

Automatic Differentiation of Optimization Algorithms with Time-Varying Updates

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Abstract

Numerous Optimization Algorithms have a time-varying update rule thanks to, for instance, a changing step size, momentum parameter or, Hessian approximation. In this paper, we apply unrolled or automatic differentiation to a time-varying iterative process and provide convergence (rate) guarantees for the resulting derivative iterates. We adapt these convergence results and apply them to proximal gradient descent with variable step size and FISTA when solving partly smooth problems. We confirm our findings numerically by solving ℓ_1 and ℓ_2 -regularized linear and logistic regression respectively. Our theoretical and numerical results show that the convergence rate of the algorithm is reflected in its derivative iterates.

1 Introduction

For some parameter $\mathbf{u} \in \mathcal{U}$, we consider the following parametric iterative process

$$\mathbf{x}^{(k+1)}(\mathbf{u}) := \mathcal{A}(\mathbf{x}^{(k)}(\mathbf{u}), \mathbf{u}), \quad (\mathcal{R})$$

for $k \geq 0$, where $\mathbf{x}^{(0)} \in \mathcal{X}$ is the initial iterate and $\mathcal{A}: \mathcal{X} \times \mathcal{U} \rightarrow \mathcal{X}$ is the update mapping. The iterates $\mathbf{x}^{(k)}(\mathbf{u})$ generated by (\mathcal{R}) depend on \mathbf{u} due to the dependence of \mathcal{A} on \mathbf{u} . The goal of performing the iterations (\mathcal{R}) is mainly to solve the non-linear equation

$$\mathbf{x} = \mathcal{A}(\mathbf{x}, \mathbf{u}), \quad (\mathcal{R}_e)$$

with respect to \mathbf{x} for each parameter \mathbf{u} . A simple example is gradient descent with appropriate step size $\alpha > 0$ where we define $\mathcal{A}(\mathbf{x}, \mathbf{u}) := \mathbf{x} - \alpha \nabla_{\mathbf{x}} F(\mathbf{x}, \mathbf{u})$ for solving a parametric optimization problem of the form

$$\min_{\mathbf{x} \in \mathcal{X}} F(\mathbf{x}, \mathbf{u}), \quad (\mathcal{P})$$

with a smooth objective $F: \mathcal{X} \times \mathcal{U} \rightarrow \mathbb{R}$. In this case (\mathcal{R}_e) reduces to the optimality condition $\nabla_{\mathbf{x}} F(\mathbf{x}, \mathbf{u}) = 0$.

Often in practice, for some smooth $\ell: \mathcal{X} \times \mathcal{U} \rightarrow \mathbb{R}$, we encounter problems of the form

$$\min_{\mathbf{u} \in \mathcal{U}} \ell(\psi(\mathbf{u}), \mathbf{u}). \quad (1)$$

where, given any $\mathbf{u} \in \mathcal{U}$, $\psi(\mathbf{u})$ is a solution of (\mathcal{R}_e) or (\mathcal{P}) . This kind of optimization, formally known as bilevel optimization [21, 22] has emerged as a crucial tool in machine learning, playing a foundational role in various applications such as hyperparameter optimization [10, 24, 44], implicit neural networks [4, 3, 5, 6, 60], meta-learning [33], and neural architecture search [42].

Solving (1) through gradient-based methods requires computing the gradient of the upper objective $\ell(\psi(\mathbf{u}), \mathbf{u})$ with respect to \mathbf{u} which, in turn, requires computing the derivative of the solution mapping $\mathbf{u} \mapsto \psi(\mathbf{u})$, that is, $D\psi(\mathbf{u})$ by using the chain rule. When ℓ and F (or \mathcal{A}) satisfy certain smoothness and regularity assumptions, this can be achieved by two different methods. (i) One is known as *Implicit Differentiation* (ID) which leverages the classical Implicit Function Theorem or IFT [25, Theorem 1B.1] applied to (\mathcal{R}_e) to estimate

$$\begin{aligned} D\psi(\mathbf{u}) &= (I - D_{\mathbf{x}}\mathcal{A}(\mathbf{x}, \mathbf{u}))^{-1} D_{\mathbf{x}}\mathcal{A}(\mathbf{x}, \mathbf{u}) \\ &= -\nabla_{\mathbf{x}}^2 F(\mathbf{x}, \mathbf{u})^{-1} D_{\mathbf{u}}\nabla_{\mathbf{x}}F(\mathbf{x}, \mathbf{u}), \end{aligned} \quad (2)$$

where $\mathbf{x} := \psi(\mathbf{u})$ (see Theorem 28 for more details). The key assumption for IFT is the strict bound on the spectral radius $\rho(D_{\mathbf{x}}\mathcal{A}(\psi(\mathbf{u}), \mathbf{u})) < 1$, which we call the contraction property since it is a sufficient condition for \mathcal{A} to be 1-Lipschitz or contractive. A direct consequence is the linear convergence of $\mathbf{x}^{(k)}(\mathbf{u})$ to $\psi(\mathbf{u})$ [51, Section 2.1.2, Theorem 1]. The output of ID (2) depends on accurately solving (\mathcal{R}_e) — possibly through (\mathcal{R}) — and inverting the linear system efficiently. (ii) The other technique is known as *Unrolled, Iterative or Automatic Differentiation* (AD) or simply *Unrolling* where $D\psi(\mathbf{u})$ is estimated by applying automatic differentiation [59, 39, 32] to the output $\mathbf{x}^{(K)}(\mathbf{u})$ of (\mathcal{R}) after $K \in \mathbb{N}$ iterations. The update rule for forward mode AD applied to $\mathbf{x}^{(K)}$ is given by

$$D\mathbf{x}^{(k+1)}(\mathbf{u}) := D_{\mathbf{x}}\mathcal{A}(\mathbf{x}^{(k)}(\mathbf{u}), \mathbf{u})D\mathbf{x}^{(k)}(\mathbf{u}) + D_{\mathbf{u}}\mathcal{A}(\mathbf{x}^{(k)}(\mathbf{u}), \mathbf{u}), \quad (\mathcal{DR})$$

for $0 \leq k < K$ where we may assume $D\mathbf{x}^{(0)}(\mathbf{u}) = 0$. The effective use of AD relies on the guarantee that $D\mathbf{x}^{(K)}(\mathbf{u})$ accurately estimates $D\psi(\mathbf{u})$ for a preferably small K . More formally, we require the convergence of $D\mathbf{x}^{(K)}(\mathbf{u})$ to $D\psi(\mathbf{u})$ as $K \rightarrow \infty$, with a convergence rate comparable to that of $\mathbf{x}^{(k)}(\mathbf{u})$. The reverse mode AD or Backpropagation [55, 7] has a different update rule, however, the result computed is the same in the end [32]. Due to the nature of the iterations (\mathcal{DR}) , we will use $\mathbf{x}^{(K)}$ and $\mathbf{x}^{(k)}$ interchangeably.

The reverse mode AD has a memory overhead since it requires storing the iterates $(\mathbf{x}^{(k)})_{0 \leq k < K}$. Even though this is in contrast with ID which only depends on $\mathbf{x}^{(K)}$, AD is still a popular choice for estimating $D\psi(\mathbf{u})$. A crucial advantage of AD is that it provides a nice blackbox implementation thanks to the powerful autograd libraries included in PyTorch [49], TensorFlow [1], and JAX [17] whereas ID requires either a custom implementation [16, see Remark 2] or using special libraries [12, 52, etc.].

1.1 Convergence of Automatic Differentiation

The convergence of the derivative sequence $D\mathbf{x}^{(k)}(\mathbf{u})$ for AD of (\mathcal{R}) were studied classically for linear [27] and general iteration maps [30]. More recently, the convergence analysis was provided for gradient descent [43, 45], the Heavy-ball method [45], proximal gradient descent for lasso-like problems [11], the Sinkhorn-Knopp algorithm [50], and super-linearly convergent algorithms [16]. The convergence results were extended to non-smooth iterative processes in [15] using conservative calculus [13, 14]. Ablin et al. [2] theoretically established the better convergence rate for computing the gradient of the value function through AD and ID. Usually, the proof of convergence of $D\mathbf{x}^{(k)}(\mathbf{u})$ relies on the contraction property in each of the above works with an exception of [50]. The linear rate of convergence requires (local) Lipschitz continuity of $D\mathcal{A}$. A slightly different line of study on the problematic behaviour of automatic differentiation in the earlier iterations was carried out in [56].

1.2 Iteration-Dependent Updates

Most iterative algorithms for solving (\mathcal{P}) which include gradient descent with line search, Nesterov’s accelerated gradient [48], and Quasi-Newton methods [20, 29, 18, 28, etc.] cannot be modelled by (\mathcal{R}) . This happens because the update mapping is changing at every iteration; \mathcal{A} in (\mathcal{R}) is replaced by $\mathcal{A}_k: \mathcal{X} \times \mathcal{U} \rightarrow \mathcal{X}$ giving us the update

$$\mathbf{x}^{(k+1)}(\mathbf{u}) := \mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}), \mathbf{u}). \quad (\mathcal{R}_k)$$

For example, for gradient descent with line search, $\mathcal{A}_k(\mathbf{x}, \mathbf{u}) := \mathbf{x} - \alpha_k \nabla_{\mathbf{x}} F(\mathbf{x}, \mathbf{u})$. When \mathcal{A}_k is C^1 -smooth for all $k \in \mathbb{N}$, the modified update rule for performing forward mode AD on (\mathcal{R}_k) reads:

$$D\mathbf{x}^{(k+1)}(\mathbf{u}) := D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}), \mathbf{u})D\mathbf{x}^{(k)}(\mathbf{u}) + D_{\mathbf{u}}\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}), \mathbf{u}). \quad (D\mathcal{R}_k)$$

Beck [9] studied this problem for the C^1 -smooth sequence of functions \mathcal{A}_k with uniformly bounded derivatives and $D\mathcal{A}_k$ converging to $D\mathcal{A}$ pointwise. They showed that for such a sequence, when $(\mathbf{x}^{(k)}(\mathbf{u}))_{k \in \mathbb{N}}$ is generated by (\mathcal{R}_k) to solve the system (\mathcal{R}_e) , then $(D\mathbf{x}^{(k)}(\mathbf{u}))_{k \in \mathbb{N}}$ generated by $(D\mathcal{R}_k)$ converges to $D\psi(\mathbf{u})$ defined in (2). *However, their results cannot account for the linear convergence of $D\mathbf{x}^{(k)}(\mathbf{u})$ in their given setting (see Section A.2). Moreover, their setting excludes the more general cases where \mathcal{A}_k does not converge, for instance, gradient descent with line search.*

Griewank et al. [31] studied the special setting for solving the non-linear system $G(\mathbf{x}, \mathbf{u}) = 0$ with respect to \mathbf{x} through preconditioned Picard iterations, that is, $\mathcal{A}_k(\mathbf{x}, \mathbf{u}) := \mathbf{x} - P_k(\mathbf{u})G(\mathbf{x}, \mathbf{u})$. The parameter-dependent preconditioner $P_k: \mathcal{U} \rightarrow \mathcal{L}(\mathcal{X}, \mathcal{X})$ is changing at every iteration and may not converge. They demonstrated linear convergence of $D\mathbf{x}^{(k)}(\mathbf{u})$ for a C^1 -smooth $G: \mathcal{X} \times \mathcal{U} \rightarrow \mathcal{X}$ with bounded maps $D_{\mathbf{x}}G$ and $(\mathbf{x}, \mathbf{u}) \mapsto D_{\mathbf{x}}G(\mathbf{x}, \mathbf{u})^{-1}$ and Lipschitz continuous map DG . The map P_k is assumed to be C^1 -smooth with bounded (potentially 0) derivative for every $k \in \mathbb{N}$.

Recently in [53, 46], AD was applied to (\mathcal{R}_k) when \mathcal{A}_k denotes the update mapping of FISTA [8] (which we will call Accelerated Proximal Gradient or APG) applied to (\mathcal{P}) for

non-smooth $F := f + g$ with step size α_k and extrapolation parameter β_k . They adapted the results of [9] and demonstrated the convergence of $D\mathbf{x}^{(k)}(\mathbf{u})$ to $D\psi(\mathbf{u})$ when f is C^2 -smooth with a Lipschitz continuous gradient, g is partly smooth [35], the sequences $(\alpha_k)_{k \in \mathbb{N}}$ and $(\beta_k)_{k \in \mathbb{N}}$ converge and F additionally satisfies restricted injectivity and non-degeneracy conditions [35]. $D\psi(\mathbf{u})$ is computed by applying the Implicit Function Theorem for partly smooth functions [35, Theorem 5.7]. Partly smooth functions are a class of special non-smooth functions which exhibit smoothness when restricted to a low-dimensional manifold \mathcal{M} and model various practical regularization functions [58]. The non-smooth or sharp behaviour occurs only when we move orthogonal to \mathcal{M} . The combination of restricted injectivity and non-degeneracy assumptions induces the contraction property in proximal gradient descent or PGD [38] and APG [37] near the solution. *The results of [53, 46] do not explain the linear convergence of AD of APG or even the convergence of AD of PGD with non-converging variable step size.*

1.3 Contributions

In this paper, we aim to resolve the theoretical gaps presented in Section 1.2 and therefore reinforce the usefulness of AD. In particular, the main contributions of this paper are the following:

- (i) We strengthen the results of [9] by providing a convergence rate analysis for $D\mathbf{x}^{(k)}(\mathbf{u})$ generated by (\mathcal{DR}_k) after equipping their setting with an additional assumption that is satisfied by most optimization algorithms (see Assumption 2.1(ii) and Remark 1).
- (ii) We establish (linear) convergence of $D\mathbf{x}^{(k)}(\mathbf{u})$ beyond the setting in (i) without the pointwise convergence condition of \mathcal{A}_k to \mathcal{A} removed (see Assumption 2.1(ii) and 2.1(iii)).
- (iii) We demonstrate the convergence of $D\mathbf{x}^{(k)}(\mathbf{u})$ for Proximal Gradient Descent [40] or PGD with variable step size and Accelerated Proximal Gradient [8] or APG by adapting the results for (ii) and (i) respectively. We show that the rate of convergence of $\mathbf{x}^{(k)}(\mathbf{u})$ is reflected in that of $D\mathbf{x}^{(k)}(\mathbf{u})$ for both algorithms.

