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 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. A diverse set of example components and architectures arising in modern deep networks intersperse the exposition 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 (Krizhevsky et al. 2012, Pennington et al. 2014, Duvenaud et al. 2015). A deep network can be framed as a chain of composition of modules, where each module is typically the composition of a non-linear function and an affine transformation. The last module in the chain is usually task-specific and can be expressed either in analytical form as in supervised classification or as the solution of an optimization problem in dimension reduction or 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 (Werbos 1994, Rumelhart et al. 1986, Lecun 1988). See also (Duda et al. 2012, Anthony & Bartlett 2009, Shalev-Shwartz & Ben-David 2014, Goodfellow et al. 2016) for an exposition and (Abadi et al. 2015, Paszke et al. 2017) for an implementation of gradient back-propagation for deep networks. 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 topology 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 (Simonyan & Zisserman 2015, Ioffe & Szegedy 2015). All proofs and notations are provided in the Appendix.
2 Problem formulation

2.1 Deep network structure

A feed-forward deep network of depth \( \tau \) can be described as a transformation of an input \( x \) into an output \( z_\tau \) 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 \( l \)th layer can be described as a function of its parameters \( v_l \) and a given input \( z_{l-1} \) that outputs \( z_l \) as

\[
    z_l = \phi_l(v_l, z_{l-1}) = a_l(b_l(v_l, z_{l-1})),
\]

where \( b_l \) is generally linear in \( v_l \) and affine in \( z_{l-1} \) and \( a_l \) is non-linear.

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

\[
    \min_{(v_1, \ldots, v_\tau) \in \mathbb{R}^{p_1} \times \cdots \times \mathbb{R}^{p_\tau}} \quad f(z^{(1)}_\tau, \ldots, z^{(n)}_\tau) + r(v_1, \ldots, v_\tau)
\]

subject to

\[
    z^{(i)}_l = \phi_l(v_l, z^{(i)}_{l-1}) \quad \text{for } l = 1, \ldots, \tau, \quad i = 1, \ldots, n,
\]

\[
    z^{(i)}_0 = x^{(i)} \quad \text{for } i = 1, \ldots, n,
\]

where \( v_l \in \mathbb{R}^{p_l} \) is the set of parameters at layer \( l \) whose dimension \( p_l \) can vary among layers and \( r \) is a regularization on the parameters of the network.

We are interested in the influence of the structure of the problem, i.e., the chain of computations defined below, on the optimization complexity of the problem.

**Definition 2.1.** A function \( \psi : \mathbb{R}^p \rightarrow \mathbb{R}^q \) is a chain of \( \tau \) computations, if it is defined by an input \( x \in \mathbb{R}^\delta \) and \( \tau \) functions

\[
    \phi_l : \mathbb{R}^{p_l} \times \mathbb{R}^{q_{l-1}} \rightarrow \mathbb{R}^{p_l} \quad \text{for } l = 1, \ldots, \tau
\]

such that \( p = \sum_{l=1}^{\tau} p_l, q = \delta, \delta = 0_0 \) and for \( w = (v_1; \ldots; v_\tau) \in \mathbb{R}^p \) with \( v_l \in \mathbb{R}^{p_l} \), the output of \( \psi \) is given by

\[
    \psi(w) = z_\tau, \quad \text{with} \quad z_l = \phi_l(v_l, z_{l-1}) \quad \text{for } l = 1, \ldots, \tau,
\]

\[
    z_0 = x.
\]

By considering the concatenation of the parameters \( w = (v_1; \ldots; v_\tau) \) and the concatenation of the transformations of each input as a single transformation, i.e., \( \psi(w) = (\psi^{(1)}(w); \ldots; \psi^{(n)}(w)) \) where \( \psi^{(i)} \) is the chain of computations defined by the input \( x^{(i)} \), the objective in (2) can be written as

\[
    \min_{w \in \mathbb{R}^p} f(\psi(w)) + r(w),
\]

where \( \psi : \mathbb{R}^p \rightarrow \mathbb{R}^q \) is a chain of \( \tau \) computations\(^2\), \( r : \mathbb{R}^p \rightarrow \mathbb{R} \) is typically a decomposable differentiable function such as \( r(w) = \sum_{l=1}^{\tau} \|v_l\|^2 \) and we present examples of learning objectives \( f : \mathbb{R}^q \rightarrow \mathbb{R} \) below. Assumptions on differentiability and smoothness of the objective are detailed in Sec. 4.

2.2 Objectives

2.2.1 Supervised learning

For supervised learning, the objective can be decomposed as

\[
    f(\psi(w)) = \frac{1}{n} \sum_{i=1}^{n} f^{(i)}(\psi^{(i)}(w)),
\]

where \( f^{(i)} \) are losses on the labels predicted by the chain of computations, i.e., \( f^{(i)}(\hat{y}^{(i)}) = \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) \) where \( y^{(i)} \) is the label of the input \( x^{(i)} \) of the chain of computations \( \psi^{(i)} \), \( \hat{y}^{(i)} = \psi^{(i)}(w) \), and \( \mathcal{L} \) is a given loss such as the squared loss and the logistic loss (see Appendix B.1).

\(^1\)We denote by semi-columns the concatenation of variables by rows.

\(^2\)Note that if \( k \) is the output dimension of each chain \( \psi^{(i)} \), the output dimension of the chain \( \psi \) scales with the number of samples as \( q = nk \).
2.2.2 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 is written

\[
f(\psi(w)) = \min_{y_1, \ldots, y_n \in \mathbb{R}^q} \frac{1}{2} \sum_{i=1}^{n} \|y^{(i)} - \psi^{(i)}(w)\|_2^2 + \sum_{i < j} \|y^{(i)} - y^{(j)}\|_2,
\]

where \(\psi^{(i)}(w)\) are \(n\) chains defined by inputs \(x^{(i)}\). See (Hocking et al. 2011, Tan & Witten 2015) for the original formulations. We consider in Appendix B.2 different clustering objectives. Note that the classical ones (\(k\)-means, spectral clustering) are inherently non-smooth, i.e., non-continuously differentiable, as they are defined as the minimization of a linear objective under constraints.

2.3 Layers

The layer \(l\) 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 \(b_l : \mathbb{R}^{m_l} \times \mathbb{R}^{d_{l-1}} \rightarrow \mathbb{R}^{n_l}\) and decomposed as

\[
b_l(v_l, z_{l-1}) = \beta_l(v_l, z_{l-1}) + \beta_v^l(v_l) + \beta_z^l(z_{l-1}) + \beta_0^l, \tag{6}
\]

where \(\beta_l\) is bilinear, \(\beta_v^l\) and \(\beta_z^l\) are linear and \(\beta_0^l\) is a constant vector,

(ii) an activation function, such as the element-wise application of a non-linear function, denoted \(\alpha_l : \mathbb{R}^{n_l} \rightarrow \mathbb{R}^{n_l}\),

(iii) a reduction of dimension, such as a pooling operation, denoted \(\pi_l : \mathbb{R}^{n_l} \rightarrow \mathbb{R}^{d_l}\),

(iv) a normalization of the output, such as batch-normalization, denoted \(\nu_l : \mathbb{R}^{d_l} \rightarrow \mathbb{R}^{d_l}\).

By concatenating the non-affine operations, i.e., defining \(a_l = \nu_l \circ \pi_l \circ \alpha_l\), a layer can be written as

\[
\phi_l(v_l, z_{l-1}) = a_l(b_l(v_l, z_{l-1})). \tag{7}
\]

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 \(a_l\) to be an arbitrary composition of functions, i.e., \(a_l = a_l,k_l \circ \ldots \circ a_{l,1}\). We present common examples of the components of a deep network, a list is detailed in Appendix B with the smoothness properties of each function.

2.3.1 Linear operations

In the following, we drop the dependency w.r.t. the layer \(l\) and denote by \(\tilde{\cdot}\) 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 a batch of \( m \) inputs of dimension \( d \) is written

\[
\tilde{Z} = W^T Z + w^0 1^T_m,
\]

where \( Z \in \mathbb{R}^{d \times m} \) is the batch of inputs, \( W \in \mathbb{R}^{d \times d} \) are the weights of the layer and \( w^0 \in \mathbb{R}^d \) define the offsets. By vectorizing the parameters and the inputs, a fully connected layer can be written as

\[
\tilde{z} = \beta(v, z) + \beta^\nu(v),
\]

where

\[
\beta(v, z) = \text{Vec}(W^T Z) \in \mathbb{R}^{md}, \quad \beta^\nu(v) = \text{Vec}(w^0 1^T_m),
\]

\[
z = \text{Vec}(Z) \in \mathbb{R}^{md}, \quad v = \text{Vec}(W; w^0) \in \mathbb{R}^{d(d+1)}.
\]

Convoluted layer. A convolutional layer convolves a batch of \( m \) inputs (images or signals) of dimension \( d \) stacked as \( Z = (z_1, \ldots, z_m) \in \mathbb{R}^{d \times m} \) with \( n^f \) affine filters of size \( s^f \) defined by weights \( W = (w_1, \ldots, w_{n^f}) \in \mathbb{R}^{s^f \times n^f} \) and offsets \( w_0 = (w_0^1, \ldots, w_0^{n^f}) \in \mathbb{R}^{n^f} \) through \( n^p \) patches. The \( k \)th output of the convolution of the \( i \)th input by the \( j \)th filter reads

\[
\Xi_{i,j,k} = w_j^T \Pi_k z_i + w_0^j,
\]

where \( \Pi_k \in \mathbb{R}^{s^f \times d} \) extracts a patch of size \( s^f \) at a given position of the input \( z_i \). The output \( \tilde{Z} = (\tilde{z}_1, \ldots, \tilde{z}_m) \) is then given by the concatenation of each input, i.e., \( \tilde{z}_{i,k+n^f(j-1)} = \Xi_{i,j,k} \). 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

\[
\tilde{z} = \beta(v, z) + \beta^\nu(v),
\]

where

\[
\beta(v, z) = (w_j^T \Pi_k z_i)_{i=1; m; j=1; n^f; k=1; n^p} \in \mathbb{R}^{mn^f n^p}, \quad \beta^\nu(v) = 1_m \otimes w^0 \otimes 1_{n^p},
\]

\[
z = \text{Vec}(Z) \in \mathbb{R}^{md}, \quad v = \text{Vec}(W; w^0) \in \mathbb{R}^{(s^f+1)n^f},
\]

\[
Z = (z_1, \ldots, z_m), \quad W = (w_1, \ldots, w_{n^f}),
\]

where \( \beta(v, z) \) is defined by concatenations of the output.

2.3.2 Activation functions

We consider differentiable element-wise activation functions \( \alpha : \mathbb{R}^n \rightarrow \mathbb{R}^n \), i.e., for a given \( z = (z_1, \ldots, z_n) \in \mathbb{R}^n \)

\[
\alpha(z) = (\bar{\alpha}(z_1), \ldots, \bar{\alpha}(z_n)),
\]

for a given scalar function \( \bar{\alpha} \) such as \( \bar{\alpha}(x) = (1 + \exp(-x))^{-1} \) 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 a batch of inputs \( Z \in \mathbb{R}^{d \times m} \), the average pooling with a patch size \( s^f \) for inputs with \( n^f \) channels and \( n^p \) coordinates such that \( d = n^f n^p \) convolves the inputs with a filter \( P = 1_{n^f} 1^T_{n^f} / s^f \). The output dimension for each input is \( \tilde{d} = n^f n^p \) and the patches, represented by some \( (\Pi_k)_{k=1}^{n^p} \) acting in Eq. (9), are chosen such that it induces a reduction of dimension, i.e., \( n^p \leq n^p \).

2.3.4 Normalization functions

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

\[
(\tilde{Z})_{ij} = \frac{Z_{ij} - \mu_i}{\sqrt{\epsilon + \sigma_i^2}},
\]

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 \( \nu(z) = \text{Vec}(\tilde{Z}) \) for \( z = \text{Vec}(Z) \).
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

All optimization oracles can be formally defined as the minimization of an approximation of the objective with an additional proximal term. For a function \( f \), we denote

\[
\ell_f(y; x) = f(x) + \nabla f(x)^\top (y-x)
\]

\[
q_f(y; x) = f(x) + \nabla f(x)^\top (y-x) + \frac{1}{2}(y-x)^\top \nabla^2 f(x)(y-x)
\]

the linear and quadratic approximations respectively of \( f \) around \( x \) provided that \( \nabla f(x), \nabla^2 f(x) \) are defined respectively. On a point \( w_t \in \mathbb{R}^p \), given a step-size \( \gamma \), for an objective of the form \( f \circ \psi + r \),

(i) a gradient step is defined as

\[
w_{t+1} = \arg\min_{w \in \mathbb{R}^p} \ell_{f \circ \psi}(w; w_t) + \ell_r(w; w_t) + \frac{1}{2\gamma} \|w - w_t\|^2_2,
\]

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

\[
w_{t+1} = \arg\min_{w \in \mathbb{R}^p} q_f(\ell_{f \circ \psi}(w; w_t); \psi(w_t)) + q_r(w; w_t) + \frac{1}{2\gamma} \|w - w_t\|^2_2,
\]

(iii) a Newton step is defined as

\[
w_{t+1} = \arg\min_{w \in \mathbb{R}^p} q_{f \circ \psi}(w; w_t) + q_r(w; w_t) + \frac{1}{2\gamma} \|w - w_t\|^2_2.
\]

All those steps amount to solving quadratic problems on a linearized network as shown in the following proposition. For a multivariate function \( f : \mathbb{R}^d \mapsto \mathbb{R}^n \), composed of \( f^{(j)} \) real functions with \( j \in \{1, \ldots, n\} \), 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 \( x \). We represent its 2nd order information by a tensor \( \nabla^2 f(x) = (\nabla^2 f^{(1)}(x), \ldots, \nabla^2 f^{(n)}(x)) \in \mathbb{R}^{d \times d \times n} \).

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

\[
\nabla f(x, y) = \begin{pmatrix} \nabla_x f(x, y) \\ \nabla_y f(x, y) \end{pmatrix}
\]

with \( \nabla_x f(x, y) \in \mathbb{R}^d, \ \nabla_y f(x, y) \in \mathbb{R}^p \).

We decompose similarly its Hessian and combine notations for multivariate functions. See Appendix A for further details on derivatives and tensor notations.

