined in line 21 of Algo. 5.

*Proof.* The cost-to-go functions satisfy the recursive equation (20) for  $t \in \{1, ..., \tau\}$ 

$$\operatorname{cost}_{t-1}(x_{t-1}) = \frac{1}{2} x_{t-1}^{\top} P_{t-1} x_{t-1} + p_{t-1}^{\top} x_{t-1} + \min_{v_t \in \mathbb{R}^{\rho_t}} \left\{ x_{t-1}^{\top} R_t v_t + \frac{1}{2} v_t^{\top} Q_t v_t + q_t^{\top} v_t + \frac{\kappa}{2} \| v_t \|_2^2 + \operatorname{cost}_t (A_t x_{t-1} + B_t v_t) \right\},$$

starting from  $\operatorname{cost}_{\tau}(x_{\tau}) = \frac{1}{2}x_{\tau}^{\top}P_{\tau}x_{\tau} + p_{\tau}^{\top}x_{\tau}$  so we get  $C_{\tau} = P_{\tau}$  and  $c_{\tau} = p_{\tau}$ . Assume that the cost-to-go function  $\operatorname{cost}_{t}$  has the form (31) for  $t \in \{1, \ldots, \tau\}$  then the recursive equation (20) reads

$$\cot_{t-1}(x_{t-1}) = \frac{1}{2} x_{t-1}^{\top} (P_{t-1} + A_t^{\top} C_t A_t) x_{t-1} + (A_t^{\top} c_t + p_{t-1})^{\top} x_{t-1} \\
+ \min_{v_t \in \mathbb{R}^{\rho_t}} \left\{ v_t^{\top} (R_t^{\top} x_{t-1} + q_t + B_t^{\top} (C_t A_t x_{t-1} + c_t)) + \frac{1}{2} v_t^{\top} (\kappa \operatorname{I} + Q_t + B_t^{\top} C_t B_t) v_t \right\}.$$

If  $\kappa \mathbf{I} + Q_t + B_t^\top C_t B_t \succeq 0$ , then the minimization problem is unbounded below and so is the original objective. If  $\kappa \mathbf{I} + Q_t + B_t^\top C_t B_t \succ 0$ , then the minimization gives us  $\operatorname{cost}_{t-1}$  as a quadratic and the corresponding minimizer  $v_t^*(x_{t-1})$  for a given  $x_{t-1}$ , i.e.

$$\begin{aligned} C_{t-1} &= P_{t-1} + A_t^{\top} C_t A_t - (R_t + A_t^{\top} C_t B_t) (\kappa \operatorname{I} + Q_t + B_t^{\top} C_t B_t)^{-1} (R_t^{\top} + B_t^{\top} C_t A_t), \\ c_{t-1} &= A_t^{\top} c_t + p_{t-1} - (R_t + A_t^{\top} C_t B_t) (\kappa \operatorname{I} + Q_t + B_t^{\top} C_t B_t)^{-1} (q_t + B_t^{\top} c_t), \\ v_t^*(x_{t-1}) &= -(\kappa \operatorname{I} + Q_t + B_t^{\top} C_t B_t)^{-1} ((R_t^{\top} + B_t^{\top} C_t A_t) x_{t-1} + q_t + B_t^{\top} c_t). \end{aligned}$$

The solution of (18) is given by computing  $cost_0(0)$  which amounts to compute, starting from  $y_0 = 0$ ,

$$v_t^* = \operatorname*{arg\,min}_{v \in \mathbb{R}^{\rho_t}} \left\{ \frac{1}{2} v^\top Q_t v + q_t^\top v + y_{t-1}^\top R_t v + \operatorname{cost}_{t+1}(A_t y_{t-1} + B_t v) \right\} = v_t^*(x_{t-1}),$$
  
$$y_t = A_t y_{t-1} + B_t v_t^*.$$

Finally we present the derivation of a gradient step, i.e., gradient back-propagation, as a dynamic programming procedure, which gives the forward-backward algorithm presented in Sec. 3 by taking r = 0,  $\kappa = -1$ .

**Proposition B.3.** Consider the gradient step (15) as formulated in (18) with  $\kappa = 1/\gamma$ . The cost-to-go functions defined as in (30) are linear of the form

$$\operatorname{cost}_t(x_t) = \lambda_t^{\top} x_t + \operatorname{cste},\tag{32}$$

where

$$\lambda_{\tau} = \nabla h(\psi(u))$$
  
$$\lambda_{t-1} = \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t) \lambda_t \quad \text{for } t \in \{1, \dots, \tau\}$$

and the solution of the step is given by

$$v_t^* = -\gamma(\nabla r(u_t) + \nabla_{u_t}\phi_t(x_{t-1}, u_t)\lambda_t).$$

*Proof.* The cost-to-go function defined in (30) for a gradient step reads for  $t = \tau$ ,  $\operatorname{cost}_{\tau}(x_{\tau}) = p_{\tau}^{\top} x_{\tau}$ , so we get Eq. (32) for  $t = \tau$  with  $\lambda_{\tau} = \nabla h(\psi(u))$ . Assume that the cost-to-go function has the form (32) for  $t \in \{1, \ldots, \tau\}$ , then the recursive equation (20) reads

$$\operatorname{cost}_{t-1}(x_{t-1}) = \min_{v_t \in \mathbb{R}^{\rho_t}} \left\{ v_t^\top q_t + \lambda_t^\top (A_t x_{t-1} + B_t v_t) + \frac{1}{2\gamma} \|v_t\|_2^2 \right\}$$

So we get that  $\text{cost}_{t-1}$  is a linear function defined by  $\lambda_{t-1} = A_t^\top \lambda_t$  and that the optimal corresponding parameter is independent of  $x_{t-1}$  and reads

$$v_t^* = -\gamma(q_t + B_t^{\top}\lambda_t).$$

Plugging the values of  $A_t, B_t, q_t$  into the solutions give the results.

#### Algorithm 5 Newton oracle by dynamic programming

- 1: Inputs: Chain of computations f defined by  $\phi_t$ , objective h, regularization r, regularization for the step  $\kappa$ , current weights  $u = (u_1; \ldots; u_\tau)$
- 2: Forward pass:
- 3: for  $t = 1, ..., \tau$  do
- 4: Compute  $x_t = \phi_t(x_{t-1}, u_t)$
- 5: Store  $A_t = \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t)^\top$ ,  $B_t = \nabla_{u_t} \phi_t(x_{t-1}, u_t)^\top$ and  $\nabla^2_{u_t u_t} \phi_t(x_{t-1}, u_t)$ ,  $\nabla^2_{u_t x_{t-1}} \phi_t(x_{t-1}, u_t)$ ,  $\nabla^2_{x_{t-1} x_{t-1}} \phi_t(x_{t-1}, u_t)$
- 6: end for
- 7: 1st Backward pass:
- 8: Initialize  $\lambda_{\tau} = \nabla h(x_{\tau}), P_{\tau} = \nabla^2 h(x_{\tau}), p_{\tau} = \nabla h(x_{\tau})$
- 9: for  $t = \tau, ..., 1$  do
- 10: Compute

$$P_{t-1} = \nabla_{x_{t-1}x_{t-1}}^2 \phi_t(x_{t-1}, u_t)[\cdot, \cdot, \lambda_t] \qquad p_{t-1} = 0$$

$$Q_t = \nabla_{u_t u_t}^2 \phi_t(x_{t-1}, u_t)[\cdot, \cdot, \lambda_t] + \nabla^2 r_t(u_t) \qquad q_t = \nabla r_t(u_t)$$

$$R_t = \nabla_{x_{t-1}u_t}^2 \phi_t(x_{t-1}, u_t)[\cdot, \cdot, \lambda_t]$$

- 11: Compute  $\lambda_{t-1} = \nabla_{x_{t-1}} \phi_t(x_{t-1}, u_t) \lambda_t$ 12: end for 13: 2nd Backward pass: 14: Initialize  $C_{\tau} = P_{\tau}, c_{\tau} = p_{\tau}$ , feasible = True 15: for  $t = \tau, \dots, 1$  do 16: if  $\kappa I + Q_t + B_t^\top C_t B_t \neq 0$  then 17: feasible = False 18: break 19: end if
- 20: Compute

$$C_{t-1} = P_{t-1} + A_t^{\top} C_t A_t - (R_t + A_t^{\top} C_t B_t) (\kappa \mathbf{I} + Q_t + B_t^{\top} C_t B_t)^{-1} (R_t^{\top} + B_t^{\top} C_t A_t)$$
  
$$c_{t-1} = A_t^{\top} c_t + p_{t-1} - (R_t + A_t^{\top} C_t B_t) (\kappa \mathbf{I} + Q_t + B_t^{\top} C_t B_t)^{-1} (q_t + B_t^{\top} c_t)$$

21: Store

$$K_t = -(\kappa \mathbf{I} + Q_t + B_t^{\top} C_t B_t)^{-1} (R_t^{\top} + B_t^{\top} C_t A_t) \qquad k_t = -(\kappa \mathbf{I} + Q_t + B_t^{\top} C_t B_t)^{-1} (q_t + B_t^{\top} c_t)$$

22: end for

23: if feasible = False then 24: Re-do 2nd backward pass with  $\kappa := 2 \cdot \kappa$ 25: end if 26: Rollout: 27: Initialize  $y_0 = 0$ 28: for  $t = 1, ..., \tau$  do 29:

$$v_t^* = K_t y_{t-1} + k_t, \qquad y_t = A_t y_{t-1} + B_t v_t$$

30: end for 31: Output:  $(v_1^*; ...; v_{\tau}^*)$ 

#### **B.3** Detailed complexities of forward and backward passes

**Definition B.4** (Sparsity of the operations). We define the sparsity  $s_{\beta}$  of a bilinear operation  $\beta$  as the number of non-zero elements in its corresponding tensor.

We define the sparsity  $s_{\alpha}$  of a function  $\alpha$  as the sparsity of its gradient, i.e., the maximal number of its non-zero elements for any inputs.

The sparsity of a bilinear operation amounts to the number of multiplications needed to compute  $\mathcal{B}[x, y, z]$ ,  $\mathcal{B}[\cdot, y, z]$ ,  $\mathcal{B}[x, \cdot, z]$  or  $\mathcal{B}[x, y, \cdot]$ , which gives us the sparsity of the two bilinear operations studied in this paper.

**Fact B.5.** For a matrix-product as in (8), we have  $s_{\beta} = m \tilde{\delta} \delta$ . For a convolution as in (9), we have  $s_{\beta} = m n^p n^f s^f$ .

We considered  $\prod_k Z_{t-1}$  as the extraction of coordinates and not a matrix-vector product. Note that the sparsity of the bilinear operation defines also the number of multiplications needed to compute gradient vector products like  $\nabla_{x_{t-1}}\beta_t(x_{t-1}, u_t)\lambda_{t+1}$  or  $\nabla_{u_t}\beta_t(x_{t-1}, u_t)\lambda_{t+1}$  for  $\lambda_{t+1} \in \mathbb{R}^{\delta_t}$ .

The sparsity of a function  $f \in \mathbb{R}^d \to \mathbb{R}^n$  naturally gives the number of multiplications needed to compute gradientvector products  $\nabla f(x)\lambda$  for any  $x \in \mathbb{R}^d$ ,  $\lambda \in \mathbb{R}^n$ . For element-wise activation functions as in (10), we have  $s_\alpha = m\delta$ , where we consider the input of the activation function to be z = Vec(Z) for  $Z \in \mathbb{R}^{m \times \delta}$ . Note that the sparsity of an activation function as defined here does not directly give the cost of computing it, neither its gradient.