1.4 Bilevel Optimization beyond Automatic and Implicit Differentiation

It is worthwhile to point out a different method for solving (1) in addition to AD and ID. The idea is to rewrite the problem by incorporating the value function through an inequality constraint [23, 41, 57]. This reduces the nested problem into a single problem which is then solved through penalty-based methods. This technique is sometimes referred to as single-loop or Hessian-free approach and has been shown to give promising results [34].

1.5 Notation

In this paper, \mathcal{X} and \mathcal{U} are Euclidean spaces and $\overline{\mathbb{R}} := [-\infty, \infty]$. With a slight abuse of notation, $\|\cdot\|$ denotes any norm on these spaces including the one induced by the inner product $\langle \cdot, \cdot \rangle$. Any operator norm on the space of linear operators between \mathcal{X} and \mathcal{U} is also denoted by $\|\cdot\|$. We say that $\mathbf{w}^{(k)} = o(\mathbf{z}^{(k)})$ iff $\|\mathbf{w}^{(k)}\| = o(\|\mathbf{z}^{(k)}\|)$ and $\mathbf{w}^{(k)} = \mathcal{O}(\mathbf{z}^{(k)})$ iff $\|\mathbf{w}^{(k)}\| = \mathcal{O}(\|\mathbf{z}^{(k)}\|)$. We use standard notions of Riemannian Geometry and partly smooth functions found in [35, 36, 58]. A C^2 -smooth embedded submanifold $\mathcal{M} \subset \mathcal{X}$ of \mathcal{X} is simply referred to as a manifold. For any $\mathbf{x} \in \mathcal{M}$, $\Pi(\mathbf{x}) := \text{proj}_{T_{\mathbf{x}}\mathcal{M}}$ and $\Pi^\perp(\mathbf{x}) := \text{proj}_{N_{\mathbf{x}}\mathcal{M}}$ denote the orthogonal projection onto $T_{\mathbf{x}}\mathcal{M}$ and $N_{\mathbf{x}}\mathcal{M}$, the tangent and normal spaces respectively and for any $\mathbf{v} \in T_{\mathbf{x}}\mathcal{M}$, $\mathfrak{W}_{\mathbf{x}}(\cdot, \mathbf{v})$ represents the Weingarten map. For any $\alpha > 0$ and proper and lower semi-continuous $g: \mathcal{X} \times U \rightarrow \overline{\mathbb{R}}$ where $g(\cdot, \mathbf{u})$ is convex for all $\mathbf{u} \in U \subset \mathcal{U}$, we define $P_{\alpha g}: \mathcal{X} \times U \rightarrow \mathcal{X}$ by $P_{\alpha g}(\cdot, \mathbf{u}) = \text{prox}_{\alpha g(\cdot, \mathbf{u})}$, that is,

$$P_{\alpha g}(\mathbf{w}, \mathbf{u}) := \underset{\mathbf{x} \in \mathcal{X}}{\text{argmin}} \alpha g(\mathbf{x}, \mathbf{u}) + \frac{1}{2} \|\mathbf{x} - \mathbf{w}\|^2. \quad (3)$$

We use the terminology of [54] for the subdifferential of g . When U is open and for any $\mathbf{x} \in \mathcal{X}$, $g(\mathbf{x}, \cdot)$ is differentiable at $\mathbf{u} \in U$, we obtain $\partial g(\mathbf{x}, \mathbf{u}) = \partial_{\mathbf{x}} g(\mathbf{x}, \mathbf{u}) \times \{\nabla_{\mathbf{u}} g(\mathbf{x}, \mathbf{u})\}$ [46, Lemma 1]. When $g|_{\mathcal{M} \times U}$ is C^2 -smooth, we follow [46, Remark 22(iv)] to denote its Riemannian gradient and Hessian.

2 Differentiation of Iteration-Dependent Algorithms

In this section, we lay down the assumptions on the sequence $(\mathcal{A}_k)_{k \in \mathbb{N}}$ and provide convergence and convergence rate guarantees for the derivative iterations defined in (\mathcal{DR}_k) . In particular we establish (i) convergence rates when \mathcal{A}_k has a pointwise limit \mathcal{A} , and (ii) convergence and convergence rates when \mathcal{A}_k does not have a pointwise limit. For a better comparison and understanding, this section is adapted to follow the same pattern as Section A.2, which summarizes the results by [9].

2.1 Problem Setting

For a given \mathbf{u}^* , we assume that \mathbf{x}^* is the solution that we are trying to estimate through (\mathcal{R}_k) . Because the pointwise limit \mathcal{A} of \mathcal{A}_k may not exist, we assume that \mathbf{x}^* is a fixed point of $\mathcal{A}_k(\cdot, \mathbf{u}^*)$ for every $k \in \mathbb{N}$. This seemingly restrictive assumption is satisfied by the optimization algorithms highlighted in Section 1.2. The application of the Implicit Function Theorem on this sequence of fixed-point equations requires the contraction property, that is, the strict bound on some operator norm $\|D_{\mathbf{x}} \mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)\| < 1$ eventually for all $k \in \mathbb{N}$. Furthermore, we assume that the sequence of affine maps $(X \mapsto D_{\mathbf{x}} \mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)X + D_{\mathbf{u}} \mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*))_{k \in \mathbb{N}}$ share a common fixed-point $X_* \in \mathcal{L}(\mathcal{X}, \mathcal{X})$ — the reason will become clear shortly. Finally, to show the convergence of the derivative sequence $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$, we assume that the sequence $(\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ converges to \mathbf{x}^* . More formally, given $(\mathbf{x}^{(0)}, \mathbf{x}^*, \mathbf{u}^*, X_*) \in \mathcal{X} \times \mathcal{X} \times \mathcal{U} \times \mathcal{L}(\mathcal{X}, \mathcal{X})$,

$V \in \mathcal{N}_{(\mathbf{x}^*, \mathbf{u}^*)}$, $(\mathcal{A}_k)_{k \in \mathbb{N}_0}$, and a norm $\|\cdot\|$ on $\mathcal{L}(\mathcal{X}, \mathcal{X})$ induced by some vector norm, we assume that the following conditions hold.

- Assumption 2.1.** (i) $\mathcal{A}_k|_V$ is C^1 -smooth for all k ,
- (ii) $\mathbf{x}^* = \mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)$ and $X_* = D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)X_* + D_{\mathbf{u}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)$ for all k ,
- (iii) $\limsup_{k \rightarrow \infty} \|D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)\| < 1$, and
- (iv) $\mathbf{x}^{(k)}(\mathbf{u}^*)$ generated by (\mathcal{R}_k) has limit \mathbf{x}^* such that $(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*) \in V$ for all k .

Remark 1. A special case of Assumption 2.1(iii) arises when for some C^1 -smooth mapping $\mathcal{A}: V \rightarrow \mathcal{X}$, we have $\mathbf{x}^* = \mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)$, $D\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*) \rightarrow D\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)$ and $\rho(D_{\mathbf{x}}\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)) < 1$.

2.2 Implicit Differentiation

Combining Assumptions 2.1(i)–(iii) allows us to invoke the Implicit Function Theorem on $\mathbf{x}^* = \mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)$ for every k large enough and obtain a C^1 -smooth fixed-point map ψ_k on a neighbourhood $U_k \in \mathcal{N}_{\mathbf{u}^*}$. In particular, we have the following result.

Lemma 2. Let $(\mathbf{x}^*, \mathbf{u}^*, X_*) \in \mathcal{X} \times \mathcal{U} \times \mathcal{L}(\mathcal{X}, \mathcal{X})$, $V \in \mathcal{N}_{(\mathbf{x}^*, \mathbf{u}^*)}$, $(\mathcal{A}_k)_{k \in \mathbb{N}_0}$, and $\|\cdot\|$ be such that Assumption 2.1 (i)–(iii) is satisfied. Then there exists $K \in \mathbb{N}$ such that $\forall k \geq K$, there exists $U_k \in \mathcal{N}_{\mathbf{u}^*}$ and a C^1 -smooth $\psi_k: U_k \rightarrow \mathcal{X}$ such that $\forall \mathbf{u} \in U_k$, $\psi_k(\mathbf{u}) = \mathcal{A}_k(\psi_k(\mathbf{u}), \mathbf{u})$, and

$$D\psi_k(\mathbf{u}) = (I - D_{\mathbf{x}}\mathcal{A}_k(\psi_k(\mathbf{u}), \mathbf{u}))^{-1} D_{\mathbf{u}}\mathcal{A}_k(\psi_k(\mathbf{u}), \mathbf{u}), \quad (4)$$

so that $D\psi_k(\mathbf{u}^*) = X_*$.

Proof. The proof is in Section B.1 in the appendix. □

Remark 3. If we replace Assumptions 2.1(ii) and 2.1(iii) by a slightly stronger assumption, that is, “there exists $U \in \mathcal{N}_{\mathbf{u}^*}$ such that for any $(\mathbf{x}, \mathbf{u}) \in \mathcal{X} \times U$, $\mathbf{x} = \mathcal{A}_k(\mathbf{x}, \mathbf{u})$ for some $k \in \mathbb{N}$ implies $\mathbf{x} = \mathcal{A}_k(\mathbf{x}, \mathbf{u})$ for every $k \in \mathbb{N}$, and $\limsup_{k \rightarrow \infty} \|D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}, \mathbf{u})\| < 1$ ”, we obtain a shared C^1 -smooth fixed-point map $\psi: U \rightarrow \mathcal{X}$, such that, $U_k = U$ and $\psi_k = \psi$ for all $k \in \mathbb{N}$.

2.3 Automatic Differentiation

In Lemma 2, we just showed that under Assumption 2.1, the common fixed-point X_* of the mappings $X \mapsto D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)X + D_{\mathbf{u}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)$ for $k \in \mathbb{N}$ represents the derivative of the solution at $\mathbf{u} = \mathbf{u}^*$. We now show that the derivative sequence generated by (\mathcal{DR}_k) for $\mathbf{u} = \mathbf{u}^*$ converges to X_* . Instead of assuming a pointwise limit for $D\mathcal{A}_k$, we assert that $D\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*) - D\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)$ tends to 0.

Assumption 2.2. The sequence $(D\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*) - D\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*))_{k \in \mathbb{N}_0}$ converges to 0.

Remark 4. (i) A sufficient condition for Assumption 2.2 is equicontinuity of $(\mathcal{A}_k)_{k \in \mathbb{N}_0}$ at $(\mathbf{x}^*, \mathbf{u}^*)$.

(ii) Combining Assumption 2.2 with the special case of Remark 1, we obtain the setting of [9], that is, $D\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*) - D\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*) \rightarrow 0$ (see also Section A.2 in the appendix).

We are now ready to establish the convergence of the derivative sequence $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ to X_* when Assumptions 2.1 and 2.2 hold.

Theorem 5. Let $(\mathbf{x}^{(0)}, \mathbf{x}^*, \mathbf{u}^*) \in \mathcal{X} \times \mathcal{X} \times \mathcal{U}$, $V \in \mathcal{N}_{(\mathbf{x}^*, \mathbf{u}^*)}$, and $(\mathcal{A}_k)_{k \in \mathbb{N}_0}$ be such that Assumptions 2.1 and 2.2 are satisfied. Then the sequence $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}_0}$ generated by (\mathcal{DR}_k) converges to X_* which is equal to $(I - D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*))^{-1} D_{\mathbf{u}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)$ for all $k \in \mathbb{N}$ (see Assumption 2.1(ii)).

Proof. The proof is in Section B.2 in the appendix. □

The derivative iterates $D\mathbf{x}^{(k)}(\mathbf{u}^*)$ additionally converge with a linear rate when the sequences $\mathbf{x}^{(k)}(\mathbf{u}^*)$ and $D\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*) - D\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)$ converge linearly.

Assumption 2.3. The sequence $(\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}_0}$ converges linearly to \mathbf{x}^* and

$$D\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*) - D\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*) = \mathcal{O}(\mathbf{x}^{(k)}(\mathbf{u}^*) - \mathbf{x}^*). \quad (5)$$

Remark 6. A sufficient condition for Assumption 2.3 is the Lipschitz continuity of $(D\mathcal{A}_k)_{k \in \mathbb{N}_0}$ in \mathbf{x} uniformly in \mathbf{u} and k .

Theorem 7. Let $(\mathbf{x}^{(0)}, \mathbf{x}^*, \mathbf{u}^*) \in \mathcal{X} \times \mathcal{X} \times \mathcal{U}$, $V \in \mathcal{N}_{(\mathbf{x}^*, \mathbf{u}^*)}$, and $(\mathcal{A}_k)_{k \in \mathbb{N}_0}$ be such that Assumptions 2.1 and 2.3 are satisfied. Then the sequence $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}_0}$ generated by (\mathcal{DR}_k) converges linearly to X_* . In particular, for all $\delta \in (0, 1 - \rho)$, there exist $C_1(\delta)$, $C_2(\delta)$ and $K \in \mathbb{N}$, such that for all $k \geq K$, we have

$$\begin{aligned} \|D\mathbf{x}^{(k)}(\mathbf{u}^*) - X_*\| &\leq C_1(\delta)(k - K)q^{k-K} \\ &\quad + C_2(\delta)(\rho + \delta)^{k-K}, \end{aligned} \quad (6)$$

where $\rho := \rho(D_{\mathbf{x}}\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*))$, $q := \max(\rho + \delta, q_{\mathbf{x}})$, and $q_{\mathbf{x}} < 1$ is the convergence rate of the sequence $(\mathbf{x}^{(k)})_{k \in \mathbb{N}_0}$.