**Proposition 3.1.** Let \( w_t = (v_1; \ldots; v_r) \) and \( z_0, \ldots, z_r \) be defined by the chain of computations in (3) applied to \( w_t \). Assume \( r \) to be decomposable as \( r(w_t) = \sum_{l=1}^r r_l(v_l) \). Gradient (12), Gauss-Newton (13) and Newton (14) steps are given as \( w_{t+1} = w_t + \tilde{w} \) where \( \tilde{w}^* = (\tilde{v}_1; \ldots; \tilde{v}_r) \) is the solution of

\[
\min_{\tilde{v}_1, \ldots, \tilde{v}_r \in \mathbb{R}^{d_1} \times \ldots \times \mathbb{R}^{d_p}} \sum_{l=1}^r \frac{1}{2} \tilde{z}_l^\top B_l \tilde{z}_l + p_l^\top \tilde{z}_l + \tilde{z}_{l-1}^\top R_l \tilde{v}_l + \frac{1}{2} \tilde{v}_l^\top Q_l \tilde{v}_l + q_l^\top \tilde{v}_l + \frac{1}{2\gamma} \|\tilde{v}_l\|^2_2
\]

subject to \( \tilde{z}_l = A_l \tilde{z}_{l-1} + B_l \tilde{v}_l \) for \( l \in \{1, \ldots, r\} \),

\( \tilde{z}_0 = 0 \).
shows that each optimization step can be chunked into smaller problems defined as the cost-to-go from (16). W e present in Appendix C the detailed computation of a Newton step. See (Dunn & Bertsekas 1989) for an alternate derivation. 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 C, a gradient step can naturally be derived as a dynamic programming procedure applied to the subproblem (15). 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 \( \psi : \mathbb{R}^p \to \mathbb{R}^q \) as defined in Def. 2.1 and \( w \in \mathbb{R}^p \), an automatic differentiation oracle is a procedure that gives access to

\[
\mu \to \nabla \psi(w) \mu \quad \text{for any } \mu \in \mathbb{R}^q.
\]

The point is that we have access to \( \nabla \psi(w) \) not as a matrix but as a linear operator. The matrix \( \nabla \psi(w) \) 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 in a 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 \( \psi(w) \) and stores the information necessary to compute gradient-vector products,
2. a backward pass that computes \( \mu \to \nabla \psi(w) \mu \) for any \( \mu \in \mathbb{R}^q \) given the information stored 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 \( \nabla \psi(w) \mu \) 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 \( \psi(w) \) and the linear operator \( \mu \to \nabla \psi(w) \mu \) is then presented in Algo. 3.

Computing the gradient \( g = \nabla (f \circ \psi)(w) \) on \( w \in \mathbb{R}^p \) amounts then to

1. computing with Algo. 3, \( (\psi(w), \mu \to \nabla \psi(w) \mu) = \text{Autodiff}(\psi, w) \),
2. computing \( \mu = \nabla f(\psi(w)) \) then \( g = \nabla \psi(w) \mu \) using the oracle \( \mu \to \nabla \psi(w) \mu \) computed by Autodiff.

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**Algorithm 1 Forward pass**

1: **Inputs:** Chain of computations \( \psi \) defined by \( (\phi_l)_{l=1,\ldots,\tau} \), input \( x \) as in Def. 2.1, variable \( w = (v_1; \ldots; v_\tau) \)
2: Initialize \( z_0 = x \)
3: for \( l = 1, \ldots, \tau \) do
4: Compute \( z_l = \phi_l(v_l, z_{l-1}) \)
5: Store \( \nabla \phi_l(v_l, z_{l-1}) \)
6: end for
7: **Output:** \( z_\tau, \nabla \phi_l(v_l, z_{l-1}) \) for \( l \in \{1, \ldots, \tau\} \).

**Algorithm 2 Backward pass**

1: **Inputs:** Slope \( \mu \), intermediate gradients \( \nabla \phi_l(v_l, z_{l-1}) \) for \( l \in \{1, \ldots, \tau\} \)
2: Initialize \( \lambda_\tau = \mu \)
3: for \( l = \tau, \ldots, 1 \) do
4: Compute \( \lambda_{l-1} = \nabla_{z_{l-1}} \phi_l(v_l, z_{l-1}) \lambda_l \)
5: Store \( g_l = \nabla_{v_l} \phi_l(v_l, z_{l-1}) \lambda_l \)
6: end for
7: **Output:** \( (g_1, \ldots, g_\tau) = \nabla \psi(w) \mu \)
2.1 C.3...

The Gauss-Newton step can also be solved by making calls to an automatic differentiation oracle as shown in (27).

For a chain of convolutional layers the space and time complexities of the forward and backward passes, Algo. 1, Algo. 2, are of the order of

\[ S = \sum_{l=1}^{\tau} (\rho_l + \delta_{l-1})\delta_l, \quad T = \sum_{l=1}^{\tau} T(\phi_l, \nabla\phi_l) + 2\sum_{l=1}^{\tau} (\delta_{l-1}\delta_l + \rho_l\delta_l), \]

respectively, where \( T(\phi_l, \nabla\phi_l) \) is the time complexity of computing \( \phi_l, \nabla\phi_l \) during the forward pass, \( T_F \) denotes the time-complexity of the forward pass and \( T_B \) denotes the time complexity of the backward pass.

For chain of computations of the form (7), the time complexity of the backward pass can be refined as shown in Appendix C.3. Specifically, we have the following corollary.

**Corollary 3.4.** For a chain of fully-connected layers (8) with element-wise activation function, no normalization or pooling, the time complexity of the backward pass \( T_B \) is of the order of

\[ T_B = \mathcal{O}\left(\sum_{l=1}^{\tau} 2md_l(d_{l-1} + 1)\right) \]

elementary operations. For a chain of convolutional layers (9) with element-wise activation function, no normalization or pooling, the time complexity of the backward pass \( T_B \) is of the order of

\[ T_B = \mathcal{O}\left(\sum_{l=1}^{\tau} (2n_l^p n_l^f s_l^f + n_l^p n_l^f + d_l)m\right) \]

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 as shown in (Roulet et al. 2019) and stated in the framework considered in this paper.

**Proposition 3.5.** Consider the Gauss-Newton-step (13) on \( w_t = (v_1; \ldots; v_\tau) \) for a convex objective \( f \), a convex decomposable regularization \( r(w) = \sum_{l=1}^{\tau} r_l(v_l) \) and a differentiable chain of computations \( \psi \). We have that

1. the Gauss-Newton-step amounts to solving

\[ \min_{\mu \in \mathbb{R}^d} \hat{q}_f^*(\mu) + \hat{q}_r^*(-\nabla\psi(w_t)\mu), \]  

where \( \hat{q}_f(y) = q_f(\psi(w_t) + y; \psi(w_t)), \hat{q}_r(w) = q_r(w_t + w; w_t) + \|w\|_2^2/2 \) and for a function \( f \) we denote by \( f^* \) its convex conjugate,

2. the Gauss-Newton-step reads \( w_{t+1} = w_t + \nabla\hat{q}_f^*(-\nabla\psi(w_t)\mu^*) \) where \( \mu^* \) is the solution of (18),

3. the dual problem (18) can be solved by \( 2q + 1 \) calls to an automatic differentiation procedure.
Proposition 3.5 shows that a Gauss-Newton step is only \(2q+1\) times more expansive than a gradient-step. Precisely, for a deep network with a supervised objective, we have \(q = nk\) 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

The convergence guarantee of a first-order method towards an \(\epsilon\)-stationary point is governed by the smoothness property of the objective, i.e., the Lipschitz continuity of the function itself or its gradient when it is defined. We study smoothness properties with respect to the Euclidean norm \(\| \cdot \|_2\), whose operator norm is denoted \(\| \cdot \|_{2,2}\). In the following, for a function \(f : \mathbb{R}^d \rightarrow \mathbb{R}^n\) and a set \(C \subset \text{dom } f \subset \mathbb{R}^d\), we denote by

\[
M^C_f = \sup_{x \in C} \| f(x) \|_2,
\]

\[
\ell^C_f = \sup_{x,y \in C \atop x \neq y} \frac{\| f(x) - f(y) \|_2}{\| x - y \|_2},
\]

\[
L^C_f = \sup_{x,y \in C \atop x \neq y} \frac{\| \nabla f(x) - \nabla f(y) \|_{2,2}}{\| x - y \|_2},
\]

(19)

a bound of \(f\) on \(C\), the Lipschitz-continuity parameter of \(f\) on \(C\) and the smoothness parameter of \(f\) on \(C\) (i.e. the Lipschitz-continuity parameter of its gradient if it exists), all with respect to \(\| \cdot \|_2\). We denote by \(m_f, \ell_f, L_f\) the same quantities defined on the domain of \(f\), e.g., \(m_f = m_{\text{dom } f}\). If these quantities are not defined, we consider them to be infinite. For example if \(f\) is not bounded, \(m_f = +\infty\) or if \(f\) is not continuously differentiable \(L_f = +\infty\).

For a given set \(C \subset \mathbb{R}^d\), we denote by \(C^C_{m,F,C,L,C}\) the class of functions \(f\) such that \(\text{dom } f \supset C\) and \(m^C_f = m^C\), \(\ell^C_f = \ell^C\), \(L^C_f = L^C\). Similarly we denote by \(C_{m,F,L}\) the class of functions \(f\) such that \(m_f = m\), \(\ell_f = \ell\), \(L_f = L\). We drop indexes to denote classes of functions for which only a subset of these parameters is defined. For example, we denote \(C\) the set of functions that are \(\ell\)-Lipschitz continuous.

#### 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** (Ghadimi et al. (2016, Theorems 1 and 2)). Consider problems of the form

\[
(i) \quad \min_{w \in \mathbb{R}^p} \left\{ F(w) := f(\psi(w)) + r(w) \right\}, \quad \text{or} \quad (ii) \quad \min_{w \in \mathbb{R}^p} \left\{ F(w) := \frac{1}{n} \sum_{i=1}^n f_i(\psi_i(w)) + r(w) \right\},
\]

subject to \(w \in C\), subject to \(w \in C\),

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

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

\[
\mathcal{O} \left( \frac{L^C_F(F(w_0) - F^*)}{\epsilon^2} \right)
\]

iterations, where \(w_0\) is the initial point and \(F^* = \min_{w \in C} F(w)\).

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

\[
\mathcal{O} \left( \frac{L^C_F(F(w_0) - F^*)}{\epsilon^2} \right)
\]

iterations, where \(w_0\) is the initial point and \(F^* = \min_{w \in C} F(w)\).

\(^3\)Recall that the norm operator of a matrix \(A : \mathbb{R}^d \rightarrow \mathbb{R}^n\) with respect to the norm \(\| \cdot \|_2\) is defined as \(\sup_{x \in \mathbb{R}^d} \| Ax \|_2/\| x \|_2\).

\(^4\)Note that if \(x = \text{Vec}(X)\) for a given matrix \(X\), \(\| x \|_2 = \| X \|_F\).
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

\[
\mathcal{O} \left( \frac{L_p \left( F(w_0) - F^* \right)}{\varepsilon^2} \right)
\]

iterations, where \(S_0 = \{ w \in \mathbb{R}^p : F(w) \leq F(w_0) \} \) is the initial sub-level set.

2. Better rates of convergence can be obtained for the finite-sum problem, see for example (Paquette et al. 2018) and references therein. They still depend on the smoothness constants of the objective or the maximal smoothness of the components on \(C\), i.e., \(\max_{i=1,\ldots,n} L_{f_i,\psi_l,\tau}^C\).

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 \(C \subset \mathbb{R}^p\), \(\psi \in C_{\ell_0}^{C_{\ell_0},\ell_0^C}\), \(r \in C_{L_r}\), and \(f \in C_{\ell_f,\ell_f}\) with \(\ell_f = +\infty\) if \(f\) is not Lipschitz-continuous. The smoothness of \(F = f \circ \psi + r\) on \(C\) is bounded as

\[
L_C^F \leq L_C^\ell f C + (\ell_C^f)^2 L_f + L_r,
\]

where \(\ell_C^f = \min(\ell_f, \min_{z \in \psi(C)} \|\nabla f(z)\|_2 + L_f \ell_C^f D^C)\), where \(D^C = \sup_{x, y \in C} \|x - y\|_2\).

It remains then to characterize the smoothness properties of a chain of computations.

### 4.2 Smoothness of chains of computations

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.

We first present a general result for chains of computations without specific structure. Although the result is not readily applicable to deep networks, it clarifies the recurrence used to compute the smoothness of a chain of computations.

**Proposition 4.3.** Consider a chain \(\psi\) of \(\tau\) computations as defined in Def. 2.1, by layers \(\phi_l \in C_{\ell_{\phi_l},L_{\phi_l}}\).

(i) An upper-bound on the Lipschitz-continuity of the chain \(\psi\) is given by \(\ell_\psi = \ell_\tau\), for where for \(l \in \{1, \ldots, \tau\}\),

\[
\ell_l = \ell_{\phi_l} + \ell_{l-1} \ell_{\phi_l}, \quad \ell_0 = 0.
\]

(ii) An upper-bound on the smoothness of the chain \(\psi\) is given by \(L_\psi = L_\tau\), where for \(l \in \{1, \ldots, \tau\}\),

\[
L_l = L_{l-1} \ell_{\phi_l} + L_{\phi_l} (1 + \ell_{l-1})^2, \quad L_0 = 0.
\]

Layers of deep networks are a priori not Lipschitz continuous. To get an estimate of their properties, we use their specific parametrization and consider their properties on compact sets as tackled in the following proposition. We denote by \(BL_L\) the set of bilinear functions that are \(L\)-smooth and by \(L_L\) the set of linear functions that are \(\ell\)-Lipschitz-continuous.