**Forward-backward detailed complexity.** We present in the next proposition the cost of computing only the backward pass to compute the whole gradient. The cost of computing the function and the gradients of the layers in the forward pass can be further detailed using the sparsity of the bilinear operation and the cost of computing the activation function and its derivatives. The detailed complexities given in Sec. 3 follow.

**Proposition B.6.** Consider a chain f of  $\tau$  layers as defined in Def. 2.1 whose layers  $\phi_t$  are defined by  $a_t, b_t$  as in (7). Then the cost of the backward pass defined in Algo. 2 is of the order of

$$\mathcal{O}\left(\sum_{t=1}^{\tau} s_{a_t} + 2s_{\beta_t} + s_{\beta_t^u} + s_{\beta_t^x}\right)$$

elementary operations.

*Proof.* If the chain of layers has the form (7), the gradient vector products during the backward pass read

$$\nabla_{x_{t-1}}\phi_t(x_{t-1}, u_t)\lambda_{t+1} = \nabla_{x_{t-1}}b_t(x_{t-1}, u_t)\nabla a_t(\omega_t)\lambda_{t+1} = (\mathcal{B}_t[\cdot, u_t, \cdot] + \nabla\beta_t^z(x_{t-1}))\nabla a_t(\omega_t)\lambda_{t+1},$$
  
$$\nabla_{u_t}\phi_t(x_{t-1}, u_t)\lambda_{t+1} = \nabla_{u_t}b_t(x_{t-1}, u_t)\nabla a_t(\omega_t)\lambda_{t+1} = (\mathcal{B}_t[x_{t-1}, \cdot, \cdot] + \nabla\beta_t^u(u_t))\nabla a_t(\omega_t)\lambda_{t+1},$$

where  $\omega_t = b_t(x_{t-1}, u_t)$ . The definitions of the sparsity of bilinear or general operations give the result by looking at each operation starting from the right.

## B.4 Gauss-Newton by axutomatic differentiation

Derivatives of the gradient vector product can then be computed themselves by back-propagation as recalled in the following lemma.

**Lemma B.7** ([21, Lemma 3.4]). Consider a differentiable chain of composition f and an input  $x_0 \in \mathbb{R}^{d_0}$  such that  $\psi = f_{x_0,\tau} : \mathbb{R}^{\sum_{t=1}^{\tau} p_t} \to \mathbb{R}^{d_{\tau}}$ . Given a variable  $u \in \mathbb{R}^{\sum_{t=1}^{\tau} p_t}$  and a decomposable differentiable function  $g : \mathbb{R}^{\sum_{t=1}^{\tau} p_t} \to \mathbb{R}$  such that  $g(u) = \sum_{t=1}^{\tau} g_t(u_t)$  for  $u = (u_1; \ldots; u_{\tau})$ , computing the derivative of  $\mu \to g(\nabla \psi(u)\mu)$  requires two calls to an automatic-differentiation procedure.

**Proposition 3.3.** Consider the Gauss-Newton oracle (16) on  $u = (u_1; ...; u_\tau)$  for a convex objective h, a convex decomposable regularization  $r(u) = \sum_{t=1}^{\tau} r_t(u_t)$  and a differentiable chain of computations f with output  $\psi = f_{x_0,\tau}$  on some input  $x_0$ . We have that

1. the Gauss-Newton oracle amounts to solving

$$\min_{\mu \in \mathbb{R}^{d_{\tau}}} \left( q_h^{\psi(u)} \right)^{\star}(\mu) + \left( q_r^u + \kappa \| \cdot \|_2^2 / 2 \right)^{\star} (-\nabla \psi(u)\mu),$$
(22)

where for a function f we denote by  $f^*$  its convex conjugate,

- 2. the Gauss-Newton oracle is  $v^* = \nabla \left(q_r^u + \kappa \|\cdot\|_2^2/2\right)^* \left(-\nabla \psi(u)\mu^*\right)$  where  $\mu^*$  is the solution of (22),
- *3. the dual problem* (22) *can be solved by*  $2d_{\tau} + 1$  *calls to an automatic differentiation procedure.*

*Proof.* The first and second claims follow from standard duality computations applied to (16), they require convexity of h and r. The third claim comes from the fact that (22) is a quadratic convex problem that can be solved in at most  $d_{\tau}$  iterations of a conjugate gradient descent. Each iteration requires to compute the gradient of  $\mu \to (q_r^u + \kappa \| \cdot \|_2^2/2)^*(-\nabla \psi(u)\mu)$  which requires two calls to an automatic differentiation procedure by Lemma B.7 and using that  $r^*$  is also decomposable. A last call to an automatic differentiation procedure is needed to compute  $\nabla \psi(u)\mu^*$ . The costs of computing  $\nabla(q_h^{\psi(u)})^*(\mu)$  for  $\mu \in \mathbb{R}^{d_{\tau}}$  and  $\nabla(q_r^u + \kappa \| \cdot \|_2^2/2)^*(u)$  for  $u \in \mathbb{R}^{\sum_{t=1}^{\tau} p_t}$  are ignored since they do not involve a chain of compositions and are assumed to be easily accessible.

## **C** Smoothness computations

## C.1 Elementary operations

Univariate functions.

**Lemma C.1.** Let  $\alpha_i \in C_{\ell_i, L_i}$  for i = 1, ..., n. Denote  $\ell = (\ell_i)_{i=1}^n$ ,  $L = (L_i)_{i=1}^n$ .

1. Assume  $\alpha_i : \mathbb{R}^{d_i} \to \mathbb{R}^{m_i}$ , then

$$a: \begin{cases} \mathbb{R}^{\sum_{i=1}^{n} d_i} & \to \mathbb{R}^{\sum_{i=1}^{n} m_i} \\ x = (x_1; \dots; x_n) & \to (\alpha_1(x_1); \dots; \alpha_n(x_n)) \end{cases}$$

is  $\|\ell\|_2$ -Lipschitz continuous and  $\|L\|_{\infty}$ -smooth.

2. Assume  $\alpha_i : \mathbb{R}^{d_i} \to \mathbb{R}^m$ , then

$$a: \begin{cases} \mathbb{R}^{\sum_{i=1}^{n} d_i} & \to \mathbb{R}^m \\ x = (x_1; \dots; x_n) & \to \sum_{i=1}^{n} \alpha_i(x_i) \end{cases}$$

is  $\|\ell\|_2$ -Lipschitz continuous and  $\|L\|_{\infty}$ -smooth.

3. Assume  $a_i : \mathbb{R}^d \to \mathbb{R}^{m_i}$ , then

$$a: \begin{cases} \mathbb{R}^d & \to \mathbb{R}^{\sum_{i=1}^n m_i} \\ x & \to (\alpha_1(x); \dots; \alpha_n(x)) \end{cases}$$

- is  $\|\ell\|_2$ -Lipschitz continuous and  $\|L\|_2$ -smooth.
- 4. Assume  $\alpha_i : \mathbb{R}^d \to \mathbb{R}^m$ , then

$$a: \begin{cases} \mathbb{R}^d & \to \mathbb{R}^m \\ x & \to \sum_{i=1}^n \alpha_i(x) \end{cases}$$

is  $\|\ell\|_1$ -Lipschitz continuous and  $\|L\|_1$ -smooth.

*Proof.* 1. We have for  $x = (x_1; \ldots; x_n) \in \mathbb{R}^{\sum_{i=1}^n d_i}$  and  $z = (z_1; \ldots; z_n) \in \mathbb{R}^{\sum_{i=1}^n m_i}$ ,

$$\|\nabla a(x)z\|_{2} = \|\sum_{i=1}^{n} \nabla \alpha_{i}(x_{i})z_{i}\|_{2} \le \sum_{i=1}^{n} \|z_{i}\|_{2} \|\nabla \alpha_{i}(x_{i})\|_{2,2} \le \|z\|_{2} \sqrt{\sum_{i=1}^{n} \ell_{i}^{2}},$$

which gives an upper bound on the Lipschitz-continuity of a. For  $x = (x_1; \ldots; x_n), y = (y_1; \ldots; y_n) \in \mathbb{R}^{\sum_{i=1}^n d_i}$ , we have

$$\|(\nabla a(x) - \nabla a(y))z\|_{2} \le \sum_{i=1}^{n} \|z_{i}\|_{2} \|\nabla \alpha_{i}(x_{i}) - \nabla \alpha_{i}(y_{i})\|_{2,2} \le \sum_{i=1}^{n} \|z_{i}\|_{2} \|x_{i} - y_{i}\|_{2} L_{i} \le \|z\|_{2} \|x - y\|_{2} \max_{i \in \{1, \dots, n\}} L_{i}$$

Hence  $\|\nabla a(x) - \nabla a(y)\|_{2,2} \le \|x - y\|_2 \max_{i \in \{1,...,n\}} L_i$  which gives an upper bound on the smoothness of a.

2. We have for  $x = (x_1; \ldots; x_n) \in \mathbb{R}^{\sum_{i=1}^n d_i}$  and  $z \in \mathbb{R}^m$ ,

$$\|\nabla a(x)z\|_{2}^{2} = \sum_{i=1}^{n} \|\nabla \alpha_{i}(x_{i})z\|_{2}^{2} \le \sum_{i=1}^{n} \ell_{i}^{2} \|z\|_{2}^{2},$$

which gives the Lipschitz-continuity parameter. Similarly we have for  $x = (x_1; \ldots; x_n), y = (y_1; \ldots; y_n) \in \mathbb{R}^{\sum_{i=1}^n d_i}$ ,

$$\|(\nabla a(x) - \nabla a(y))z\|_{2}^{2} = \sum_{i=1}^{n} \|(\nabla \alpha_{i}(x_{i}) - \nabla \alpha_{i}(y_{i}))z\|_{2}^{2} \le \sum_{i=1}^{n} L_{i}^{2} \|x_{i} - y_{i}\|_{2}^{2} \|z\|_{2}^{2} \le \max_{i \in \{1, \dots, n\}} L_{i}^{2} \|x - y\|_{2}^{2} \|z\|_{2}^{2},$$

which gives the smoothness constant of a.

3. The bound on the Lipschitz-continuity parameter follows from the same argument as in 1. For the smoothness parameter, we have for  $x, y \in \mathbb{R}^d$  and  $z = (z_1; \ldots; z_n) \in \mathbb{R}^{\sum_{i=1}^n m_i}$ ,

$$\|(\nabla a(x) - \nabla a(y))z\|_{2} \le \sum_{i=1}^{n} \|z_{i}\|_{2} \|\nabla \alpha_{i}(x) - \nabla \alpha_{i}(y)\|_{2,2} \le \sum_{i=1}^{n} \|z_{i}\|_{2} \|x - y\|_{2} L_{i} \le \|z\|_{2} \|x - y\|_{2} \sqrt{\sum_{i=1}^{n} L_{i}^{2}}.$$

Hence the result as in 1.

4. Clear by linearity of the gradient and triangular inequality.

#### **Bilinear functions.**

**Lemma C.2.** Consider  $s \times t$  bilinear functions  $\beta_{i+(j-1)s} : \mathbb{R}^{d_i} \times \mathbb{R}^{p_j} \to \mathbb{R}^{m_{i+(j-1)s}}$  for  $i \in \{1, \ldots s\}, j \in \{1, \ldots t\}$  then

$$\beta: \begin{cases} \mathbb{R}^{\sum_{i=1}^{s} d_i} \times \mathbb{R}^{\sum_{j=1}^{t} p_j} & \to \mathbb{R}^{\sum_{k=1}^{st} m_k} \\ (x, u) & \to (\beta_1(x_1, u_1); \dots; \beta_s(x_s, u_1); \beta_{s+1}(x_1, u_2); \dots; \beta_{st}(x_s, u_t)) \end{cases}$$

is  $L_{\beta} = \max_{k \in \{1, \dots, st\}} L_{\beta_k}$  smooth.