Proof. The proof is in Section B.3 in the appendix. □

Owing to Corollary 25 and our discussion in Remark 1, the following result shows that the work of [9] is reproduced and strengthened with a convergence rate guarantee under the additional requirement of Assumption 2.1(ii).

Corollary 8. The conclusions of Theorems 5 and 7 also hold when, in their respective hypotheses, Assumption 2.1(iii) is replaced by “there exists a C^1 -smooth $\mathcal{A}: V \rightarrow \mathcal{X}$, such that $D\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)$ converges to $D\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)$ and $\rho(D_{\mathbf{x}}\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)) < 1$ ”.

Remark 9. The conclusions of Theorems 5 and 7 and Corollary 8 do not require the neighbourhood V of $(\mathbf{x}^*, \mathbf{u}^*)$ to be a connected set as long as Assumptions 2.2 and 2.3 are respectively satisfied along with Assumption 2.1(iv).

3 Differentiation of Proximal Gradient-type Methods

We now turn our attention to unrolling PGD with variable step size and APG when solving

$$\min_{\mathbf{x} \in \mathcal{X}} F(\mathbf{x}, \mathbf{u}), \quad F := f + g, \quad (7)$$

and aim at providing convergence (rate) guarantees for the corresponding derivative sequences. The idea is to consider the class of partly smooth functions [35] which models a wide range of non-smooth regularizers and constraints appearing in practice [58]. Furthermore, this setting (see Assumption 3.1) under some additional assumptions (see Assumptions 3.2 and 3.3) yields a more general IFT (see Theorem 10) for differentiating the solution mapping of (7). This in turn allows us to differentiate the update mappings of PGD (see Theorem 13) and APG (see Theorem 19), since they are also the solution mappings of partly smooth functions (see Equations 3, 9 and 11).

3.1 Problem Setting

We first define our setting in a more precise manner. Let \mathcal{M} be a C^2 -smooth manifold and $\Omega \subset \mathcal{U}$ be an open set, we need f and g to satisfy the following assumption.

Assumption 3.1 (Convex Partly Smooth Objective). $f: \mathcal{X} \times \mathcal{U} \rightarrow \mathbb{R}$ is C^2 -smooth, $g: \mathcal{X} \times \mathcal{U} \rightarrow \overline{\mathbb{R}}$ is partly smooth relative to $\mathcal{M} \times \Omega$ and for every $\mathbf{u} \in \Omega$, $f(\cdot, \mathbf{u})$ and $g(\cdot, \mathbf{u})$ are convex, $f(\cdot, \mathbf{u})$ has an L -Lipschitz continuous gradient, and $g(\cdot, \mathbf{u})$ has a simple proximal mapping.

Let $\mathbf{x}^* \in \mathcal{M}$ be a solution of (7) at $\mathbf{u}^* \in \Omega$. When $g = 0$, IFT requires $\nabla_{\mathbf{x}} f(\mathbf{x}^*, \mathbf{u}^*) \succ 0$ which is also a sufficient condition for the linear convergence of gradient descent and the Heavy-ball method [51]. When g is partly smooth, IFT requires positive definiteness of $\nabla_{\mathcal{M}}^2 F(\mathbf{x}^*, \mathbf{u}^*)$ [35] while the linear convergence of PGD and APG is established by the positive definiteness of $\Pi(\mathbf{x}^*) \nabla_{\mathbf{x}}^2 f(\mathbf{x}^*, \mathbf{u}^*) \Pi(\mathbf{x}^*)$ [38, 37].

Assumption 3.2 (Restricted Positive Definiteness). Let $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be a given point.

- (i) The Hessian $\nabla_{\mathcal{M}}^2 F(\mathbf{x}^*, \mathbf{u}^*)$ is positive definite on $T_{\mathbf{x}^*} \mathcal{M}$, that is,

$$\nabla_{\mathcal{M}}^2 F(\mathbf{x}^*, \mathbf{u}^*) \succ 0. \quad (\text{RPD-i})$$

- (ii) Moreover, $\Pi(\mathbf{x}^*) \nabla_{\mathbf{x}}^2 f(\mathbf{x}^*, \mathbf{u}^*)$ is positive definite on $T_{\mathbf{x}^*} \mathcal{M}$, that is,

$$\Pi(\mathbf{x}^*) \nabla_{\mathbf{x}}^2 f(\mathbf{x}^*, \mathbf{u}^*)|_{T_{\mathbf{x}^*} \mathcal{M}} \succ 0. \quad (\text{RPD-ii})$$

Finally, for partly smooth problems, IFT and linear convergence of PGD and APG also require a non-degeneracy assumption to hold which ensures that the solution stays in \mathcal{M} for any \mathbf{u} near \mathbf{u}^* .

Assumption 3.3 (Non-degeneracy). The non-degeneracy condition is satisfied at $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$, that is,

$$0 \in \text{ri } \partial_{\mathbf{x}} F(\mathbf{x}^*, \mathbf{u}^*). \quad (\text{ND})$$

3.2 Implicit Function Theorem

The following theorem is thanks to [35] which furnishes a C^1 -smooth solution map for (7) near \mathbf{u}^* . The expression for the derivative can be found in [58, 46].

Theorem 10 (Differentiation of Solution Map). Let f and g satisfy Assumption 3.1 and $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be such that Assumptions 3.2(i) and 3.3 are satisfied. Then there exist an open neighbourhood $U \subset \Omega$ of \mathbf{u}^* and a continuously differentiable mapping $\psi: U \rightarrow \mathcal{M}$ such that for all $\mathbf{u} \in U$,

- (i) $\psi(\mathbf{u})$ is the unique minimizer of $F(\cdot, \mathbf{u})|_{\mathcal{M}}$,
- (ii) (ND) and (RPD-i) are satisfied at $(\psi(\mathbf{u}), \mathbf{u})$, and
- (iii) the derivative of ψ is given by

$$D\psi(\mathbf{u}) = -\nabla_{\mathcal{M}}^2 F(\psi(\mathbf{u}), \mathbf{u})^\dagger D_{\mathbf{u}} \nabla_{\mathcal{M}} F(\psi(\mathbf{u}), \mathbf{u}), \quad (8)$$

where $\nabla_{\mathcal{M}}^2 F(\psi(\mathbf{u}), \mathbf{u})^\dagger$ denotes the pseudoinverse of $\nabla_{\mathcal{M}}^2 F(\psi(\mathbf{u}), \mathbf{u})$.

3.3 The Extrapolated Proximal Gradient Algorithm

Although Theorem 10 is not practical when computing the derivative of the solution map, it allows us to differentiate the update mappings of PGD and APG as we will see shortly. Algorithm 1 provides the update procedure for proximal gradient with extrapolation where $P_{\alpha g}$ is defined in (3). This algorithm reduces to (i) PGD when $\beta_k = 0$ for all $k \in \mathbb{N}$, and (ii) APG when the sequence β_k ensures acceleration in PGD [8, 19].

Algorithm 1.

- **Initialization:** $\mathbf{x}^{(0)} = \mathbf{x}^{(-1)} \in \mathcal{X}$, $\mathbf{u} \in \mathcal{U}$, $0 < \underline{\alpha} \leq \bar{\alpha} < 2/L$.
- **Parameter:** $(\alpha_k)_{k \in \mathbb{N}} \in [\underline{\alpha}, \bar{\alpha}]$ and $(\beta_k)_{k \in \mathbb{N}} \in [0, 1]$.
- **Update** $k \geq 0$:

$$\begin{aligned} \mathbf{y}^{(k)} &:= (1 + \beta_k) \mathbf{x}^{(k)} - \beta_k \mathbf{x}^{(k-1)} \\ \mathbf{w}^{(k)} &:= \mathbf{y}^{(k)} - \alpha_k \nabla_{\mathbf{x}} f(\mathbf{y}^{(k)}, \mathbf{u}) \\ \mathbf{x}^{(k+1)} &:= P_{\alpha_k g}(\mathbf{w}^{(k)}, \mathbf{u}). \end{aligned} \quad (\text{APG})$$

3.4 Proximal Gradient Descent

We first extend our results from Section 2 and provide convergence rate guarantees for AD of PGD. For a given step size $\alpha > 0$, we write the update mapping for PGD in a more compact manner through the map $\mathcal{A}_\alpha: \mathcal{X} \times \Omega \rightarrow \mathcal{X}$ defined by

$$\mathcal{A}_\alpha(\mathbf{x}, \mathbf{u}) := \text{P}_{\alpha g}(\mathbf{x} - \alpha \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{u}), \mathbf{u}), \quad (9)$$

Liang et al. [38] established that under Assumptions 3.1, 3.2(ii) and 3.3, all the iterates $\mathbf{x}^{(k)}(\mathbf{u}^*)$ of PGD lie on \mathcal{M} after a finite number of iterations and exhibit a local linear convergence behaviour as summarized by the following lemma.

Lemma 11 (Activity Identification and Linear Convergence of PGD). Let f and g satisfy Assumption 3.1 and $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be such that Assumption 3.3 is satisfied. For $\alpha_k \in [\underline{\alpha}, \bar{\alpha}]$ and $\beta_k := 0$, let the sequence $(\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ generated by Algorithm 1 converges to \mathbf{x}^* . Then there exists $K \in \mathbb{N}$, such that $\mathbf{x}^{(k)}(\mathbf{u}^*) \in \mathcal{M}$ for all $k \geq K$. Moreover when Assumption 3.2(ii) is also satisfied and $\bar{\alpha} < 2M/L^2$ where $M := \lambda_{\max}(\Pi(\mathbf{x}^*) \nabla_{\mathbf{x}} f(\mathbf{x}^*, \mathbf{u}^*) \Pi(\mathbf{x}^*))$, then $\mathbf{x}^{(k)}(\mathbf{u}^*)$ converge linearly to \mathbf{x}^* .

Remark 12. The precise rate of convergence of PGD can be found in [38, Theorem 3.1].

Mehmood and Ochs [46, Theorem 34] provide a foundation for proving the following crucial differentiability result for \mathcal{A}_α by combining Theorem 10 and Lemma 11. However, the result below is novel since it establishes differentiability of \mathcal{A}_{α_k} at the iterates $\mathbf{x}^{(k)}(\mathbf{u}^*)$ of PGD for all $k \in \mathbb{N}$ and also shows that the derivative sequence $D\mathcal{A}_{\alpha_k}$ is well-behaved.

Theorem 13. Let f and g satisfy Assumption 3.1 and $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be such that Assumption 3.3 are satisfied. For $\alpha_k \in [\underline{\alpha}, \bar{\alpha}]$ and $\beta_k := 0$, let the sequence $(\mathbf{x}^{(k)} := \mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ generated by Algorithm 1 converges to \mathbf{x}^* . Then there exists $K \in \mathbb{N}$, such that,

- (i) the mapping $(\mathbf{x}, \mathbf{u}, \alpha) \mapsto \mathcal{A}_\alpha(\mathbf{x}, \mathbf{u})$ defined in (9) is C^1 -smooth near $(\mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k)$ and $(\mathbf{x}^*, \mathbf{u}^*, \alpha_k)$ for all $k \geq K$,
- (ii) $(D\mathcal{A}_{\alpha_k}(\mathbf{x}^{(k)}, \mathbf{u}^*) - D\mathcal{A}_{\alpha_k}(\mathbf{x}^*, \mathbf{u}^*))_{k \geq K}$ converges to 0, and
- (iii) additionally, when \mathcal{M} is C^3 -smooth, $\nabla_{\mathcal{M}} g$, $\nabla_{\mathbf{x}}^2 f$, $\nabla_{\mathcal{M}}^2 g$, $D_{\mathbf{u}} \nabla_{\mathbf{x}} f$, and $D_{\mathbf{u}} \nabla_{\mathcal{M}} g$ are locally Lipschitz continuous near $(\mathbf{x}^*, \mathbf{u}^*)$ and $(\mathbf{x}^{(k)})_{k \in \mathbb{N}}$ converges linearly, then $D\mathcal{A}_{\alpha_k}(\mathbf{x}^{(k)}, \mathbf{u}^*) - D\mathcal{A}_{\alpha_k}(\mathbf{x}^*, \mathbf{u}^*) = \mathcal{O}(\mathbf{x}^{(k)} - \mathbf{x}^*)$.

Proof. The proof is in Section C.1 in the appendix. □

Remark 14. The C^3 -smoothness of \mathcal{M} is a sufficient condition for the local Lipschitz continuity of the Weingarten map $(\mathbf{x}, \mathbf{v}) \mapsto \mathfrak{W}_{\mathbf{x}}(\cdot, \mathbf{v})$.

3.4.1 Implicit Differentiation

Under Assumptions 3.1–3.3, Mehmood and Ochs [46, Theorem 34] provided an IFT for the fixed-point equation of PGD which is more practical for using ID than (8) and is restated below.

Theorem 15. Let f and g satisfy Assumption 3.1 and $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be such that Assumptions 3.2(ii) and 3.3 are satisfied. Then for any $\alpha \in [\underline{\alpha}, \bar{\alpha}]$, $\rho(D_{\mathbf{x}}\mathcal{A}_{\alpha}(\mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*)) < 1$. Additionally when Assumption 3.2(i) is also satisfied, the (possibly reduced) neighbourhood U and the mapping ψ from Theorem 10 satisfy $\mathbf{x} = \mathcal{A}_{\alpha}(\mathbf{x}, \mathbf{u})$ and

$$D\psi(\mathbf{u}) = (I - D_{\mathbf{x}}\mathcal{A}_{\alpha}(\mathbf{x}, \mathbf{u})\Pi(\mathbf{x}))^{-1} D_{\mathbf{u}}\mathcal{A}_{\alpha}(\mathbf{x}, \mathbf{u}), \quad (10)$$

for all $\mathbf{u} \in U$ and $\mathbf{x} := \psi(\mathbf{u})$.

3.4.2 Automatic Differentiation

Using Theorems 13, and 15 and our results from Section 2, we obtain the convergence (rate) guarantees for AD of PGD.