**Proposition 4.4.** Consider a chain \(\psi\) of \(\tau\) computations as defined in Def. 2.1 whose layers \(\phi_l\) for \(l \in \{1, \ldots, \tau\}\) are defined by

\[
\phi_l(v_l, z_{l-1}) = a_l(b_l(v_l, z_{l-1})),
\]

where \(b_l\) is decomposed as

\[
b_l(v_l, z_{l-1}) = \beta_l(v_l, z_{l-1}) + \beta_l^1(v_l) + \beta_l^2(z_{l-1}) + \beta_l^3,
\]

with \(\beta_l \in BL_{L_{\beta_l}}, \beta_l^1 \in L_{\ell_{\beta_l}}, \beta_l^2 \in L_{\ell_{\beta_l}}, \beta_l^3\) is a constant vector, and \(a_l\) is decomposed as

\[
a_l = a_{l,1} \circ \ldots \circ a_{l,1},
\]

with \(a_{l,1} \in C_{m_{a_{l,1}}} L_{a_{l,1}}\). Consider \(C = \{ w = (v_1; \ldots, v_\tau) \in \mathbb{R}^p : \forall l \in \{1, \ldots, \tau\}, \|v_l\| \leq R\}\).
(i) An upper-bound on the output of the chain $\psi$ on $C$ is given by $m^C_\psi \leq m_\tau$ where for $l \in \{1, \ldots, \tau\}$,

\[
m_l = m_{l,k_1}, \quad m_{l,j} = \min\{m_{a_{l,j}(0)}, \|a_{l,j}(0)\|_2 + \epsilon_{a_{l,j}} m_{l,j-1}, \|a_{l,j}(0)\|_2 + (\|\nabla a_{l,j}(0)\|_2 + L_{a_{l,j}}) m_{l,j-1}\} \text{ for } j=1, \ldots, k_l,
\]

\[
m_{l,0} = L_{\beta_l} R m_{l-1} + \epsilon_{\beta_l} R + \epsilon_{\beta_l}^a m_{l-1} + \|\beta^a\|_2,
\]

\[
m_0 = \|x\|_2.
\]

(ii) An upper-bound on the Lipschitz-continuity of the chain $\psi$ on $C$ is given by $\ell_\psi(C) \leq \ell_\tau$, where for $l \in \{1, \ldots, \tau\}$,

\[
\ell_l = \left(\prod_{j=1}^{k_l} \ell_{l,j}\right) \left((L_{\beta_l} R + L_{\beta_l}^a) \ell_{l-1} + m_{l-1} L_{\beta_l} + \ell_{\beta_l}\right)
\]

\[
\ell_{l,j} = \min\{\epsilon_{a_{l,j}}, \|\nabla a_{l,j}(0)\|_2 + L_{a_{l,j}} m_{l,j-1}\}, \text{ for } j=1, \ldots, k_l,
\]

\[
\ell_0 = 0.
\]

(iii) An upper-bound on the smoothness of the chain $\psi$ on $C$ is given by $L_\psi(C) \leq L_\tau$, where for $l \in \{1, \ldots, \tau\}$,

\[
L_l = L_{l-1}(L_{\beta_l} R + L_{\beta_l}^a) \left(\prod_{j=1}^{k_l} \ell_{l,j}\right) + \left((L_{\beta_l} R + L_{\beta_l}^a)^2 L_{l,k_1} \ell_{l-1}^2\right) + 2 \left((L_{\beta_l} m_{l-1} + L_{\beta_l}^a)(L_{\beta_l} R + L_{\beta_l}^a)L_{l,k_1} + L_{\beta_l} \left(\prod_{j=1}^{k_l} \ell_{l,j}\right)\right) \ell_{l-1} + \left((L_{\beta_l} m_{l-1} + L_{\beta_l}^a)^2 L_{l,k_1}\right)
\]

\[
L_{l,k_1} = \sum_{j=1}^{k_l} L_{a_{l,j}} \left(\prod_{i=1}^{j-1} \ell_{l,i}\right)^2 \left(\prod_{i=j+1}^{k_l} \ell_{l,i}\right).
\]

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

**Corollary 4.5.** Consider a chain $\psi$ of $\tau$ computations as defined in Prop. 4.4 and $w^* = (v_1^*, \ldots, v_\tau^*) \in \mathbb{R}^p$. The smoothness properties of $\psi$ on $C' = \{w = (v_1; \ldots; v_\tau) \in \mathbb{R}^p : \forall l \in \{1, \ldots, \tau\}, \|v_l - v_l^*\| \leq R\}$ are given as in Prop. 4.4 by considering

\[
R' \text{ in place of } R,
\]

\[
\ell_{\beta_l} + L_{\beta_l}\|v_l^*\|_2 \text{ in place of } \ell_{\beta_l},
\]

\[
\|\beta_l^a\|_2 + L_{\beta_l}^a\|v_l^*\|_2 \text{ in place of } \|\beta_l^a\|_2.
\]

5 **Application**

We apply our framework to assess the smoothness properties of the Visual Geometry Group (VGG) deep network used for image classification (Simonyan & Zisserman 2015).

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 below in our framework. We consider the smooth version of VGG where the original max pooling and ReLU operations are replaced by average pooling and soft-plus activation respectively. 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 $d_{out}$.

0. $x_i \in \mathbb{R}^{n^p \times n^f}$ with $n^p = 224 \times 224$ and $n^f = 3$,
1. $\phi_1(v, z) = \alpha_{\text{softplus}}(b_{\text{conv}}(v, z))$
   
   \[ n^p_{\text{conv}} = 224 \times 224, \ n^f_{\text{conv}} = 64, \]
2. $\phi_2(v, z) = \pi_{\text{avgpool}}(\alpha_{\text{softplus}}(b_{\text{conv}}(v, z)))$
   
   \[ n^p_{\text{conv}} = 224 \times 224, \ n^f_{\text{conv}} = 64, \ n^p_{\text{avgpool}} = 112 \times 112, \ n^f_{\text{avgpool}} = 64, \]
3. $\phi_3(v, z) = \alpha_{\text{softplus}}(b_{\text{conv}}(v, z))$
   
   \[ n^p_{\text{conv}} = 112 \times 112, \ n^f_{\text{conv}} = 128 \]
4. $\phi_4(v, z) = \pi_{\text{avgpool}}(\alpha_{\text{softplus}}(b_{\text{conv}}(v, z)))$
   
   \[ n^p_{\text{conv}} = 112 \times 112, \ n^f_{\text{conv}} = 128, \ n^p_{\text{avgpool}} = 56 \times 56, \ n^f_{\text{avgpool}} = 128, \]
5. $\phi_5(v, z) = \alpha_{\text{softplus}}(b_{\text{conv}}(v, z))$
   
   \[ n^p_{\text{conv}} = 56 \times 56, \ n^f_{\text{conv}} = 256, \]
6. $\phi_6(v, z) = \alpha_{\text{softplus}}(b_{\text{conv}}(v, z))$
   
   \[ n^p_{\text{conv}} = 56 \times 56, \ n^f_{\text{conv}} = 256, \]
7. $\phi_7(v, z) = \pi_{\text{avgpool}}(\alpha_{\text{softplus}}(b_{\text{conv}}(v, z)))$
   
   \[ n^p_{\text{conv}} = 56 \times 56, \ n^f_{\text{conv}} = 256, \ n^p_{\text{avgpool}} = 28 \times 28, \ n^f_{\text{avgpool}} = 256, \]
8. $\phi_8(v, z) = \alpha_{\text{softplus}}(b_{\text{conv}}(v, z))$
   
   \[ n^p_{\text{conv}} = 28 \times 28, \ n^f_{\text{conv}} = 512, \]
9. $\phi_9(v, z) = \alpha_{\text{softplus}}(b_{\text{conv}}(v, z))$
   
   \[ n^p_{\text{conv}} = 28 \times 28, \ n^f_{\text{conv}} = 512, \]
10. $\phi_{10}(v, z) = \pi_{\text{avgpool}}(\alpha_{\text{softplus}}(b_{\text{conv}}(v, z)))$
    
    \[ n^p_{\text{conv}} = 28 \times 28, \ n^f_{\text{conv}} = 512, \ n^p_{\text{avgpool}} = 14 \times 14, \ n^f_{\text{avgpool}} = 512, \]
11. $\phi_{11}(v, z) = \alpha_{\text{softplus}}(b_{\text{conv}}(v, z))$
    
    \[ n^p_{\text{conv}} = 14 \times 14, \ n^f_{\text{conv}} = 512, \]
12. $\phi_{12}(v, z) = \alpha_{\text{softplus}}(b_{\text{conv}}(v, z))$
    
    \[ n^p_{\text{conv}} = 14 \times 14, \ n^f_{\text{conv}} = 512, \]
13. $\phi_{13}(v, z) = \pi_{\text{avgpool}}(\alpha_{\text{softplus}}(b_{\text{conv}}(v, z)))$
    
    \[ n^p_{\text{conv}} = 14 \times 14, \ n^f_{\text{conv}} = 512, \ n^p_{\text{avgpool}} = 7 \times 7, \ n^f_{\text{avgpool}} = 512, \]
14. $\phi_{14}(v, z) = \alpha_{\text{softplus}}(b_{\text{full}}(v, z))$
    
    \[ d_{out} = 4096, \]
15. $\phi_{15}(v, z) = \alpha_{\text{softplus}}(b_{\text{full}}(v, z))$
    
    \[ d_{out} = 4096, \]
16. $\phi_{16}(v, z) = \alpha_{\text{softmax}}(b_{\text{full}}(v, z))$
    
    \[ d_{out} = 1000, \]
17. $f(\hat{y}) = \sum_{i=1}^{k} \log(\hat{y}_i, y_i) / n$ for $k = 1000$ classes.

We consider in the following smoothness properties for mini-batches with size $m = 128$, i.e., by concatenating $m$ chains of computations $\psi^{(i)}$ 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 $\beta^v$. The smoothness constants of interest are

1. $\ell_{\text{conv}} = \sqrt{mn^f}, \ L_{\text{conv}} = \sqrt{n^p}$,
2. $\ell_{\text{full}} = \sqrt{m}, \ L_{\text{full}} = 1$,
3. $\ell_{\text{softplus}} = 1, \ L_{\text{softplus}} = 1/4$,
4. $\ell_{\text{softmax}} = 2, \ L_{\text{softmax}} = 4$,
5. $\ell_{\text{avgpool}} = 1, \ L_{\text{avgpool}} = 0$. 

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A Lipschitz-continuity estimate of this architecture can then be computed using Prop. 4.4 on a Cartesian product of balls \( C = \{ w = (v_1; \ldots; v_{16}) : \|v_l\|_2 \leq R \} \) for \( R = 1 \) for example.

### 5.2 Variations of VGG

**Batch-normalization effect.** We can also compare the smoothness properties of the VGG 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 B, the batch-normalization satisfies

1. \( m_{\text{batch}} = dm, \ell_{\text{batch}} = 2e^{-1/2}, L_{\text{batch}} = 2m^{-1/2}e^{-1} \).

Denoting \( \ell_{\text{VGG}}, L_{\text{VGG}} \) and \( \ell_{\text{VGG-batch}}, L_{\text{VGG-batch}} \) the Lipschitz-continuity and smoothness estimates of the VGG network with and without batch-normalization respectively on a Cartesian product of balls \( C = \{ w = (v_1; \ldots; v_{16}) : \|v_l\|_2 \leq 1 \} \) with \( \|x\|_2 = 1 \), we get using Prop. 4.4,

\[
\begin{align*}
\ell_{\text{VGG}} & \leq \ell_{\text{VGG-batch}} \\
L_{\text{VGG}} & \leq L_{\text{VGG-batch}} \\
\ell_{\text{VGG}} & \geq \ell_{\text{VGG-batch}} \\
L_{\text{VGG}} & \geq L_{\text{VGG-batch}}
\end{align*}
\]

Intuitively, the batch-norm bounds the output of each layer, mitigating the increase of \( m_l \) in Eq. (20) and (21). 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).

**Acknowledgments.** This work was supported by NSF CCF-1740551, NSF DMS-1839371, the program “Learning in Machines and Brains”, and faculty research awards.

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A Notations

A.1 Matrices

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

A.2 Tensors

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

\[
\mathcal{A}[P, Q, R] = \left( \sum_{k=1}^p R_{k,1} P^T A_k Q, \ldots, \sum_{k=1}^p R_{k,p'} P^T A_k Q \right) \in \mathbb{R}^{d' \times n' \times p'}.
\]

If \( P, Q \) or \( R \) are identity matrices, we use the symbol ‘⋯’ in place of the identity matrix. For example, we denote \( \mathcal{A}[P, Q, I_p] = \mathcal{A}[P, Q, ] = (P^T A_1 Q, \ldots, P^T A_p Q) \). 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

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

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

For a tensor \( \mathcal{A} = (A_1, \ldots, A_p) \in \mathbb{R}^{d \times n \times p} \) we denote \( \mathcal{A}^T = (A_1^T, \ldots, A_p^T) \in \mathbb{R}^{n \times d \times p} \). 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

\[
(x \boxtimes y \boxtimes z)_{ijk} = x_i y_j z_k.
\]

We define the norm of a tensor \( \mathcal{A} \) induced by the Euclidean norm as follows

**Definition A.1.** The norm of a tensor \( \mathcal{A} \) induced by the Euclidean norm is defined as

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

**Fact A.2.** 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. \( \|\mathcal{A}[P, Q, R]\|_{2,2,2} \leq \|\mathcal{A}\|_{2,2,2} \|P\|_{2,2} \|Q\|_{2,2} \|R\|_{2,2} \) 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 \( f : \mathbb{R}^d \rightarrow \mathbb{R}^n \), composed of \( f^{(j)} \) real functions with \( j \in \{1, \ldots, n\} \), 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 \( x \), \( \nabla f(x) = (\frac{\partial f^{(j)}}{\partial x_i}(x))_{1 \leq i \leq d, 1 \leq j \leq n} \in \mathbb{R}^{d \times n} \). 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.3. We have for \( f : \mathbb{R}^d \to \mathbb{R}^n \), twice differentiable, and \( C \subset \text{dom} \ f \) convex,
\[
\ell_f^C = \sup_{x, y \in C, x \neq y} \frac{\|f(x) - f(y)\|_2}{\|x - y\|_2} = \sup_{x \in C} \|\nabla f(x)\|_{2,2}, \quad L_f^C = \sup_{x, y \in C, x \neq y} \frac{\|\nabla f(x) - \nabla f(y)\|_2}{\|x - y\|_2} = \sup_{x \in C} \|\nabla^2 f(x)\|_{2,2,2},
\]
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 \( x, y \in C \),
\[
\|f(x) - f(y)\|_2 = \left\| \int_0^1 \nabla f(x + t(y - x)) \, dt \right\|_2 \leq \sup_{x \in C} \|\nabla f(x)\|_{2,2} \|x - y\|_2,
\]
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, \( f : \mathbb{R}^{d+p} \to \mathbb{R} \), whose value is denoted \( f(x,y) \), we decompose its gradient \( \nabla f(x,y) \in \mathbb{R}^{d+p} \) on \((x,y) \in \mathbb{R}^{d+p}\) 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 \( \nabla^2 f(x,y) \) as
\[
\nabla^2 f(x,y) = \begin{pmatrix} \nabla^2_{xx} f(x,y) & \nabla^2_{xy} f(x,y) \\ \nabla^2_{yx} f(x,y) & \nabla^2_{yy} f(x,y) \end{pmatrix}.
\]