*Proof.* By Lemma A.7, we have that  $L_{\beta} = \sup_{x,u} \|\beta(x,u)\|_2 / \|x\|_2 \|u\|_2$ . Now

$$\|\beta(x,u)\|_{2}^{2} = \sum_{i=1}^{s} \sum_{j=1}^{t} \|\beta_{i+s(j-1)}(x_{i},u_{j})\|_{2}^{2}$$
  
$$\leq \sum_{i=1}^{s} \sum_{j=1}^{t} L_{\beta_{i+s(j-1)}} \|x_{i}\|_{2}^{2} \|u_{j}\|_{2}^{2} \leq \max_{k \in \{1,...,st\}} L_{\beta_{k}} \|x\|_{2}^{2} \|u\|_{2}^{2}.$$

#### C.2 Compositions

The smoothness properties of the functions can be derived by bounding appropriately their first and second order information. Even if e.g. the functions are not twice differentiable, the same results would apply by decomposing carefully the terms, we directly use the second order information as it directly gives what we are interested in.

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For a smooth function, an upper bound on the Lipschitz continuity of the function on a bounded set can be estimated even if the function is not Lipschitz continuous. Similarly a bound on the function a bounded set can be refined as defined below.

**Fact C.3.** For a function  $f \in \mathcal{C}_{m_f,\ell_f,L_f}$  and R > 0. Denoting  $B_R = \{x \in \text{dom } f : ||x||_2 \le R\}$ , we have that

$$\ell_f^{B_R} \le \ell_f(R) := \min\{\ell_f, \|\nabla f(0)\|_{2,2} + RL_f\},\$$
$$m_f^{B_R} \le m_f(R) := \min\{m_f, \|f(0)\|_2 + R\ell_f(R)\}$$

For a sequence of compositions we have the following result.

#### Lemma C.4. Consider

 $a = a_k \circ \ldots \circ a_1$ with  $a_j \in \mathcal{C}_{m_{a_j}, \ell_{a_j}, L_{a_j}}$  for  $j \in \{1, \ldots, k\}$  and  $a : \mathbb{R}^d \to \mathbb{R}^n$ . Denote  $B_R = \{x \in \mathbb{R}^d : ||x||_2 \leq R\}$ , and for  $j \in \{1, \ldots, k\}$ ,

$$m_{j} = m_{a_{j}}(m_{t-1}),$$
  

$$\ell_{j} = \ell_{j-1}\ell_{a_{j}}(m_{j-1}),$$
  

$$L_{j} = L_{a_{j}}\ell_{j-1}^{2} + L_{j-1}\ell_{a_{j}}(m_{j-1}),$$

with  $m_0 = R, \ell_0 = 1, L_0 = 0$ . We have

$$m_a^{B_R} \le m_\tau, \qquad \ell_a^{B_R} \le \ell_\tau = \prod_{j=1}^k \ell_{a_j}(m_{j-1}), \qquad L_a^{B_R} \le L_\tau = \sum_{j=1}^k L_{a_j}\left(\prod_{i=1}^{j-1} \ell_{a_i}(m_{i-1})\right)^2 \left(\prod_{i=j+1}^k \ell_{a_i}(m_{i-1})\right).$$

*Proof.* The bound on the output is a direct iterative application of Fact C.3. We have for  $x \in \mathbb{R}^d$ ,

$$\nabla a(x) = \prod_{j=1}^{k} g_j(x), \quad \text{where} \quad g_j(x) = \nabla a_j(a_{j-1} \circ \ldots \circ a_1(x)) \quad \text{for } j \in \{1, \ldots, k\}.$$

We have

$$\sup_{x \in \mathbb{R}^d: \|x\|_2 \le R} \|g_j(x)\|_{2,2} \le \min\{\ell_{a_j}, \|\nabla a_j(0)\|_{2,2} + L_{a_j} m_{a_{j-1} \circ \dots \circ a_1}^{B_R}\}$$

Therefore

$$\ell_a^{B_R} \le \prod_{j=1}^k \ell_{a_j}(m_{j-1}).$$

We have for  $x \in \mathbb{R}^d$ ,

$$\nabla^2 a(x) = \sum_{j=1}^k \nabla^2 a_j(x) \left[ \left( \prod_{i=1}^{j-1} g_i(x) \right)^\top, \left( \prod_{i=1}^{j-1} g_i(x) \right)^\top, \prod_{i=j+1}^k g_i(x) \right]$$

Therefore

$$L_a^{B_R} \le \sum_{j=1}^k L_{a_j} \left( \prod_{i=1}^{j-1} \ell_{a_i}(m_{i-1}) \right)^2 \left( \prod_{i=j+1}^k \ell_{a_i}(m_{i-1}) \right).$$

Lemma C.4 can be used to estimate the smoothness of a chain of computations with respect to its input for fixed parameters.

**Corollary C.5.** Consider a chain f of  $\tau$  computations  $\phi_t \in C_{m_{\phi_t}, \ell_{\phi_t}, L_{\phi_t}}$  with given parameters  $u = (u_1; \ldots; u_{\tau})$ .

Denote  $\phi_{t,u_t} = \phi_t(\cdot, u_t)$ . Denote  $B_R = \{x \in \mathbb{R}^d : ||x||_2 \le R\}$ , and for  $j \in \{1, ..., k\}$ ,

$$m_{j} = m_{\phi_{t}(\cdot, u_{t})}(m_{t-1}),$$
  

$$\ell_{j} = \ell_{j-1}\ell_{\phi_{j}(\cdot, u_{j})}(m_{j-1}),$$
  

$$L_{j} = L_{\phi_{j}(\cdot, u_{j})}\ell_{j-1}^{2} + L_{j-1}\ell_{\phi_{j}(\cdot, u_{j})}(m_{j-1})$$

with  $m_0 = R, \ell_0 = 1, L_0 = 0$ . We have

$$m_{f_{\tau,u}}^{B_R} \le m_{\tau}, \quad \ell_{f_{\tau,u}}^{B_R} \le \ell_{\tau} = \prod_{j=1}^k \ell_{\phi_j(\cdot,u_j)}(m_{j-1}),$$
$$L_{f_{\tau,u}}^{B_R} \le L_{\tau} = \sum_{j=1}^k L_{\phi_j(\cdot,u_j)} \left( \prod_{i=1}^{j-1} \ell_{\phi_i(\cdot,u_i)}(m_{i-1}) \right)^2 \left( \prod_{i=j+1}^k \ell_{\phi_i(\cdot,u_i)}(m_{i-1}) \right).$$

### C.3 Chains of computations

We have the following result for smooth and Lipschitz continuous chains of computations.

**Lemma 4.3.** Consider a chain f of  $\tau$  computations  $\phi_t \in C_{\ell_{\phi_t}, L_{\phi_t}}$  initialized at some  $x_0 \in \mathbb{R}^{d_0}$ . (i) We have  $\ell_{f_{\tau, x_0}} \leq \ell_{\tau}$ , where

$$\ell_0 = 0, \ \ell_t = \ell_{\phi_t} + \ell_{t-1}\ell_{\phi_t}, \ for \ t \in \{1, \dots, \tau\}.$$

(ii) We have  $L_{f_{\tau,x_0}} \leq L_{\tau}$ , where

$$L_0 = 0, \ L_t = L_{t-1}\ell_{\phi_t} + L_{\phi_t}(1+\ell_{t-1})^2, \ for \ t \in \{1,\ldots,\tau\}$$

Proof. The first claim follows directly from Lemma B.1. For the second claim we have that (27) gives

$$L_{f_t} \le L_{f_{t-1}} \ell_{\phi_t} + L_{\phi_t} \ell_{f_{t-1}}^2 + 2L_{\phi_t} \ell_{f_{t-1}} + L_{\phi_t},$$

which simplifies to give the result.

For a bivariate function  $\phi(x, u) : \mathbb{R}^d \times \mathbb{R}^p \to \mathbb{R}^\eta$ , we define

$$\ell_\phi^u = \sup_{u \in \mathbb{R}^p, x \in \mathbb{R}^d} \ell_{\phi(x, u+\cdot)}, \qquad \ell_\phi^x = \sup_{u \in \mathbb{R}^p, x \in \mathbb{R}^d} \ell_{\phi(x+\cdot, u)}.$$

Moreover if the function is continuously differentiable, we define

$$\begin{split} L^{uu}_{\phi} &= \sup_{u \in \mathbb{R}^p, x \in \mathbb{R}^d} \ell_{\nabla_u \phi(x, u+\cdot)}, \qquad L^{xu}_{\phi} &= \sup_{u \in \mathbb{R}^p, x \in \mathbb{R}^d} \ell_{\nabla_u \phi(x+\cdot, u)}, \\ L^{ux}_{\phi} &= \sup_{u \in \mathbb{R}^p, x \in \mathbb{R}^d} \ell_{\nabla_x \phi(x, u+\cdot)}, \qquad L^{xx}_{\phi} &= \sup_{u \in \mathbb{R}^p, x \in \mathbb{R}^d} \ell_{\nabla_x \phi(x+\cdot, u)}. \end{split}$$

For a bivariate continuosuly differentiable function  $\phi(x, u) : \mathbb{R}^p \times \mathbb{R}^d \to \mathbb{R}^\eta$ , we have that

$$\ell_{\phi}^{u} = \sup_{u \in \mathbb{R}^{p}, x \in \mathbb{R}^{d}} \|\nabla_{u}\phi(x, u)\|_{2, 2}, \qquad \ell_{\phi}^{x} = \sup_{u \in \mathbb{R}^{p}, x \in \mathbb{R}^{d}} \|\nabla_{x}\phi(x, u)\|_{2, 2}.$$

If the function  $\phi$  is twice continuously differentiable, we have that

$$\begin{split} L_{\phi}^{uu} &= \sup_{u \in \mathbb{R}^{p}, x \in \mathbb{R}^{d}} \|\nabla_{uu}^{2} \phi(x, u)\|_{2, 2, 2}, \qquad L_{\phi}^{xu} &= \sup_{u \in \mathbb{R}^{p}, x \in \mathbb{R}^{d}} \|\nabla_{xu}^{2} \phi(x, u)\|_{2, 2, 2}, \\ L_{\phi}^{ux} &= \sup_{u \in \mathbb{R}^{p}, x \in \mathbb{R}^{d}} \|\nabla_{uu}^{2} \phi(x, u)\|_{2, 2, 2}, \qquad L_{\phi}^{xx} &= \sup_{u \in \mathbb{R}^{p}, x \in \mathbb{R}^{d}} \|\nabla_{uu}^{2} \phi(x, u)\|_{2, 2, 2}. \end{split}$$

Finally for  $R_x \ge 0, R_u \ge 0$ , we have

$$\sup_{(x,u)\in B_{R_x}\times B_{R_u}} \|\nabla_u \phi(x,u)\|_{2,2} \le \ell_\phi^u(R_x,R_u) := \min\{\ell_\phi^u, \|\nabla_u \phi(0,0)\|_{2,2} + L_\phi^{uu}R_u + L_\phi^{xu}R_x\}$$
(33)

 $\sup_{(x,u)\in B_{R_x}\times B_{R_u}} \|\nabla_x \phi(x,u)\|_{2,2} \le \ell_{\phi}^x(R_x,R_u) := \min\{\ell_{\phi}^x, \|\nabla_x \phi(0,0)\|_{2,2} + L_{\phi}^{xx}R_u + L_{\phi}^{ux}R_x\}.$ 

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We then have the following.