Theorem 16. Let f and g satisfy Assumption 3.1 and $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be such that Assumptions 3.2 and 3.3 are satisfied. Let $\alpha_k \in [\underline{\alpha}, \bar{\alpha}]$, $\beta_k := 0$ and the sequence $(\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ generated by Algorithm 1 converges to \mathbf{x}^* with $\mathbf{x}^{(0)}$ sufficiently close to \mathbf{x}^* . Then the sequence $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ converges to $D\psi(\mathbf{u}^*)$. Additionally $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ converges linearly with rate $\max(q_{\mathbf{x}}, \limsup_{k \rightarrow \infty} \rho(D_{\mathbf{x}}\mathcal{A}_{\alpha_k}(\mathbf{x}^*, \mathbf{u}^*)))$ when \mathcal{M} is C^3 -smooth, $\nabla_{\mathcal{M}}g$, $\nabla_{\mathbf{x}}^2 f$, $\nabla_{\mathcal{M}}^2 g$, $D_{\mathbf{u}}\nabla_{\mathbf{x}}f$, and $D_{\mathbf{u}}\nabla_{\mathcal{M}}g$ are locally Lipschitz continuous near $(\mathbf{x}^*, \mathbf{u}^*)$ and $(\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ converges with rate $q_{\mathbf{x}} < 1$.

Proof. The proof is in Section C.2 in the appendix. □

Remark 17. (i) Because $\mathbf{x}^{(0)}$ is not close enough to \mathbf{x}^* in practice, one may resort to late-starting [46, Section 1.4.2].

(ii) In practice, we do not need $\mathbf{x}^{(0)}$ to be close enough to \mathbf{x}^* because even when the update map \mathcal{A}_{α_k} is not differentiable in the earlier iterations of Algorithm 1, the autograd libraries still yield a finite output as the derivative [13, 14]. Hence, AD of Algorithm 1 can still recover a good estimate of $D\psi(\mathbf{u})$ as long as Algorithm 1 is run for sufficiently large number of iterations [46, Remark 45(i)].

(iii) When α_k is generated through line-search methods, it also depends on \mathbf{u} in a possibly non-differentiable way. Therefore, the total derivative of $\mathbf{x}^{(k)}$ with respect to \mathbf{u} may not make sense. However computing $D\mathbf{x}^{(k)}(\mathbf{u})$ by ignoring this dependence — for instance, in practice, through routines like `stop_gradient` [17, 1] and `detach` [49] — the true derivative is still recovered in the limit provided that conditions of Theorem 16 are met. This fact was first explored in [31].

3.5 Accelerated Proximal Gradient

We similarly compute AD of APG and show (linear) convergence of the corresponding derivative iterates. Given step size $\alpha > 0$ and extrapolation parameter $\beta \in [0, 1]$, we define the update mapping $\mathcal{A}_{\alpha,\beta}: \mathcal{X} \times \mathcal{X} \times \mathcal{U} \rightarrow \mathcal{X} \times \mathcal{X}$ by

$$\mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u}) := (\mathcal{A}_\alpha(\mathbf{x}_1 + \beta(\mathbf{x}_1 - \mathbf{x}_2), \mathbf{u}), \mathbf{x}_1), \quad (11)$$

for $\mathbf{z} := (\mathbf{x}_1, \mathbf{x}_2) \in \mathcal{X} \times \mathcal{X}$. Just like PGD, APG also exhibit activity identification property and local linear convergence under Assumptions 3.1, 3.2(ii), and 3.3 [37].

Lemma 18 (Activity Identification and Linear Convergence of APG). Let f and g satisfy Assumption 3.1 and $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be such that Assumption 3.3 is satisfied. For $\alpha_k \in [\underline{\alpha}, \bar{\alpha}]$ and $\beta_k \in [0, 1]$, let the sequence $(\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ generated by Algorithm 1 converges to \mathbf{x}^* . Then there exists $K \in \mathbb{N}$, such that $\mathbf{x}^{(k)}(\mathbf{u}^*) \in \mathcal{M}$ for all $k \geq K$. Moreover when Assumption 3.2(ii) is also satisfied, $\alpha_k \rightarrow \alpha_*$ and $\beta_k \rightarrow \beta_*$ such that $-1/(1 + 2\beta_*) < \lambda_{\min}(D_{\mathbf{x}}\mathcal{A}_{\alpha_*}(\mathbf{x}^*, \mathbf{u}^*))$, then $\mathbf{x}^{(k)}(\mathbf{u}^*)$ converge linearly to \mathbf{x}^* with rate $\rho(D_{\mathbf{z}}\mathcal{A}_{\alpha_*,\beta_*}(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*, \mathbf{x}^*))$.

Using Theorem 10, and Lemma 18, we can differentiate $\mathcal{A}_{\alpha_k,\beta_k}$ near $(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*)$ for all $k \in \mathbb{N}$. The following result is mostly derived from [46, Theorem 39].

Theorem 19. Let f and g satisfy Assumption 3.1 and $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be such that Assumption 3.3 are satisfied. For $[\underline{\alpha}, \bar{\alpha}] \ni \alpha_k \rightarrow \alpha_*$ and $[0, 1] \ni \beta_k \rightarrow \beta_*$, let the sequence $(\mathbf{x}^{(k)} := \mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ generated by Algorithm 1 converges to \mathbf{x}^* . Then there exist $V_{\alpha_*} \in \mathcal{N}_{(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*, \alpha_*)}$ and $K \in \mathbb{N}$, such that

- (i) the mapping $(\mathbf{z}, \mathbf{u}, \alpha) \mapsto \mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u})$ defined in (11) is C^1 -smooth on V_{α_*} and $(\mathbf{z}^{(k)}, \mathbf{u}^*, \alpha_k) \in V_{\alpha_*}$ for all $k \geq K$,
- (ii) $(D\mathcal{A}_{\alpha_k,\beta_k}(\mathbf{z}^{(k)}, \mathbf{u}^*) - D\mathcal{A}_{\alpha_k,\beta_k}(\mathbf{z}^*, \mathbf{u}^*))_{k \geq K}$ converges to 0, and $(D\mathcal{A}_{\alpha_k,\beta_k}(\mathbf{z}^*, \mathbf{u}^*))_{k \geq K}$ converges to $D\mathcal{A}_{\alpha_*,\beta_*}(\mathbf{z}^*, \mathbf{u}^*)$, and
- (iii) additionally, when \mathcal{M} is C^3 -smooth, $\nabla_{\mathcal{M}}g$, $\nabla_{\mathbf{x}}^2 f$, $\nabla_{\mathcal{M}}^2 g$, $D_{\mathbf{u}}\nabla_{\mathbf{x}}f$, and $D_{\mathbf{u}}\nabla_{\mathcal{M}}g$ are locally Lipschitz continuous near $(\mathbf{x}^*, \mathbf{u}^*)$ and $(\mathbf{x}^{(k)})_{k \in \mathbb{N}}$ converges linearly, then $D\mathcal{A}_{\alpha_k,\beta_k}(\mathbf{z}^{(k)}, \mathbf{u}^*) - D\mathcal{A}_{\alpha_k,\beta_k}(\mathbf{z}^*, \mathbf{u}^*) = \mathcal{O}(\mathbf{x}^{(k)} - \mathbf{x}^*)$,

where $\mathbf{z} := (\mathbf{x}_1, \mathbf{x}_2)$, $\mathbf{z}^{(k)} := (\mathbf{x}^{(k)}, \mathbf{x}^{(k-1)})$, and $\mathbf{z}^* := (\mathbf{x}^*, \mathbf{x}^*)$

Proof. The proof is in Section C.3 in the appendix. □

3.5.1 Implicit Differentiation

Similarly Theorems 10, and 19 can be used to yield an IFT for the fixed-point equation of APG [46, Theorem 39], which we recall below.

Theorem 20. Let f and g satisfy Assumption 3.1 and $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be such that Assumptions 3.2(ii) and 3.3 are satisfied. Then for any $\alpha \in [\underline{\alpha}, \bar{\alpha}]$ and $\beta \in [0, 1]$ with $-1/(1+2\beta) < \lambda_{\min}(D_{\mathbf{x}}\mathcal{A}_{\alpha}(\mathbf{x}^*, \mathbf{u}))$, we have $\rho(D_{\mathbf{z}}\mathcal{A}_{\alpha,\beta}(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*, \mathbf{x}^*)) < 1$. Additionally when Assumption 3.2(i) is also satisfied, the (possibly reduced) neighbourhood U and the mapping ψ from Theorem 10 satisfy $\mathbf{z} = \mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u})$ and

$$\begin{bmatrix} D\psi(\mathbf{u}) \\ D\psi(\mathbf{u}) \end{bmatrix} = (I - D_{\mathbf{z}}\mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u})\Pi(\mathbf{z}))^{-1} D_{\mathbf{u}}\mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u}), \quad (12)$$

for all $\mathbf{u} \in U$ and $\mathbf{z} := (\psi(\mathbf{u}), \psi(\mathbf{u}))$.

3.5.2 Automatic Differentiation

Mehmood and Ochs [46, see Theorem 44] established the convergence of the derivative iterates of APG. We strengthen their results by providing convergence rate guarantees in our final result below.

Theorem 21. Let f and g satisfy Assumption 3.1 and $(\mathbf{x}^*, \mathbf{u}^*) \in \mathcal{M} \times \Omega$ be such that Assumption 3.3 are satisfied. For $[\underline{\alpha}, \bar{\alpha}] \ni \alpha_k \rightarrow \alpha_*$ and $[0, 1] \ni \beta_k \rightarrow \beta_*$, let the sequence $(\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ generated by Algorithm 1 converges to \mathbf{x}^* with $\mathbf{x}^{(0)}$ sufficiently close to \mathbf{x}^* . Then the sequence $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ converges to $D\psi(\mathbf{u}^*)$. Additionally $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ converges linearly with rate $\max(q_{\mathbf{x}}, \rho(D_{\mathbf{z}}\mathcal{A}_{\alpha_*,\beta_*}(\mathbf{x}^*, \mathbf{u}^*)))$ when \mathcal{M} is C^3 -smooth, $\nabla_{\mathcal{M}}g$, $\nabla_{\mathbf{x}}^2 f$, $\nabla_{\mathcal{M}}^2 g$, $D_{\mathbf{u}}\nabla_{\mathbf{x}}f$, and $D_{\mathbf{u}}\nabla_{\mathcal{M}}g$ are locally Lipschitz continuous near $(\mathbf{x}^*, \mathbf{u}^*)$ and $(\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ converges with rate $q_{\mathbf{x}} < 1$.

Proof. The proof is in Section C.4 in the appendix. □

Remark 22. The arguments made in Remark 17 naturally extend to Theorem 21.

4 Experiments

To test our results, we provide numerical demonstration on one smooth and one non-smooth example from classical Machine Learning. These include logistic regression with ℓ_2 regularization, that is,

$$\min_{\mathbf{x}} \frac{1}{M} \sum_{i=1}^M \log(1 + \exp(-b_i \mathbf{a}_i^T \mathbf{x})) + \frac{1}{2} \lambda \|\mathbf{x}\|_2^2, \quad (13)$$

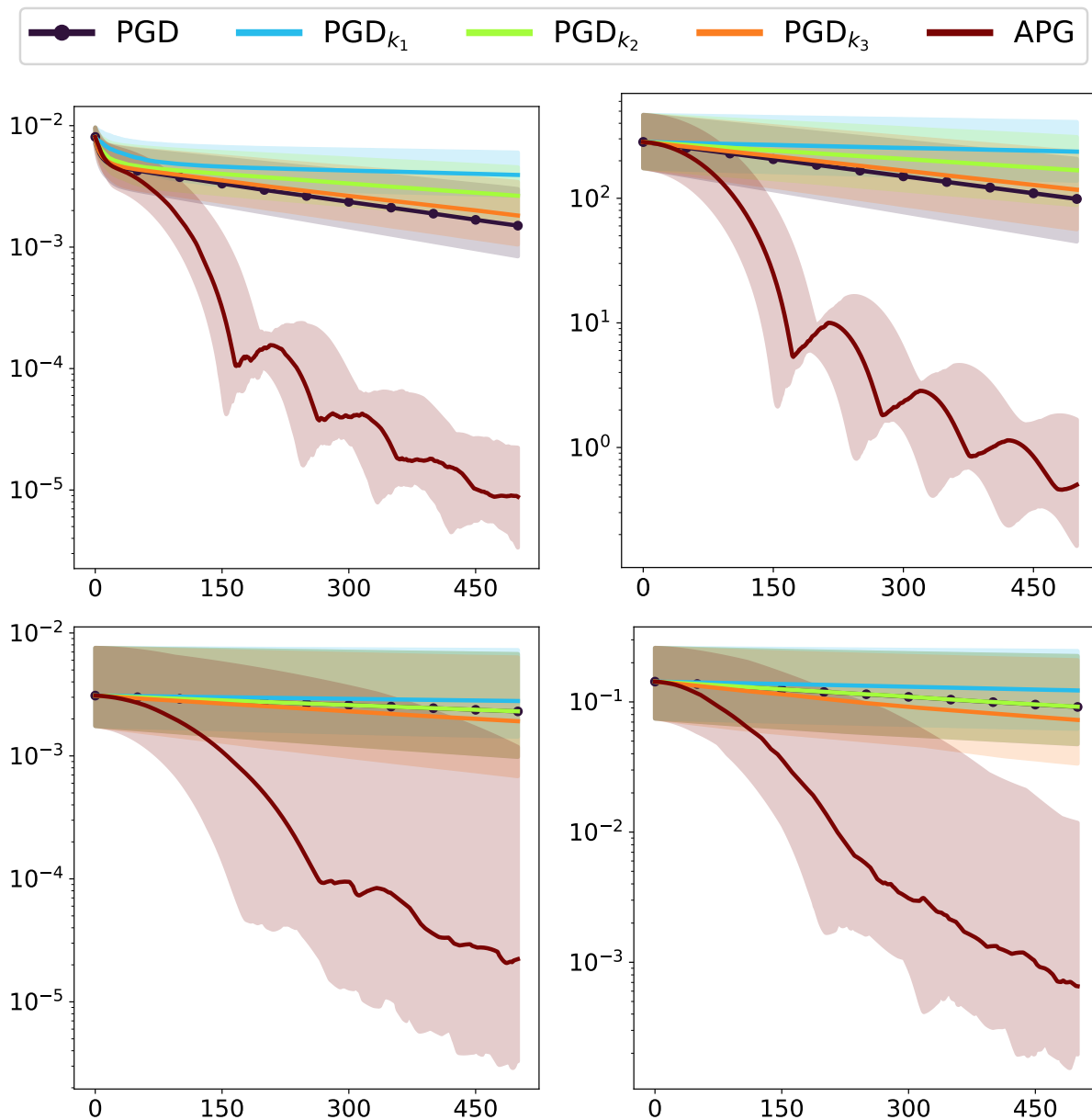


Figure 1: Error plots of iterates (left column) of PGD and APG for Logistic (top row) and Lasso (bottom row) Regression along with their derivative iterates (right column). Similarity in the convergence rates of the original and the derivative iterates is clearly visible.

with parameters $\mathbf{u} := (A, \lambda)$ and linear regression with ℓ_1 regularization, that is,

$$\min_{\mathbf{x}} \frac{1}{2} \|A\mathbf{x} - \mathbf{b}\|_2 + \lambda \|\mathbf{x}\|_1, \quad (14)$$

with parameters $\mathbf{u} := (A, \mathbf{b}, \lambda)$. All the parameters are selected in such a way that Assumptions 3.1–3.3 are satisfied.