Given a function \( f : \mathbb{R}^{d+p} \to \mathbb{R}^n \) and \((x,y)\), we define \( \nabla f(x,y) = (\nabla f_1(x,y), \ldots, \nabla f_n(x,y)) \in \mathbb{R}^{d+n} \). For its second order information we define \( \nabla^2 f(x,y) = (\nabla^2 f_1(x,y), \ldots, \nabla^2 f_n(x,y)) \), similarly for \( \nabla^2 y f(x,y) \) and \( \nabla^2 x f(x,y) \). Dimensions of these definitions are
\[
\nabla f_1(x,y) \in \mathbb{R}^{d \times n}, \quad \nabla f_n(x,y) \in \mathbb{R}^{p \times n},
\]
\[
\nabla^2 f_1(x,y) \in \mathbb{R}^{d \times d \times n}, \quad \nabla^2 f_n(x,y) \in \mathbb{R}^{p \times p \times n},
\]
\[
\nabla^2 x f(x,y) \in \mathbb{R}^{d \times p \times n}, \quad \nabla^2 y f(x,y) \in \mathbb{R}^{p \times d \times n}.
\]

A.4 Bilinear functions

Definition A.4. A function \( \beta : \mathbb{R}^d \times \mathbb{R}^n \to \mathbb{R}^p \) is bilinear if it is represented by a tensor \( B \in \mathbb{R}^{d \times n \times p} \) such that for any \( x \in \mathbb{R}^d, y \in \mathbb{R}^n \),
\[
\beta(x,y) = B[x,y,\cdot].
\]

The gradient of a bilinear function \( \beta \) represented by a tensor \( B \in \mathbb{R}^{d \times n \times p} \) at a point \((x,y)\) is given by
\[
\nabla_x \beta(x,y) = B[\cdot,y,\cdot] \in \mathbb{R}^{d \times p}, \quad \nabla_y \beta(x,y) = B[\cdot,\cdot,\cdot] \in \mathbb{R}^{n \times p}.
\]

The Hessian of the bilinear function is given by
\[
\nabla^2_{xx} \beta(x,y) = 0, \quad \nabla^2_{yy} \beta(x,y) = 0, \quad \nabla^2_{yx} \beta(x,y) = B, \quad \nabla^2_{xy} \beta(x,y) = B^\top.
\]

A bilinear function is not Lipschitz continuous as can be seen from Eq. (23). It is smooth w.r.t. the Euclidean norm with a smoothness constant given by the tensor norm of \( B \) as shown in the following proposition.
Proposition A.5. The smoothness of a bilinear function $\beta$ defined by a tensor $B$ is given by $L_\beta = \|B\|_{2,2,2}$.

Proof. We have
\[
\|\nabla^2 \beta(x,y)\|_{2,2,2} = \sup_{z \neq 0} \frac{\| \sum_{k=1}^p z_k \hat{B}_k \|_{2,2}}{\|z\|_2},
\]
where $\nabla^2 \beta(x,y) = (\hat{B}_1, \ldots, \hat{B}_p)$. We have by Eq. (24) that $\sum_{k=1}^p z_k \hat{B}_k$ is of the form
\[
\sum_{k=1}^p z_k \hat{B}_k = \left( \begin{array}{cc}
\sum_{k=1}^p z_k B_k^\top & 0 \\
0 & \sum_{k=1}^p z_k B_k
\end{array} \right),
\]
where $B = (B_1, \ldots, B_p)$. Using that $\| \sum_{k=1}^p z_k \hat{B}_k \|_{2,2} = \| \sum_{k=1}^p z_k B_k \|_{2,2}$, (Horn & Johnson 2012, Theorem 7.3.3.), we get
\[
\|\nabla^2 \beta(x,y)\|_2 = \sup_{z \neq 0} \frac{\| \sum_{k=1}^p z_k \hat{B}_k \|_{2,2}}{\|z\|_2} = \sup_{z \neq 0} \frac{\| \sum_{k=1}^p z_k B_k \|_{2,2}}{\|z\|_2} = \|B\|_{2,2,2}.
\]

\[\square\]

### B List of objectives and layers

#### B.1 Supervised objectives

Recall that the supervised objectives read
\[
f(\psi(w)) = \frac{1}{n} \sum_{i=1}^n f_i(\psi_i(w)),
\]
such that $f : \mathbb{R}^{nq} \to \mathbb{R}$ reads for $\hat{y} = (\hat{y}_1; \ldots; \hat{y}_n)$ with $\hat{y}_i \in \mathbb{R}^q$,
\[
f(\hat{y}) = \frac{1}{n} \sum_{i=1}^n f_i(\hat{y}_i),
\]
and $\psi : \mathbb{R}^p \to \mathbb{R}^{nq}$ is defined by
\[
\psi(w) = (\psi_1(w); \ldots; \psi_n(w)),
\]
for chains $\psi_i : \mathbb{R}^p \to \mathbb{R}^q$ defined as in Def. 2.1.

We are interested in this section in the smoothness $\ell_f(C)$ and Lipschitz-continuity $\ell_f(C)$ of the objective $f$ 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. We denote by
\[
\rho_C = \max_{x \in C} \|x\|_2,
\]
a bound on the size of the set. The smoothness and Lipschitz-continuity of the objective are given by the Lipschitz-continuity and smoothness constants of the components $f_i$. Precisely we have\(^5\)
\[
\ell_f(C) \leq \max_{i \in \{1, \ldots, n\}} \ell_{f_i}(C), \quad L_f(C) \leq \max_{i \in \{1, \ldots, n\}} L_{f_i}(C).
\]
The Lipschitz and smoothness constants boil down to the choice of the loss since we have $f_i(\hat{y}_i) = \mathcal{L}(\hat{y}_i, y_i)$, i.e.,
\[
\ell_f(C) \leq \ell_\mathcal{L}(C), \quad L_f(C) \leq L_\mathcal{L}(C),
\]
where Lipschitz continuity and smoothness of the losses are defined w.r.t. its first argument.

\(^5\)Note that for the smoothness constant, a sharper bound is given by $L_f \leq \frac{1}{n} \max_{i \in \{1, \ldots, n\}} L_{f_i}$ for twice differentiable functions using that the spectral norm of a block diagonal matrix is given by the maximal spectral norm of its components.
**Square loss.** Assume that the labels belong to a compact set $\mathcal{Y}$ and denote $\rho_\mathcal{Y} = \max_{y \in \mathcal{Y}} \|y\|_2$. The square loss is defined by $\mathcal{L}_{sq}(\hat{y}, y) = (\hat{y} - y)^2 / 2$. We have then

$$\ell_{sq}(C) = \rho_C + \rho_\mathcal{Y}, \quad \mathcal{L}_{sq} = 1.$$ 

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

$$\nabla f(\hat{y}) = -y + \frac{\exp(\hat{y})}{\exp(\hat{y})^\top 1_q}, \quad \nabla^2 f(\hat{y}) = \text{diag}(\exp(\hat{y})) \frac{\exp(\hat{y})}{\exp(\hat{y})^\top 1_q} - \frac{\exp(\hat{y}) \exp(\hat{y})^\top}{(\exp(\hat{y})^\top 1_q)^2}.$$ 

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

$$\ell_{log} \leq 2, \quad L_{log} \leq 2.$$ 

**B.2 Unsupervised objectives**

In the following, denote $k$ the number of classes that the unsupervised objective aims to cluster and

$$\mathcal{Y} = \{Y = (y_1, \ldots, y_n)^\top \in \{0, 1\}^{n \times k} \text{ s.t. } Y 1_k = 1_n\}, \quad \Psi(w) = (\psi_1(w), \ldots, \psi_n(w)) \in \mathbb{R}^{q \times n}.$$ 

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

$$f(\psi(w)) = \min_{C \in \mathbb{R}^{q \times k}} \sum_{i=1}^n \|C y_i - \psi_i(w)\|_2^2.$$ 

Minimization in $C$ can be performed analytically such that the problem can be rewritten

$$f(\psi(w)) = \min_{N \in \mathcal{N}} \text{Tr}((I_n - N)\Psi(w)^\top \Psi(w)),$$

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

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

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

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

$$f(\psi(w)) = \min_{P \in \mathcal{P}} \text{Tr}((I_n - P)\Psi(w)^\top \Psi(w))$$

is then given by finding the $k$ largest eigenvectors of the Gram matrix $\Psi(w)^\top \Psi(w)$. Formally the objective is written

$$f(\psi(w)) = \sum_{i=n-k+1}^n \sigma_i^2(\Psi(w)),$$

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

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Convex clustering. The convex clustering objective reads

$$f(\psi(w)) = \min_{y_1, \ldots, y_n \in \mathbb{R}^n} \sum_{i=1}^{n} \frac{1}{2} \| y_i - \psi_i(w) \|^2_2 + \sum_{i<j} \| y_i - y_j \|^2_2.$$  \hfill (25)

Denoting $\psi(w) = (\psi_1(w); \ldots; \psi_n(w)) \in \mathbb{R}^{qn}$, $y = (y_1; \ldots; y_n) \in \mathbb{R}^{qn}$, the objective reads

$$f(\psi(w)) = \min_{y \in \mathbb{R}^{qn}} \frac{1}{2} \| y - \psi(w) \|^2_2 + \| Dy \|_G,$$

where $D \in \mathbb{R}^{qn(n-1)/2 \times qn}$ maps $y$ to the concatenation of all possible $y_i - y_j$ for $i < j$ and $\| \cdot \|_G$ is a group norm, i.e., $\| x \|_G = \sum_{g \in G} \| x_g \|_2$ where $G$ is a partition of $\{1, \ldots, N\}$ for $x \in \mathbb{R}^N$ and $x_g \in \mathbb{R}^s$ is the vector corresponding to the group $g$ of size $s_g$. Here the groups are defined by all possible differences for $i < j$ in Eq. (25).

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

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

is convex, Lipschitz-continuous and smooth with parameters

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

respectively.

**Proof.** The convex clustering objective $f$ is the Moreau envelope of the function $\Omega : y \to \| D y \|_G$. It is therefore convex and 1-smooth, i.e.,

$$L_f = 1.$$

Moreover, the Moreau envelope can be rewritten

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

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

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

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

$$\nabla f(\hat{y}) \in \text{dom}(\Omega^*) \subset B_2 \left(0, \frac{n(n-1)}{2}\right),$$

where $B_2(0, \frac{n(n-1)}{2})$ is the Euclidean ball centered at 0 with radius $\frac{n(n-1)}{2}$.

**B.3 Bilinear and linear layers.** 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 $\mathcal{M} = ((I_d \otimes e_{(q \mod n) + 1})(f^q_{[0:n]} \otimes I_d))_{q=1,\ldots,np} \in \mathbb{R}^{nd \times dp \times np}$ where $e_i$ is the $i$th canonical vector in $\mathbb{R}^n$ and $f_j$ is the $j$th canonical vector in $\mathbb{R}^p$ such that

$$\text{Vec}(AB) = \mathcal{M}[\text{Vec}(A), \text{Vec}(B), \cdot].$$  \hfill (26)

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

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

$$= \text{Vec}(A)^\top (I_d \otimes e_i)(f_j^\top \otimes I_d)\text{Vec}(B)$$

$$= (\mathcal{M}[\text{Vec}(A), \text{Vec}(B), \cdot])_q.$$
Smoothness of fully-connected layer. Consider a fully-connected layer as in (8). As the matrix multiplication satisfies \(\|AB\|_F \leq \|A\|_F \|B\|_F\), we deduce that \(L_{\beta_l} = 1\). For the linear part we have \(\beta_n^{\ell}(y) = (1_n \otimes I_d)w_\ell^T\), so we get \(\ell_{\beta_l} = \sqrt{m}\). To summarize denoting \(L_{\text{full}}\) the smoothness of the bilinear operation and \(\ell_{\text{full}}\) the Lipschitz-constant of the linear operation,

\[
L_{\text{full}} = 1, \quad \ell_{\text{full}} = \sqrt{m}.
\]

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 \(C\) filters \(\mathcal{F}_1, \ldots, \mathcal{F}_C \in \mathbb{R}^{C \times K \times K}\) of patch size \(K\) and the biases are given by \(b \in \mathbb{R}^C\). The convolution of the image by a filter \(\mathcal{F}_c\), with \(c \in \{1, \ldots, C\}\) with additional bias \(b_c\), is given at point \(i, j\) as

\[
C_{c,i,j} = \sum_{c=1}^{C} \langle \mathcal{F}_c[i, \cdot, \cdot], E_{\text{row},i}\mathcal{I}[c, \cdot, \cdot] \rangle E_{\text{col},j} + b_c,
\]

where \(\mathcal{F}_c[i, \cdot, \cdot]\) is the filter of size \(K \times K\) in channel \(c\) of filter \(\mathcal{F}_c\) and \(\mathcal{I}[c, \cdot, \cdot]\) is the image in channel \(c\).

The matrices \(E_{\text{row},i} \in \mathbb{R}^{H \times K}\) and \(E_{\text{col},j} \in \mathbb{R}^{B \times K}\) extract rows and columns of \(\mathcal{I}[c, \cdot, \cdot]\). They are bands with a diagonal of \(K\) ones centered at positions \(i\) or \(j\). If the pattern of the patch is given as \(P = 1_K \otimes 1_K\), the extraction matrices read \(E_{\text{row},i} = e_i \otimes 1_K \in \mathbb{R}^{H \times K}\), \(e_i \in \mathbb{R}^H\) for \(i \in \{1, \ldots, H\}\), similarly \(E_{\text{col},j} = e_j \otimes 1_K \in \mathbb{R}^{B \times K}\). They satisfy \(E_{\text{row},i}E_{\text{row},i}^\top = 1_{K^2}\) and \(E_{\text{row},i}E_{\text{row},j}^\top \in \mathbb{R}^{H \times H}\) is a projector. Similarly facts apply for \(E_{\text{col},j}\) except that one replaces \(H\) by \(B\). The output of the convolution with all filters is then a tensor \(\mathcal{C} \in \mathbb{R}^{H \times B \times C}\) where \(\hat{H}\) and \(\hat{B}\) depend on the choices of the stride chosen in the convolution.

