

PRIMAL-DUAL EXTRAGRADIENT METHODS FOR NONLINEAR NONSMOOTH PDE-CONSTRAINED OPTIMIZATION

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Abstract We study the extension of the Chambolle–Pock primal-dual algorithm to non-smooth optimization problems involving nonlinear operators between function spaces. Local convergence is shown under technical conditions including metric regularity of the corresponding primal-dual optimality conditions. We also show convergence for a Nesterov-type accelerated variant provided one part of the functional is strongly convex. We show the applicability of the accelerated algorithm to examples of inverse problems with L^1 and L^∞ fitting terms as well as of state-constrained optimal control problems, where convergence can be guaranteed after introducing an (arbitrary small, still nonsmooth) Moreau–Yosida regularization. This is verified in numerical examples.

1 INTRODUCTION

This work is concerned with the numerical solution of optimization problems of the form

$$(1.1) \quad \min_{u \in X} F(K(u)) + G(u),$$

where $F : Y \rightarrow \overline{\mathbb{R}} := \mathbb{R} \cup \{+\infty\}$ and $G : X \rightarrow \overline{\mathbb{R}}$ are proper, convex, and lower semicontinuous functionals, and $K : X \rightarrow Y$ is a (nonlinear) Fréchet-differentiable operator between two Hilbert spaces X and Y with locally Lipschitz-continuous derivative K' . Such problems arise for example in inverse problems with nonsmooth discrepancy or regularization terms or in optimal control problems subject to state or control constraints. We are particularly interested in the situation where K is a *nonlinear* operator involving the solution of a partial differential equation and F is a *nonsmooth* discrepancy or tracking term.

To fix ideas, a prototypical example is the L^1 fitting problem

$$(1.2) \quad \min_{u \in L^2(\Omega)} \|S(u) - y^\delta\|_{L^1} + \frac{\alpha}{2} \|u\|_{L^2}^2,$$

i.e., $G(u) = \frac{\alpha}{2} \|u\|_{L^2}^2$, $F(y) = \|y\|_{L^1}$, and $K(u) = S(u) - y^\delta$, where S maps u to the solution y of $-\Delta y + uy = f$ for given f and y^δ is a given noisy measurement; see [7]. This problem

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occurs in parameter identification from data corrupted by impulsive noise instead of the usual Gaussian noise. Other examples are the L^∞ fitting problem from [6] or optimal control with state constraints; see Section 3 for details.

One possible approach to solving (1.1) is to apply a Moreau–Yosida regularization to the nonsmooth functional F , which allows deriving classical first-order necessary optimality conditions that can be solved by a semismooth Newton method in function spaces; see, e.g. [12, 19] for semismooth Newton methods in general as well as [6, 7, 11] for their application to L^1 fitting, L^∞ fitting, and optimal control with state constraints, respectively. Such methods are very efficient due to their superlinear convergence and mesh independence; however, they suffer from local convergence, with the convergence region depending strongly on the choice of the Moreau–Yosida parameter. For this reason, usually continuation methods are employed where a sequence of minimization problems with gradually diminishing parameter are solved, although the range of parameter values for which convergence can be observed is still limited in practice.

An alternative approach which has become very popular in the context of imaging problems are primal-dual extragradient methods. One widely used example, introduced in [3] for linear operators and extended in [20] to nonlinear operators, applied to (1.1) reads as follows.

Algorithm 1 Nonlinear primal-dual extragradient method

- 1: choose u^0, v^0
 - 2: **for** $i = 0, \dots$ **do**
 - 3: $u^{i+1} = \text{prox}_{\tau G}(u^i - \tau K'(u^i)^* v^i)$
 - 4: $\bar{u}^{i+1} = 2u^{i+1} - u^i$
 - 5: $v^{i+1} = \text{prox}_{\sigma F^*}(v^i + \sigma K(\bar{u}^{i+1}))$
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Here, $\sigma, \tau > 0$ are appropriately chosen step lengths, $K'(u)^*$ denotes the adjoint of the Fréchet derivative of K , and prox_{F^*} denotes the proximal mapping of the Fenchel conjugate of F ; we postpone precise definitions to later and only remark that if F^* is the indicator function of a convex set C , the proximal mapping coincides with the metric projection onto C . Such methods do not require (for linear K) choosing the initial guess sufficiently close to the solution to ensure convergence or solving—possibly ill-conditioned—linear systems in each iteration. Consequently, they recently have received increasing interest also in the context of optimal control; see, e.g., [13, 15]. In addition, other proximal point methods for optimal control problems have been treated in [1] and [18]; in particular, the latter is concerned with classical forward–backward splitting for sparse control of linear elliptic PDEs. However, so far these methods have only been considered in the finite-dimensional setting, i.e., after discretizing (1.1), or for specific (linear) problems. One of the goals of this work is therefore to show convergence of Algorithm 1 in Hilbert spaces and to demonstrate that it can be applied to problems of the form (1.2).

While the general convergence theory is a straightforward extension of the analysis in [20] (in fact, the proof is virtually identical), it requires verifying a set-valued Lipschitz property—known as the *Aubin* or *pseudo-Lipschitz property*—on the inverse of a monotone operator $H_{\bar{u}}$ encoding the optimality conditions. This is also called *metric regularity* of $H_{\bar{u}}$. This verification is significantly more involved in infinite dimensions. For problems of the form (1.1) where F and G are given by integral functionals for regular integrands, we can apply the theory from [9] to obtain an explicit, verifiable, condition for metric regularity to hold. While our analysis will show

that for problems such as (1.2), this condition does in fact not hold in general unless a Moreau–Yosida regularization is introduced—or the data y^δ and the fitting term are finite-dimensional—we do obtain convergence for arbitrarily small regularization parameter, and numerical examples show that this can be observed in practice independent of the discretization. Similarly, although for nonlinear operators, the convergence is only local since smallness conditions on the distance to the solution enter via bounds on the nonlinearity of the operator, in contrast to semismooth Newton methods we actually observe convergence for any starting point and arbitrarily small regularization parameter without the need for continuation.

In addition, Moreau–Yosida regularization results in a strongly convex functional, which can be exploited for accelerating [Algorithm 1](#) as in [4] via adaptive step length and extrapolation parameters. This leads to the following iteration.

Algorithm 2 Accelerated nonlinear primal-dual extragradient method

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1: choose  $u^0, v^0$ 
2: for  $i = 0, \dots$  do
3:    $u^{i+1} = \text{prox}_{\tau G}(u^i - \tau K'(u^i)^* v^i)$ 
4:    $\omega_i = 1/\sqrt{1 + 2\mu\sigma_i}, \quad \tau_{i+1} = \tau_i/\omega_i, \quad \sigma_{i+1} = \sigma_i\omega_i$ 
5:    $\bar{u}^{i+1} = u^{i+1} + \omega_i(u^{i+1} - u^i)$ 
6:    $v^{i+1} = \text{prox}_{\sigma F^*}(v^i + \sigma K(\bar{u}^{i+1}))$ 

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Here, $\mu \geq 0$ is a fixed acceleration parameter; setting $\mu = 0$ coincides with the unaccelerated [Algorithm 1](#). The appropriate choice for $\mu > 0$ is related to the constant of strong convexity of F^* , and in the convex case yields the optimal convergence rate of $\mathcal{O}(1/k^2)$ for the functional values rather than the rate $\mathcal{O}(1/k)$ for the original version; see [3, 4, 21]. A similar acceleration is possible if G is strongly convex by swapping the roles of σ_i and τ_i in [Line 4](#); we will refer to both variants as [Algorithm 2](#) in the following. Such an acceleration was not considered in [20]. While a proof of the optimal convergence rate is outside the scope of this work, we show that [Algorithm 2](#) converges (locally) in infinite-dimensional Hilbert spaces under the same conditions as for [Algorithm 1](#) and demonstrate the accelerated convergence in numerical examples.