We solve the two problems through PGD with four different choices of step sizes and APG with fixed step size and $\beta_k := (k - 1)/(k + 5)$ (depicted by APG in Figure 1). This generates five different algorithm sequences $(\mathbf{x}^{(k)}(\mathbf{u}))_{k \in \mathbb{N}}$ for each problem. The four step size options for PGD include $\alpha_k := \alpha_*$ (depicted by PGD in Figure 1), $\alpha_k \sim U(0, \frac{2}{3L})$ (depicted by PGD_{k1}), $\alpha_k \sim U(\frac{2}{3L}, \frac{4}{3L})$ (depicted by PGD_{k2}), and $\alpha_k \sim U(\frac{4}{3L}, \frac{2}{L})$ (depicted by PGD_{k3}) where α_* is the optimal step size for each problem. We solve each problem for 50 different instances of the parameters and plot the median error. For each problem, we initialize $\mathbf{x}^{(0)} \in B_{10^{-2}}(\mathbf{x}^*)$ by first solving it partially.

In Figure 1, the left column shows the median error plots of the five algorithms and the right column shows the errors of the corresponding derivatives with the same colour. The top and bottom rows correspond to the error plots for (13) and (14) respectively. The figure clearly shows that the derivative error decays as fast as the algorithm error for each problem.

5 Conclusion

We applied automatic differentiation on the iterative processes with time-varying update mappings. We strengthened a previous result [9] with convergence rate guarantee and extended them to a new setting. As an example for each setting, we adapted our results to proximal gradient descent with variable step size and its accelerated counterpart, that is, FISTA. We showed that the convergence rate of the algorithm is simply mirrored in its derivative iterates which was supported through experiments on toy problems.

A Preliminaries & Related Work

Before we move on to the proofs of our main results, we present some preliminary results which will be useful later. We also provide a recap of the results of [9] for a better understanding of our work.

A.1 Matrix Analysis

This section provides a few preliminary results on Matrix Analysis. We start by recalling a classical result from Linear Algebra which forms the foundation for the implicit differentiation applied to (\mathcal{R}_e) when combined with the Implicit Function Theorem [25, Theorem 1B.1].

Lemma 23. For any linear operator $B: \mathcal{X} \rightarrow \mathcal{X}$ with $\rho(B) < 1$, the linear operator $I - B$ is invertible.

We now provide some results which will be used in the proofs of convergence of automatic differentiation of the fixed-point iterations. In particular, we provide convergence guarantees of sequences generated through linear iterative procedures including (18), and (15) which bear strong resemblance with (DR) and (DR_k) (see the proofs of Theorems 30 and 5 for a more detailed comparison). These convergence results are mainly derived from [51, Section 2.1.2, Theorem 1], [53, Proposition 2.7], and [46, Theorem 8]. The following theorem will be used to prove convergence results in Section 2.

Theorem 24. Let $(B_k)_{k \in \mathbb{N}_0}$, $(C_k)_{k \in \mathbb{N}_0}$ and $(\mathbf{d}^{(k)})_{k \in \mathbb{N}_0}$ be sequences in $\mathcal{L}(\mathcal{X}, \mathcal{X})$, $\mathcal{L}(\mathcal{X}, \mathcal{X})$ and \mathcal{X} respectively such that $C_k \rightarrow 0$, $\mathbf{d}^{(k)} \rightarrow 0$ and $\rho := \limsup_{k \rightarrow \infty} \|B_k\| < 1$ where $\|\cdot\|$ is a norm on $\mathcal{L}(\mathcal{X}, \mathcal{X})$ induced by some vector norm. Then the sequence $(\mathbf{e}^{(k)})_{k \in \mathbb{N}_0}$, with $\mathbf{e}^{(0)} \in \mathcal{X}$, generated by

$$\mathbf{e}^{(k+1)} := B_k \mathbf{e}^{(k)} + C_k \mathbf{e}^{(k)} + \mathbf{d}^{(k)}, \quad (15)$$

converges to 0. The convergence is linear when C_k and $\mathbf{d}^{(k)}$ converge linearly with rates q_C and $q_{\mathbf{d}}$ respectively. In fact, for all $\varepsilon \in (0, 1 - \rho)$, there exist $C_1(\varepsilon)$, $C_2(\varepsilon)$ and $K \in \mathbb{N}$, such that for all $k \geq K$, we have

$$\|\mathbf{e}^{(k)}\| \leq C_1(\varepsilon)(k - K)q^{k-K} + C_2(\varepsilon)(\rho + \varepsilon)^{k-K}, \quad (16)$$

where $q := \max(\rho + \varepsilon, q_C, q_{\mathbf{d}})$.

Proof. From classical analysis, given $\varepsilon \in (0, 1 - \rho)$, there exists $K \in \mathbb{N}$ such that $\|B_k\| < \rho + \varepsilon/2$ for all $k \geq K$. Also, with K large enough we have $\|C_k \mathbf{e}^{(k)}\| / \|\mathbf{e}^{(k)}\| \leq \varepsilon/2$ since $C_k \rightarrow 0$. Therefore, from (15), we get

$$\begin{aligned} \|\mathbf{e}^{(k+1)}\| &\leq (\rho + \varepsilon/2)\|\mathbf{e}^{(k)}\| + \|C_k \mathbf{e}^{(k)}\| + \|\mathbf{d}^{(k)}\| \\ &\leq (\rho + \varepsilon)\|\mathbf{e}^{(k)}\| + \|\mathbf{d}^{(k)}\|. \end{aligned}$$

The convergence of $\mathbf{e}^{(k)}$ then follows from the arguments following Equation 34 in the proof of Theorem 8 in [46].

For the rate of convergence, we note that $\boldsymbol{\varepsilon}^{(k)} := C_k \mathbf{e}^{(k)} + \mathbf{d}^{(k)}$ converges linearly to 0 with rate $\max(q_C, q_{\mathbf{d}})$ and for $K \in \mathbb{N}$ sufficiently large we can write $\|\boldsymbol{\varepsilon}^{(k)}\| \leq \max(q_C, q_{\mathbf{d}})^{k-K} \|\boldsymbol{\varepsilon}^{(K)}\|$ for all $k \geq K$. Thus, for any $k \geq K$, we expand the expression $\mathbf{e}^{(k+1)} = B_k \mathbf{e}^{(k)} + \boldsymbol{\varepsilon}^{(k)}$ to obtain

$$\mathbf{e}^{(k+1)} = B_{k:K} \mathbf{e}^{(K)} + \sum_{i=K}^k B_{k:i+1} \boldsymbol{\varepsilon}^{(i)}$$

where $B_{k:i}$ denotes the ordered product $B_k B_{k-1} \cdots B_{i+1} B_i$ when $i \leq k$ and identity operator I when $i > k$. Observe that, for any $\varepsilon \in (0, 1 - \rho)$ and $K \in \mathbb{N}$ large enough, $\|B_k\| < \rho + \varepsilon$ for all $k \geq K$ and therefore for any $K \leq i \leq k + 1$, we have $\|B_{k:i}\| \leq (\rho + \varepsilon)^{k-i+1}$. Therefore,

setting $q := \max(\rho + \varepsilon, q_C, q_d)$, we end up with

$$\begin{aligned}
 \|\mathbf{e}^{(k+1)}\| &\leq \|B_{k:K}\| \|\mathbf{e}^{(K)}\| + \sum_{i=K}^k \|B_{k:i+1}\| \|\boldsymbol{\varepsilon}^{(i)}\| \\
 &\leq \|\mathbf{e}^{(K)}\| (\rho + \varepsilon)^{k-K+1} + \sum_{i=K}^k (\rho + \varepsilon)^{k-i} \|\boldsymbol{\varepsilon}^{(K)}\| \max(q_C, q_d)^{i-K} \\
 &\leq \|\mathbf{e}^{(K)}\| (\rho + \varepsilon)^{k-K+1} + \|\boldsymbol{\varepsilon}^{(K)}\| \sum_{i=K}^k q^{k-K} \\
 &\leq \|\mathbf{e}^{(K)}\| (\rho + \varepsilon)^{k-K+1} + \|\boldsymbol{\varepsilon}^{(K)}\| (k - K + 1) q^{k-K}.
 \end{aligned} \tag{17}$$

□

The result below is a direct consequence of the above theorem and will find its use when proving Corollary 8.

Corollary 25. The conclusion of Theorem 24 also holds when the assumptions on the sequence $(B_k)_{k \in \mathbb{N}_0}$ are replaced with $B_k \rightarrow B \in \mathcal{L}(\mathcal{X}, \mathcal{X})$ and $\rho(B) < 1$.

Proof. This is a special case of Theorem 24 because for any $\delta \in (0, 1 - \rho(B))$, there exists a norm on $\mathcal{L}(\mathcal{X}, \mathcal{X})$ induced by some vector norm, both denoted by $\|\cdot\|_\delta$, such that $\|B\|_\delta \leq \rho(B) + \delta$ and $\rho := \lim_{k \rightarrow \infty} \|B_k\|_\delta = \|B\|_\delta \leq \rho(B) + \delta < 1$. □

The following result is a special case of the setting of Corollary 25 and is straightforward to show.

Corollary 26. The conclusion of Theorem 24 also holds when the assumptions on the sequence $(B_k)_{k \in \mathbb{N}_0}$ are replaced with $B_k := B \in \mathcal{L}(\mathcal{X}, \mathcal{X})$ for all $k \in \mathbb{N}$ and $\rho(B) < 1$.

Using Corollary 26, we can prove the following statement which will be useful in the convergence proofs of Section A.2.

Theorem 27. Let $(B_k)_{k \in \mathbb{N}_0}$ and $(\mathbf{b}^{(k)})_{k \in \mathbb{N}_0}$ be sequences in $\mathcal{L}(\mathcal{X}, \mathcal{X})$ and \mathcal{X} with limits B and \mathbf{b} , respectively. If $\rho = \rho(B) < 1$, the sequence $(\mathbf{x}^{(k)})_{k \in \mathbb{N}_0}$, with $\mathbf{x}^{(0)} \in \mathcal{X}$, generated by

$$\mathbf{x}^{(k+1)} := B_k \mathbf{x}^{(k)} + \mathbf{b}^{(k)}, \tag{18}$$

converges to $\mathbf{x} := (I - B)^{-1} \mathbf{b}$. The convergence is linear when $(B_k)_{k \in \mathbb{N}_0}$ and $(\mathbf{b}^{(k)})_{k \in \mathbb{N}_0}$ converge linearly with rates q_B and q_b , respectively. In fact, for all $\delta \in (0, 1 - \rho)$, there exist $C_1(\delta)$, $C_2(\delta)$ and $K \in \mathbb{N}$, such that for all $k \geq K$, we have

$$\|\mathbf{x}^{(k)} - \mathbf{x}\| \leq C_1(\delta)(k - K)q^{k-K} + C_2(\delta)(\rho + \delta)^{k-K}, \tag{19}$$

where $q := \max(\rho + \delta, q_B, q_b)$.

Proof. The expression $\mathbf{x} = (I - B)^{-1}\mathbf{b}$ is well-defined thanks to Lemma 23 and solves the linear equation $\mathbf{x} = B\mathbf{x} + \mathbf{b}$ for \mathbf{x} . By setting $\mathbf{e}^{(k)} := \mathbf{x}^{(k)} - \mathbf{x}$, $C_k := B_k - B$, and $\mathbf{d}^{(k)} := (B_k - B)\mathbf{x} + \mathbf{b}^{(k)} - \mathbf{b}$, we obtain,

$$\begin{aligned} \mathbf{e}^{(k+1)} &= (B_k\mathbf{x}^{(k)} + \mathbf{b}^{(k)}) - (B\mathbf{x} + \mathbf{b}) \\ &= B\mathbf{e}^{(k)} + C_k\mathbf{e}^{(k)} + \mathbf{d}^{(k)}. \end{aligned}$$

Since the above recursion matches (15) and the setting of Corollary 26 applies, the result follows. \square

A.2 Differentiation of Iteration-Dependent Algorithms: Classical Results

In this section, we briefly recap the results of [9] in a way that aligns with those of Section 2, allowing for a clearer comparison between the two sets of results. We first lay down the assumptions on the sequence of mappings \mathcal{A}_k in (\mathcal{R}_k) and the mapping \mathcal{A} in (\mathcal{R}_e) which will ensure the convergence of the sequence $D\mathbf{x}^{(k)}(\mathbf{u})$ generated by (\mathcal{DR}_k) . The main requirement in the work of [9] is that of the pointwise convergence of the sequence $D\mathcal{A}_k$ to $D\mathcal{A}$.