Smoothness of convolutional layer. Consider a convolutional layer as in (9). We have that its output without the offset term denoted \(\hat{Z}\) has a Frobenius norm bounded as

\[
\|\hat{Z}\|_F^2 = \sum_{i,j,k} (W^{(j)} \Pi_k Z^{(i)})^2 \leq \sum_{i,j,k} \|W^{(j)}\|_F^2 \|\Pi_k\|_2^2 \|Z^{(i)}\|_F^2 \leq \|W\|_F^2 \|Z\|_F^2 \sum_k \|\Pi_k\|_2^2
\]

\[
\leq n^p \|W\|_F^2 \|Z\|_F^2,
\]

where we used that the patch matrices \(\Pi_k\) satisfy \(\Pi_k \Pi_k^\top = I_d\). We deduce then \(L_{\beta} = \sqrt{n^p}\) where \(n^p\) is the number of patches defining the convolution. For the linear part, bounding the part that depends on the offset as above, we get \(\ell_{\beta} \leq \sqrt{n^p m}\). To summarize denoting \(L_{\text{conv}}\) the smoothness of the bilinear operation and \(\ell_{\text{conv}}\) the Lipschitz-constant of the linear operation,

\[
L_{\text{conv}} = \sqrt{n^p}, \quad \ell_{\text{conv}} = \sqrt{n^p m}.
\]

### B.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 \(\tilde{\alpha}_t\) 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 \(\tilde{\alpha}(x) = f(x)\), we get

\[
\ell_{\text{softplus}} = 1, \quad L_{\text{softplus}} = 1/4.
\]

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

\[
\ell_{\text{sig}} = 1/4, \quad L_{\text{sig}} = 1/10.
\]
Proposition B.2. The batch normalization operation \( \nu_{\text{batch}} : \mathbb{R}^{dm} \to \mathbb{R}^{dm} \) defined as in (11) is

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

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

\[
\nu_1(z) = \text{Vec} \left( Z - Z \frac{1_m 1_m^\top}{m} \right)
\]

and a normalization step

\[
\nu_2(\tilde{z}) = \text{Vec} \left( \text{diag} \left( \left( \frac{1}{m} \text{diag}(\tilde{Z} \tilde{Z}^\top) + \epsilon 1_d \right)^{-1/2} \right) \tilde{Z} \right),
\]

where here and thereafter \( Z, \tilde{Z} \in \mathbb{R}^{d \times m} \), \( z = \text{Vec}(Z) \), \( \tilde{z} = \text{Vec}(\tilde{Z}) \).

The centering step is an orthonormal projection, i.e., \( \nu_1(z) = \text{Vec}(Z \Pi_m) = (\Pi_m \otimes I_m) z \) where \( \Pi_m = I_m - \frac{1_m 1_m^\top}{m} \) 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 \( \tilde{x} = (x_1; \ldots; x_d) \in \mathbb{R}^{md} \) with \( x_i \in \mathbb{R}^m \),

\[
f(x) = \sqrt{\frac{1}{m} \|x\|^2_2 + \epsilon}, \quad g(x) = \left( \frac{x_i}{f(x)} \right)_{i=1,\ldots,m}, \quad \bar{g}(\tilde{x}) = (g(x_1); \ldots; g(x_d)) \in \mathbb{R}^{md},
\]

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

\[
\|\bar{g}(\tilde{x})\|_2 \leq d \max_{i \in \{1, \ldots, d\}} \|g(x_i)\|_2 \leq dm^{1/2},
\]

such that

\[
m_{\nu_2} \leq dm^{1/2}.
\]

Then the gradients can be computed as

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

\[
\nabla g(x) = \frac{f(x) I_m - \nabla f(x)x^\top}{f(x)^2} = \frac{mf(x)^2 I_m - xx^\top}{mf(x)^3} \in \mathbb{R}^{m \times m},
\]

\[
\nabla \bar{g}(\tilde{x}) = \text{diag}(\nabla g(x_1), \ldots, \nabla g(x_m)) \in \mathbb{R}^{md \times md},
\]

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

\[
\text{diag}(X_1, \ldots, X_\tau) = \\
\begin{pmatrix}
X_1 & 0 & \ldots & 0 \\
0 & \ddots & & \\
\vdots & \ddots & \ddots & 0 \\
0 & \ldots & 0 & X_\tau
\end{pmatrix} \in \mathbb{R}^{d\tau \times p\tau},
\]
The second order tensor of $\gamma > T$ spectral norm of its block diagonal components. Since with Lipschitz constant one, the step-size must be chosen small enough such that the Newton step is a convex problem.

$c$ where

$$\nabla^2 g(x) = \frac{3}{m^2 f(x)^5} x \otimes x \otimes x - \frac{1}{m f(x)^3} \left( \sum_{i=1}^{m} x \otimes e_i \otimes e_i + e_i \otimes x \otimes e_i + e_i \otimes e_i \otimes x \right) \in \mathbb{R}^{m \times m \times m},$$

$$\nabla^2 \tilde{g}(\bar{x}) = \text{diag}^3(\nabla^2 g(x_1), \ldots, \nabla^2 g(x_d)),$$

where $e_i \in \mathbb{R}^m$ is the $i$th canonical vector in $\mathbb{R}^m$ and for a sequence of tensors $X_1, \ldots, X_d$ we denote by $X = \text{diag}^3(X_1, \ldots, X_d) \in \mathbb{R}^{dm \times dm \times dm}$ the tensor whose diagonal is composed of the tensors $X_1, \ldots, X_d$ such that $X_{i+(m-1)p+(m-1)p+k+(m-1)p} = (X_r)_{ijk}$ and 0 outside the diagonal. We then by definition of the tensor norm,

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

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

$$L_{avg} \leq 2dm^{-1/2} \epsilon^{-1}.$$  

\[\Box\]

### B.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.

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

### C Oracle arithmetic complexity proofs

#### C.1 Feasibility of the optimization oracle steps

The gradient step (12) is always feasible for any $\gamma > 0$, the gauss-newton step (13) is feasible for any $\gamma > 0$ if $f, r$ are convex and the Newton step is feasible for any $\gamma > 0$ if $f \circ \psi$ and $r$ are convex. A sufficient condition for the Newton step to be feasible if $f \circ \psi$ is not convex but $f \circ \psi$ and $r$ are smooth is to choose $\gamma < (L_f \psi + L_r)^{-1}$. In other words, the step-size must be chosen small enough such that the Newton step is a convex problem.
C.2 Optimization oracles as linear quadratic control problems

Proposition 3.1. Let \( w_t = (v_1; \ldots; v_\tau) \) and \( z_0, \ldots, z_\tau \) be defined by the chain of computations in (3) applied to \( w_t \). Assume \( r \) to be decomposable as \( r(w_t) = \sum_{l=1}^{\tau} r_l(v_l) \). Gradient (12), Gauss-Newton (13) and Newton (14) steps are given as \( w_{t+1} = w_t + \tilde{w}^* \) where \( \tilde{w}^* = (\tilde{v}_1; \ldots; \tilde{v}_\tau) \) is the solution of

\[
\min_{\tilde{v}_1, \ldots, \tilde{v}_\tau \in \mathbb{R}^{p_1} \times \cdots \times \mathbb{R}^{p_\tau}} \sum_{l=1}^{\tau} \frac{1}{2} \tilde{v}_l^T P_l \tilde{z}_l + p_l^T \tilde{z}_l + \tilde{z}_{l-1}^T R_l \tilde{v}_l + \frac{1}{2} \tilde{v}_l^T Q_l \tilde{v}_l + q_l^T \tilde{v}_l + \frac{1}{2\gamma} \|	ilde{v}_l\|^2 \quad (15)
\]

subject to \( \tilde{z}_l = A_l \tilde{z}_{l-1} + B_l \tilde{v}_l \) for \( l \in \{1, \ldots, \tau\} \),

where

\[
A_l = \nabla_{z_{l-1}} \phi_l(v_l, z_{l-1})^T, \quad B_l = \nabla_{v_l} \phi_l(v_l, z_{l-1})^T, \quad p_l = \nabla f(\psi(w_t)), \quad p_l = 0 \quad \text{for } l \neq \tau, \quad q_l = \nabla r_l(v_l),
\]

1. for gradient steps (12),

\[
P_l = 0, R_l = 0, Q_l = 0,
\]

2. for Gauss-Newton steps (13),

\[
P_l = \nabla^2 f(\psi(w_t)), \quad P_l = 0 \quad \text{for } l \neq \tau, \quad R_l = 0, Q_l = \nabla^2 r_l(v_l),
\]

3. for Newton steps (14), defining

\[
\lambda_l = \nabla f(\psi(w_t)), \quad \lambda_{l-1} = \nabla_{z_{l-1}} \phi_l(v_l, z_{l-1}) \lambda_l \quad \text{for } l \in \{1, \ldots, \tau\},
\]

we have

\[
P_l = \nabla^2 f(\psi(w_t)), \quad P_l = 0 = \nabla^2 f(\psi(w_t)) \lambda_l \quad \text{for } l \in \{1, \ldots, \tau\},
\]

\[
R_l = \nabla^2_{z_{l-1}v_l} \phi_l(v_l, z_{l-1}) \lambda_l, \quad Q_l = \nabla^2 r_l(v_l) + \nabla^2_{w_l} \phi_l(v_l, z_{l-1}) \lambda_l.
\]

Proof. By considering \( w = w_t + \tilde{w} \) in the minimizations of (12), (13), (14), the optimization oracles can be rewritten as follows:

1. the gradient step (12) is given by

\[
w_{t+1} = w_t + \arg \min_{\tilde{w} \in \mathbb{R}^p} \left\{ \nabla f(\psi(w_t))^T \nabla \psi(w_t)^T \tilde{w} + \nabla r(w_t)^T \tilde{w} + \frac{1}{2\gamma} \|	ilde{w}\|_2^2 \right\}, \quad (27)
\]

2. the Gauss-Newton step (13) is given by

\[
w_{t+1} = w_t + \arg \min_{\tilde{w} \in \mathbb{R}^p} \left\{ \frac{1}{2} \tilde{w}^T \nabla^2 f(\psi(w_t)) \nabla \psi(w_t)^T \tilde{w} + \nabla f(\psi(w_t))^T \nabla \psi(w_t)^T \tilde{w} \right.
\]

\[
+ \frac{1}{2} \tilde{w}^T \nabla^2 r(w_t) \tilde{w} + \nabla r(w_t)^T \tilde{w} + \frac{1}{2\gamma} \|	ilde{w}\|_2^2 \right\}, \quad (28)
\]

3. the Newton step (14) is given by

\[
w_{t+1} = w_t + \arg \min_{\tilde{w} \in \mathbb{R}^p} \left\{ \frac{1}{2} \tilde{w}^T \nabla^2 f(\psi(w_t)) \nabla \psi(w_t)^T \tilde{w} + \frac{1}{2} \nabla^2 \psi(w_t) \tilde{w}, \tilde{w}, \nabla f(\psi(w_t)) \right\}
\]

\[
+ \nabla f(\psi(w_t))^T \nabla \psi(w_t)^T \tilde{w} + \frac{1}{2} \tilde{w}^T \nabla^2 r(w_t) \tilde{w} + \nabla r(w_t)^T \tilde{w} + \frac{1}{2\gamma} \|	ilde{w}\|_2^2 \right\}. \quad (29)
\]

To reformulate the optimization oracle problems as quadratic problems with linear dynamics we reformulate \( \nabla \psi(w_t)^T \tilde{w} \) as a linear chain of compositions and \( \nabla^2 \psi(w_t) \tilde{w}, \tilde{w}, \nabla f(\psi(w_t)) \) as a quadratic on the linear trajectory defined
by the gradient and the parameters. We denote simply $w = w_l$ in the following. For $w = (v_1; \ldots; v_\tau)$, define $\tilde{z}(w) = (\tilde{z}_1(w); \ldots; \tilde{z}_\tau(w))$ by

$$\tilde{z}_l(w) = \phi_l(v_l, \tilde{z}_{l-1}(w)) = \phi_l(E_l^T w, \tilde{z}_{l-1}(w)),$$

(30)

with $\tilde{z}_0(w) = x$, such that $\psi(w) = \tilde{z}_\tau(w)$ where here and thereafter, unless specified, the recursion is for $l \in \{1, \ldots, \tau\}$ and $E_l = (0_{p_l, p_1}; \ldots; 1_{p_l, p_1}; \ldots; 0_{p_\tau, p_{\tau-1}}) \in \mathbb{R}^{p \times p}$ is such that $E_l^T w = v_l$. We have from (30),

$$\nabla \tilde{z}_l(w) = \nabla \tilde{z}_{l-1}(w) \phi_l(E_l^T w, \tilde{z}_{l-1}(w)) + E_l \nabla_v \phi_l(E_l^T w, \tilde{z}_{l-1}(w)).$$

(31)

with $\nabla \tilde{z}_0(w) = 0$, where we simplified the gradient notations by dropping the dependencies w.r.t. the layers and the variable $w$ for the latent variables, for example $\nabla \phi_l(E_l^T w, \tilde{z}_{l-1}(w)) = \nabla \tilde{z}_{l-1}(w) \phi_l(E_l^T w, \tilde{z}_{l-1}(w))$. Therefore for $w = (v_1, \ldots; v_\tau)$ and $\tilde{w} = (\tilde{v}_1; \ldots; \tilde{v}_\tau)$, denoting $\tilde{z}(w) = (z_1; \ldots; z_\tau)$ and $\nabla \tilde{z}(w)^T \tilde{w} = (\tilde{z}_1; \ldots; \tilde{z}_\tau)$, we have

$$\nabla \psi(w)^T \tilde{w} = \tilde{z}_\tau$$

with

$$\tilde{z}_l = \nabla \phi_l(v_l, z_{l-1})^T \tilde{z}_{l-1} + \nabla_v \phi_l(v_l, z_{l-1})^T \tilde{v}_l,$$

for $l \in \{1, \ldots, \tau\}$

(32)

$$\tilde{z}_0 = 0,$$

where $z_0 = x$. For the second order derivatives, from (31), we have

$$\nabla^2 \tilde{z}_l(w) = \nabla^2 \tilde{z}_{l-1}[\cdot, \cdot, \nabla \phi_l(v_l, z_{l-1})]$$

(33)

$$+ \nabla^2_{zz} \phi_l(v_l, z_{l-1})[\nabla \tilde{z}_{l-1}(w)^T, \nabla \tilde{z}_{l-1}(w)^T, \cdot]$$

$$+ \nabla^2_{zv} \phi_l(v_l, z_{l-1})[\nabla \tilde{z}_{l-1}(w)^T, E_l^T, \cdot]$$

$$+ \nabla^2_{vv} \phi_l(v_l, z_{l-1})[E_l^T, \nabla \tilde{z}_{l-1}(w)^T, \cdot]$$

$$+ \nabla^2_{vv} \phi_l(v_l, z_{l-1})[E_l^T, E_l^T, \cdot].$$

where $\nabla^2 \tilde{z}_0(w) = 0, \nabla \tilde{z}_0(w) = 0$. Therefore for $\tilde{w} = (\tilde{v}_1; \ldots; \tilde{v}_\tau)$,

$$\frac{1}{2} \nabla^2 \psi(w)(\tilde{w}, \tilde{w}, \nabla f(\psi(w))) = \sum_{l=1}^\tau \frac{1}{2} \nabla^2_{zz} \phi_l(v_l, z_{l-1})[\tilde{z}_{l-1}, \tilde{z}_{l-1}, \lambda_l]$$

(34)

$$+ \nabla^2_{zv} \phi_l(v_l, z_{l-1})[\tilde{z}_{l-1}, \tilde{v}_l, \lambda_l]$$

$$+ \nabla^2_{vv} \phi_l(v_l, z_{l-1})[\tilde{v}_l, \tilde{v}_l, \lambda_l]$$

where $\tilde{z}_l$ are given in (32) and $\lambda_l$ are defined by

$$\lambda_\tau = \nabla f(\psi(w))$$

$$\lambda_{l-1} = \nabla \phi_l(v_l, z_{l-1}) \lambda_l$$

for $l \in \{1, \ldots, \tau\}$.