This work is organized as follows. In the remainder of this section, we summarize some notations and definitions necessary for what follows. [Section 2](#) is concerned with the convergence analysis of the accelerated [Algorithm 2](#) in infinite-dimensional Hilbert spaces, where we discriminate the case of F^* ([Section 2.1](#)) or G ([Section 2.2](#)) being strongly convex. We also briefly address the verification of metric regularity for functionals of the form (1.1) in [Section 2.3](#). A more detailed discussion for the specific case of the motivating problems (L^1 fitting, L^∞ fitting, and optimal control with state constraints) is given in [Section 3](#), where we also derive the explicit form of the accelerated [Algorithm 2](#) in these cases. [Section 4](#) concludes with numerical examples for the three model problems.

1.1 NOTATION AND DEFINITIONS

Convex analysis We assume $G : X \rightarrow \overline{\mathbb{R}}$ and $F : Y \rightarrow \overline{\mathbb{R}}$ to be convex, proper, lower semicontinuous functionals on Hilbert spaces X and Y , satisfying $\text{int dom } G \neq \emptyset$ and $\text{int dom } F \neq$

0. We call, e.g., F strongly convex with constant $\gamma_F > 0$ if

$$(1.3) \quad F(v') - F(v) \geq \langle z, v' - v \rangle + \frac{\gamma_F}{2} \|v' - v\|^2 \quad (v, v' \in Y; z \in \partial F(v)),$$

where ∂F denotes the convex subdifferential of F . We denote by

$$F^* : Y^* \rightarrow \overline{\mathbb{R}}, \quad F^*(p) = \sup_{y \in Y} \langle p, y \rangle_Y - F(y),$$

the *Fenchel conjugate* of F , which is convex, proper, and lower semicontinuous. As usual, we identify the topological dual Y^* of Y with itself. The *Moreau–Yosida* regularization of F for the parameter $\gamma > 0$ is defined as

$$(1.4) \quad F_\gamma(y) := \min_{y' \in Y} F(y') + \frac{1}{2\gamma} \|y' - y\|^2,$$

whose Fenchel conjugate is (cf., e.g., [2, Prop. 13.21 (i)])

$$(1.5) \quad F_\gamma^*(p) = F^*(p) + \frac{\gamma}{2} \|p\|^2.$$

Note that F_γ^* is strongly convex with constant at least γ .

For convex F, G and continuously Fréchet-differentiable K , we can apply the calculus of Clarke's generalized derivative (which reduces to the convex subdifferential for convex functionals; see, e.g., [5, Chap. 2.3]) to deduce for (1.1) the overall system of critical point conditions

$$(1.6) \quad \begin{cases} K(\widehat{u}) \in \partial F^*(\widehat{v}), \\ -K'(\widehat{u})^* \widehat{v} \in \partial G(\widehat{u}). \end{cases}$$

Algorithm 1 can be derived from these conditions with the help of the *proximal mapping* (or *resolvent*) of G ,

$$\text{prox}_G(v) = \arg \min_{w \in X} \frac{1}{2} \|w - v\|_X^2 + G(w) = (\text{Id} + \partial G)^{-1}(v),$$

and similarly for F^* . We recall the following useful calculus rules for proximal mappings, e.g., from [2, Prop. 23.29 (i), (viii)]:

(P1) For any $\sigma > 0$ it holds that

$$\text{prox}_{\sigma F^*}(v) = v - \sigma \text{prox}_{\sigma^{-1}F}(\sigma^{-1}v).$$

(P2) For any $\gamma > 0$ it holds that

$$\text{prox}_{F_\gamma^*}(v) = \text{prox}_{(1+\gamma)^{-1}F^*}((1+\gamma)^{-1}v).$$

Set-valued analysis We first define for $U \subset X$ the set of *Fréchet (or regular) normals* to U at $u \in U$ by

$$\widehat{N}(u; U) := \left\{ z \in X \mid \limsup_{U \ni u' \rightarrow u} \frac{\langle z, u' - u \rangle}{\|u' - u\|} \leq 0 \right\}$$

and the set of *tangent vectors* by

$$T(u; U) := \left\{ z \in X \mid \text{exist } \tau^i \searrow 0 \text{ and } u^i \in U \text{ such that } z = \lim_{i \rightarrow \infty} \frac{u^i - u}{\tau^i} \right\}.$$

For a convex set U , these coincide with the usual normal and tangent cones of convex analysis.

For any cone $V \subset X$, we also define the *polar cone*

$$V^\circ := \{z \in X \mid \langle z, z' \rangle \leq 0 \text{ for all } z' \in V\}.$$

We use the notation $R : Q \rightrightarrows W$ to denote a set-valued mapping R from Q to W ; i.e., for every $q \in Q$ holds $R(q) \subset W$. For $R : Q \rightrightarrows W$, we define the domain $\text{dom } R := \{q \in Q \mid R(q) \neq \emptyset\}$ and graph $\text{Graph } R := \{(q, w) \in Q \times W \mid w \in R(q)\}$. The regular coderivatives of such maps are defined graphically with the help of the normal cones. Let Q and W be Hilbert spaces, and $R : Q \rightrightarrows W$ with $\text{dom } R \neq \emptyset$. We then define the *regular coderivative* $\widehat{D}^*R(q|w) : W \rightrightarrows Q$ of R at $q \in Q$ for $w \in W$ as

$$\widehat{D}^*R(q|w)(\Delta w) := \left\{ \Delta q \in Q \mid (\Delta q, -\Delta w) \in \widehat{N}((q, w); \text{Graph } R) \right\}.$$

We also define the *graphical derivative* $DR(q|w) : Q \rightrightarrows W$ by

$$DR(q|w)(\Delta q) := \{\Delta w \in W \mid (\Delta q, \Delta w) \in T((q, w); \text{Graph } R)\}$$

and its convexification $\widetilde{DR}(q|w)$ via

$$\text{Graph } \widetilde{DR}(q|w) = \text{conv Graph}[DR(q|w)].$$

Finally, we say that the set-valued mapping $R : Q \rightrightarrows W$ is *metrically regular* at \widehat{w} for \widehat{q} if $\text{Graph } R$ is locally closed and there exist $\rho, \delta, \ell > 0$ such that

$$\inf_{p : w \in R(p)} \|q - p\| \leq \ell \|w - R(q)\| \quad \text{for any } q, w \text{ such that } \|q - \widehat{q}\| \leq \delta, \|w - \widehat{w}\| \leq \rho.$$

We note that metric regularity of R is equivalent to the *Aubin property* of R^{-1} . Hence, for the sake of consistency with [9], we denote the infimum over valid constants ℓ by $\ell_{R^{-1}}(\widehat{w}|\widehat{q})$, or $\ell_{R^{-1}}$ for short when there is no ambiguity about the point $(\widehat{w}, \widehat{q})$. Metric regularity is then equivalent to $\ell_{R^{-1}}(\widehat{w}|\widehat{q}) > 0$.