A.2.1 Problem Setting

Given $\mathbf{u}^* \in \mathcal{X}$, we assume that \mathbf{x}^* solves (\mathcal{R}_e) for \mathbf{x} with $\mathbf{u} = \mathbf{u}^*$ and is the desired limit of $\mathbf{x}^{(k)}(\mathbf{u}^*)$ generated by (\mathcal{R}_k) . Furthermore, we assume that for all k , \mathcal{A}_k and \mathcal{A} are C^1 -smooth near $(\mathbf{x}^*, \mathbf{u}^*)$ and the contraction property holds for $D_x\mathcal{A}$ at $(\mathbf{x}^*, \mathbf{u}^*)$. In particular, given $(\mathbf{x}^{(0)}, \mathbf{x}^*, \mathbf{u}^*) \in \mathcal{X} \times \mathcal{X} \times \mathcal{U}$, $V \in \mathcal{N}_{(\mathbf{x}^*, \mathbf{u}^*)}$, and $(\mathcal{A}_k)_{k \in \mathbb{N}_0}$, we assume that the following assumption holds.

Assumption A.1. (i) $\mathcal{A}_k|_V$ and $\mathcal{A}|_V$ are C^1 -smooth for all k ,

(ii) $\mathbf{x}^* = \mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)$,

(iii) $\rho(D_x\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)) < 1$, and

(iv) $\mathbf{x}^{(k)}(\mathbf{u}^*)$ generated by (\mathcal{R}_k) has limit \mathbf{x}^* such that $(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*) \in V$ for all $k \in \mathbb{N}$.

A.2.2 Implicit Differentiation

From Assumption A.1, Lemma 23, and [25, Theorem 1B.1], we obtain the Implicit Function Theorem for (\mathcal{R}_e) .

Theorem 28 (Implicit Function Theorem). For some $(\mathbf{x}^*, \mathbf{u}^*)$, let \mathcal{A} be C^1 -smooth near $(\mathbf{x}^*, \mathbf{u}^*)$, $\mathbf{x}^* = \mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)$ and $\rho(D_x\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)) < 1$. Then $\exists U \in \mathcal{N}_{\mathbf{u}^*}$ and a C^1 -smooth mapping $\psi: U \rightarrow \mathcal{X}$ such that $\forall \mathbf{u} \in U$, $\psi(\mathbf{u}) = \mathcal{A}(\psi(\mathbf{u}), \mathbf{u})$, and

$$D\psi(\mathbf{u}) = (I - D_x\mathcal{A}(\psi(\mathbf{u}), \mathbf{u}))^{-1}D_u\mathcal{A}(\psi(\mathbf{u}), \mathbf{u}). \quad (20)$$

A.2.3 Automatic Differentiaion

As stated in Section A.1, the update procedure to generate the derivative iterates in (\mathcal{DR}_k) takes after the iterative process defined by (18) in Theorem 27. That is, for some $\mathbf{u}^* \in \mathcal{U}$ and $\dot{\mathbf{u}} \in \mathcal{U}$, if we set $B_k := D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*)$ and $\mathbf{b}^{(k)} := D_{\mathbf{u}}\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*)\dot{\mathbf{u}}$, the resulting sequence is $\mathbf{y}^{(k)} = D\mathbf{x}^{(k)}(\mathbf{u}^*)\dot{\mathbf{u}}$. Similarly, the limit $\mathbf{y}^* := (I - B)^{-1}\mathbf{b}$ of the sequence $\mathbf{y}^{(k)}$ generated by (18) matches $D\psi(\mathbf{u}^*)\dot{\mathbf{u}}$ from (20), if we set $B := D_{\mathbf{x}}\mathcal{A}(\psi(\mathbf{u}^*), \mathbf{u}^*)$ and $\mathbf{b} := D_{\mathbf{u}}\mathcal{A}(\psi(\mathbf{u}^*), \mathbf{u}^*)\dot{\mathbf{u}}$. One way to prove the convergence of $D\mathbf{x}^{(k)}(\mathbf{u}^*)\dot{\mathbf{u}}$ to $D\psi(\mathbf{u}^*)\dot{\mathbf{u}}$ is by asserting that $D\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*)$ converges to $D\mathcal{A}(\psi(\mathbf{u}^*), \mathbf{u}^*)$.

Assumption A.2. The sequence $(D\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*))_{k \in \mathbb{N}_0}$ converges to $D\mathcal{A}(\psi(\mathbf{u}^*), \mathbf{u}^*)$.

Remark 29. When the sequence of functions $(D\mathcal{A}_k)_{k \in \mathbb{N}}$ is equicontinuous at $(\mathbf{x}^*, \mathbf{u}^*)$ and has a pointwise limit $D\mathcal{A}$ near $(\mathbf{x}^*, \mathbf{u}^*)$, then Assumption A.2 naturally holds.

The main result of [9] can then be stated below.

Theorem 30. Let $(\mathbf{x}^{(0)}, \mathbf{x}^*, \mathbf{u}^*)$ be such that Assumptions A.1 and A.2 are satisfied by \mathcal{A}_k and \mathcal{A} . Then the sequence $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}_0}$ generated by (\mathcal{DR}_k) converges to $D\psi(\mathbf{u}^*)$.

Proof. The proof is a direct consequence of Assumptions A.1 and A.2, Theorem 27 and the arguments following Theorem 27. \square

For linear convergence we require a stronger assumption on $D\mathcal{A}_k$, that is its linear convergence as given below.

Assumption A.3. The sequence $(\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}_0}$ converges linearly to \mathbf{x}^* and

$$D\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*) - D\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*) = \mathcal{O}(\mathbf{x}^{(k)}(\mathbf{u}^*) - \mathbf{x}^*). \quad (21)$$

Theorem 31. Let $(\mathbf{x}^{(0)}, \mathbf{x}^*, \mathbf{u}^*)$ be such that Assumptions A.1 and A.3 are satisfied by \mathcal{A}_k and \mathcal{A} . Then the sequence $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}_0}$ generated by (\mathcal{DR}_k) converges linearly to $D\psi(\mathbf{u}^*)$. In particular, when the sequence $(\mathbf{x}^{(k)})_{k \in \mathbb{N}_0}$ converges with rate $q_{\mathbf{x}} < 1$, then for all $\delta \in (0, 1 - \rho)$, there exist $C_1(\delta)$, $C_2(\delta)$ and $K \in \mathbb{N}$, such that for all $k \geq K$, we have

$$\|D\mathbf{x}^{(k)}(\mathbf{u}^*) - D\psi(\mathbf{u}^*)\| \leq C_1(\delta)(k - K)q^{k-K} + C_2(\delta)(\rho + \delta)^{k-K}, \quad (22)$$

where $\rho := \rho(D_{\mathbf{x}}\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*))$ and $q := \max(\rho + \delta, q_{\mathbf{x}})$.

Proof. Assumption A.3 asserts that the sequences $D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*)$ and $D_{\mathbf{u}}\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*)\dot{\mathbf{u}}$ respectively converge to $D_{\mathbf{x}}\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)$ and $D_{\mathbf{u}}\mathcal{A}(\mathbf{x}^*, \mathbf{u}^*)\dot{\mathbf{u}}$ for any $\dot{\mathbf{u}} \in \mathcal{U}$. Furthermore, the rate of convergence of the two sequences is linear and is the same as that of $\mathbf{x}^{(k)}$, that is, $q_{\mathbf{x}}$. Therefore, the proof follows by simply invoking the second part of Theorem 27. \square

Remark 32. Assumption A.3 is not practical and therefore we rarely see any application of the above result in practice. For instance, for gradient descent with line search, it requires linear convergence of the step size sequence which does not hold in general.

B Proofs of Section 2

B.1 Proof of Lemma 2

Proof. From Assumption 2.1(iii), given $\varepsilon \in (0, 1 - \rho)$, there exists $K \in \mathbb{N}$ such that $\rho(D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)) \leq \|D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)\| < \rho + \varepsilon$ for all $k \geq K$, where $\rho := \limsup_{k \rightarrow \infty} \|D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)\|$. The existence of the neighbourhood U and the C^1 -smooth mapping $\psi: U \rightarrow \mathcal{X}$ is guaranteed by Theorem 28 applied to \mathcal{A}_n for some $n \geq K$, thanks to Assumption 2.1 (i)–(ii). In particular, for all $\mathbf{u} \in U$, $\psi(\mathbf{u}) = \mathcal{A}_n(\psi(\mathbf{u}), \mathbf{u})$ and $D\psi(\mathbf{u})$ is given by (20) with \mathcal{A} replaced by \mathcal{A}_n . From Assumption 2.1(ii), for any $k \geq K$ and $\mathbf{u} \in U$, we have $\psi(\mathbf{u}) = \mathcal{A}_n(\psi(\mathbf{u}), \mathbf{u}) = \mathcal{A}_k(\psi(\mathbf{u}), \mathbf{u})$ and with U possibly reduced, $\rho(D_{\mathbf{x}}\mathcal{A}_k(\psi(\mathbf{u}), \mathbf{u})) < 1$. Therefore, by using the Chain rule and Lemma 23, we obtain the expression in (4). \square

B.2 Proof of Theorem 5

Proof. From Lemma 2 and Remark 3, there exists $K \in \mathbb{N}$ such that for any $k \geq K$, the fixed-point mapping ψ_k of $\mathcal{A}_k(\cdot, \mathbf{u})$ is C^1 -smooth near \mathbf{u}^* and $D\psi_k(\mathbf{u}^*) = X_*$ (see Assumption 2.1(ii)). We denote $\mathbf{x}^{(k)} := \mathbf{x}^{(k)}(\mathbf{u}^*)$ for simplicity and define

$$\begin{aligned} \mathbf{e}^{(k)} &:= (D\mathbf{x}^{(k)}(\mathbf{u}^*) - X_*) \dot{\mathbf{u}} \\ B_k &:= D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*) \\ C_k &:= D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^{(k)}, \mathbf{u}^*) - D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*) \\ \mathbf{d}^{(k)} &:= (D\mathcal{A}_k(\mathbf{x}^{(k)}, \mathbf{u}^*) - D\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*)) \begin{bmatrix} X_* \dot{\mathbf{u}} \\ \dot{\mathbf{u}} \end{bmatrix}, \end{aligned} \quad (23)$$

to obtain

$$\begin{aligned} \mathbf{e}^{(k+1)} &= \left(D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^{(k)}, \mathbf{u}^*) D\mathbf{x}^{(k)}(\mathbf{u}^*) \dot{\mathbf{u}} + D_{\mathbf{u}}\mathcal{A}_k(\mathbf{x}^{(k)}, \mathbf{u}^*) \dot{\mathbf{u}} \right) - \\ &\quad \left(D_{\mathbf{x}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*) X_* \dot{\mathbf{u}} + D_{\mathbf{u}}\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*) \dot{\mathbf{u}} \right) \\ &= B_k \mathbf{e}^{(k)} + C_k \mathbf{z}^{(k)} + \mathbf{d}^{(k)}. \end{aligned} \quad (24)$$

From Assumption 2.2 and the definitions of C_k and $\mathbf{y}^{(k)}$, we note that $C_k \rightarrow 0$ and $\mathbf{d}^{(k)} \rightarrow 0$. Therefore, from Theorem 24, $(D\mathbf{x}^{(k)}(\mathbf{u}^*) \dot{\mathbf{u}})_{k \in \mathbb{N}_0}$ converges to $X_* \dot{\mathbf{u}}$ for any $\dot{\mathbf{u}} \in \mathcal{U}$. \square

B.3 Proof of Theorem 7

Proof. From Assumption 2.3, we have $D\mathcal{A}_k(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{u}^*) - D\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*) \rightarrow 0$ and the rate of convergence of the two sequences is $q_{\mathbf{x}}$. For any $\dot{\mathbf{u}} \in \mathcal{U}$, by using the definitions in (23), we note that both C_k and $\mathbf{y}^{(k)}$ converge linearly with rate $q_{\mathbf{x}}$. Thus, invoking the second part of Theorem 24, we obtain the asymptotic and the non-asymptotic convergence rate of $(D\mathbf{x}^{(k)}(\mathbf{u}^*) \dot{\mathbf{u}})_{k \in \mathbb{N}_0}$. \square

C Proofs of Section 3

C.1 Proof of Theorem 13

The proof of Theorem 13 relies on the following preliminary result from set-valued analysis.

Lemma 33. Given a sequence of non-empty, closed, convex sets $C_k \subset \mathcal{X}$ which converges to $C \subset \mathcal{X}$. Let $\mathbf{x}^{(k)} \in C_k$ be a sequence with limit $\mathbf{x} \in \text{ri} C$. Then there exists $K \in \mathbb{N}$ such that $\mathbf{x}^{(k)} \in \text{ri} C_k$ for all $k \geq K$.