The results follow by using the decomposability of $r$ and inserting (32) and (34) in the steps detailed in (27), (28) and (29).

We present the resolution of the Newton step by dynamic programming in Algo. 4 whose implementation is justified in Proposition C.1. 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 C.1. Consider problem (15) and assume it is bounded below, then the cost-to-go functions defined for $l \in \{0, \ldots, \tau\}$ and $z_l \in \mathbb{R}^{d_l}$ as

$$\text{cost}(z_l) = \min_{\tilde{z}_{l+1}, \ldots, \tilde{z}_\tau} \sum_{l'=1}^l \frac{1}{2} \tilde{z}_{l'}^T P_{l'} \tilde{z}_{l'} + P_{l'}^T \tilde{z}_{l'} + \sum_{l'=l+1}^\tau \tilde{z}_{l'}^T R_{l'} \tilde{v}_{l'} + \frac{1}{2} \tilde{v}_{l'}^T Q_{l'} \tilde{v}_{l'} + q_{l'}^T \tilde{v}_{l'} + \frac{1}{2\gamma} ||\tilde{v}_{l'}||^2_2$$

(35)

subject to

$$\tilde{z}_{l'} = A_{l'} \tilde{z}_{l'+1} + B_{l'} \tilde{v}_{l'}$$

for $l' \in \{l + 1, \ldots, \tau\}$,

$$\tilde{z}_l = z_l,$$
where \( P_0 = 0, p_0 = 0 \), are quadratics of the form
\[
\text{cost}(z_l) = \frac{1}{2} z_l^T C_l z_l + c_l^T z_l + \text{const},
\]
where \( C_l, c_l \) are defined recursively in line 20 Algo. 4 with \( C_l = C_l^T \) and const is a constant. The solution of (15) is given by, starting from \( \tilde{z}_0 = 0 \),
\[
\tilde{v}_l^* = K_l \tilde{z}_{l-1} + k_l \quad \tilde{z}_l = A_l \tilde{z}_{l-1} + B_l \tilde{v}_l^*,
\]
where \( K_l \) and \( k_l \) are defined in line 21 of Algo. 4.

**Proof.** The cost-to-go functions satisfy the Bellman equation for \( l \in \{1, \ldots, \tau\} \)
\[
\text{cost}_{l-1}(z_{l-1}) = \frac{1}{2} \tilde{z}_{l-1}^T P_{l-1} \tilde{z}_{l-1} + p_{l-1}^T \tilde{z}_{l-1} + \min_{\tilde{v}_l \in \mathbb{R}^l} \left\{ z_{l-1}^T R_l \tilde{v}_l + \frac{1}{2} \tilde{v}_l^T Q_l \tilde{v}_l + \frac{1}{2} \gamma \| \tilde{v}_l \|^2 \right\}
\]
starting from \( \text{cost}_{\tau}(z_{\tau}) = \frac{1}{2} z_{\tau}^T P_{\tau} z_{\tau} + p_{\tau}^T z_{\tau} \) so we get \( C_{\tau} = P_{\tau} \) and \( c_{\tau} = p_{\tau} \). Assume that the cost-to-go function \( \text{cost}_l \) has the form (36) for \( l \in \{1, \ldots, \tau\} \) then the Bellman equation reads
\[
\text{cost}_{l-1}(z_{l-1}) = \frac{1}{2} \tilde{z}_{l-1}^T (P_{l-1} + A_l^T C_l A_l) \tilde{z}_{l-1} + (A_l^T c_l + p_{l-1})^T \tilde{z}_{l-1}
\]
\[
+ \min_{\tilde{v}_l \in \mathbb{R}^l} \left\{ \tilde{v}_l^T (R_l \tilde{z}_{l-1} + q_l + B_l^T (C_l A_l \tilde{z}_{l-1} + c_l)) + \frac{1}{2} \tilde{v}_l^T (\gamma^{-1} I + Q_l + B_l^T C_l B_l) \tilde{v}_l \right\}.
\]
If \( \gamma^{-1} I + Q_l + B_l^T C_l B_l \succeq 0 \), then the minimization problem is unbounded below and so is the original objective. If \( \gamma^{-1} I + Q_l + B_l^T C_l B_l \succ 0 \), then the minimization gives us \( \text{cost}_{l-1} \) as a quadratic and the corresponding minimizer \( \tilde{v}_l^* \) for a given \( \tilde{z}_{l-1} \), i.e.
\[
C_{l-1} = P_{l-1} + A_l^T C_l A_l - (R_l + A_l^T C_l B_l) (\gamma^{-1} I + Q_l + B_l^T C_l B_l)^{-1} (R_l + B_l^T C_l A_l),
\]
\[
c_{l-1} = A_l^T c_l + p_{l-1} - (R_l + A_l^T C_l B_l) (\gamma^{-1} I + Q_l + B_l^T C_l B_l)^{-1} (q_l + B_l^T c_l),
\]
\[
\tilde{v}_l^* (z_{l-1}) = - (\gamma^{-1} I + Q_l + B_l^T C_l B_l)^{-1} (R_l^T + B_l^T C_l A_l) z_{l-1} + q_l + B_l^T c_l).
\]
The solution of (15) is given by computing \( \text{cost}_0(0) \) which amounts to compute, starting from \( \tilde{z}_0 = 0 \),
\[
\tilde{v}_l = \arg \min_{\tilde{v}_l \in \mathbb{R}^l} \left\{ \frac{1}{2} \tilde{v}_l^T Q_l \tilde{v}_l + \frac{1}{2} \tilde{v}_l^T R_l \tilde{v}_l + \text{cost}_{l+1}(A_l \tilde{z}_{l-1} + B_l \tilde{v}_l) \right\} = \tilde{v}_l^* (z_{l-1}),
\]
\[
\tilde{z}_l = A_l \tilde{z}_{l-1} + B_l \tilde{v}_l^*.
\]
\[\square\]

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 \( r = 0, \gamma = -1 \).

**Proposition C.2.** Consider the gradient step (12) as formulated in (15). The cost-to-go functions defined in (35) are linear of the form
\[
\text{cost}_l(z_l) = \lambda_l^T z_l + \text{const},
\]
where
\[
\lambda_l = \nabla f(\psi(w))
\]
\[
\lambda_{l-1} = \nabla z_{l-1} \psi_l(v_l, z_{l-1}) \lambda_l \quad \text{for } l \in \{1, \ldots, k\}
\]
and the solution of the step is given by
\[
\tilde{v}_l^* = - \gamma (\nabla r(u_l) + \nabla \psi_l(u_l, z_{l-1}) \lambda_l).
\]

**Proof.** The cost-to-go function defined in (35) for a gradient step reads for \( l = \tau \), \( \text{cost}_\tau(z_\tau) = p_\tau^T z_\tau \), so we get Eq. (37) for \( l = \tau \) with \( \lambda_\tau = \nabla f(\psi(w)) \). Assume that the cost-to-go function has the form (37) for \( l \in \{1, \ldots, \tau\} \),
Algorithm 4 Newton step by dynamic programming

1: **Inputs:** Chain of layers $\psi$ defined by layers $\phi_l$, objective $f$, regularization $r$, step-size $\gamma$, current weights $w_t = (v_1; \ldots; v_\tau)$

2: **Forward pass:**
3: for $l = 1, \ldots, \tau$ do
4: Compute $z_l = \phi_l(v_l, z_{l-1})$
5: Store $A_l = \nabla^2_{v_l z_{l-1}} \phi_l(v_l, z_{l-1}) \top$, $B_l = \nabla_{v_l} \phi_l(v_l, z_{l-1}) \top$
6: and $\nabla^2_{v_l z_{l-1}} \phi_l(v_l, z_{l-1}), \nabla^2_{v_l z_{l-1}} \phi_l(v_l, z_{l-1}), \nabla^2_{z_{l-1} z_{l-1}} \phi_l(v_l, z_{l-1})$
7: end for

8: **1st Backward pass:**
9: Initialize $\lambda_\tau = \nabla f(\psi(w)), P_\tau = \nabla^2 f(\psi(w)), p_\tau = \nabla f(\psi(w))$
10: for $l = \tau, \ldots, 1$ do
11: Compute $P_{l-1} = \nabla^2_{z_{l-1} z_{l-1}} \phi_l(v_l, z_{l-1})[:, \cdot, \cdot, \lambda_l]$ $p_{l-1} = 0$
12: $Q_l = \nabla^2_{v_l z_{l-1}} \phi_l(v_l, z_{l-1})[:, \cdot, \lambda_l] + \nabla^2 r_l(v_l)$ $q_l = \nabla r_l(v_l)$
13: $R_l = \nabla^2_{z_{l-1} z_{l-1}} \phi_l(v_l, z_{l-1})[:, \cdot, \cdot, \cdot, \cdot, \lambda_l]$ $r_l = \nabla r_l(v_l)$
14: until $\lambda_{l-1} = \nabla_{z_{l-1}} \phi_l(v_l, z_{l-1})\lambda_l$
15: end for

16: **2nd Backward pass:**
17: Initialize $C_\tau = P_\tau, c_\tau = p_\tau, \text{feasible} = True$
18: for $l = \tau, \ldots, 1$ do
19: if $\gamma^{-1} I + Q_l + B_l \top C_l B_l \not\geq 0$ then
20: feasible = False
21: break
22: end if
23: Compute $C_{l-1} = P_{l-1} + A_l \top C_l A_l - (R_l + A_l \top C_l B_l)(\gamma^{-1} I + Q_l + B_l \top C_l B_l)^{-1}(R_l \top + B_l \top C_l A_l)$
24: $c_{l-1} = A_l \top c_l + p_{l-1} - (R_l + A_l \top C_l B_l)(\gamma^{-1} I + Q_l + B_l \top C_l B_l)^{-1}(q_l + B_l \top c_l)$
25: until $\lambda_{l-1} = \nabla_{z_{l-1}} \phi_l(v_l, z_{l-1})\lambda_l$
26: end for
27: if feasible = False then
28: Re-do 2nd backward pass with $\gamma := \gamma/2$
29: end if

30: **Rollout:**
31: Initialize $\hat{z}_0 = 0$
32: for $l = 1, \ldots, \tau$ do
33: $\hat{v}^*_l = K_l \hat{z}_{l-1} + k_l, \quad \hat{z}_l = A_l \hat{z}_{l-1} + B_l \hat{v}_l$
34: end for

35: **Output:** $w_{t+1} = w_t + (\hat{v}^*_1; \ldots; \hat{v}^*_\tau)$
then the Bellman equation reads
\[ \text{cost}_{t-1}(z_{t-1}) = \min_{\hat{v}_t \in \mathbb{R}^n} \left\{ \hat{v}_t^T q_t + \lambda_t^T (A_t z_{t-1} + B_t \hat{v}_t) + \frac{1}{2\gamma} \| \hat{v}_t \|_2^2 \right\} \]
So we get that $\text{cost}_{t-1}$ is a linear function defined by $\lambda_{t-1} = A_t^T \lambda_t$ and that the optimal corresponding parameter is independent of $z_{t-1}$ and reads
\[ \hat{v}_t^* = -\gamma (q_t + B_t^T \lambda_t). \]

**Proof.** The matrices stored during the forward pass are matrices $A_t$ and $B_t$, $q_t$ respectively, where $\lambda_{t-1}$ denotes the time complexity of the backward pass. The backward pass amounts to (i) computing matrix vector products $A_t \hat{v}_t + B_t \hat{v}_t$, (ii) computing matrix vector products $B_t \hat{v}_t$, (iii) computing matrix vector products $A_t \hat{v}_t$, (iv) computing matrix vector products $B_t \hat{v}_t$, (v) computing matrix vector products $A_t \hat{v}_t + B_t \hat{v}_t$, (vi) computing matrix vector products $B_t \hat{v}_t$. The time complexity of the backward pass follows. The time complexity of the backward pass is given by the definition of $T(\phi_t, \nabla \phi_t)$.

**C.3 Complexity of the forward and backward passes**

We first detail the generic complexity of the forward-backward passes.

**Proposition 3.3.** The space and time complexities of the forward and backward passes, Algo. 1, Algo. 2, are of the order of
\[ S = \sum_{l=1}^\tau (\rho_l + \delta_{l-1}) \delta_l, \quad T = \sum_{l=1}^\tau T(\phi_l, \nabla \phi_l) + 2 \sum_{l=1}^\tau (\delta_{l-1} \delta_l + \rho_l \delta_l), \]
respectively, where $T(\phi_l, \nabla \phi_l)$ is the time complexity of computing $\phi_l$, $\nabla \phi_l$ during the forward pass, $T_F$ denotes the time complexity of the forward pass and $T_B$ denotes the time complexity of the backward pass.

**Proof.** The matrices stored during the forward pass are $\nabla \phi_l(v_l, z_{l-1}) \in \mathbb{R}^{(\rho_l + \delta_{l-1}) \times \delta_l}$ for $l \in \{1, \ldots, \tau\}$. The space complexity of the forward-backward passes follows. The backpass amounts to (i) computing matrix vector products $\nabla z_{l-1} \phi_l(v_l, z_{l-1}) \lambda_l$ for $l \in \{1, \ldots, \tau\}$, each costing $2 \delta_{l-1} \delta_l$, (ii) computing matrix vector products $\nabla v_l \phi_l(v_l, z_{l-1}) \lambda_l$ for $l \in \{1, \ldots, \tau\}$, each costing $2 \rho_l \delta_l$. The time complexity of the backward pass follows. The time complexity of the forward pass is given by the definition of $T(\phi_l, \nabla \phi_l)$.

**Sparsity of the inner operations.**

**Definition C.3 (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 $B[x, y, z]$, $B[x, y, z]$, $B[x, y, z]$ or $B[x, y, z]$, which gives us the sparsity of the two bilinear operations studied in this paper.