2 CONVERGENCE

We now show the convergence in infinite-dimensional Hilbert spaces of [Algorithm 2](#), where the acceleration is stopped at some iteration N . We begin by observing from the definition of the proximal mapping that [Algorithm 2](#) may be written in the form

$$(2.1) \quad 0 \in H_{u^i}(q^{i+1}) + v^i + M_i(q^{i+1} - q^i)$$

for the family, over a base point $\bar{u} \in X$, of monotone operators

$$H_{\bar{u}}(u, v) := \begin{pmatrix} \partial G(u) + K'(\bar{u})^* v \\ \partial F^*(v) - K'(\bar{u})u - c_{\bar{u}} \end{pmatrix} \quad \text{where} \quad c_{\bar{u}} := K(\bar{u}) - K'(\bar{u})\bar{u},$$

the preconditioning operator

$$M_i := \begin{pmatrix} \tau_i^{-1} \text{Id} & -K'(u^i)^* \\ -K'(u^i) & \sigma_i^{-1} \text{Id} \end{pmatrix},$$

and the discrepancy term

$$v^i := \bar{v}^i + v_{\omega}^i := \underbrace{\begin{pmatrix} 0 \\ K'(u^i)\bar{u}^{i+1} + c_{u^i} - K(\bar{u}^{i+1}) \end{pmatrix}}_{\text{linearization discrepancy}} + \underbrace{\begin{pmatrix} 0 \\ (1 - \omega_i)K'(u^i)(u^{i+1} - u^i) \end{pmatrix}}_{\text{acceleration discrepancy}}.$$

Observe (or see [20, Lem. 3.2]) that $|v^i| \leq C|u^{i+1} - u^i|$ for some constant $C > 0$. This is the only property needed from v^i for the convergence proof. Therefore v^i can also incorporate further discrepancies, e.g., from inexact evaluation of K which can be useful in the context of PDE-constrained optimization.

Throughout, we set

$$q = (u, v) \in X \times Y \quad \text{and} \quad w = (\xi, \eta) \in X \times Y,$$

extending this notation to \widehat{q} , etc., in the obvious way. Here we fix $R > 0$ such that there exists a solution \widehat{q} to

$$(2.2a) \quad 0 \in H_{\widehat{u}}(\widehat{q}) \quad \text{with} \quad \|\widehat{q}\| \leq R/2.$$

Note that the condition $0 \in H_{\widehat{u}}(\widehat{q})$ is equivalent to the necessary optimality condition (1.6) for (1.1). Regarding the operator $K : X \rightarrow Y$ and the step length parameters $\sigma_i, \tau_i > 0$, we require that K is Fréchet-differentiable with locally Lipschitz-continuous derivative K' satisfying

$$(2.2b) \quad \sigma_i \tau_i \left(\sup_{\|u\| \leq R} \|K'(u)\|^2 \right) < 1.$$

Observe that $\sigma_i \tau_i = \sigma_0 \tau_0$ is maintained under acceleration schemes such as the one in [Algorithm 2](#); it is therefore sufficient to ensure this condition for the initial choice. We denote by L_2 the local Lipschitz factor of $u \mapsto K'(u)$ on the closed ball $B(0, R) \subset X$. We define the uniform condition number

$$(2.2c) \quad \kappa := \Theta/\theta$$

based on Θ and θ from the condition

$$(2.3) \quad \theta^2 \text{Id} \leq M_i \leq \Theta^2 \text{Id}.$$

If $\tau_i, \sigma_i > 0$ are constant, $\|u^i\| \leq R$, and (2.2b) holds, such θ and Θ exist [20, Lem. 3.1]. Easily this extends to $0 < C_1 \leq \tau_i, \sigma_i \leq C_2 < \infty$.

Remark 2.1. *The bound (2.3), on which the analysis from [20] depends, is the reason we need to stop the acceleration: Since $\tau_i \rightarrow 0$ and $\sigma_i \rightarrow \infty$, no uniform bound exists for M_i if the acceleration is not stopped. Possibly the convergence proofs from [20] can be extended to the fully accelerated case, but such an endeavour is outside the scope of the present work. In numerical practice, in any case, we stop the algorithm—and hence a fortiori the acceleration—at a suitable iteration N .*

We now distinguish whether F^* or G is strongly convex. The former is always guaranteed by Moreau–Yosida regularization of F , while the latter—if it holds in addition, which is the case in the examples considered here—might allow stronger acceleration, independent of the Moreau–Yosida parameter. In both cases, the convergence proof follows closely the original proof in [20, § 2–3]. Although this was stated in finite-dimensional spaces, none of the arguments rely on this fact. Aside from the inverse mapping theorem for set-valued functions extracted from [20, Lem. 3.8], which holds in general complete metric spaces, the arguments are entirely algebraic manipulations. They therefore hold in infinite-dimensional Hilbert spaces as well.

Some modifications are, however, necessary since the accelerated step sizes are no longer constant. The original proof starts with a basic descent inequality obtained from the monotonicity of H and assumes strong convexity properties. It then modifies this inequality through a sequence of lemmas to obtain an estimate from which a generic telescoping result quickly produces convergence [20, Thm. 2.1]. In the following, we detail the first two elementary steps which contain changes to the original proof (for F^* strongly convex only the second step changes, for G strongly convex both do). The remaining steps heavily employ the metric regularity of H and are unchanged and therefore only summarized briefly.

2.1 CONVERGENCE FOR STRONGLY CONVEX F^*

We begin by considering the case of F^* being strongly convex, which is closest to the setting of [20]. In this case, we chose for $\mu \geq 0$ the acceleration sequence

$$(2.4) \quad \sigma_{i+1} := \omega_i \sigma_i \quad \text{and} \quad \tau_{i+1} := \tau_i / \omega_i \quad \text{with} \quad \omega_i := 1 / \sqrt{1 + 2\mu\sigma_i}.$$

Under the above assumptions, and if metric regularity holds for $H_{\bar{u}}$, [Algorithm 2](#) locally converges to a solution of (2.2a).

We begin from the basic descent estimate obtained from the monotonicity of H_{u^i} and the assumed strong convexity.

Lemma 2.2 ([20, Lem. 2.1]). *Let $q^i \in X \times Y$ and $\bar{u} \in X$. Suppose $q^{i+1} \in X \times Y$ solves (2.1) and that $\tilde{q}^i \in X \times Y$ is a solution to*

$$0 \in H_{u^i}(\tilde{q}^i) + v^i.$$

If F^ is strongly convex on Y with constant $\gamma_{F^*} > 0$, then we have*

$$(\widehat{\mathbb{D}^2\text{-loc-}\gamma\text{-}F^*}) \quad \|q^i - \tilde{q}^i\|_{M_i}^2 \geq \|q^{i+1} - q^i\|_{M_i}^2 + \|q^{i+1} - \tilde{q}^i\|_{M_i}^2 + \gamma_{F^*} \|v^{i+1} - \tilde{v}^i\|^2.$$

Remark 2.3. *Strong convexity of F^* with factor γ_{F^*} is equivalent [10] to strong monotonicity of ∂F^* in the sense that*

$$\langle \partial F^*(v') - \partial F^*(v), v' - v \rangle \geq \gamma_{F^*} \|v' - v\|^2 \quad (v', v \in Y),$$

observing that there is no factor 1/2 in the latter unlike mistakenly written at [20, the end of page 7]. Hence the slight difference in the statement of $(\widehat{\mathbb{D}^2}\text{-loc-}\gamma\text{-F}^*)$ in comparison to the similarly-named equation in [20]. In the cited article, the exact factors make no difference however; in the present work they do for the acceleration.