Proof. Because $\mathbf{x}^{(k)} \rightarrow \mathbf{x}$ and $\mathbf{x} \in \text{ri} C$, there exists a compact set V and $K \in \mathbb{N}$ such that $\mathbf{x}^{(k)}, \mathbf{x} \in \text{int} V \neq \emptyset$ for all $k \geq K$ and $V \cap \text{aff} C \subset C$. Moreover, the convergence of C_k implies $\text{aff} C_k \rightarrow \text{aff} C$ which implies $V \cap \text{aff} C_k \rightarrow V \cap \text{aff} C$ [47, Lemma 1.4]. Once we show that $V \cap \text{aff} C_k \subset C_k$ eventually, we are done. Assume for contradiction, that there exists a subsequence $(C_{k_i})_{i \in \mathbb{N}}$ such that for all $i \in \mathbb{N}$, $\mathbf{y}^{(i)} \in V \cap \text{aff} C_{k_i}$ and $\mathbf{y}^{(i)} \notin C_{k_i}$. The compactness of V and convergence of $V \cap \text{aff} C_{k_i}$ implies the existence of $\mathbf{y} \in V \cap \text{aff} C$ such that $\mathbf{y}^{(i)} \rightarrow \mathbf{y}$, possibly through a subsequence. We define the bounded sequence $\mathbf{b}^{(i)} := \mathbf{a}^{(i)} / \|\mathbf{a}^{(i)}\|$ where $\mathbf{a}^{(i)} := \mathbf{y}^{(i)} - \text{proj}_{C_{k_i}}(\mathbf{y}^{(i)})$ which lies in $\text{par} C_{k_i}$ and has limit $0 \neq \mathbf{b} \in \text{par} C$, again, possibly through a subsequence. For all $i \in \mathbb{N}$ and for all $\mathbf{w} \in C_{k_i}$,

$$\begin{aligned} \langle \mathbf{b}^{(i)}, \mathbf{w} - \mathbf{y}^{(i)} \rangle &= -\frac{1}{\|\mathbf{a}^{(i)}\|} \left(\langle \mathbf{a}^{(i)}, \mathbf{y}^{(i)} - \text{proj}_{C_{k_i}}(\mathbf{y}^{(i)}) \rangle + \langle \mathbf{a}^{(i)}, \text{proj}_{C_{k_i}}(\mathbf{y}^{(i)}) - \mathbf{w} \rangle \right) \\ &\leq -\frac{1}{2} \|\mathbf{a}^{(i)}\| \leq 0, \end{aligned}$$

where the inequality follows because $\mathbf{a}^{(i)} \in N_{C_{k_i}}(\text{proj}_{C_{k_i}}(\mathbf{y}^{(i)}))$. The above inequality leads to $\langle \mathbf{b}, \mathbf{w} - \mathbf{y} \rangle \leq 0$ for all $\mathbf{w} \in C$. In other words, we obtain $0 \neq \mathbf{b} \in N_C(\mathbf{y}) \cap \text{par} C$ which is a contradiction because $\mathbf{y} \in \text{ri} C$. \square

Proof. [Proof of Theorem 13]

- (i) From the convergence of $\mathbf{x}^{(k)} := \mathbf{x}^{(k)}(\mathbf{u}^*)$, Lemma 18 ensures that for $\delta > 0$ small enough, there exists $K \in \mathbb{N}$, such that $\mathbf{x}^{(k)} \in \mathcal{M} \cap B_\delta(\mathbf{x}^*)$ for all $k \geq K$. We define the maps $G: \mathcal{X} \times \Omega \times (0, 2/L) \rightarrow \mathcal{X}$ by $G(\mathbf{x}, \mathbf{u}, \alpha) = \mathbf{x} - \alpha \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{u})$ and $H: \mathcal{X} \times \mathcal{X} \times \Omega \times (0, 2/L) \rightarrow \overline{\mathbb{R}}$ by

$$H(\mathbf{y}, \mathbf{x}, \mathbf{u}, \alpha) := \alpha g(\mathbf{y}, \mathbf{u}) + \frac{1}{2} \|\mathbf{y} - \mathbf{x} + \alpha \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{u})\|^2,$$

and note that $\mathbf{x}^{(k+1)} = \mathcal{A}_{\alpha_k}(\mathbf{x}^{(k)}, \mathbf{u}^*) = \text{argmin}_{\mathbf{y}} H(\mathbf{y}, \mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k)$, which is equivalent to $0 \in \partial_{\mathbf{y}} H(\mathbf{x}^{(k+1)}, \mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k)$ or $\boldsymbol{\mu}^{(k)} \in \partial_{\mathbf{x}} F(\mathbf{x}^{(k+1)}, \mathbf{u}^*)$ from Fermat's rule, where

$$\boldsymbol{\mu}^{(k)} := \frac{1}{\alpha_k} \left(G(\mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k) - G(\mathbf{x}^{(k+1)}, \mathbf{u}^*, \alpha_k) \right). \quad (25)$$

Notice that $\boldsymbol{\mu}^{(k)} \rightarrow 0$ because $G(\cdot, \mathbf{u}^*, \alpha)$ is non-expansive when $\alpha \in (0, 2/L)$ and we have $\|\boldsymbol{\mu}^{(k)}\| \leq \frac{1}{\underline{\alpha}} \|\mathbf{x}^{(k)} - \mathbf{x}^{(k+1)}\|$. Therefore, from (ND) and Lemma 33, we have $\boldsymbol{\mu}^{(k)} \in \text{ri } \partial_{\mathbf{x}} F(\mathbf{x}^{(k+1)}, \mathbf{u}^*)$ or $0 \in \text{ri } \partial_{\mathbf{y}} H(\mathbf{x}^{(k+1)}, \mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k)$, for all $k \in \mathbb{N}$ large enough. Since H is partly smooth relative to $\mathcal{M} \times \mathcal{X} \times \Omega \times (0, 2/L)$ and $H(\cdot, \mathbf{x}, \mathbf{u}, \alpha)$ is strongly convex for all $(\mathbf{x}, \mathbf{u}, \alpha) \in \mathcal{X} \times \Omega \times (0, 2/L)$, and non-degeneracy condition holds, the C^1 -smoothness of the update map near $(\mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k)$ follows by invoking Theorem 10. The C^1 -smoothness of \mathcal{A}_α near $(\mathbf{x}^*, \mathbf{u}^*, \alpha)$ under given assumptions was shown in [46, Corollary 32] for any $\alpha \in [\underline{\alpha}, \bar{\alpha}]$.

(ii) We define

$$\begin{aligned} Q_k &:= \nabla_{\mathcal{M}}^2 H(\mathbf{x}^{(k+1)}, \mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k), & \tilde{Q}_k &:= \nabla_{\mathcal{M}}^2 H(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*, \alpha_k) \\ P_{\omega, k} &:= D_\omega \nabla_{\mathcal{M}} H(\mathbf{x}^{(k+1)}, \mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k), & \tilde{P}_{\omega, k} &:= D_\omega \nabla_{\mathcal{M}} H(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*, \alpha_k) \\ \Pi_k &:= \Pi(\mathbf{x}^{(k)}), & \Pi_* &:= \Pi(\mathbf{x}^*), & \Pi_k^\perp &:= \Pi^\perp(\mathbf{x}^{(k)}), & \Pi_*^\perp &:= \Pi^\perp(\mathbf{x}^*), \end{aligned}$$

where $\omega \in \{\mathbf{x}, \mathbf{u}, \alpha\}$ and evaluate Q_k to obtain

$$\begin{aligned} Q_k &= \alpha_k \nabla_{\mathcal{M}}^2 g(\mathbf{x}^{(k+1)}, \mathbf{u}^*) + \Pi_{k+1} + \mathfrak{W}_{\mathbf{x}^{(k+1)}}(\cdot, \Pi_{k+1}^\perp(\mathbf{x}^{(k+1)} - G(\mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k))) \\ &= \alpha_k \nabla_{\mathcal{M}}^2 g(\mathbf{x}^*, \mathbf{u}^*) + \alpha_k \mathfrak{W}_{\mathbf{x}^{(k+1)}}(\cdot, \Pi_{k+1}^\perp \nabla_{\mathbf{x}} f(\mathbf{x}^{(k+1)}, \mathbf{u}^*)) + \Pi_{k+1} + \\ &\quad \mathfrak{W}_{\mathbf{x}^{(k+1)}}(\cdot, \Pi_{k+1}^\perp(G(\mathbf{x}^{(k+1)}, \mathbf{u}^*, \alpha_k) - G(\mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k))) \\ &= \alpha_k \nabla_{\mathcal{M}}^2 F(\mathbf{x}^*, \mathbf{u}^*) - \Pi_{k+1} \nabla_{\mathbf{x}}^2 f(\mathbf{x}^{(k+1)}, \mathbf{u}^*) \Pi_{k+1} + \Pi_{k+1} + \\ &\quad \mathfrak{W}_{\mathbf{x}^{(k+1)}}(\cdot, \Pi_{k+1}^\perp(G(\mathbf{x}^{(k+1)}, \mathbf{u}^*, \alpha_k) - G(\mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k))). \end{aligned}$$

Similarly, \tilde{Q}_k is given by

$$\tilde{Q}_k = \alpha_k \nabla_{\mathcal{M}}^2 F(\mathbf{x}^*, \mathbf{u}^*) - \alpha_k \Pi_* \nabla_{\mathbf{x}}^2 f(\mathbf{x}^*, \mathbf{u}^*) \Pi_* + \Pi_*.$$

From [37, Lemma 4.3], $\alpha_k \nabla_{\mathcal{M}}^2 F(\mathbf{x}^*, \mathbf{u}^*) - \alpha_k \Pi_* \nabla_{\mathbf{x}}^2 f(\mathbf{x}^*, \mathbf{u}^*) \Pi_*$ is positive semi-definite and the eigenvalues of \tilde{Q}_k^\dagger lie in $(0, 1]$. Moreover, the non-expansiveness of $G(\cdot, \mathbf{u}^*, \alpha_k)$ and the continuity of $(\mathbf{x}, \mathbf{v}) \mapsto \mathfrak{W}_{\mathbf{x}}(\cdot, \mathbf{v})$ due to the C^2 -smoothness of \mathcal{M} implies that $\mathfrak{W}_{\mathbf{x}^{(k+1)}}(\cdot, \Pi_{k+1}^\perp(G(\mathbf{x}^{(k+1)}, \mathbf{u}^*, \alpha_k) - G(\mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k))) \rightarrow 0$. This entails that $Q_k - \tilde{Q}_k \rightarrow 0$ and the eigenvalues of Q_k^\dagger are also eventually bounded. Hence, $Q_k^\dagger - \tilde{Q}_k^\dagger$, which can be rewritten as

$$\begin{aligned} Q_k^\dagger - \tilde{Q}_k^\dagger &= Q_k^\dagger - Q_k^\dagger \Pi_* + Q_k^\dagger \Pi_* - \Pi_k \tilde{Q}_k^\dagger + \Pi_k \tilde{Q}_k^\dagger - \tilde{Q}_k^\dagger \\ &= Q_k^\dagger \Pi_k - Q_k^\dagger \Pi_* + Q_k^\dagger \tilde{Q}_k \tilde{Q}_k^\dagger - Q_k^\dagger Q_k Q_k^\dagger + \Pi_k \tilde{Q}_k^\dagger - \tilde{Q}_k^\dagger \Pi_* \\ &= Q_k^\dagger (\Pi_k - \Pi_*) - Q_k^\dagger (Q_k - \tilde{Q}_k) \tilde{Q}_k^\dagger + (\Pi_k - \Pi_*) \tilde{Q}_k^\dagger, \end{aligned}$$

also converges to 0. Similarly $P_{\omega, k} - \tilde{P}_{\omega, k} \rightarrow 0$ for all $\omega \in \{\mathbf{x}, \mathbf{u}, \alpha\}$ because

$$\begin{aligned} P_{\mathbf{x}, k} - \tilde{P}_{\mathbf{x}, k} &= \Pi_{k+1} (I - \alpha_k \nabla_{\mathbf{x}}^2 f(\mathbf{x}^{(k)}, \mathbf{u}^*)) - \Pi_* (I - \alpha_k \nabla_{\mathbf{x}}^2 f(\mathbf{x}^*, \mathbf{u}^*)) \\ &= (\Pi_{k+1} - \Pi_*) - \alpha_k (\Pi_{k+1} \nabla_{\mathbf{x}}^2 f(\mathbf{x}^{(k)}, \mathbf{u}^*) - \Pi_* \nabla_{\mathbf{x}}^2 f(\mathbf{x}^*, \mathbf{u}^*)) \\ P_{\mathbf{u}, k} - \tilde{P}_{\mathbf{u}, k} &= \alpha_k (D_{\mathbf{u}} \nabla_{\mathcal{M}} g(\mathbf{x}^{(k+1)}, \mathbf{u}^*) + D_{\mathbf{u}} \Pi_{k+1} \nabla_{\mathbf{x}} f(\mathbf{x}^{(k)}, \mathbf{u}^*) - D_{\mathbf{u}} \nabla_{\mathcal{M}} F(\mathbf{x}^*, \mathbf{u}^*)) \\ P_{\alpha, k} - \tilde{P}_{\alpha, k} &= \nabla_{\mathcal{M}} g(\mathbf{x}^{(k+1)}, \mathbf{u}^*) + \Pi_{k+1} \nabla_{\mathbf{x}} f(\mathbf{x}^{(k)}, \mathbf{u}^*) - \nabla_{\mathcal{M}} F(\mathbf{x}^*, \mathbf{u}^*) \end{aligned}$$

This concludes the proof because from (8), $D\mathcal{A}_\alpha(\mathbf{x}, \mathbf{u})$ is given by,

$$D\mathcal{A}_\alpha(\mathbf{x}, \mathbf{u}) = -\nabla_{\mathcal{M}}^2 H(\mathcal{A}_\alpha(\mathbf{x}, \mathbf{u}), \mathbf{x}, \mathbf{u}, \alpha)^\dagger D_{(\mathbf{x}, \mathbf{u}, \alpha)} \nabla_{\mathcal{M}} H(\mathcal{A}_\alpha(\mathbf{x}, \mathbf{u}), \mathbf{x}, \mathbf{u}, \alpha). \quad (26)$$

(iii) The expressions for $Q_k - \tilde{Q}_k$ and $P_{\omega, k} - \tilde{P}_{\omega, k}$ for $\omega \in \{\mathbf{x}, \mathbf{u}, \alpha\}$ clearly indicate that these sequences converge linearly under the given assumptions.