**Fact C.4.** For a matrix-product as in (8), we have $s_\beta = m d d$. For a convolution as in (9), we have $s_\beta = m n p n f s f$.

We considered $\Pi_k Z_{t-1}$ 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 $\nabla_{x_{l-1}} \beta_l(v_l, z_{l-1}) \lambda_{t+1}$ or $\nabla_{x_{l-1}} \beta_l(v_l, z_{l-1}) \lambda_{t+1}$ for $\lambda_{t+1} \in \mathbb{R}^n$.

The sparsity of a function $f \in \mathbb{R}^d \rightarrow \mathbb{R}^n$ naturally gives the number of multiplications needed to compute gradient-vector 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 $s_\alpha = m d$, where we consider the input of the activation function to be $z = \text{Vec}(Z)$ for $Z \in \mathbb{R}^{m \times d}$. 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 Cor. 3.4 follow.
Proposition C.5. Consider a chain \( \psi \) of \( \tau \) layers as defined in Def. 2.1 whose layers \( \psi_l \) are defined by \( a_l, b_l \) as in (7). The time complexity of the backward pass defined in Algo. 2 is of the order of

\[
T_B = \mathcal{O} \left( \sum_{l=1}^{\tau} s_{a_l} + 2s_{\beta_l} + s_{\beta_l^r} \right)
\]

elementary operations, where \( s_f \) is the sparsity of an operation \( f \) as defined in Def. C.3.

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

\[
\nabla_{z_{l-1}} \psi_l(v_l, z_{l-1}) \lambda_{l+1} = \nabla_{z_{l-1}} b_l(v_l, z_{l-1}) \nabla a_l(\omega_l) \lambda_{l+1} = (B_l[v_l, \cdot, \cdot] + \nabla \beta_l^r(z_{l-1})) \nabla a_l(\omega_l) \lambda_{l+1},
\]

\[
\nabla_{v_l} \psi_l(v_l, z_{l-1}) \lambda_{l+1} = \nabla_{v_l} b_l(v_l, z_{l-1}) \nabla a_l(\omega_l) \lambda_{l+1} = (B_l[v_l, z_{l-1}, \cdot] + \nabla \beta_l^r(v_l)) \nabla a_l(\omega_l) \lambda_{l+1},
\]

where \( \omega_l = b_l(v_l, z_{l-1}) \). The definitions of the sparsity of bilinear or general operations give the result by looking at each operation starting from the right. \( \square \)

C.4 Gauss-Newton by automatic differentiation

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

Lemma C.6 ((Roulet et al. 2019, Lemma 3.4)). Given a differentiable chain of composition \( \psi : R^p \rightarrow R^q \) as defined in Def. 2.1, a variable \( w \) and a decomposable differentiable function \( g : \mathbb{R}^p \rightarrow \mathbb{R} \) such that \( g(w) = \sum_{l=1}^{\tau} g_l(w_l) \) for \( w = (v_1; \ldots; v_\tau) \), computing the derivative of \( \mu \rightarrow g(\nabla \psi(w)\mu) \) requires two calls to an automatic-differentiation procedure.

Proposition 3.5. Consider the Gauss-Newton-step (13) on \( w_t = (v_1; \ldots; v_\tau) \) for a convex objective \( f \), a convex decomposable regularization \( r(w) = \sum_{l=1}^{\tau} r_l(w_l) \) and a differentiable chain of computations \( \psi \). We have that

1. the Gauss-Newton-step amounts to solving

\[
\min_{\mu \in \mathbb{R}^q} \tilde{q}_f^*(\mu) + \tilde{q}_r^*(-\nabla \psi(w_t)\mu), \tag{18}
\]

where \( \tilde{q}_f(y) = q_f(\psi(w_t) + y; \psi(w_t)) \), \( \tilde{q}_r(w) = q_r(w_t + w; w_t) + \|w\|^2/2 \) and for a function \( f \) we denote by \( f^* \) its convex conjugate,

2. the Gauss-Newton-step reads \( w_{t+1} = w_t + \nabla \tilde{q}^*_r(-\nabla \psi(w_t)\mu^*) \) where \( \mu^* \) is the solution of (18),

3. the dual problem (18) can be solved by 2\( q \) + 1 calls to an automatic differentiation procedure.

Proof. The first and second claims follow from standard duality computations applied to (28), they require convexity of \( f \) and \( r \). The third claim comes from the fact that (18) is a quadratic convex problem that can be solved in at most \( q \) iterations of a conjugate gradient descent. Each iteration requires to compute the gradient of \( z \rightarrow \tilde{q}^*_r(-\nabla \psi(w)\mu) \) which requires two calls to an automatic differentiation procedure by Lemma C.6 and using that \( r^* \) is also decomposable. A last call to an automatic differentiation procedure is needed to compute \( \nabla \psi(w)\mu^* \). The costs of computing \( \nabla \tilde{q}^*_f(\mu) \) for \( \mu \in \mathbb{R}^q \) and \( \nabla \tilde{q}^*_r(w) \) for \( w \in \mathbb{R}^q \) are ignored since they do not involve a chain of compositions and are assumed to be easily accessible. \( \square \)

D Optimization complexity proofs

D.1 Smoothness of the objective

Proposition D.1. Consider a closed convex set \( C \subset \mathbb{R}^p, \psi \in \mathcal{C}_{w_C, \ell_C}^r \mathcal{L}_C^r, r \in \mathcal{C}_r, \) and \( f \in \mathcal{C}_f \) with \( \ell_f = +\infty \) if \( f \) is not Lipschitz-continuous. The smoothness of \( F = f \circ \psi + r \) on \( C \) is bounded as

\[
\mathcal{L}_C^C \leq \mathcal{L}_\psi^C \mathcal{L}_f^C + (\mathcal{L}_C^r)^2 L_f + L_r,
\]

where \( \mathcal{L}_f^C = \min\{\ell_f, \min_{x \in \psi(C)} \|\nabla f(z)\|_2 + L_f \mathcal{L}_\psi^C D_C \} \), where \( D_C = \sup_{x, y \in C} \|x - y\|_2 \).
Proof. Consider \( f, \psi \) to be twice differentiable. Same results can be obtained by considering differences of gradients. We get for \( w \in \mathbb{R}^p, \)

\[
\nabla^2 (f \circ \psi)(w) = \nabla^2 \psi(w)[\nabla f(\psi(w)) + \nabla \psi(w)] + \nabla \psi(w) \nabla^2 f(\psi(w)) \nabla \psi(w)^T.
\]

The norm of \( \nabla f(\psi(w)) \) can either be directly bounded by \( \ell_\psi \) or by using that for any \( w, w' \in C, \| \nabla f(\psi(w)) \|_2 \leq \| \nabla f(\psi(w')) \|_2 + L_f \| \psi(w) - \psi(w') \|_2. \) By choosing \( w' = \arg \min_{w' \in C} \| \nabla f(\psi(w)) \|_2 \) and bounding the second term by the diameter of \( C, \) we get a bound on \( \sup_{w \in C} \| \nabla f(\psi(w)) \|_2. \) The result follows using Fact. A.3 and the definitions of the norms used to bound \( \ell_f, L_f \) for a given function \( f. \)

D.2 Smoothness of chain of layers

**Proposition 4.3.** Consider a chain \( \psi \) of \( \tau \) computations as defined in Def. 2.1, by layers \( \phi_l \in C_{\ell_{\phi_l}}, L_{\phi_l}. \)

(i) An upper-bound on the Lipschitz-continuity of the chain \( \psi \) is given by \( \ell_\psi = \ell_\tau, \) where for \( l \in \{1, \ldots, \tau\}, \)

\[
\ell_l = \ell_{\phi_l} + \ell_{\phi_{l-1}}, \quad \ell_0 = 0.
\]

(ii) An upper-bound on the smoothness of the chain \( \psi \) is given by \( L_\psi = L_\tau, \) where for \( l \in \{1, \ldots, \tau\}, \)

\[
L_l = L_{l-1} \ell_{\phi_l} + L_{\phi_l}(1 + \ell_{l-1})^2, \quad L_0 = 0.
\]

**Proof.** For \( w = (v_1; \ldots; v_\tau), \) define

\[
\hat{z}_l(w) = \phi_l(v_l, \hat{z}_{l-1}(w)), \quad \text{for } l = 1, \ldots, \tau,
\]

with \( \hat{z}_0(w) = x. \) We can bound the gradients obtained in Eq. (31) to get

\[
\ell_{\hat{z}_l} \leq \ell_{\phi_l} + \ell_{\hat{z}_{l-1}} \ell_{\phi_l},
\]

with \( \ell_{\hat{z}_0} = 0. \) To compute the smoothness of the function we bound the Hessians. If the functions are not twice differentiable, the same results can be obtained by considering differences of gradients. From Eq. (33), we get

\[
\begin{align*}
L_{\hat{z}_l} & \leq L_{\phi_l} + L_{\phi_l} \ell_{\hat{z}_{l-1}} + \ell_{\hat{z}_{l-1}} L_{\phi_l} + \ell_{\hat{z}_l} \ell_{\phi_l} L_{\phi_l} L_{\hat{z}_{l-1}} L_{\phi_l} \\
& = L_{\phi_l} + 2 L_{\phi_l} \ell_{\hat{z}_{l-1}} + L_{\phi_l} (\ell_{\hat{z}_{l-1}})^2 + L_{\hat{z}_{l-1}} L_{\phi_l},
\end{align*}
\]

with \( L_{\hat{z}_0} = 0. \) The Lipschitz-continuity and the smoothness of the chain are given by \( \ell_{\hat{z}} \) and \( L_{\hat{z}}, \) respectively.

**Lemma D.2.** Consider

\[
a = a_k \circ \ldots \circ a_1
\]

with \( a_j \in C_{m_j, \ell_{a_j}, L_{a_j}} \) 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 \( j \in \{1, \ldots, k\}, \)

\[
\begin{align*}
\hat{m}_j(R) & = \min\{ m_{a_j}, \| a_j(0) \|_2 + \ell_{a_j} \hat{m}_{j-1}(R), \| a_j(0) \|_2 + (\| \nabla a_j(0) \|_2 + L_{a_j} \hat{m}_{j-1}(R)) \hat{m}_{j-1}(R) \} \\
\hat{\ell}_j(R) & = \min\{ \ell_{a_j}, \| \nabla a_j(0) \|_2, \ell_{a_j} \hat{m}_{j-1}(R) \}
\end{align*}
\]

with \( \hat{m}_0(R) = R. \) We have

\[
\begin{align*}
m^B_a & \leq \hat{m}_k(R), \\
\ell^B_a & \leq \prod_{j=1}^k \hat{\ell}_j(R), \\
L^B_a & \leq \sum_{j=1}^k L_{a_j} \left( \prod_{i=1}^{j-1} \hat{\ell}_i(R) \right)^2 \left( \prod_{i=j+1}^k \hat{\ell}_i(R) \right).
\end{align*}
\]

Therefore \( a \) is bounded on \( B_R \) if \( \forall i \in \{1, \ldots, k\} \) \( m_{a_i}, \ell_{a_i} \) or \( L_{a_i} \) is finite, it is Lipschitz-continuous on \( B_R \) if \( \forall i \in \{1, \ldots, k\} \) \( \ell_{a_i} \) or \( L_{a_i} \) is finite and it is smooth on \( B_R \) if \( \forall i \in \{1, \ldots, k\} \) \( L_{a_i} \) is finite.
Proof. Denote

\[
m_{a_j\circ\cdots\circ a_1}^{BR} = \sup_{x \in \mathbb{R}^d, \|x\|_2 \leq R} \|a_j \circ \cdots \circ a_1(x)\|_2 \quad \text{for } j \in \{1, \ldots, k\}.
\]

We have for \( j = 1, \ldots, k, \)

\[
m_{a_j\circ\cdots\circ a_1}^{BR} \leq \min\{m_{a_j}, \|a_j(0)\|_2 + \ell_{a_j} m_{a_{j-1}\circ\cdots\circ a_1}^{BR}, \|a_j(0)\|_2 + (\|\nabla a_j(0)\|_{2,2} + L_{a_j} m_{a_{j-1}\circ\cdots\circ a_1}^{BR}) m_{a_{j-1}\circ\cdots\circ a_1}^{BR}\},
\]

where \( m_{id}^{BR} = R, \) which gives

\[
m_{a_j\circ\cdots\circ a_1}^{BR} \leq \tilde{m}_j(R),
\]

where for \( j = 1, \ldots, k, \)

\[
\tilde{m}_j(R) = \min\{m_{a_j}, \|a_j(0)\|_2 + \ell_{a_j} \tilde{m}_{j-1}(R), \|a_j(0)\|_2 + (\|\nabla a_j(0)\|_{2,2} + L_{a_j} \tilde{m}_{j-1}(R)) \tilde{m}_{j-1}(R)\},
\]

with \( \tilde{m}_0(R) = R \) and in particular \( m_{a_j}^{BR} = \tilde{m}_k(R). \) We have for \( x \in \mathbb{R}^d, \)

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

We have

\[
\sup_{x \in \mathbb{R}^d, \|x\|_2 \leq R} \|g_j(x)\|_{2,2} \leq \min\{\ell_{a_j}, \|\nabla a_j(0)\|_{2,2} + L_{a_j} m_{a_{j-1}\circ\cdots\circ a_1}^{BR}\}.
\]

Therefore

\[
\ell_{a_j}^{BR} \leq \prod_{j=1}^{k} \tilde{\ell}_j(R),
\]

where

\[
\tilde{\ell}_j(R) = \min\{\ell_{a_j}, \|\nabla a_j(0)\|_{2,2} + L_{a_j} \tilde{m}_{j-1}(R)\} \quad \text{for } j \in \{1, \ldots, k\}.
\]

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

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

Therefore

\[
L_{a_j}^{BR} \leq \sum_{j=1}^{k} L_{a_j} \left( \prod_{i=1}^{j-1} \tilde{\ell}_i(R) \right)^2 \left( \prod_{i=j+1}^{k} \tilde{\ell}_i(R) \right).
\]

\[
\Box
\]