Note that $(\widehat{\mathbb{D}^2}\text{-loc-}\gamma\text{-F}^*)$ still uses the old norm $\|\cdot\|_{M_i}$ for the new iterate. To pass to $\|\cdot\|_{M_{i+1}}$ under acceleration requires replacing [20, Lem. 3.6]. For this, we first need the following bound on the step lengths.

Lemma 2.4. *If $\{\sigma_i\}_{i \in \mathbb{N}}$ satisfies (2.4), then $\mu + (\sigma_i^{-1} - \sigma_{i+1}^{-1}) \geq 0$.*

Proof. We first note that

$$2\mu + (\sigma_i^{-1} - \sigma_{i+1}^{-1}) = \sigma_i^{-1}(2\mu\sigma_i + 1 - \omega_i^{-1}).$$

Thus the claim holds if

$$2\mu\sigma_i + 1 - \omega_i^{-1} \geq \mu\sigma_i,$$

i.e., after multiplying both sides by ω_i^2 and using the definition of ω_i ,

$$1 - \omega_i \geq \mu\omega_i^2\sigma_i.$$

In other words, we need to show that

$$(2.5) \quad \mu \leq \frac{1 - \omega_i}{\omega_i^2\sigma_i} = \frac{\omega_i^{-1} - 1}{\omega_i\sigma_i}.$$

But using the concavity of the square root, we can estimate

$$\omega_i^{-1} - 1 = (-\sqrt{1}) - (-\sqrt{1 + 2\mu\sigma_i}) \geq -\frac{1}{2\sqrt{1 + 2\mu\sigma_i}}(1 - (1 + 2\mu\sigma_i)) = \mu\sigma_i\omega_i.$$

This proves (2.5). □

The following lemma is the crucial step towards extending the results of [20] to the accelerated case.

Lemma 2.5. *Suppose (2.2) and $(\widehat{\mathbb{D}^2}\text{-loc-}\gamma\text{-F}^*)$ hold. Let R, L_2, κ be as in (2.2), and choose $\xi_1 \in (0, 1)$. If*

$$(2.6) \quad \|q^i - \widehat{q}\| \leq R/4 \quad \text{and} \quad \|q^i - \widetilde{q}^i\| \leq C$$

for a suitable constant $C = C(\gamma_{F^*}, \mu, \xi_1, \theta, L_2, \kappa, R)$, then

$$(\widehat{\mathbb{D}^2}\text{-M}) \quad \|q^i - \widetilde{q}^i\|_{M_i}^2 \geq \xi_1 \|q^{i+1} - q^i\|_{M_i}^2 + \|q^{i+1} - \widetilde{q}^i\|_{M_{i+1}}^2.$$

holds.

Proof. Using (2.6) and the property $\|\widehat{q}\| \leq R/2$ from (2.2a), we have

$$(2.7) \quad \|q^i\| \leq \|q^i - \widehat{q}\| + \|\widehat{q}\| \leq 3R/4.$$

The estimate $(\widehat{D^2}\text{-loc-}\gamma\text{-F}^*)$ implies

$$\|q^{i+1} - q^i\| \leq \kappa \|\widetilde{q}^i - q^i\|.$$

Choosing $C \leq R/(4\kappa)$ and using (2.6) and (2.7), we thus get

$$\|q^{i+1}\| \leq \|q^{i+1} - q^i\| + \|q^i\| \leq \kappa \|\widetilde{q}^i - q^i\| + \|q^i\| \leq R.$$

As both $\|q^i\| \leq R$ and $\|q^{i+1}\| \leq R$, by local Lipschitz continuity of K' we have again

$$(2.8) \quad \|K'(u^{i+1}) - K'(u^i)\| \leq L_2 \|u^{i+1} - u^i\|.$$

We now expand

$$\begin{aligned} \|q^{i+1} - \widetilde{q}^i\|_{M_i}^2 - \|q^{i+1} - \widetilde{q}^i\|_{M_{i+1}}^2 &= -2\langle v^{i+1} - \widetilde{v}^i, (K'(u^{i+1}) - K'(u^i))(u^{i+1} - \widetilde{u}^i) \rangle \\ &\quad + (\tau_i^{-1} - \tau_{i+1}^{-1}) \|u^{i+1} - \widetilde{u}^i\|^2 + (\sigma_i^{-1} - \sigma_{i+1}^{-1}) \|v^{i+1} - \widetilde{v}^i\|^2 \\ &\geq -2\langle v^{i+1} - \widetilde{v}^i, (K'(u^{i+1}) - K'(u^i))(u^{i+1} - \widetilde{u}^i) \rangle \\ &\quad + (\sigma_i^{-1} - \sigma_{i+1}^{-1}) \|v^{i+1} - \widetilde{v}^i\|^2. \end{aligned}$$

In the final step, we have used the fact that $\{\tau_i\}_{i \in \mathbb{N}}$ is non-decreasing. Using (2.8), we further derive by application of Young's inequality

$$(2.9) \quad \|q^{i+1} - \widetilde{q}^i\|_{M_i}^2 - \|q^{i+1} - \widetilde{q}^i\|_{M_{i+1}}^2 \geq (\sigma_i^{-1} - \sigma_{i+1}^{-1}) \|v^{i+1} - \widetilde{v}^i\|^2 - 2L_2 \|v^{i+1} - \widetilde{v}^i\| \|q^{i+1} - q^i\| \|q^{i+1} - \widetilde{q}^i\|.$$

Using once more Young's inequality, (2.9), and Lemma 2.4, we deduce

$$(2.10) \quad \begin{aligned} \|q^{i+1} - \widetilde{q}^i\|_{M_i}^2 - \|q^{i+1} - \widetilde{q}^i\|_{M_{i+1}}^2 + \gamma_{F^*} \|v^{i+1} - \widetilde{v}^i\|^2 &\geq (\mu + \sigma_i^{-1} - \sigma_{i+1}^{-1}) \|v^{i+1} - \widetilde{v}^i\|^2 \\ &\quad - \frac{L_2^2}{\gamma_{F^*} - \mu} \|q^{i+1} - q^i\|^2 \|q^{i+1} - \widetilde{q}^i\|^2 \\ &\geq -\frac{L_2^2}{\gamma_{F^*} - \mu} \|q^{i+1} - q^i\|^2 \|q^{i+1} - \widetilde{q}^i\|^2. \end{aligned}$$

By application of (2.3) and $(\widehat{D^2}\text{-loc-}\gamma\text{-F}^*)$, we bound

$$\|q^{i+1} - \widetilde{q}^i\|^2 \leq \theta^{-2} \|q^{i+1} - \widetilde{q}^i\|_{M_i}^2 \leq \kappa^2 \|q^i - \widetilde{q}^i\|^2$$

and

$$\|q^{i+1} - q^i\|^2 \leq \theta^{-2} \|q^{i+1} - q^i\|_{M_i}^2.$$

Setting

$$c := \frac{L_2^2}{\gamma_{F^*} - \mu} \quad \text{and} \quad C := (1 - \xi_1) \frac{\theta^2}{c\kappa^2}$$

and using (2.6) therefore yields

$$c \|q^{i+1} - q^i\|^2 \|q^{i+1} - \tilde{q}^i\|^2 \leq \frac{c\kappa^2}{\theta^2} \|q^{i+1} - q^i\|_{M_i}^2 \|q^i - \tilde{q}^i\|^2 \leq (1 - \xi_1) \|q^{i+1} - q^i\|_{M_i}^2.$$