**Lemma C.6.** Let f be a chain of  $\tau$  computations  $\phi_t \in C_{m_{\phi_t},\ell_{\phi_t}^u,L_{\phi_t}^u,L_{\phi_t}^{xu},L_{\phi_t}^{xu},L_{\phi_t}^{xu}}$ , initialized at some  $x_0$  such that  $\|x_0\|_2 \leq R_0$ . Let  $C = \bigotimes_{t=1}^{\tau} B_{R_t}(\mathbb{R}^{p_t}) = \{u = (u_1;\ldots;u_{\tau}) \in \mathbb{R}^{\sum_{t=1}^{\tau} p_t} : u_t \in \mathbb{R}^{p_t}, \|u_t\|_2 \leq R_t\}$ . Define for  $t \in \{1,\ldots,\tau\}$ ,

$$m_{t} = \min\{m_{\phi_{t}}, \|\phi_{t}(0,0)\|_{2} + \ell_{\phi_{t}}^{u}(m_{t-1},R_{t})R_{t} + \ell_{\phi_{t}}^{x}(m_{t-1},R_{t})m_{t-1}\}$$
  

$$\ell_{t} = \ell_{\phi_{t}}^{u}(m_{t-1},R_{t}) + \ell_{t-1}\ell_{\phi_{t}}^{x}(m_{t-1},R_{t}),$$
  

$$L_{t} = L_{t-1}\ell_{\phi_{t}}^{x}(m_{t-1},R_{t}) + L_{\phi_{t}}^{xx}\ell_{t-1}^{2} + (L_{\phi_{t}}^{xu} + L_{\phi_{t}}^{ux})\ell_{t-1} + L_{\phi_{t}}^{uu}.$$

with  $m_0 = R_0$ ,  $\ell_0 = 0$ ,  $L_0 = 0$ . We have that

$$m_{f_{\tau},x_0}^C \le m_{\tau}, \quad \ell_{f_{\tau},x_0}^C \le \ell_{\tau}, \quad L_{f_{\tau},x_0}^C \le L_{\tau}.$$

*Proof.* The result directly follows from Lemma B.1, with the Lipschitz-continuity constants derived in (33).

*Proof.* The proof relies on Lemma C.6, where the smoothness of the inner compositions are computed according to Lemma C.4. Namely, we have

$$\ell_{\phi_t}^u(R_x, R_u) \le \ell_{a_t}(m_{b_t}(R_x, R_u))\ell_{b_t}^u(R_x, R_u), \qquad \ell_{\phi_t}^x(R_x, R_u) \le \ell_{a_t}(m_{b_t}(R_x, R_u))\ell_{b_t}^x(R_x, R_u)$$

with

$$\ell_{b_t}^u(R_x, R_u) = L_{b_t}R_x + l_{b_t}^u, \qquad \ell_{b_t}^x(R_x, R_u) = L_{b_t}R_u + l_{b_t}^x,$$
$$m_{b_t}(R_x, R_u) = \ell_{b_t}^u(R_x, R_u)R_u + \ell_{b_t}^x(R_x, R_u)R_x + \|b_t(0, 0)\|_2$$

and  $\ell_{a_t}$  can be computed as in Lemma. C.4. On the other hand, denoting  $L_{\phi_t}^{xx}(R_x, R_u) = \sup_{(x,u)\in B_{R_x}\times B_{R_u}} \|\nabla_{xx}^2\phi_t(x, u)\|_{2,2,2}$ (and similarly for  $L_{\phi_t}^{uu}, L_{\phi_t}^{ux}, L_{\phi_t}^{xu}$ ), we have

$$L_{\phi_t}^{xx}(R_x, R_u) \leq L_{a_t}(m_{b_t}(R_x, R_u))\ell_{b_t}^x(R_x, R_u)^2$$
$$L_{\phi_t}^{uu}(R_x, R_u) \leq L_{a_t}(m_{b_t}(R_x, R_u))\ell_{b_t}^u(R_x, R_u)^2$$
$$L^{xu}(R_x, R_u) = L^{ux}(R_x, R_u) = L_{b_t}\ell_{a_t}(m_{b_t}(R_x, R_u)) + L_{a_t}(m_{b_t}(R_x, R_u))\ell_{b_t}^u(R_x, R_u)\ell_{b_t}^x(R_x, R_u),$$

where  $L_{a_t}(m_{b_t}(R_x, R_u))$  is computed by Lemma C.4.

## **D** Smoothness of objectives and layers

### **D.1** Supervised objectives

For supervised objectives  $h : \mathbb{R}^{nd_{\tau}} \to \mathbb{R}$  that reads for  $\hat{y} = (\hat{y}_1; \ldots; \hat{y}_n)$  with  $\hat{y}_i \in \mathbb{R}^{d_{\tau}}$ ,

$$h(\hat{y}) = \frac{1}{n} \sum_{i=1}^{n} h_i(\hat{y}_i),$$

we only need to compute the smoothness of  $h_i(\hat{y}_i)$  (see Lemma C.1) which is usually defined by a loss  $h_i(\hat{y}_i) = \mathcal{L}(\hat{y}_i, y_i)$ . We are interested in this section in the smoothness  $L_h(C)$  and Lipschitz-continuity  $\ell_h(C)$  of the objective h on a set C. We omit the dependency on the set C if Lipschitz-continuity or smoothness properties of the functions are defined on its whole domain.

**Square loss.** Assume that the labels belong to a compact set  $\mathcal{Y}$ . The square loss is defined by  $h(\hat{y}) = \mathcal{L}_{sq}(\hat{y}, y) = (\hat{y} - y)^2/2$ . We have then

$$\ell_{\mathrm{sq}}(C) = \rho_C + \rho_{\mathcal{Y}}, \qquad L_{\mathrm{sq}} = 1.$$

where  $\rho_C = \max_{x \in C} \|x\|_2$  and  $\rho_{\mathcal{Y}} = \max_{y \in \mathcal{Y}} \|y\|_2$ .

**Logistic loss.** Consider  $y \in \{0,1\}^q$ , the logistic loss is defined as  $h(\hat{y}) = \mathcal{L}_{\log}(\hat{y}, y) = -y^\top \hat{y} + \log\left(\sum_{j=1}^q \exp(\hat{y}_j)\right)$ . We have then, denoting  $\exp(y) = (\exp(y_i))_{i=1,\dots,q}$ ,

$$\nabla h(\hat{y}) = -y + \frac{\exp(\hat{y})}{\exp(\hat{y})^{\top} \mathbf{1}_q}, \qquad \nabla^2 h(\hat{y}) = \frac{\operatorname{diag}(\exp(\hat{y}))}{\exp(\hat{y})^{\top} \mathbf{1}_q} - \frac{\exp(\hat{y})\exp(\hat{y})^{\top}}{(\exp(\hat{y})^{\top} \mathbf{1}_q)^2}.$$

Therefore using that  $y \in \{0,1\}^q$  and that  $\|\exp(\hat{y})\|_2 \le \|\exp(\hat{y})\|_1$ ,

$$\ell_{\log} \le 2, \qquad L_{\log} \le 2.$$

### **D.2** Unsupervised objectives

For the k-means and spectral clustering objectives, we consider the outputs of the chains of the computations to form a matrix  $F(\bar{x}, u) = (f(\bar{x}^{(1)}, u), \dots, f(\bar{x}^{(n)}, u)) \in \mathbb{R}^{q \times n}$  where  $q = d_{\tau}$  and n to be the number of samples. The objectives are then  $h : \mathbb{R}^{q \times n} \to \mathbb{R}$  and we denote by  $Z \in \mathbb{R}^{q \times n}$  their variables. The overall objective is  $h(F(\bar{x}, u))$  for  $\bar{x} = (\bar{x}^{(1)}; \dots; \bar{x}^{(n)})$ . We denote k the number of classes that the unsupervised objective aims to cluster and

$$\mathcal{Y} = \{ Y = (y_1, \dots, y_n)^\top \in \{0, 1\}^{n \times k} \text{ s.t. } Y \mathbf{1}_k = \mathbf{1}_n \}.$$

K-means clustering. The K-means clustering objective reads

$$h(Z) = \min_{\substack{Y \in \mathcal{Y} \\ C \in \mathbb{R}^{q \times k}}} \sum_{i=1}^{n} \|Cy_i - z_i\|_2^2$$

for  $Z = (z_1, \ldots, z_n) \in \mathbb{R}^{q \times n}$ . Minimization in C can be performed analytically such that the problem can be rewritten

$$h(Z) = \min_{N \in \mathcal{N}} \operatorname{Tr}((\mathbf{I}_n - N)Z^{\top}Z),$$

where  $\mathcal{N} = \{N = Y(Y^{\top}Y)^{-1}Y^{\top} \in \mathbb{R}^{n \times n}$  for  $Y \in \mathcal{Y}, \quad Y^{\top}Y \succ 0\}$  is the set of normalized equivalence matrices.

Spectral clustering. A natural relaxation of K-means is spectral clustering, that considers

$$\mathcal{P} = \{ P \in \mathbb{R}^{n \times n} \quad \text{s.t. } P \succeq 0, \ P^2 = P, \ \mathbf{Rank}(P) = k \} \supset \mathcal{N}$$

instead of the set of normalized equivalence matrices. The solution of

$$h(Z) = \min_{P \in \mathcal{P}} \operatorname{Tr}((\mathbf{I}_n - P)Z^{\top}Z)$$

is then given by finding the k largest eigenvectors of the Gram matrix  $Z^{\top}Z$ . Formally the objective is written

$$h(Z) = \sum_{i=n-k+1}^{n} \sigma_i^2(Z),$$

where for a matrix A,  $\sigma_1(A) \ge \ldots, \ge \sigma_n(A)$  are the singular values of A in decreasing order. The objective h is then a spectral function of the matrix Z.

**Convex clustering.** The convex clustering objective reads for  $\hat{y} = (\hat{y}_1; \ldots; \hat{y}_n) \in \mathbb{R}^{qn}$ 

$$h(\hat{y}) = \min_{y^{(1)}, \dots, y^{(n)} \in \mathbb{R}^q} \sum_{i=1}^n \frac{1}{2} \|y^{(i)} - \hat{y}^{(i)}\|_2^2 + \sum_{i < j} \|y^{(i)} - y^{(j)}\|_2,$$

$$= \min_{y \in \mathbb{R}^{q_n}} \frac{1}{2} \|y - \hat{y}\|_2^2 + \|Dy\|_G$$
(34)

where  $y = (y_1; \ldots; y_n) \in \mathbb{R}^{qn}$  and  $D \in \mathbb{R}^{qn(n-1)/2 \times qn}$  maps y to the concatenation of all possible  $y_i - y_j$  for i < jand  $\|\cdot\|_G$  is a group norm, i.e.,  $\|x\|_G = \sum_{g \in \mathcal{G}} \|x_g\|_2$  where  $\mathcal{G}$  is a partition of  $\{1, \ldots, N\}$  for  $x \in \mathbb{R}^N$  and  $x_g \in \mathbb{R}^{s_g}$  is the vector corresponding to the group g of size  $s_q$ . Here the groups are defined by all possible differences for i < jin Eq. (34).