**Proposition 4.4.** Consider a chain \( \psi \) of \( \tau \) computations as defined in Def. 2.1 whose layers \( \phi_l \) for \( l \in \{1, \ldots, \tau\} \) are defined by

\[
\phi_l(v_l, z_{l-1}) = a_l(b_l(v_l, z_{l-1})),
\]

where \( b_l \) is decomposed as

\[
b_l(v_l, z_{l-1}) = \beta_l(v_l, z_{l-1}) + \beta_l^t(v_l) + \beta_l^v(z_{l-1}) + \beta_l^0,
\]

with \( \beta_l \in \mathcal{B}L_{\ell_{B1}}, \beta_l^t \in \mathcal{B}L_{\ell_{B2}}, \beta_l^v \in \mathcal{B}L_{\ell_{B3}}, \beta_l^0 \) is a constant vector, and \( a_l \) is decomposed as

\[
a_l = a_{t1} \circ \cdots \circ a_{t1},
\]

with \( a_{t1} \in \mathcal{C}_{\ell_{B1}, \ell_{B2}, \ell_{B3}}. \) Consider \( C = \{w = (v_1; \ldots; v_\tau) \in \mathbb{R}^p : \forall l \in \{1, \ldots, \tau\}, \|v_l\| \leq R\}. \)
(i) An upper-bound on the output of the chain $\psi$ on $C$ is given by $m^c_{\psi} \leq m_\tau$ where for $l \in \{1, \ldots, \tau\}$,

$$m_l = m_{l,k_l},$$

$$m_{l,j} = \min\{m_{a_{l,j}}, \|a_{l,j}(0)\|_2 + \ell_{a_{l,j}}, m_{l,j-1}, \|a_{l,j}(0)\|_2 + (\|\nabla a_{l,j}(0)\|_2, 2 + L_{a_{l,j}} m_{l,j-1}) \} \text{ for } j = 1, \ldots, k_l,$$

$$m_{l,0} = L_{\beta_l} R m_{l-1} + \ell_{\beta_l} R + \ell_{\beta_l} m_{l-1} + \|\beta_0\|_2,$$

$$m_0 = \|x\|_2.$$

(ii) An upper-bound on the Lipschitz-continuity of the chain $\psi$ on $C$ is given by $\ell_{\psi}(C) \leq \ell_\tau$, where for $l \in \{1, \ldots, \tau\}$,

$$\ell_l = \left(\prod_{j=1}^{k_l} \ell_{l,j}\right) \left( (L_{\beta_l} R + \ell_{\beta_l}^2) + \ell_{l-1} L_{\beta_l} + \ell_{\beta_l} \right)$$

$$\ell_{l,j} = \min\{\ell_{a_{l,j}}, \|\nabla a_{l,j}(0)\|_2, 2 + L_{a_{l,j}} m_{l,j-1}\}, \text{ for } j = 1, \ldots, k_l,$$

$$\ell_0 = 0.$$

(iii) An upper-bound on the smoothness of the chain $\psi$ on $C$ is given by $L_{\psi}(C) \leq L_\tau$, where for $l \in \{1, \ldots, \tau\}$,

$$L_l = L_{l-1} (L_{\beta_l} R + \ell_{\beta_l}^2) \left(\prod_{j=1}^{k_l} \ell_{l,j}\right) + \ell_{l-1} \left( L_{\beta_l} + \ell_{\beta_l} \right),$$

$$L_{l,k_l} = \left( \sum_{j=1}^{k_l} L_{a_{l,j}} \left( \prod_{i=1}^{j-1} \ell_{l,i} \right)^2 \right)^{1/2} \left( \prod_{i=1}^{k_l} \ell_{l,i} \right).$$

**Proof.** For $w = (v_1; \ldots; v_\tau)$, define

$$\tilde{z}_l(w) = a_l(\zeta_l(w)), \text{ for } l = 1, \ldots, \tau,$$

$$\zeta_l(w) = b_l(v_l, \tilde{z}_{l-1}(w)), \text{ for } l = 1, \ldots, \tau,$$

with $\tilde{z}_0(w) = x$. Denote $B_l$ the tensor defining $\beta_l$ and $B_l^x$, $B_l^{\ell}$ the matrices defining $\beta_l^x$ and $\beta_l^{\ell}$ respectively. By assumption, we have $\|B_l\|_2, 2 = L_{\beta_l}$ (see Prop. A.5), $\|B_l^x\|_2, 2 = \ell_{\beta_l}^x$, $\|B_l^{\ell}\|_2, 2 = \ell_{\beta_l}^{\ell}$. For $l \in \{1, \ldots, \tau\}$, denote as in Lemma (D.2), for $j \in \{1, \ldots, k_l\}$,

$$\tilde{m}_{l,j}(R') = \min\{m_{a_{l,j}}, \|a_{l,j}(0)\|_2 + \ell_{a_{l,j}} \tilde{m}_{l,j-1}(R')\},$$

$$\ell_{l,j}(R') = \min\{\ell_{a_{l,j}}, \|\nabla a_{l,j}(0)\|_2 + L_{a_{l,j}} \tilde{m}_{l,j-1}(R')\}.$$

with $\tilde{m}_{l,0}(R') = R'$.

We have, using Lemma C.6,

$$m^c_{\tilde{z}_l} = m^c_{a_l}(C) \leq \tilde{m}_{l,k_l} \left( \sup_{w \in C} \|\zeta_l(w)\|_2 \right) \leq \tilde{m}_{l,k_l} (L_{\beta_l} R m^c_{\tilde{z}_{l-1}} + \ell_{\beta_l} R + \ell_{\beta_l} m^c_{\tilde{z}_{l-1}} + \|\beta_0\|_2).$$

Denoting

$$m_l = \tilde{m}_{l,k_l} (L_{\beta_l} R m_{l-1} + \ell_{\beta_l} R + \ell_{\beta_l} m_{l-1} + \|\beta_0\|_2),$$

with $m_0 = \|x\|_2$, we get $m^c_{\tilde{z}_l} \leq m_l$ and in particular $m^c_{\psi} \leq m_\tau$.

The gradients of the dynamics are given by (dropping the dependency w.r.t. the layer in the gradient notations in
the following)

\[
\nabla_v \phi_l(v_l, z_{l-1}) = (B_l[\cdot, z_{l-1}, \cdot] + B_{\beta_l}^v)\nabla a_l(\omega_l),
\]

\[
\nabla_z \phi_l(v_l, z_{l-1}) = (B_l[v_l, \cdot, \cdot] + B_{\beta_l}^z)\nabla a_l(\omega_l),
\]

where we denoted \( \omega_l = b_l(v_l, z_{l-1}) \). Therefore for \( v_l \in \mathbb{R}^m \) such that \( \|v_l\|_2 \leq R \) and \( z_{l-1} \in \tilde{z}_{l-1}(C) \), we get

\[
\|\nabla_v \phi_l(v_l, z_{l-1})\|_2 \leq (m_{\omega_l}^C L_{\beta_l} + \ell_{\beta_l}^z)\ell_{\alpha_l}^C(C),
\]

\[
\|\nabla_z \phi_l(v_l, z_{l-1})\|_2 \leq (R L_{\beta_l} + \ell_{\beta_l}^v)\ell_{\alpha_l}^C(C).
\]

Plugging this into Eq. (31), we get for any \( l \in \{1, \ldots, \tau\} \), denoting \( \ell_{20} = 0 \),

\[
\ell_{C_l}^C \leq \ell_{\alpha_l}^C(C) \left( (R L_{\beta_l} + \ell_{\beta_l}^v)\ell_{\alpha_l}^C(C) + m_{\omega_l}^C L_{\beta_l} + \ell_{\beta_l}^z \right).
\]

Now we have by Lemma D.2

\[
\ell_{\alpha_l}^C(C) \leq \left( \prod_{j=1}^{k_l} \ell_{j,l}(L_{\beta_l} R m_{\tilde{z}_{l-1}}^C + \ell_{\beta_l}^z R + \ell_{\beta_l}^v m_{\tilde{z}_{l-1}}^C + \|\beta_0^l\|_2) \right).
\]

Therefore, denoting

\[
\ell_l = \left( \prod_{j=1}^{k_i} \ell_{j,l}(L_{\beta_l} R m_{\tilde{z}_{l-1}}^C + \ell_{\beta_l}^z R + \ell_{\beta_l}^v m_{\tilde{z}_{l-1}}^C + \|\beta_0^l\|_2) \right) \left( (R L_{\beta_l} + \ell_{\beta_l}^v)\ell_{l-1} + m_{l-1} L_{\beta_l} + \ell_{\beta_l}^z \right),
\]

with \( \ell_0 = 0 \), we get \( \ell_{C_l}^C \leq \ell_l \) and in particular \( \ell_{C_{\tau}}^C \leq \ell_{\tau} \).

Finally we consider the Hessians of the dynamics. The claims of the proposition can also be obtained by looking at the difference of the gradients. We have

\[
\nabla^2_{vv} \phi_l(v_l, z_{l-1}) = \nabla^2 a_l(\omega_l)((B_l[\cdot, z_{l-1}, \cdot] + B_{\beta_l}^v)^T, (B_l[\cdot, z_{l-1}, \cdot] + B_{\beta_l}^v)^T, \cdot),
\]

\[
\nabla^2_{zz} \phi_l(v_l, z_{l-1}) = \nabla^2 a_l(\omega_l)((B_l[v_l, \cdot, \cdot] + B_{\beta_l}^z)^T, (B_l[v_l, \cdot, \cdot] + B_{\beta_l}^z)^T, \cdot) + B_l[\cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot],
\]

\[
\nabla^2_{vz} \phi_l(v_l, z_{l-1}) = \nabla^2 a_l(\omega_l)((B_l[v_l, \cdot, \cdot] + B_{\beta_l}^z)^T, (B_l[v_l, \cdot, \cdot] + B_{\beta_l}^z)^T, \cdot) + B_l[\cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot, \cdot],
\]

Therefore for \( v_l \in \mathbb{R}^m \) such that \( \|v_l\|_2 \leq R \) and \( z_{l-1} \in \tilde{z}_{l-1}(C) \),

\[
\|\nabla^2_{vv} \phi_l(v_l, z_{l-1})\|_{2,2,2} \leq (L_{\beta_l} m_{\tilde{z}_{l-1}}^C + \ell_{\beta_l}^z)^2 L_{\alpha_l}^C(C),
\]

\[
\|\nabla^2_{zz} \phi_l(v_l, z_{l-1})\|_{2,2,2} \leq (L_{\beta_l} R + \ell_{\beta_l}^v)(L_{\beta_l} m_{\tilde{z}_{l-1}}^C + \ell_{\beta_l}^z) L_{\alpha_l}^C(C),
\]

\[
\|\nabla^2_{vz} \phi_l(v_l, z_{l-1})\|_{2,2,2} \leq (L_{\beta_l} m_{\tilde{z}_{l-1}}^C + \ell_{\beta_l}^z)(L_{\beta_l} R + \ell_{\beta_l}^v) L_{\alpha_l}^C(C) + L_{\beta_l} \ell_{\alpha_l}^C(C),
\]

\[
\|\nabla^2_{zz} \phi_l(v_l, z_{l-1})\|_{2,2,2} \leq (L_{\beta_l} R + \ell_{\beta_l}^v)^2 L_{\alpha_l}^C(C).
\]

Plugging this is Eq. (33), we get, denoting \( L_{20} = 0 \),

\[
L_{\tilde{z}_{l+1}}^{\alpha} \leq \left( L_{\tilde{z}_{l-1}}^{\alpha} + (R L_{\beta_l} + \ell_{\beta_l}^z)\ell_{\alpha_l}^C(C) \right) + (L_{\beta_l} R + \ell_{\beta_l}^v)^2 L_{\alpha_l}^C(C)(\ell_{\tilde{z}_{l-1}}^{\alpha})^2,
\]

\[
+ 2((L_{\beta_l} m_{\tilde{z}_{l-1}}^{\alpha} + \ell_{\beta_l}^z)(L_{\beta_l} R + \ell_{\beta_l}^v) L_{\alpha_l}^C(C) + L_{\beta_l} \ell_{\alpha_l}^C(C))\ell_{\tilde{z}_{l-1}}^{\alpha} + (L_{\beta_l} m_{\tilde{z}_{l-1}}^{\alpha} + \ell_{\beta_l}^z)^2 L_{\alpha_l}^C(C).
\]

The result follows using Lemma D.2 and \( m_{\tilde{z}_{l+1}}^{\alpha} \leq m_l, \ell_{\tilde{z}_{l+1}} \leq \ell_l \).

\[\square\]

**Corollary 4.5.** Consider a chain \( \psi \) of \( \tau \) computations as defined in Prop. 4.4 and \( w^* = (v_1^*; \ldots; v_{\tau}^*) \in \mathbb{R}^p \). The smoothness properties of \( \psi \) on \( C' = \{ w = (v_1; \ldots; v_{\tau}) \in \mathbb{R}^p : \forall l \in \{1, \ldots, \tau\}, \|v_l - v_l^*\| \leq R' \} \) are given as in
Prop. 4.4 by considering

\[ R' \text{ in place of } R, \]
\[ \ell_{\beta^*_l} + L_{\beta^*_l} \|v^*_l\|_2 \text{ in place of } \ell_{\beta^*_l}, \]
\[ \|\beta^{0}_l\|_2 + \ell_{\beta^*_l} \|v^*_l\|_2 \text{ in place of } \|\beta^{0}_l\|_2. \]

Proof. The smoothness properties of \( \hat{\psi} \) on \( C' \) are given by considering \( \hat{\psi}(\Delta) = \psi(w^* + \Delta) = \psi(w) \) where \( \Delta = w - w^* \) with \( \|\Delta\|_2 \leq R' \). Defining, as previously,

\[ \tilde{z}_l(w) = \phi_l(v_l, \tilde{z}_{l-1}(w)), \quad \text{for } l = 1, \ldots, \tau. \]

with \( \tilde{z}_0(w) = x \), and denoting \( \hat{z}_l(\Delta) = \hat{z}_l(w^* + \Delta) = \hat{z}_l(w) \), we get

\[ \hat{\psi}(\Delta) = \hat{z}_\tau(\Delta) \]
\[ \text{where } \hat{z}_l(\Delta) = a_l(b_l(v^*_l + \Delta_l, \hat{z}_{l-1}(\Delta))). \]

This means that \( \hat{\psi}(\Delta) \) is a chain of compositions defined by the same non-linearities \( a_l \) and by bi-affine functions \( b_l \) modified as

\[ \hat{b}_l(\Delta, z_{l-1}) = b_l(v^*_l + \Delta_l, z_{l-1}) \]
\[ = \beta_l(\Delta_l, z_{l-1}) + \beta^{0}_l(\Delta_l), \]

where

\[ \beta^{0}_l(\Delta) = \beta^{0}_l(z_{l-1}) + \beta_l(v^*_l, z_{l-1}) \quad \hat{\beta}^{0}_l = \hat{\beta}^{0}_l + \beta^{*}_l(v^*_l). \]

\( \square \)