Using (2.10) and this estimate in $(\widehat{D}^2\text{-loc-}\gamma\text{-}F^*)$, we obtain $(\widehat{D}^2\text{-}M)$. \square

The remaining proof now proceeds as in [20]. Metric regularity—whose verification is the main difficulty in function spaces and will be investigated based on the results of [9] at the end of this section—allows removing the squares from $(\widehat{D}^2\text{-loc-}\gamma\text{-}F^*)$ and bridging from the perturbed local solutions \tilde{q}^i to local solutions \hat{q}^i . This is done through a sequence of technical lemmas in [20, § 3.4–3.8] which culminate in the general descent estimate (\widehat{D}) of [20, Thm. 3.1]. From there, a generic telescoping argument given in [20, Thm. 2.1] yields convergence, which we summarize in the following statement.

Theorem 2.6. *Let (2.2) be satisfied with the corresponding constants R , Θ , κ and L_2 , and suppose F^* is strongly convex with factor γ_{F^*} . Let \hat{q} solve $0 \in H_{\hat{u}}(\hat{q})$ and $H_{\hat{u}}$ be metrically regular at 0 for \hat{q} with*

$$(2.11) \quad \ell_{H_{\hat{u}}^{-1}\kappa L_2} \|\hat{v}\| < 1 - 1/\sqrt{1 + 1/(2\ell_{H_{\hat{u}}^{-1}}^2 \Theta^4)}.$$

If $\mu \in [0, \gamma_{F^})$ and we use the rule (2.4) for $i = 1, \dots, N$ for some $N \in \mathbb{N}$, after which $\tau_i = \tau_N$ and $\sigma_i = \sigma_N$ for $i > N$, there exists $\delta > 0$ such that for any $q^1 \in X \times Y$ with*

$$\|q^1 - \hat{q}\| \leq \delta,$$

the iterates $q^{i+1} = (u^{i+1}, v^{i+1})$ generated by Algorithm 2 converge to a solution $q^ = (u^*, v^*)$ of (1.6).*

Proof. The proof is identical to that of [20, Thm. 2.1] and given here for the sake of completeness. Under the given assumptions, we can, for some $\xi > 0$, obtain from $(\widehat{D}^2\text{-}M)$ as in the proof of [20, Thm. 3.1] the inequality

$$(\widehat{D}) \quad \|q^i - \hat{q}^i\|_{M_i} \geq \xi \|q^{i+1} - q^i\|_{M_i} + \|q^{i+1} - \hat{q}^{i+1}\|_{M_{i+1}}.$$

It follows from (\widehat{D}) that

$$\sum_{i=1}^{\infty} \|q^{i+1} - q^i\|_{M_i} < \infty,$$

and consequently an application of (2.3) shows that

$$\sum_{i=1}^{\infty} \|q^{i+1} - q^i\| \leq \Theta \sum_{i=1}^{\infty} \|q^{i+1} - q^i\|_{M_i} < \infty.$$

This says that $\{q^i\}_{i=1}^\infty$ is a Cauchy sequence and hence converges to some \widehat{q} . It also implies that

$$\|M_i(q^{i+1} - q^i)\| \leq \Theta \|q^{i+1} - q^i\| \rightarrow 0.$$

Now [20, Lem. 3.5] states that under the given assumptions, it follows from (\widehat{D}) that $v^i \rightarrow 0$ and hence that

$$z^i := v^i + M_i(q^{i+1} - q^i) \rightarrow 0.$$

By (2.1), we moreover have $-z^i \in H_{u^i}(q^{i+1})$. Using $K \in C^1(X; Y)$ and the outer semicontinuity of the subgradient mappings ∂G and ∂F^* , we see that

$$\limsup_{i \rightarrow \infty} H_{u^i}(q^{i+1}) \subset H_{\widehat{u}}(\widehat{q}).$$

Here the lim sup is in the sense of an outer limit [17], consisting of the limits of all converging subsequences of elements $v^i \in H_{u^i}(q^{i+1})$. As by (2.1) we have $-z^i \in H_{u^i}(q^{i+1})$, it follows in particular that $0 \in H_{\widehat{u}}(\widehat{q})$, which is precisely (1.6). \square

Remark 2.7. *Theorem 2.6 holds if F^* is merely strongly convex on the “nonlinear” subspace*

$$Y_{NL} := \{y \in Y : \langle z, K(\cdot) \rangle \in L(X, Y)\}^\perp,$$

i.e., if (1.3) holds merely for all $v, v' \in Y_{NL}$. In this case, \widehat{v} in (2.11) can be replaced by $P_{NL}\widehat{v}$, the orthogonal projection of \widehat{v} on Y_{NL} . Indeed, [20, Lem. 2.1] directly applies to $V = Y_{NL} \subseteq Y$ to yield $(\widehat{D}^2\text{-loc-}\gamma\text{-}F^)$ for $P_{NL}(v^{i+1} - \widehat{v}^i)$, and a straightforward modification of Lemma 2.5 yields $(\widehat{D}^2\text{-}M)$. Since the Moreau–Yosida regularization, required for metric regularity in our examples, already implies strong convexity on the full space, we do not treat this more general case in detail.*

2.2 CONVERGENCE FOR STRONGLY CONVEX G

In this case, we chose for $\mu \geq 0$ the acceleration sequence

$$(2.12) \quad \sigma_{i+1} := \sigma_i / \omega_i \quad \text{and} \quad \tau_{i+1} := \tau_i \omega_i \quad \text{with} \quad \omega_i := 1 / \sqrt{1 + 2\mu\tau_i}.$$

Under the above assumptions, and if metric regularity holds for $H_{\widehat{u}}$, Algorithm 2 converges to a solution of (2.2a) as before. First, a trivial modification of the proof of [20, Lem. 2.1] yields again the basic descent estimate.

Lemma 2.8. *Let $q^i \in X \times Y$ and $\widehat{u} \in X$. Suppose $q^{i+1} \in X \times Y$ solves (2.1) and that $\widehat{q}^i \in X \times Y$ is a solution to*

$$0 \in H_{u^i}(\widehat{q}^i) + v^i.$$

If G is strongly convex on X with constant $\gamma_G > 0$, then we have

$$(\widehat{D}^2\text{-loc-}\gamma\text{-}G) \quad \|q^i - \widehat{q}^i\|_{M_i}^2 \geq \|q^{i+1} - q^i\|_{M_i}^2 + \|q^{i+1} - \widehat{q}^i\|_{M_i}^2 + \gamma_G \|u^{i+1} - \widehat{u}^i\|^2.$$

Analogously to Lemma 2.4, one now derives the following bounds.

Lemma 2.9. *Let $\{\tau_i\}_{i \in \mathbb{N}}$ satisfy (2.12). Then $\mu + (\tau_i^{-1} - \tau_{i+1}^{-1}) \geq 0$.*

We can now show the main lemma to account for the acceleration in the case of strongly convex G .