**Proposition D.1.** The convex-clustering objective

$$h(\hat{y}) = \min_{y \in \mathbb{R}^{qn}} \frac{1}{2} \|y - \hat{y}\|_2^2 + \|Dy\|_G$$

is convex, Lipschitz-continuous and smooth with parameters

$$\ell_{\text{cvx-cluster}} \leq \frac{n(n-1)}{2}, \qquad L_{\text{cvx-cluster}} \leq 1.$$

*Proof.* The convex clustering objective h is the Moreau envelope of the function  $\Omega: y \to ||Dy||_G$ . It is therefore convex and 1-smooth, i.e.,  $L_h = 1$ . Moreover, the Moreau envelope can be rewritten

$$h(\hat{y}) = \sup_{z \in \operatorname{dom}(\Omega^*)} \hat{y}^\top z - \Omega^*(z) - \frac{1}{2} \|z\|_2^2,$$

where  $\Omega^*$  is the convex conjugate of  $\Omega$ . Therefore  $\nabla h(\hat{y}) \in \operatorname{dom}(\Omega^*)$ . We have that

$$\Omega^*(z) = \sup_{y \in \mathbb{R}^q} z^\top y - \|Dy\|_G \ge \sup_{y \in \mathbb{R}^q} z^\top y - \frac{n(n-1)}{2} \|y\|_2,$$

such that the supremum is finite only if  $||z||_2 > \frac{n(n-1)}{2}$ . Therefore

$$\nabla h(\hat{y}) \in \operatorname{dom}(\Omega^*) \subset \mathcal{B}_2\left(0, \frac{n(n-1)}{2}\right)$$

where  $\mathcal{B}_2(0, \frac{n(n-1)}{2})$  is the Euclidean ball centered at 0 with radius  $\frac{n(n-1)}{2}$ .

#### **D.3 Bilinear and linear layers**

Vectorized matrix-products as a bilinear operation. Given two matrices  $A \in \mathbb{R}^{n \times d}$  and  $B \in \mathbb{R}^{d \times p}$ , the matrix product AB is defined by a tensor  $\mathcal{M} = ((I_d \otimes e_{(q \mod n)+1})(f_{\lceil q/n \rceil}^\top \otimes I_d))_{q=1,...,np} \in \mathbb{R}^{nd \times dp \times np}$  where  $e_i$  is the i<sup>th</sup> canonical vector in  $\mathbb{R}^n$  and  $f_i$  is the j<sup>th</sup> canonical vector in  $\mathbb{R}^p$  such that

$$\operatorname{Vec}(AB) = \mathcal{M}[\operatorname{Vec}(A), \operatorname{Vec}(B), \cdot].$$

$$\operatorname{This} \operatorname{can} \operatorname{be} \operatorname{checked} \operatorname{as} \operatorname{for} q = i + n(j-1) \in \{1, \dots, np\}, \text{ with } i \in \{1, \dots, n\}, j \in \{1, \dots, p\},$$

$$\operatorname{Vec}(AB)_q = (AB)_{ij} = \operatorname{Vec}(e_i^{\top}A)^{\top} \operatorname{Vec}(Bf_j)$$

$$= \operatorname{Vec}(A)^{\top}(\operatorname{I}_d \otimes e_i)(f_j^{\top} \otimes \operatorname{I}_d) \operatorname{Vec}(B)$$

$$= (\mathcal{M}[\operatorname{Vec}(A), \operatorname{Vec}(B), \cdot])_q.$$

$$(35)$$

Convolutional layer detailed. For completeness we detail the convolution for an image. For a convolutional layer, the input is an image  $\mathcal{I} \in \mathbb{R}^{C \times H \times B}$  with C channels each composed of a matrix of height H and breadth B the weights are given by  $\tilde{C}$  filters  $\mathcal{F}_1, \ldots, \mathcal{F}_{\tilde{C}} \in \mathbb{R}^{C \times K \times K}$  of patch size K and the biases are given by  $b \in \mathbb{R}^{\tilde{C}}$ . The convolution of the image by a filter  $\mathcal{F}_{\tilde{c}}$ , with  $\tilde{c} \in \{1, \dots, \tilde{C}\}$  with additional bias  $b_{\tilde{c}}$ , is given at point i, j as

$$\mathcal{C}_{\tilde{c},i,j} = \sum_{c=1}^{C} \langle \mathcal{F}_{\tilde{c}}[c,\cdot,\cdot], E_{row,i}^{\top} \mathcal{I}[c,\cdot,\cdot] E_{col,j} \rangle + b_{\tilde{c}},$$

where  $\mathcal{F}_{\tilde{c}}[c,\cdot,\cdot]$  is the filter of size  $K \times K$  in channel c of filter  $\mathcal{F}_{\tilde{c}}$  and  $I[c,\cdot,\cdot]$  is the image in channel c. The matrices  $E_{row,i} \in \mathbb{R}^{H \times K}$  and  $E_{col,j} \in \mathbb{R}^{B \times K}$  extract rows and columns of  $I[c,\cdot,\cdot]$ . They are bands with a diagonal of K ones centered at positions i or j. If the pattern of the patch is given as  $P = \mathbf{1}_K \mathbf{1}_K^{\top}$ , the extraction matrices read  $E_{row,i} = e_i \otimes \mathbf{1}_K^{\top} \in \mathbb{R}^{H \times K}$ ,  $e_i \in \mathbb{R}^H$  for  $i \in \{1, \ldots, H\}$ , similarly  $E_{col,j} = e_j \otimes \mathbf{1}_K^{\top} \in \mathbb{R}^{W \times K}$ . They satisfy  $E_{row,i}^{\top} E_{row,i} = \mathbf{I}_{K^2}$  and  $E_{row,i} E_{row,i}^{\top} \in \mathbb{R}^{H \times H}$  is a projector. Similarly facts apply for  $E_{col,j}$  except that one

6)

replaces H by B. The output of the convolution with all filters is then a tensor  $C \in \mathbb{R}^{\tilde{H} \times \tilde{B} \times \tilde{C}}$  where  $\tilde{H}$  and  $\tilde{B}$  depend on the choices of the stride chosen in the convolution.

Smoothness of fully-connected layer. For a fully connected layer, the bilinear function  $\beta(x, u) \to U^{\top} X$  for u = Vec(U), x = Vec(X) is clearly 1-smooth (because  $||U^{\top}X||_F \leq ||U||_F ||X||_F$ ). The linear part  $\beta^u$  is clearly 1-Lipschitz continuous. So we get

$$L_{full} = 1, \quad l^u_{full} = 1.$$

**Smoothness of convolutional layer.** For a convolution, by Lemma C.2, we only need to compute the smoothness of the convolution of an image with one filter. This is done by the following Lemma.

**Lemma D.2.** Consider p subsets  $S_k$  of  $\{1, \ldots, n\}$  of size  $|S_k| = d$ . Denote  $\Pi_k \in \{0, 1\}^{d \times n}$  the linear form that extracts the  $S_k$  coordinates of a vector of size n, i.e.,  $\Pi_k z = z_{S_k}$  for  $z \in \mathbb{R}^n$ . The convolution of  $z \in \mathbb{R}^n$  by  $w \in \mathbb{R}^d$  through the p subsets  $S_k$  defined as

$$\beta(z,w) = (w^{\top}\Pi_1 z; \dots; w^{\top}\Pi_p z)$$

is  $L_{\beta} = \sqrt{\max_{i=1,\dots,n} |V_i|}$ -smooth where  $V_i = \{S_j : i \in S_j\}$ .

Proof. We have

$$\begin{split} \|\beta(z,w)\|_{2}^{2} &= \sum_{j=1}^{p} (w^{\top} \Pi_{j} z)^{2} \leq \sum_{j=1}^{p} \|w\|_{2}^{2} \|z_{S_{j}}\|_{2}^{2} \\ &= \|w\|_{2}^{2} \sum_{i=1}^{d} \sum_{S_{j} \in V_{i}} z_{i}^{2} \leq \|w\|_{2}^{2} \max_{i=1,\dots,n} |V_{i}|\|z\|_{2}^{2}. \end{split}$$

Concretely, for a convolution such that at most p patches contain a coordinate i the convolution is  $\sqrt{p}$ -smooth. If the patches do not overlap then the convolution is 1-smooth. If the convolution has a stride of 1 and the operation is normalized by the size of the filters then the convolution has again a smoothness constant of 1. Generally for a 2d convolution with a kernel of size  $k \times k$  and a stride of s, we have  $\max_{i=1,...,n} |V_i| = \left\lceil \frac{k}{s} \right\rceil^2$  and so

$$L_{\rm conv} = \left\lceil \frac{k}{s} \right\rceil, \quad l_{\rm conv} = \left\lceil \frac{k}{s} \right\rceil.$$

**Batch of inputs.** For batch of inputs, the smoothness constants of the non-linear and bilinear parts do not change by Lemmas C.1 and C.2. The Lipschitz-constant of the linear part of the biaffine function is modified using Lemma C.1 item 3. Namely for a batch of size m, the fully connected layers or the convolutional layers have a linear part whose Lipschitz constant is given by  $l_b = \sqrt{m}$ .

#### **D.4** Activation functions

The Lipschitz and smoothness constants of an element-wise activation  $\alpha_t$  function are defined by the Lipschitz and smoothness constant of the scalar function  $\bar{\alpha}_t$  from which it is defined. Denote by  $f(x) := \log(1 + \exp(x))$ , we have  $f'(x) = (1 + \exp(-x))^{-1}$ ,  $f''(x) = (2 + 2\cosh(x))^{-1}$ ,  $f'''(x) = -\sinh(x)/(2(1 + \cosh(x)^2))$ .

**Soft-plus.** For  $\alpha$  defined by element-wise application of  $\bar{\alpha}(x) = f(x)$ , we get

$$\ell_{\text{softplus}} = 1, \qquad L_{\text{softplus}} = 1/4.$$

**Sigmoid.** For  $\alpha$  defined by the element-wise application of  $\bar{\alpha}(x) = f'(x)$ , we get

$$\ell_{\rm sig} = 1/4, \qquad L_{\rm sig} = 1/10.$$

**ReLU.** For  $\alpha$  defined by the element-wise application of  $\bar{\alpha}(x) = \max(0, x)$ , we get

$$\ell_{\text{ReLu}} = 1, \quad L_{\text{ReLu}} \text{ not defined},$$

since the function is not continuously differentiable.

**Soft-max layer.** A soft-max layer takes as input  $x \in \mathbb{R}^d$  and outputs  $f(x) = \exp(x)/(\exp(x)^\top \mathbf{1}_d)$  where  $\exp(x)$  is the element-wise application of exp. Its gradient is given by

$$\nabla f(x) = \frac{\operatorname{\mathbf{diag}}(\exp(\hat{y}))}{\exp(\hat{y})^{\top} \mathbf{1}_{q}} - \frac{\exp(\hat{y}) \exp(\hat{y})^{\top}}{(\exp(\hat{y})^{\top} \mathbf{1}_{q})^{2}}.$$

Its second-order information can be computed as for the batch-normalization layer, we get then

$$\ell_{\text{softmax}} = 2, \qquad L_{\text{softmax}} = 4.$$

### **D.5** Normalization layers

**Proposition D.3.** The batch normalization operation  $\nu_{\text{batch}} : \mathbb{R}^{\delta m} \to \mathbb{R}^{\delta m}$  defined as in (11) is

- (i) bounded by  $m_{\text{batch}} = \delta m$ ,
- (ii) Lipschitz-continuous with a constant  $\ell_{\text{batch}} = 2\epsilon^{-1/2}$ ,
- (iii) smooth with a constant  $L_{\text{batch}} = 2\delta m^{-1/2} \epsilon^{-1}$ .