□

C.2 Proof of Theorem 16

Proof. We again set $\mathbf{x}^{(k)} := \mathbf{x}^{(k)}(\mathbf{u}^*)$ for simplicity. Thanks to Theorem 13(i), \mathcal{A}_{α_k} are C^1 -smooth near $(\mathbf{x}^{(k)}, \mathbf{u}^*, \alpha_k)$ for all $k \in \mathbb{N}$ provided that $\mathbf{x}^{(0)}$ is sufficiently close to \mathbf{x}^* . Differentiation of the fixed-point iteration $\mathbf{x}^{(k+1)} := \mathcal{A}_{\alpha_k}(\mathbf{x}^{(k)}, \mathbf{u}^*)$ with respect to \mathbf{u} yields

$$D\mathbf{x}^{(k+1)}(\mathbf{u}^*) = D_{\mathbf{x}}\mathcal{A}_{\alpha_k}(\mathbf{x}^{(k)}, \mathbf{u}^*)\Pi(\mathbf{x}^{(k)})D\mathbf{x}^{(k)}(\mathbf{u}^*) + D_{\mathbf{u}}\mathcal{A}_{\alpha_k}(\mathbf{x}^{(k)}, \mathbf{u}^*), \quad (27)$$

and Theorem 15 asserts that under the given assumptions, for all $k \in \mathbb{N}$,

$$D\psi(\mathbf{u}^*) = D_{\mathbf{x}}\mathcal{A}_{\alpha_k}(\mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*)D\psi(\mathbf{u}^*) + D_{\mathbf{u}}\mathcal{A}_{\alpha_k}(\mathbf{x}^*, \mathbf{u}^*). \quad (28)$$

Just like the arguments made in the proof of Theorem 30, for any $\dot{\mathbf{u}} \in \mathcal{U}$, if we define

$$\begin{aligned} \mathbf{e}^{(k)} &:= D\mathbf{x}^{(k)}(\mathbf{u}^*)\dot{\mathbf{u}} - D\psi(\mathbf{u}^*)\dot{\mathbf{u}} \\ B_k &:= D_{\mathbf{x}}\mathcal{A}_{\alpha_k}(\mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*) \\ C_k &:= D_{\mathbf{x}}\mathcal{A}_{\alpha_k}(\mathbf{x}^{(k)}, \mathbf{u}^*)\Pi(\mathbf{x}^{(k)}) - D_{\mathbf{x}}\mathcal{A}_{\alpha_k}(\mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*) \\ \mathbf{d}^{(k)} &:= (D\mathcal{A}_k(\mathbf{x}^{(k)}, \mathbf{u}^*) - D\mathcal{A}_k(\mathbf{x}^*, \mathbf{u}^*))(D\psi(\mathbf{u}^*)\dot{\mathbf{u}}, \dot{\mathbf{u}}), \end{aligned}$$

and subtract (28) from (27), we obtain the recursion $\mathbf{e}^{(k+1)} = B_k\mathbf{e}^{(k)} + C_k\mathbf{e}^{(k)} + \mathbf{d}^{(k)}$. From Theorem 15, the continuity of ρ and $D\mathcal{A}_\alpha$, $\sup_{k \in \mathbb{N}} \|B_k\| < 1$ for all $k \in \mathbb{N}$ and from Theorem 13(ii), $C_k \rightarrow 0$ and $\mathbf{d}^{(k)} \rightarrow 0$. Under the additional assumptions, C_k and $\mathbf{d}^{(k)}$ converge linearly with rate $q_{\mathbf{x}}$ due to Theorem 13(i). Therefore, the (linear) convergence of the derivative sequence $(D\mathbf{x}^{(k)}(\mathbf{u}^*))_{k \in \mathbb{N}}$ follows from Theorem 24. □

C.3 Proof of Theorem 19

Proof. (i) This part follows from [46, Corollary 33] and the convergence of $\mathbf{x}^{(k)}(\mathbf{u}^*)$ and α_k .

- (ii) We set $\mathbf{z} := (\mathbf{x}_1, \mathbf{x}_2)$, and $\mathbf{y} := \mathbf{x}_1 + \beta(\mathbf{x}_1 - \mathbf{x}_2)$ and write the expression for $D\mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u})$ for $(\mathbf{z}, \mathbf{u}, \alpha, \beta) \in V_{\alpha_*} \times [0, 1]$:

$$\begin{aligned} D_{\mathbf{z}}\mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u}) &= \begin{bmatrix} (1 + \beta)D_{\mathbf{x}}\mathcal{A}_{\alpha}(\mathbf{y}, \mathbf{u}) & -\beta D_{\mathbf{x}}\mathcal{A}_{\alpha}(\mathbf{y}, \mathbf{u}) \\ I & 0 \end{bmatrix} \\ D_{\mathbf{u}}\mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u}) &= \begin{bmatrix} D_{\mathbf{u}}\mathcal{A}_{\alpha}(\mathbf{y}, \mathbf{u}) \\ 0 \end{bmatrix} \\ D_{\alpha}\mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u}) &= \begin{bmatrix} D_{\alpha}\mathcal{A}_{\alpha}(\mathbf{y}, \mathbf{u}) \\ 0 \end{bmatrix}, \end{aligned}$$

as provided in [46, Corollary 33], where $D\mathcal{A}_{\alpha}(\mathbf{y}, \mathbf{u})$ is given in (26). It is easy to see that the mapping $(\mathbf{z}, \mathbf{u}, \alpha, \beta) \mapsto D\mathcal{A}_{\alpha,\beta}(\mathbf{z}, \mathbf{u})$ is continuous on $V_{\alpha_*} \times [0, 1]$. Therefore, the sequences $(D\mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}^{(k)}(\mathbf{u}^*), \mathbf{x}^{(k-1)}(\mathbf{u}^*), \mathbf{u}^*))_{k \geq K}$ and $(D\mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*))_{k \geq K}$ both converge to $D\mathcal{A}_{\alpha_*, \beta_*}(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*)$ and their difference converges to 0.

- (iii) Because $\beta_k \in [0, 1]$ and under the additional assumptions, $D\mathcal{A}_{\alpha_k}(\mathbf{y}^{(k)}, \mathbf{u}^*) - D\mathcal{A}_{\alpha_k}(\mathbf{x}^*, \mathbf{u}^*) = \mathcal{O}(\mathbf{y}^{(k)} - \mathbf{x}^*)$ as established in Theorem 13(iii), where $\mathbf{y}^{(k)} := \mathbf{x}^{(k)}(\mathbf{u}^*) + \beta_k(\mathbf{x}^{(k)}(\mathbf{u}^*) - \mathbf{x}^{(k-1)}(\mathbf{u}^*))$, the result follows directly from the expressions of $D\mathcal{A}_{\alpha,\beta}$. □

C.4 Proof of Theorem 21

Proof. From Theorem 19 the mapping $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{u}, \alpha) \mapsto \mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{u}, \alpha)$ is C^1 -smooth on V_{α_*} . Therefore, when $\mathbf{x}^{(0)}$ is close enough to \mathbf{x}^* , we have $(\mathbf{x}^{(k)}, \mathbf{x}^{(k-1)}, \mathbf{u}^*, \alpha_k) \in V_{\alpha_*}$ where $\mathbf{x}^{(k)} := \mathbf{x}^{(k)}(\mathbf{u}^*)$ and we obtain the following recursion for the derivative iterates

$$\begin{bmatrix} D\mathbf{x}^{(k+1)}(\mathbf{u}^*) \\ D\mathbf{x}^{(k)}(\mathbf{u}^*) \end{bmatrix} = D_{\mathbf{z}}\mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}^{(k)}, \mathbf{u}^*)\Pi(\mathbf{x}^{(k)}, \mathbf{x}^{(k-1)}) \begin{bmatrix} D\mathbf{x}^{(k)}(\mathbf{u}^*) \\ D\mathbf{x}^{(k-1)}(\mathbf{u}^*) \end{bmatrix} + D_{\mathbf{u}}\mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}^{(k)}, \mathbf{u}^*)$$

From Theorem 20, we have

$$\begin{bmatrix} D\psi(\mathbf{u}^*) \\ D\psi(\mathbf{u}^*) \end{bmatrix} = D_{\mathbf{z}}\mathcal{A}_{\alpha, \beta}(\mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*, \mathbf{x}^*) \begin{bmatrix} D\psi(\mathbf{u}^*) \\ D\psi(\mathbf{u}^*) \end{bmatrix} + D_{\mathbf{u}}\mathcal{A}_{\alpha, \beta}(\mathbf{x}^*, \mathbf{u}^*),$$

for $\beta = \beta_*$ and $\beta = \beta_k$ for all $k \in \mathbb{N}$. Therefore, for any $\dot{\mathbf{u}} \in \mathcal{U}$, we define

$$\begin{aligned} \mathbf{e}^{(k)} &:= (D\mathbf{x}^{(k)}(\mathbf{u}^*) - D\psi(\mathbf{u}^*), D\mathbf{x}^{(k-1)}(\mathbf{u}^*) - D\psi(\mathbf{u}^*))\dot{\mathbf{u}} \\ B_k &:= D_{\mathbf{x}}\mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*, \mathbf{x}^*), \quad B_* := D_{\mathbf{x}}\mathcal{A}_{\alpha_*, \beta_*}(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*, \mathbf{x}^*) \\ C_k &:= D_{\mathbf{x}}\mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}^{(k)}, \mathbf{x}^{(k-1)}, \mathbf{u}^*)\Pi(\mathbf{x}^{(k)}, \mathbf{x}^{(k-1)}) - D_{\mathbf{x}}\mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*)\Pi(\mathbf{x}^*, \mathbf{x}^*) \\ \mathbf{d}^{(k)} &:= (D\mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}^{(k)}, \mathbf{x}^{(k-1)}, \mathbf{u}^*) - D\mathcal{A}_{\alpha_k, \beta_k}(\mathbf{x}^*, \mathbf{x}^*, \mathbf{u}^*))(D\psi(\mathbf{u}^*)\dot{\mathbf{u}}, D\psi(\mathbf{u}^*)\dot{\mathbf{u}}, \dot{\mathbf{u}}) \end{aligned}$$

and obtain the recursion $\mathbf{e}^{(k+1)} = B_k \mathbf{e}^{(k)} + C_k \mathbf{e}^{(k)} + \mathbf{d}^{(k)}$. Notice that $\rho(B_*) < 1$ from Theorem 20 and $B_k \rightarrow B_*$ from Theorem 19(i). Moreover $C_k \rightarrow 0$, and $\mathbf{d}^{(k)} \rightarrow 0$ owing to Theorem 19(ii) and under the additional assumptions, the convergence of C_k and $\mathbf{d}^{(k)}$ is linear with rate q_x thanks to Theorem 19(iii). Therefore, from Corollary 25, the sequence $D\mathbf{x}^{(k)}(\mathbf{u}^*)\dot{\mathbf{u}}$ converges (linearly) to $D\psi(\mathbf{u}^*)\dot{\mathbf{u}}$ for all $\dot{\mathbf{u}} \in \mathcal{U}$. \square

D Experimental Details

In this section, we fill out some missing details from Section 4. For (13), we use MADELON dataset [26] where $A \in \mathbb{R}^{M \times N}$ and $\mathbf{b} \in \{-1, +1\}^M$ where $M = 2000$ and $N = 501$ without any feature transformation apart from batch normalization. For 50 set of experiments, we sample $\lambda \sim \mathcal{N}(0, 10^{-3})$ and perturb each element of A with a Gaussian noise with standard deviation 10^{-3} . The problem is μ -strongly convex and has an L -Lipschitz continuous gradient where $\mu = \lambda$ and $L = \rho(A^T A) + \lambda$. For (14), the dataset $(A, \mathbf{b}) \in \mathbb{R}^{M \times N} \times \mathbb{R}^M$ with $70 \leq M \leq 90$ and $N = 200$ is artificially generated. In particular, for each of the 50 problems, we generate A and a sparse vector $\mathbf{x}' \in \mathbb{R}^N$ with only 50 non-zero elements. We sample each element of A and each non-zero element of \mathbf{x}' from $U(0, 1)$ and $\mathcal{N}(0, 1)$ respectively. We then generate \mathbf{b} by computing $A\mathbf{x} + \boldsymbol{\varepsilon}$ where $\boldsymbol{\varepsilon} \sim \mathcal{N}(0, 10^{-3}I)$. The problem has an L -Lipschitz continuous gradient with $L = \rho(A^T A)$ but is not even strictly convex. However, for each choice of $\lambda \sim U(0, 10)$, A , and \mathbf{b} , Assumptions 3.2 and 3.3 were satisfied for each experiment.

We obtain a very good estimate of \mathbf{x}^* for (13) by using Newton's method with backtracking line search and for (14) by running APG for sufficiently large number of iterations. The derivative of the solution $D\psi(\mathbf{u}^*)$ is computed by solving the linear system (2) for logistic regression and solving the reduced system (8) after identifying the support for lasso regression [11]. For each problem and for each experiment, we run PGD with four different choices of step size, namely, (i) $\alpha_k = 2/(L + m)$ for (13) and $\alpha_k = 1/L$ for (14), (ii) $\alpha_k \sim U(0, \frac{2}{3L})$, (iii) $\alpha_k \sim U(\frac{2}{3L}, \frac{4}{3L})$, and (iv) $\alpha_k \sim U(\frac{4}{3L}, \frac{2}{L})$, for each $k \in \mathbb{N}$. We also run APG with $\alpha_k = 1/L$ and $\beta_k = (k - 1)/(k + 5)$. Before starting each algorithm, we obtain $\mathbf{x}^{(0)} \in B_{10^{-2}}(\mathbf{x}^*)$ by partially solving each problem through APG. For computational reasons, instead of generating the sequence $D\mathbf{x}^{(k)}(\mathbf{u})$ where $\mathbf{u} = (A, \lambda)$ and $\mathbf{u} = (A, \mathbf{b}, \lambda)$ respectively for the two problems, we compute the directional derivative $D\mathbf{x}^{(k)}(\mathbf{u})\dot{\mathbf{u}}$. The vector $\dot{\mathbf{u}}$ belongs to the same space as \mathbf{u} and is fixed for the 5 different algorithms being compared for each experiment and problem.

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