Lemma 2.10. *Suppose (2.2) and $(\widehat{D}^2\text{-loc-}\gamma\text{-}G)$ hold. Let R, L_2, κ be as in (2.2), and choose $\xi_1 \in (0, 1)$. If*

$$\|q^i - \widehat{q}\| \leq R/4 \quad \text{and} \quad \|q^i - \widetilde{q}^i\| \leq C$$

for a suitable constant $C = C(\gamma_G, \mu, \xi_1, \theta, L_2, \kappa, R)$, then $(\widehat{D}^2\text{-}M)$ holds.

Proof. Proceeding as in the proof of Lemma 2.5, since now $\{\sigma_i\}_{i \in \mathbb{N}}$ is non-decreasing, we derive from $(\widehat{D}^2\text{-loc-}\gamma\text{-}G)$ instead of (2.9) the estimate

$$(2.13) \quad \begin{aligned} \|q^{i+1} - \widetilde{q}^i\|_{M_i}^2 - \|q^{i+1} - \widetilde{q}^i\|_{M_{i+1}}^2 &\geq (\tau_i^{-1} - \tau_{i+1}^{-1}) \|u^{i+1} - \widetilde{u}^i\|^2 \\ &\quad - 2L_2 \|q^{i+1} - \widetilde{q}^i\| \|q^{i+1} - q^i\| \|u^{i+1} - \widetilde{u}^i\|. \end{aligned}$$

Applying Young's inequality, (2.13), and Lemma 2.9, we deduce

$$(2.14) \quad \begin{aligned} \|q^{i+1} - \widetilde{q}^i\|_{M_i}^2 - \|q^{i+1} - \widetilde{q}^i\|_{M_{i+1}}^2 + \gamma_G \|u^{i+1} - \widetilde{u}^i\|^2 \\ \geq (\mu + \tau_i^{-1} - \tau_{i+1}^{-1}) \|u^{i+1} - \widetilde{u}^i\|^2 - \frac{L_2^2}{\gamma_G - \mu} \|q^{i+1} - q^i\|^2 \|q^{i+1} - \widetilde{q}^i\|^2 \\ \geq -\frac{L_2^2}{\gamma_G - \mu} \|q^{i+1} - q^i\|^2 \|q^{i+1} - \widetilde{q}^i\|^2. \end{aligned}$$

We now conclude analogously to the proof of Lemma 2.5. □

The remaining proof now follows as in the case of strongly convex F^* , and we obtain the following convergence result.

Theorem 2.11. *Let (2.2) be satisfied with the corresponding constants R, Θ, κ and L_2 , and suppose G is strongly convex with factor γ_G . Let \widehat{q} solve $0 \in H_{\widehat{q}}(\widehat{q})$ and $H_{\widehat{q}}$ be metrically regular at 0 for \widehat{q} with*

$$\ell_{H_{\widehat{q}}^{-1}} \kappa L_2 \|\widehat{v}\| < 1 - 1/\sqrt{1 + 1/(2\ell_{H_{\widehat{q}}^{-1}}^2 \Theta^4)}.$$

If $\mu \in [0, \gamma_G)$ and we use the rule (2.12) for $i = 1, \dots, N$ for some $N \in \mathbb{N}$, after which $\tau_i = \tau_N$ and $\sigma_i = \sigma_N$ for $i > N$, there exists $\delta > 0$ such that for any $q^1 \in X \times Y$ with

$$\|q^1 - \widehat{q}\| \leq \delta,$$

the iterates $q^{i+1} = (u^{i+1}, v^{i+1})$ generated by Algorithm 2 converge to a solution $q^* = (u^*, v^*)$ of (1.6).

2.3 METRIC REGULARITY

We finally address the verification of metric regularity in infinite-dimensional Hilbert spaces required for the convergence of Algorithm 2. Motivated by the problems considered in the next section, we assume that

$$F^*(v) = \int_{\Omega} f^*(v(x)) dx$$

for a proper, convex, lower semicontinuous f^* and (after rescaling $F + G$, see below)

$$G(u) = \frac{1}{2} \|u\|_{L^2}^2.$$

We wish to apply the results from [9]. Towards this end, we consider the Moreau–Yosida regularization (1.4) of F for some parameter $\gamma > 0$, and assume (using (1.5)) that the convexified graphical derivative of the regularized subdifferential satisfies at least at non-degenerate points for some cone $V_{\partial F^*}(v|\eta)$ and a pointwise-defined self-adjoint positive semi-definite linear superposition operator $T_v : L^2(\Omega) \rightarrow L^2(\Omega)$ —i.e., $[T_v v](x) = t_{v(x)}(x)v(x)$ for some $t : \mathbb{R} \rightarrow \mathbb{R}$ —the expression

$$(2.15) \quad \widetilde{D[\partial F^*]}(v|\eta)(\Delta v) = \begin{cases} T_v \Delta v + V_{\partial F^*}(v|\eta)^\circ, & \Delta v \in V_{\partial F^*}(v|\eta), \\ \emptyset, & \Delta v \notin V_{\partial F^*}(v|\eta). \end{cases}$$

Using the sum rule for graphical coderivatives from [9, Cor. 2.3], we deduce that $\widetilde{D[\partial F_\gamma^*]}$ has the same type of structure with

$$\widetilde{D[\partial F_\gamma^*]}(v|\eta)(\Delta v) = \widetilde{D[\partial F^*]}(v|\eta)(\Delta v) + \gamma \Delta v.$$

For the Moreau–Yosida regularized problem, we denote the corresponding operator $H_{\hat{u}}$ by $H_{Y, \hat{u}}$. Then we have the following result.

Proposition 2.12 ([9, Prop. 4.3]). *Assume (2.15) holds and $K \in C^1(X; Y)$. Suppose further that \hat{q} solves $0 \in H_{Y, \hat{u}}(\hat{q})$ for some $\bar{F} \geq 0$. Then $H_{Y, \hat{u}}$ is metrically regular at 0 for \hat{q} if and only if $T_v + \gamma I \geq \beta I$ for some $\beta > 0$, or*

$$\bar{b}(\hat{q}|0; H_{\hat{u}}) := \sup_{t>0} \inf \left\{ \frac{\|K'(\hat{u})K'(\hat{u})^* z - v\|}{\|z\|} \left| \begin{array}{l} 0 \neq z \in V_{\partial F^*}(v'|\eta'), v \in V_{\partial F^*}(v'|\eta')^\circ, \\ \eta' \in \partial F^*(v'), \|v' - \hat{v}\| < t, \\ \|\eta' - K(\hat{u})\| < t \end{array} \right. \right\} > 0.$$

Proof. In [9, Prop. 4.3], we actually take $T_v = 0$. However, the only place where this specific structure is used is [9, Lem. 4.1]. In Lemma A.1 in Appendix A, we have updated the sufficient conditions of the former to be able to deal with general $T_v \geq 0$. \square

This implies convergence for any choice of the Moreau–Yosida regularization parameter $\gamma > 0$. On the other hand, if $\gamma = 0$, we typically have to prove existence of a lower bound for \bar{b} . This is significantly more difficult. We will address the issue of verifying—or disproving—the lower bound on \bar{b} with specific examples in the next section.

3 APPLICATION TO PDE-CONSTRAINED OPTIMIZATION PROBLEMS

We now discuss the application of the preceding analysis to the motivating examples of L^1 fitting, L^∞ fitting, and optimal control with state constraints. Since this will depend on the specific structure of the mapping S , we consider as a concrete example the problem of recovering the potential term in an elliptic equation.