*Proof.* The batch-normalization layer as defined in (11) is the composition  $\nu = \nu_2 \circ \nu_1$  of a centering step

$$\nu_1(x) = \operatorname{Vec}\left(Z - Z \frac{\mathbf{1}_m \mathbf{1}_m^\top}{m}\right)$$

and a normalization step

$$\nu_2(\tilde{x}) = \operatorname{Vec}\left(\operatorname{diag}\left(\left(\frac{1}{m}\operatorname{diag}(\tilde{Z}\tilde{Z}^{\top}) + \epsilon \,\mathbf{1}_{\delta}\right)^{-1/2}\right)\tilde{Z}\right),$$

where here and thereafter  $Z, \tilde{Z} \in \mathbb{R}^{\delta \times m}$ ,  $x = \operatorname{Vec}(Z), \tilde{x} = \operatorname{Vec}(\tilde{Z})$ .

The centering step is an orthonormal projection, i.e.,  $\nu_1(x) = \operatorname{Vec}(Z\Pi_m) = (\Pi_m \otimes I_{\delta})x$  where  $\Pi_m = I_m - \frac{\mathbf{1}_m \mathbf{1}_m'}{m}$  is an orthonormal projector and so is  $(\Pi_m \otimes I_m)$ . Therefore we have  $\ell_{\nu_1} \leq 1$  and  $L_{\nu_1} = 0$ . For the normalizations step denote for  $x \in \mathbb{R}^m$ , and  $\bar{x} = (x_1; \ldots; x_{\delta}) \in \mathbb{R}^{m\delta}$  with  $x_i \in \mathbb{R}^m$ ,

$$f(x) = \sqrt{\frac{1}{m} \|x\|_2^2 + \epsilon}, \qquad g(x) = \left(\frac{x_i}{f(x)}\right)_{i=1,\dots,m}, \qquad \bar{g}(\bar{x}) = (g(x_1);\dots;g(x_{\delta})) \in \mathbb{R}^{m\delta},$$

such that  $\nu_2(\tilde{x}) = T_{m,d}\bar{g}(T_{d,m}\tilde{x})$ , where  $T_{d,m}$  is the linear operator such that  $T_{d,m}\operatorname{Vec}(Z) = \operatorname{Vec}(Z^{\top})$  for any  $Z \in \mathbb{R}^{d \times m}$ . First we have that

$$\|\bar{g}(\bar{x})\|_2 \le \delta \max_{i \in \{1,...,d\}} \|g(x_i)\|_2 \le \delta m^{1/2}$$

such that

$$m_{\nu_2} \le \delta m^{1/2}$$

Then the gradients can be computed as

$$\nabla f(x) = \frac{x}{mf(x)} = \frac{g(x)}{m} \in \mathbb{R}^m,$$
  

$$\nabla g(x) = \frac{f(x) \operatorname{I}_m - \nabla f(x) x^\top}{f(x)^2} = \frac{mf(x)^2 \operatorname{I}_m - x x^\top}{mf(x)^3} \in \mathbb{R}^{m \times m},$$
  

$$\nabla \bar{g}(\bar{x}) = \operatorname{diag}(\nabla g(x_1), \dots, \nabla g(x_m)) \in \mathbb{R}^{md \times md},$$

where for a sequence of matrices  $X_1, \ldots X_\tau \in \mathbb{R}^{d \times p}$  we denote by

$$\operatorname{diag}(X_1,\ldots,X_{\tau}) = \begin{pmatrix} X_1 & 0 & \ldots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & X_{\tau} \end{pmatrix} \in \mathbb{R}^{d\tau \times p\tau},$$

the corresponding block diagonal matrix. Therefore we get

$$\begin{aligned} \|\nabla g(x)\|_{2,2} &\leq \frac{mf(x)^2 + \|x\|_2^2}{mf(x)^3} \leq \frac{2m^{-1}\|x\|^2 + \epsilon}{(m^{-1}\|x\|_{2,2}^2 + \epsilon)^{3/2}} \leq c\epsilon^{-1/2}, \\ \|\nabla \bar{g}(\bar{x})\|_2 &\leq c\epsilon^{-1/2}, \end{aligned}$$

where  $c = 2/(3/2)^{3/2} \approx 1.1$  and we used that the spectral norm of the block-diagonal matrix is given by the maximal spectral norm of its block diagonal components. Since  $T_{m,d}$ ,  $T_{d,m}$  are orthonormal operators, we get

$$\ell_{\nu_2} \le 2\epsilon^{-1/2}$$

The second order tensor of g reads

$$\nabla^2 g(x) = \frac{3}{m^2 f(x)^5} x \boxtimes x \boxtimes x - \frac{1}{m f(x)^3} \left( \sum_{i=1}^m x \boxtimes e_i \boxtimes e_i + e_i \boxtimes x \boxtimes e_i + e_i \boxtimes x \right) \in \mathbb{R}^{m \times m \times m},$$
$$\nabla^2 \bar{g}(\bar{x}) = \operatorname{diag}^3(\nabla^2 g(x_1), \dots, \nabla^2 g(x_d)),$$

where  $e_i \in \mathbb{R}^m$  is the i<sup>th</sup> canonical vector in  $\mathbb{R}^m$  and for a sequence of tensors  $\mathcal{X}_1, \ldots, \mathcal{X}_d$  we denote by  $\mathcal{X} = \operatorname{diag}^3(\mathcal{X}_1, \ldots, \mathcal{X}_d) \in \mathbb{R}^{dm \times dm \times dm}$  the tensor whose diagonal is composed of the tensors  $\mathcal{X}_1, \ldots, \mathcal{X}_d$  such that  $\mathcal{X}_{i+(m-1)p,j+(m-1)p,k+(m-1)p} = (\mathcal{X}_p)_{ijk}$  and 0 outside the diagonal. We get then by definition of the tensor norm,

$$\begin{aligned} \|\nabla^2 g(x)\|_{2,2,2} &\leq \frac{3\|x\|_2^3}{m^2 f(x)^5} + \frac{3\|x\|_2}{mf(x)^3} = \frac{3\|x\|_2 (\|x\|_2^2 + mf(x)^2)}{m^2 f(x)^5} = \frac{3\|x\|_2 (2\|x\|_2^2 + m\epsilon)}{m^2 (m^{-1}\|x\|_2^2 + \epsilon)^{5/2}} \\ &\leq \frac{3}{m^{-1/2}} \frac{\sqrt{c}(2c+1)}{(c+1)^{5/2}} (m\epsilon)^{-1} \end{aligned}$$

where  $c = (1 + \sqrt{5})/4$  such that  $3\frac{\sqrt{c}(2c+1)}{(c+1)^{5/2}} \approx 1.6$ . Therefore we get  $\|\nabla \bar{g}(\bar{x})\|_{2,2,2} \leq \delta \max_{i \in \{1,...,\delta\}} \|\nabla^2 g(x_i)\|_{2,2,2}$  and

$$L_{\nu_2} \le 2\delta m^{-1/2} \epsilon^{-1}.$$

#### **D.6** Pooling layers

We consider pooling layers for which the patches do not coincide such that they amount to a (potentially non-linear) projection.

**Average pooling.** The average pooling layer is a linear operation. If the patches do not coincide, it is a projection with Lipschitz constant one.

$$\ell_{\text{avg}} = 1, \qquad L_{\text{avg}} = 0.$$

**Max-pooling.** Given an image  $\mathcal{I} \in \mathbb{R}^{C \times H \times B}$  with C channels each composed of a matrix of height H and breadth B, the max pooling layer extracts  $n^p$  patches of the form  $P^{i,j} = E_{row,i}^{\top} \mathcal{I}[c, \cdot, \cdot] E_{col,j}$  where  $E_{row,i} \in \mathbb{R}^{H \times K}$  and  $E_{col,j} \in \mathbb{R}^{B \times K}$  extract rows and columns of  $I[c, \cdot, \cdot]$  respectively. On each of this patch their maximum value is taken as the output, namely, the output image reads  $\tilde{\mathcal{I}}_{c,i,j} = \max_{k,l} P_{k,l}^{i,j}$ . It is naturally non-continuously differentiable and

it is 1-Lipschitz continuous if the patches do not coincide.

 $\ell_{\text{maxpool}} = 1$   $L_{\text{maxpool}}$  not defined.

## D.7 Auto-encoders, composition of chains of computations

For  $\tau$  vectors  $(u_1; \ldots; u_{\tau}) \in \mathbb{R}^{\sum_{t=1}^{\tau} p_t}$  and  $1 \leq s \leq t \leq \tau$ , we denote  $u_{s:t} = (u_s; \ldots; u_t) \in \mathbb{R}^{\sum_{r=s}^{t} p_r}$ . For  $\tau$  functions  $\phi_t : \mathbb{R}^{d_{t-1}} \times \mathbb{R}^{p_t} \to \mathbb{R}^{d_t}$ , we can split the chain of computations of the  $\tau$  functions  $\phi_t$  into smaller chains of computations. Namely, for  $1 \leq s \leq t \leq \tau$ , we denote the output of the chain of computations defined by  $\phi_s, \ldots, \phi_t$  as

$$\phi_{s \to t}(x_{s-1}, u_{s:t}) = x_t$$
  
s.t.  $x_r = \phi_r(x_{r-1}, u_r)$  for  $r \in \{s, \dots, t\}$ .

In particular, we have  $\phi_t = \phi_{t \to t}$ . The output of the chain of computations of the  $\tau$  functions  $\phi_t$  can then be split as

$$\phi_{1 \to \tau}(x_0, u_{1:\tau}) = \phi_{t+1 \to \tau}(\phi_{1 \to t}(x_0, u_{1:t}), u_{t+1:\tau}) \quad \text{for any } t \in \{1, \dots, \tau-1\}.$$

On the other hand, the composition of two chains of computations can readily be seen as a chain of computations. Namely, for two chains of computations f and g with computations  $(\phi_t^f)_{t=1}^{\tau_f}$  and  $(\psi_t^g)_{t=1}^{\tau_g}$ , parameters u and v respectively, the composition of f and g is

$$h(x_0, u) = g(f(x_0, u), v).$$

It is a chain of  $\tau_f + \tau_g$  computations

$$\chi_t = \begin{cases} \phi_t & \text{for } t \in \{1, \dots, \tau_f\} \\ \psi_{t-\tau_f} & \text{for } t \in \{\tau_f + 1, \tau_f + \tau_g\} \end{cases}$$

with input  $x_0$  and parameters  $w = (u; v) \in \mathbb{R}^{\sum_{t=1}^{\tau_f} p_t^f + \sum_{t=1}^{\tau_g} p_t^g}$  such that

$$w_t = \begin{cases} u_t & \text{for } t \in \{1, \dots, \tau_f\} \\ v_{t-\tau_f} & \text{for } t \in \{\tau_f + 1, \tau_f + \tau_g\} \end{cases}.$$

### **D.8 Residual Networks**

Recall the architecture of a residual network

$$x_t = a_t(b_t(x_{t-1}, u_t) + x_{t-2})$$
 for  $t = 1, \dots, \tau$   
 $x_0 = x, \quad x_{-1} = 0,$ 

where we assume  $b_t : \mathbb{R}^{d_{t-1}} \times \mathbb{R}^{p_t} \to \mathbb{R}^{\eta_t}$  such that  $x_{t-1} \in \mathbb{R}^{d_{t-1}}, x_{t-2} \in \mathbb{R}^{\eta_t}$  and

$$b_t(x_{t-1}, u_t) = \mathcal{B}_t[x_{t-1}, u_t, \cdot] + B_t^u u_t + B_t^x x_{t-1} + \beta_t^0$$

where  $\mathcal{B} = (B_{t,1}, \dots, B_{t,\eta_t})$  is a tensor. They can be expressed in terms of the variable  $\bar{x}_t = (x_t, x_{t-1})$  as

$$\bar{\phi}_t(\bar{x}_{t-1}, u_t) = \bar{a}_t(\bar{b}_t(\bar{x}_{t-1}, u_t)), \tag{36}$$

where  $\bar{b}_t$  is defined as

$$\begin{split} b_t(\bar{x}_{t-1}, u_t) &= \beta_t(\bar{x}_{t-1}, u_t) + \beta_t^{\ u}(u_t) + \beta_t^{\ v}(\bar{x}_{t-1}) + \beta_t^0 \\ &= \bar{\mathcal{B}}_t[\bar{x}_{t-1}, u_t, \cdot] + \bar{\mathcal{B}}_t^u u_t + \bar{\mathcal{B}}_t^x \bar{x}_{t-1} + \bar{\beta}^0_t, \\ \bar{\mathcal{B}}_t &= (\bar{\mathcal{B}}_{t,1}, \dots, \bar{\mathcal{B}}_{t,\eta_t}, \underbrace{0_{p_t \times (d_{t-1} + \eta_t)}, \dots, 0_{p_t \times (d_{t-1} + \eta_t)}}_{d_{t-1}}), \\ \bar{\mathcal{B}}_{t,j} &= (B_{t,j}, 0_{p_t \times \eta_t}) \quad \text{for } j \in \{1, \dots, d_{t-1}\}, \\ \bar{\mathcal{B}}_t^u &= \begin{pmatrix} B_t^u \\ 0_{d_{t-1} \times p_t} \end{pmatrix}, \\ \bar{\mathcal{B}}_t^x &= \begin{pmatrix} B_t^x & \mathbf{I}_{\eta_t} \\ \mathbf{I}_{d_{t-1}} & 0_{d_{t-1} \times \eta_t} \end{pmatrix}, \\ \bar{\mathcal{B}}_t^0 &= \begin{pmatrix} \beta_t^0 \\ 0_{d_{t-1}} \end{pmatrix}. \end{split}$$

Denoting  $\bar{\omega}_t = (\omega_{t,1}, \omega_{t,2}) = \bar{b}_t(\bar{x}_{t-1}, u_t)$ , we have

$$\bar{a}_t(\bar{\omega}_t) = (a(\omega_{t,1}), \omega_{t,2})$$

We can derive the smoothness constants of the layers of a residual network expressed as in (36) as

$$\begin{split} L_{\bar{\beta}_t} &= L_{\beta_t}, \qquad l_{\bar{\beta}_t^u} = l_{\beta_t^u}, \qquad l_{\bar{\beta}_t^x} \le l_{\beta_t^x} + 1, \qquad \|\bar{\beta}_t^0\|_2 = \|\beta_t^0\|_2, \\ m_{\bar{a}_t} &\le (1 + m_{a_t}), \qquad \ell_{\bar{a}_t} \le \max(1, \ell_{a_t}), \qquad L_{\bar{a}_t} = L_{a_t}. \end{split}$$

Proposition 4.5 can then be applied in this setting.

#### **D.9** Implicit functions

The smoothness constants of an implicit function are given in the following lemma. They can easily be refined by considering smoothness properties w.r.t. to each of the variables  $\alpha$  and  $\beta$  of the function  $\zeta$  defining the problem.

**Lemma D.4.** Let  $\zeta : (\alpha, \beta) \to \zeta(\alpha, \beta) \in \mathbb{R}$  for  $\alpha \in \mathbb{R}^a, \beta \in \mathbb{R}^b$  be s.t.  $\zeta(\alpha, \cdot)$  is  $\mu_{\zeta}$ -strongly convex for any  $\alpha$ . Denote  $g(\alpha) = \arg \min_{\beta \in \mathbb{R}^b} \zeta(\alpha, \beta)$ . Provided that  $\zeta$  has a  $L_{\zeta}$ -Lipschitz gradient and a  $H_{\zeta}$ -Lipschitz Hessian, the smoothness constants of g are bounded as

$$\ell_g \le L_{\zeta} \mu_{\zeta}^{-1}, \qquad \qquad L_g \le H_{\zeta} \mu_{\zeta}^{-1} (1+\ell_g) (1+L_{\zeta} \mu_{\zeta}^{-1}) \le H_{\zeta} \mu_{\zeta}^{-1} (1+L_{\zeta} \mu_{\zeta}^{-1})^2.$$

*Proof.* By the implicit function theorem,  $g(\alpha)$  is uniquely defined and its gradient is given by

$$\nabla g(\alpha) = -\nabla_{\alpha}\xi(\alpha, g(\alpha))\nabla_{\beta}\xi(\alpha, g(\alpha))^{-1} = -\nabla^{2}_{\alpha,\beta}\zeta(\alpha, g(\alpha))\nabla^{2}_{\beta,\beta}\zeta(\alpha, g(\alpha))^{-1}$$

where  $\xi(\alpha, \beta) = \nabla_{\beta} \zeta(\alpha, \beta)$ . The Lipschitz constant of g follows from that. For the smoothness we compute its second order information and bound the corresponding tensors. Note that the same results can be obtained by simply splitting the functions in appropriate terms. We have

$$\nabla g(\alpha) = h(\alpha, g(\alpha)),$$
  
where  $h(\alpha, \beta) = -\nabla_{\alpha} \xi(\alpha, \beta) \nabla_{\beta} \xi(\alpha, \beta)^{-1} = -\nabla_{\alpha, \beta}^{2} \zeta(\alpha, \beta) \nabla_{\beta, \beta}^{2} \zeta(\alpha, \beta)^{-1}$ 

Using Lemma D.5, we get

$$\begin{aligned} \nabla^2 g(\alpha) &= \nabla_\alpha h(\alpha, g(\alpha)) + \nabla_\beta h(\alpha, g(\alpha)) [\nabla g(\alpha), \cdot, \cdot] \\ &= -\nabla^2_{\alpha\alpha} \xi(\alpha, g(\alpha)) [\cdot, \cdot, \nabla_\beta \xi(\alpha, g(\alpha))^{-1}] \\ &- \nabla^2 \xi_{\alpha\beta}(\alpha, g(\alpha)) [\cdot, \nabla_\beta \xi(\alpha, g(\alpha))^{-1} \nabla_\alpha \xi(\alpha, g(\alpha))^\top, \nabla_\beta \xi(\alpha, g(\alpha))^{-1}] \\ &- \nabla^2_{\beta\alpha} \xi(\alpha, g(\alpha)) [\nabla g(\alpha), \cdot, \nabla_\beta \xi(\alpha, g(\alpha))^{-1}] \\ &- \nabla^2 \xi_{\beta\beta}(\alpha, g(\alpha)) [\nabla g(\alpha), \nabla_\beta \xi(\alpha, g(\alpha))^{-1} \nabla_\alpha \xi(\alpha, g(\alpha))^\top, \nabla_\beta \xi(\alpha, g(\alpha))^{-1}]. \end{aligned}$$

The result follows by using Facts A.4 and A.3. We observe that second derivatives of  $\xi$  correspond to third derivatives of  $\zeta$ , whose norms are bounded by  $H_{\zeta}$  by assumption. Moreover we have that  $\|\nabla_{\beta}\xi(\alpha, g(\alpha))^{-1}\|_{2} = \|\nabla_{\beta,\beta}^{2}\zeta(\alpha, \beta)^{-1}\|_{2} \le \mu_{\zeta}^{-1}$  by assumption.

The approximation error of the gradient when using an approximate minimizer inside the expression of the gradient is provided in the following lemma. It follows from smoothness considerations.

**Lemma 2.2.** Let  $\zeta : (\alpha, \beta) \to \zeta(\alpha, \beta) \in \mathbb{R}$  for  $\alpha \in \mathbb{R}^a, \beta \in \mathbb{R}^b$  be s.t.  $\zeta(\alpha, \cdot)$  is  $\mu_{\zeta}$ -strongly convex for any  $\alpha$  and denote  $\xi(\alpha, \beta) = \nabla_{\beta}\zeta(\alpha, \beta)$ . Denote  $g(\alpha) = \arg \min_{\beta \in \mathbb{R}^b} \zeta(\alpha, \beta)$  and  $\hat{g}(\alpha) \approx \arg \min_{\beta \in \mathbb{R}^b} \zeta(\alpha, \beta)$  be an approximate minimizer. Provided that  $\zeta$  has a  $L_{\zeta}$ -Lipschitz gradient and a  $H_{\zeta}$ -Lipschitz Hessian, the approximation error of using

$$\widehat{\nabla}\widehat{g}(\alpha) = -\nabla_{\alpha}\xi(\alpha,\widehat{g}(\alpha))\nabla_{\beta}\xi(\alpha,\widehat{g}(\alpha))^{-1}$$

instead of  $\nabla g(\alpha)$  is bounded as

$$\|\widehat{\nabla}\widehat{g}(\alpha) - \nabla g(\alpha)\|_2 \le H_{\zeta} \mu_{\zeta}^{-1} (1 + L_{\zeta} \mu_{\zeta}^{-1}) \|\widehat{g}(\alpha) - g(\alpha)\|_2.$$

*Proof.* Denote  $h(\alpha, \beta) = -\nabla_{\alpha}\xi(\alpha, \beta)\nabla_{\beta}\xi(\alpha, \beta)^{-1} = -\nabla_{\alpha,\beta}^{2}\zeta(\alpha, \beta)\nabla_{\beta,\beta}^{2}\zeta(\alpha, \beta)^{-1}$  such that  $\widehat{\nabla}\hat{g}(\alpha) = h(\alpha, \hat{g}(\alpha))$  and  $\nabla g(\alpha) = h(\alpha, g(\alpha))$ . The approximation error is given by computing the smoothness constant of  $h(\alpha, \cdot)$  for any  $\alpha$ . We bound the gradient of  $h(\alpha, \cdot)$  (same results can be obtained by considering differences of the functions). From Lemma D.5, we have

$$\nabla_{\beta}h(\alpha,\beta) = -\nabla_{\beta\alpha}^{2}\xi(\alpha,\beta)[\cdot,\cdot,\nabla_{\beta}\xi(\alpha,\beta)^{-1}] - \nabla^{2}\xi_{\beta\beta}(\alpha,\beta)[\cdot,\nabla_{\beta}\xi(\alpha,\beta)^{-1}\nabla_{\alpha}\xi(\alpha,g(\alpha))^{\top},\nabla_{\beta}\xi(\alpha,\beta)^{-1}].$$

The result follows by using Facts A.4 and A.3. We observe that second derivatives of  $\xi$  correspond to third derivatives of  $\zeta$ , whose norms are bounded by  $H_{\zeta}$  by assumption. Moreover we have that  $\|\nabla_{\beta}\xi(\alpha, g(\alpha))^{-1}\|_{2} = \|\nabla_{\beta,\beta}^{2}\zeta(\alpha, \beta)^{-1}\|_{2} \le \mu_{\zeta}^{-1}$  by assumption.

**Lemma D.5.** Let  $\xi : (\alpha, \beta) \to \xi(\alpha, \beta) \in \mathbb{R}^b$  for  $\alpha \in \mathbb{R}^a, \beta \in \mathbb{R}^b$  such that  $\nabla_\beta \xi(\alpha, \beta) \in \mathbb{R}^{b \times b}$  is positive definite for all  $\alpha \in \mathbb{R}^a, \beta \in \mathbb{R}^b$ . Denoting  $h(\alpha, \beta) = \nabla_\alpha \xi(\alpha, \beta) \nabla_\beta \xi(\alpha, \beta)^{-1} \in \mathbb{R}^{a \times b}$  we have

$$\nabla_{\alpha}h(\alpha,\beta) = \nabla_{\alpha\alpha}^{2}\xi(\alpha,\beta)[\cdot,\cdot,\nabla_{\beta}\xi(\alpha,\beta)^{-1}] + \nabla^{2}\xi_{\alpha\beta}(\alpha,\beta)[\cdot,\nabla_{\beta}\xi(\alpha,\beta)^{-1}\nabla_{\alpha}\xi(\alpha,\beta)^{\top},\nabla_{\beta}\xi(\alpha,\beta)^{-1}],$$
  
$$\nabla_{\beta}h(\alpha,\beta) = \nabla_{\beta\alpha}^{2}\xi(\alpha,\beta)[\cdot,\cdot,\nabla_{\beta}\xi(\alpha,\beta)^{-1}] + \nabla^{2}\xi_{\beta\beta}(\alpha,\beta)[\cdot,\nabla_{\beta}\xi(\alpha,\beta)^{-1}\nabla_{\alpha}\xi(\alpha,\beta)^{\top},\nabla_{\beta}\xi(\alpha,\beta)^{-1}].$$

Proof. This follows from the product rule, Fact A.5, Lemma D.6 and Fact A.1.