Let $\Omega \subset \mathbb{R}^d$, $d \leq 3$, be an open bounded domain with a Lipschitz boundary $\partial\Omega$, and set $X := L^2(\Omega)$ as well as

$$U := \{v \in L^\infty(\Omega) : v(x) \geq \varepsilon \text{ for a.e. } x \in \Omega\} \subset X$$

for some $\varepsilon > 0$. For a given coefficient $u \in U$ and $f \in L^2(\Omega)$ fixed, denote by $S(u) := y \in H^1(\Omega) \subset L^2(\Omega) =: Y$ the weak solution of

$$(3.1) \quad \langle \nabla y, \nabla v \rangle + \langle uy, v \rangle = \langle f, v \rangle \quad (v \in H^1(\Omega)).$$

This operator has the following useful properties [16]:

(A1) The operator S is uniformly bounded in $U \subset X$ and completely continuous: If for $u \in U$, the sequence $\{u_n\} \subset U$ satisfies $u_n \rightharpoonup u$ in X , then

$$S(u_n) \rightarrow S(u) \quad \text{in } Y.$$

(A2) S is twice Fréchet differentiable.

(A3) There exists a constant $C > 0$ such that

$$\|S'(u)h\|_{L^2} \leq C\|h\|_X \quad (u \in U, h \in X).$$

(A4) There exists a constant $C > 0$ such that

$$\|S''(u)(h, h)\|_{L^2} \leq C\|h\|_X^2 \quad (u \in U, h \in X).$$

Furthermore, from the implicit function theorem, the directional Fréchet derivative $S'(u)h$ at $u \in U$ for given $h \in X$ can be computed as the solution $w \in H^1(\Omega)$ to

$$\langle \nabla w, \nabla v \rangle + \langle uw, v \rangle = \langle -yh, v \rangle \quad (v \in H^1(\Omega)).$$

Similarly, the directional adjoint derivative $S'(u)^*h$ is given by yz , where $z \in H^1(\Omega)$ solves

$$\langle \nabla z, \nabla v \rangle + \langle uz, v \rangle = \langle -h, v \rangle \quad (v \in H^1(\Omega)).$$

Similar expressions hold for $S''(u)(h_1, h_2)$ and $(S'(u)^*h_1)'h_2$. Hence, assumptions (A3–A4) hold for S'^* and $(S'(u)^*v)'$ for given v as well.

Other operators satisfying the above assumptions are mappings from a Robin or diffusion coefficient to the solution of the corresponding elliptic partial differential equation; cf. [7].

3.1 L^1 FITTING

First, we consider the L^1 fitting problem (1.2). In order to make use of the strong convexity of the penalty term for the acceleration, we rewrite this equivalently as

$$(3.2) \quad \min_{u \in L^2} \frac{1}{\alpha} \|S(u) - y^\delta\|_{L^1} + \frac{1}{2} \|u\|_{L^2}^2,$$

i.e., we set $G(u) = \frac{1}{2}\|u\|_{L^2}^2$, $K(u) = S(u) - y^\delta$, and $F(y) = \frac{1}{\alpha}\|y\|_{L^1}$ in (1.1). Hence

$$[F^*(p)](x) = \iota_{[-\alpha^{-1}, \alpha^{-1}]}(p(x)) \quad (\text{a.e. } x \in \Omega),$$

where ι_C denotes the indicator function of the convex set C in the sense of convex analysis [10].

To guarantee metric regularity, we replace F by its Moreau–Yosida regularization, which coincides with the well-known Huber norm, i.e.,

$$F_Y(y) = \int_{\Omega} |y(x)|_Y dx, \quad |t|_Y = \begin{cases} \frac{1}{2\gamma}|t|^2 & \text{if } |t| \leq \frac{\gamma}{\alpha}, \\ \frac{1}{\alpha}|t| - \frac{\gamma}{2\alpha} & \text{if } |t| > \frac{\gamma}{\alpha}. \end{cases}$$

Using the calculus of Clarke’s generalized derivative and (1.5), i.e., $\partial F_Y^*(p) = \partial F^*(p) + \{\gamma p\}$, we obtain the corresponding regularized optimality conditions (cf. also [7, Thm. 2.7])

$$(3.3) \quad \begin{cases} S(u_Y) - y^\delta - \gamma p_Y \in \partial F^*(p_Y), \\ -S'(u_Y)^* p_Y = u_Y. \end{cases}$$

For G and F^* as above, the proximal mappings are given by

$$\begin{aligned} [\text{prox}_{\tau G}(u)](x) &= \frac{1}{1+\tau}u(x), \\ [\text{prox}_{\sigma F^*}(v)](x) &= \text{proj}_{[-\alpha^{-1}, \alpha^{-1}]}(v(x)). \end{aligned}$$

Using rule (P2) above, we thus obtain for the Moreau–Yosida regularization F_Y^*

$$[\text{prox}_{\sigma F_Y^*}(v)](x) = \text{proj}_{[-\alpha^{-1}, \alpha^{-1}]} \left(\frac{1}{1+\sigma\gamma}v(x) \right).$$

Since G is strongly convex with constant $\gamma_G = 1$, we can use the acceleration scheme (2.12) for any $\mu < 1$. Algorithm 2 thus has the following explicit form, where we denote the dual variable with p instead of v to be consistent with the notation in this section.

Algorithm 3 Accelerated primal-dual algorithm for L^1 fitting

- 1: choose u^0, p^0
 - 2: **for** $i = 0, \dots, N$ **do**
 - 3: $z^{i+1} = S'(u^i)^* p^i$
 - 4: $u^{i+1} = \frac{1}{1+\tau_i}(u^i - \tau_i z^{i+1})$
 - 5: $\omega_i = 1/\sqrt{1+2\mu\tau_i}$, $\tau_{i+1} = \omega_i \tau_i$, $\sigma_{i+1} = \sigma_i/\omega_i$
 - 6: $\bar{u}^{i+1} = u^{i+1} + \omega_i(u^{i+1} - u^i)$
 - 7: $p^{i+1} = \text{proj}_{[-\alpha^{-1}, \alpha^{-1}]} \left(\frac{1}{1+\sigma_{i+1}\gamma}(p^i + \sigma_{i+1}(S(\bar{u}^{i+1}) - y^\delta)) \right)$
-

To show convergence of Algorithm 3 using Theorem 2.11 and Proposition 2.12, we have to verify the expression (2.15) for $D[\partial F^*]$. This is the content of [9, Cor. 2.11]. However, as discussed in [9, § 5.1], for $\gamma = 0$ (i.e., no regularization), we in general have $\bar{b}(\widehat{q}|0; H_{\bar{u}}) = 0$.

(We remark that in the case of finite-dimensional data $y^\delta \in Y_h \subset Y$, replacing F by $F \circ P_h$ where P_h denotes the orthogonal projection onto Y_h , there exists a constant $c > 0$ such that $\bar{b}(\widehat{q}|0; H_{\bar{u}, h}) \geq c > 0$ holds; see [9, § 5.3]. Hence, regularization is not necessary in this case.)

We summarize the above discussion on the convergence for the infinite-dimensional L^1 fitting problem (3.2) in the next corollary.