**Lemma D.6.** Let  $g : \mathbb{R}^d \to S_n^{++}$  be differentiable and  $h(x) = (g(x))^{-1}$ . Then  $\nabla h(x) = \nabla g(x)[\cdot, g(x)^{-1}, g(x)^{-1}]$ .

*Proof.* Let  $x \in \mathbb{R}^d$  and  $\delta \in \mathbb{R}^d$ . Consider first d = 1, such that  $\nabla g(x) \in \mathbb{R}^{n \times n}$ .

$$h(x+\delta) = (g(x) + \delta \nabla g(x) + o(\delta))^{-1} = g(x)^{-1} - \delta g(x)^{-1} \nabla g(x) g(x)^{-1} + o(\delta).$$

So in this case  $\nabla h(x) = g(x)^{-1} \nabla g(x) g(x)^{-1} \in \mathbb{R}^{n \times n}$ . The result follows for n = d by concatenating this result in a tensor such that for d > 1,  $\nabla h(x) = \nabla g(x)[\cdot, g(x)^{-1}, g(x)^{-1}]$ . Alternatively it can directly be seen from the following first order approximation for d > 1,

$$h(x+\delta) = (g(x) + \nabla g(x)[\delta, \cdot, \cdot] + o(\|\delta\|_2))^{-1} = g(x)^{-1} - g(x)^{-1} \nabla g(x)[\delta, \cdot, \cdot]g(x)^{-1} + o(\|\delta\|_2).$$

## **E** Optimization complexity proofs

#### **E.1** Smoothness of the objective

**Proposition 4.2.** Consider a closed convex set  $C \subset \mathbb{R}^p$ ,  $\psi \in \mathcal{C}_{m_{\psi}^C, \ell_{\psi}^C, L_{\psi}^C}^C$ ,  $r \in \mathcal{C}_{L_r}$  and  $h \in \mathcal{C}_{\ell_h, L_h}$  with  $\ell_h = +\infty$  if h is not Lipschitz-continuous. The smoothness of  $F = h \circ \psi + r$  on C is bounded as

$$L_F^C \le L_{\psi}^C \tilde{\ell}_h^C + \left(\ell_{\psi}^C\right)^2 L_h + L_r,$$

where  $\tilde{\ell}_h^C = \min\{\ell_h, \min_{z \in \psi(C)} \|\nabla h(z)\|_2 + L_h \ell_\psi^C D^C\}$ , where  $D^C = \sup_{x,y \in C} \|x-y\|_2$ .

*Proof.* Consider h, f to be twice differentiable. Same results can be obtained by considering differences of gradients. We get for  $u \in \mathbb{R}^p$ ,

 $\nabla^2 (h \circ f)(u) = \nabla^2 f(u)[\cdot, \cdot, \nabla h(f(u))] + \nabla f(u) \nabla^2 h(f(u)) \nabla f(u)^\top.$ 

The norm of  $\nabla h(f(u))$  can either be directly bounded by  $\ell_h$  or by using that for any  $u, u' \in C$ ,  $\|\nabla h(f(u))\|_2 \leq \|\nabla h(f(u'))\|_2 + L_h \|f(u) - f(u')\|_2$ . By choosing  $u' \in \arg \min_{u \in C} \|\nabla h(f(u))\|_2$  and bounding the second term by the diameter of C, we get a bound on  $\sup_{u \in C} \|\nabla h(f(u))\|_2$ . The result follows using Fact. A.4 and the definitions of the norms used to bound  $\ell_f$ ,  $L_f$  for a given function f.

**Corollary 4.6.** Consider a chain f of  $\tau$  computations as defined in Prop. 4.5 and  $u^* = (u_1^*; \ldots, u_{\tau}^*) \in \mathbb{R}^p$ . The smoothness properties of f on  $C' = \{u = (u_1; \ldots; u_{\tau}) \in \mathbb{R}^p : \forall t \in \{1, \ldots, \tau\}, \|u_t - u_t^*\| \leq R_t'\}$  are given as in Prop. 4.5 by considering

$$\begin{aligned} R'_t & \text{ in place of } \quad R_t, \\ l_{\beta_t^x} + L_{\beta_t} \| u_t^* \|_2 & \text{ in place of } \quad l_{\beta_t^x}, \\ |\beta_t^0\|_2 + l_{\beta_t^u} \| u_t^* \|_2 & \text{ in place of } \quad \|\beta_t^0\|_2 \end{aligned}$$

*Proof.* The smoothness properties of  $f_{x_0}$  on C' are given by considering  $\hat{f}_{x_0}(\Delta) = f_{x_0}(u^* + \Delta) = f_{x_0}(u)$  where  $\Delta = u - u^*$  with  $\|\Delta_t\|_2 \leq R'$ . The shifted chain of computations is given by

$$\hat{f}_{x_0,t}(\Delta) = a_t(b_t(\hat{f}_{x_0,t-1}(\Delta), u_t^* + \Delta_t))$$

This means that  $\hat{f}_{x_0}(\Delta)$  is a chain of compositions defined by the same non-linearities  $a_t$  and bi-affine functions  $\hat{b}_t$  modified as

$$\hat{b}_t(x_{t-1}, \Delta) = b_t(x_{t-1}, u_t^* + \Delta_t) = \beta_t(x_{t-1}, \Delta_t) + \beta_t^u(\Delta_t) + \hat{\beta}_t^x(x_{t-1}) + \beta_t^0,$$

where

$$\hat{\beta}_t^x(x_{t-1}) = \beta_t^x(x_{t-1}) + \beta_t(u_t^*, x_{t-1}) \qquad \hat{\beta}_t^0 = \beta_t^0 + \beta_t^u(u_t^*).$$

## **F** Detailed network

**VGG network.** The VGG Network is a benchmark network for image classification with deep networks. The objective is to classify images among 1000 classes. Its architecture is composed of 16 layers described below. We drop the dependency to the layers in their detailed formulation. We precise the number of patches  $n^p$  of the pooling or convolution operation, which, multiplied by the number of filters  $n^f$  gives the output dimension of these operations.

For a fully connected layer we precise the output dimension  $\delta_{out}$ .

- 0.  $x_i \in \mathbb{R}^{n^p n^f}$  with  $n^p = 224 \times 224$  and  $n^f = 3$ ,
- 1.  $\phi_1(x, u) = \alpha_{\text{ReLu}}(b_{\text{conv}}(x, u))$ with  $n_{\text{conv}}^p = 224 \times 224$ ,  $n_{\text{conv}}^f = 64$ , 2.  $\phi_2(x, u) = \pi_{\text{maxpool}}(\alpha_{\text{ReLu}}(b_{\text{conv}}(x, u)))$ with  $n_{\text{conv}}^p = 224 \times 224$ ,  $n_{\text{conv}}^f = 64$ ,  $n_{\text{maxpool}}^p = 112 \times 112$ ,  $n_{\text{maxpool}}^f = 64$ , 3.  $\phi_3(x, u) = \alpha_{\text{ReLu}}(b_{\text{conv}}(x, u))$ with  $n_{\text{conv}}^p = 112 \times 112$ ,  $n_{\text{conv}}^f = 128$ 4.  $\phi_4(x, u) = \pi_{\text{maxpool}}(\alpha_{\text{ReLu}}(b_{\text{conv}}(x, u)))$ with  $n_{\text{conv}}^p = 112 \times 112$ ,  $n_{\text{conv}}^f = 128$ ,  $n_{\text{maxpool}}^p = 56 \times 56$ ,  $n_{\text{maxpool}}^f = 128$ , 5.  $\phi_5(x, u) = \alpha_{\text{ReLu}}(b_{\text{conv}}(x, u))$ with  $n_{\text{conv}}^p = 56 \times 56$ ,  $n_{\text{conv}}^f = 256$ , 6.  $\phi_6(x, u) = \alpha_{\text{ReLu}}(b_{\text{conv}}(x, u))$ with  $n_{\text{conv}}^p = 56 \times 56$ ,  $n_{\text{conv}}^f = 256$ ,

7. 
$$\phi_7(x, u) = \pi_{\text{maxpool}}(\alpha_{\text{ReLu}}(b_{\text{conv}}(x, u)))$$
  
with  $n_{\text{conv}}^p = 56 \times 56$ ,  $n_{\text{conv}}^p = 256$ ,  $n_{\text{maxpool}}^p = 28 \times 28$ ,  $n_{\text{maxpool}}^f = 256$ ,  
8.  $\phi_8(x, u) = \alpha_{\text{ReLu}}(b_{\text{conv}}(x, u))$   
with  $n_{\text{conv}}^p = 28 \times 28$ ,  $n_{\text{conv}}^f = 512$ ,  
9.  $\phi_9(x, u) = \alpha_{\text{ReLu}}(b_{\text{conv}}(x, u))$   
with  $n_{\text{conv}}^p = 28 \times 28$ ,  $n_{\text{conv}}^f = 512$ ,  
10.  $\phi_{10}(x, u) = \pi_{\text{maxpool}}(\alpha_{\text{ReLu}}(b_{\text{conv}}(x, u)))$   
with  $n_{\text{conv}}^p = 28 \times 28$ ,  $n_{\text{conv}}^f = 512$ ,  $n_{\text{maxpool}}^p = 14 \times 14$ ,  $n_{\text{maxpool}}^f = 512$ ,  
11.  $\phi_{11}(x, u) = \alpha_{\text{ReLu}}(b_{\text{conv}}(x, u))$   
with  $n_{\text{conv}}^p = 14 \times 14$ ,  $n_{\text{conv}}^f = 512$ ,  
12.  $\phi_{12}(x, u) = \alpha_{\text{ReLu}}(b_{\text{conv}}(x, u))$   
with  $n_{\text{conv}}^p = 14 \times 14$ ,  $n_{\text{conv}}^f = 512$   
13.  $\phi_{13}(x, u) = \pi_{\text{maxpool}}(\alpha_{\text{ReLu}}(b_{\text{conv}}(x, u)))$   
with  $n_{\text{conv}}^p = 14 \times 14$ ,  $n_{\text{conv}}^f = 512$ ,  
14.  $\phi_{14}(x, u) = \alpha_{\text{ReLu}}(b_{\text{full}}(x, u))$   
with  $\delta_{\text{out}} = 4096$ ,  
15.  $\phi_{15}(x, u) = \alpha_{\text{ReLu}}(b_{\text{full}}(x, u))$   
with  $\delta_{\text{out}} = 4096$ ,  
16.  $\phi_{16}(x, u) = \alpha_{\text{softmax}}(b_{\text{full}}(x, u))$   
with  $\delta_{\text{out}} = 1000$ .  
17.  $h(\hat{y}) = \sum_{i=1}^n \mathcal{L}_{\log}(\hat{y}_i, y_i)/n$  for  $k = 1000$  classes.