Corollary 3.1. *Let $\gamma > 0$ and $\mu \in [0, 1)$ be arbitrary (setting $\mu = 0$ after a finite number of iterations). Let $(u_\gamma, p_\gamma) \in L^2(\Omega)^2$ be a solution to (3.3), and take $\tau_0, \sigma_0 > 0$ satisfying (2.2b) for $K(u) = S(u) - \gamma^\delta$. Then there exists $\delta > 0$ such that for any initial iterate $(u^1, p^1) \in L^2(\Omega)^2$ with $\|(u^1, p^1) - (u_\gamma, p_\gamma)\| \leq \delta$, the iterates (u^k, p^k) generated by Algorithm 3 converge to a solution (u^*, p^*) to (3.3).*

Proof. Note that G is strongly convex with factor 1, while Moreau–Yosida regularization makes F_γ^* strongly convex with factor γ . By Proposition 2.12, $H_{\gamma, \hat{u}}$ is metrically regular at 0 for \hat{q} . The claim now follows from Theorem 2.11. \square

Remark 3.2. *In general, ensuring that the iterates generated by Algorithm 3 remain feasible, i.e., satisfy $u^i \in U$, requires adding an explicit constraint to (3.2). This would lead to a nonsmooth $G(u) = \frac{1}{2}\|u\|_{L^2}^2 + \iota_{[\varepsilon, \infty)}(u)$ (where the indicator function is to be understood pointwise almost everywhere), which was not considered in [9]. The analysis there could be extended to cover this case; specifically, all non-degenerate cases would be covered by improving [9, Lem. 4.1] to include the case $V_{\hat{G}} = \{0\}$ instead of just $V_{\hat{G}} = X$, see Lemma A.1 in Appendix A.*

However, to be able to directly apply the theory as stated in [9], and since in our numerical examples the iterates are always feasible as long as the minimizer and the initial guess are sufficiently far from the lower bound, we omit the constraint in our model problems.

3.2 L^∞ FITTING

We next consider the L^∞ fitting (“Morozov”) problem from [6],

$$(3.4) \quad \min_u \frac{1}{2} \|u\|_{L^2}^2 \quad \text{s. t.} \quad |[S(u)](x) - \gamma^\delta(x)| \leq \delta \quad \text{a. e. in } \Omega,$$

i.e., now $F(v) = \iota_{[-\delta, \delta]}(v)$ (again to be understood pointwise almost everywhere) with G and K as before.

Again, it is well-known that the Moreau–Yosida regularization of pointwise constraints is given by its quadratic penalization, i.e.,

$$F_\gamma(y) = \frac{1}{2\gamma} \|\max\{0, |y| - \delta\}\|_{L^2}^2.$$

Hence,

$$(3.5) \quad \begin{cases} S(u_\gamma) - \gamma^\delta - \gamma p_\gamma \in \partial F^*(p_\gamma), \\ -S'(u_\gamma)^* p_\gamma = u_\gamma, \end{cases}$$

where now $F^*(v) = \delta \|v\|_{L^1}$.

In this case, the proximal mapping of F^* is given by

$$[\text{prox}_{\sigma F^*}(v)](x) = (|v(x)| - \delta\sigma)^+ \text{sign}(v(x)).$$

For the Moreau–Yosida regularization F_γ^* , we obtain after some simplification

$$[\text{prox}_{\sigma F_\gamma^*}(v)](x) = \frac{1}{1 + \sigma\gamma} (|v(x)| - \delta\sigma)^+ \text{sign}(v(x)).$$

Again, we use the acceleration scheme (2.12) for $\mu < \gamma_G = 1$. Algorithm 2 now has the following explicit form.

Algorithm 4 Accelerated primal-dual algorithm for L^∞ fitting

- 1: choose u^0, p^0
 - 2: **for** $i = 0, \dots, N$ **do**
 - 3: $z^{i+1} = S'(u^i)^* p^i$
 - 4: $u^{i+1} = \frac{1}{1+\tau_i}(u^i - \tau_i z^{i+1})$
 - 5: $\omega_i = 1/\sqrt{1+2\mu\tau_i}, \quad \tau_{i+1} = \omega_i \tau_i, \quad \sigma_{i+1} = \sigma_i/\omega_i$
 - 6: $\bar{u}^{i+1} = u^{i+1} + \omega_i(u^{i+1} - u^i)$
 - 7: $p^{i+1} = \frac{1}{1+\sigma_i\gamma}(|r^{i+1}| - \delta\sigma_i)^+ \text{sign}(r^{i+1})$
-

As before, we deduce from the characterization of $\widetilde{D[\partial F^*]}$ from [9, Cor. 2.13] that (2.15) holds for F^* , while the discussion in [9, § 5.2] shows that metric regularity of $H_{Y, \bar{u}}$ only holds for $\gamma > 0$ (or finite-dimensional data). Summarizing, we have the following convergence result for the infinite-dimensional L^∞ fitting problem (3.4).

Corollary 3.3. *Let $\gamma > 0$ and $\mu \in [0, 1)$ be arbitrary (setting $\mu = 0$ after a finite number of iterations). Furthermore, let $(u_\gamma, p_\gamma) \in L^2(\Omega)^2$ be a solution to (3.5), and take $\tau_0, \sigma_0 > 0$ satisfying (2.2b) for $K(u) = S(u) - y^\delta$. Then there exists $\delta > 0$ such that for any initial iterate $(u^1, p^1) \in L^2(\Omega)^2$ with $\|(u^1, p^1) - (u_\gamma, p_\gamma)\| \leq \delta$, the iterates (u^k, p^k) generated by Algorithm 4 converge to a solution (u^*, p^*) to (3.5).*

3.3 STATE CONSTRAINTS

Finally, we address the state-constrained optimal control problem

$$(3.6) \quad \min_{u \in L^2} \frac{1}{2\alpha} \|S(u) - y^d\|_{L^2}^2 + \frac{1}{2} \|u\|_{L^2}^2 \quad \text{s. t.} \quad [S(u)](x) \leq c \quad \text{a. e. in } \Omega.$$

In this case, G is as before and $F(y) = \frac{1}{2\alpha} \|v - y^d\|_{L^2}^2 + \iota_{(-\infty, c]}(y)$ with $K(u) = S(u)$. For simplicity, we assume here that the upper bound c is constant; the extension to variable $c \in L^\infty(\Omega)$ (as well as lower bounds) is straightforward.

For F_γ , we directly use the definition (1.4) to compute pointwise

$$f_\gamma(x, v) = \begin{cases} \frac{1}{2\alpha} |c - y^d(x)|^2 + \frac{1}{2\gamma} |v - c|^2 & \text{if } v > (1 + \frac{\alpha}{\gamma})c - \frac{\alpha}{\gamma} y^d(x), \\ \frac{1}{2(\alpha+\gamma)} |v - y^d(x)|^2 & \text{if } v \leq (1 + \frac{\alpha}{\gamma})c - \frac{\alpha}{\gamma} y^d(x), \end{cases}$$

and obtain

$$F_\gamma(y) = \int_{\Omega} f_\gamma(x, y(x)) dx.$$

The corresponding regularized optimality conditions are again given by

$$(3.7) \quad \begin{cases} S(u_\gamma) - y^\delta - \gamma p_\gamma \in \partial F^*(p_\gamma), \\ -S'(u_\gamma)^* p_\gamma = u_\gamma. \end{cases}$$

It remains to compute F^* . Since $y^d \in L^2(\Omega)$ is measurable,

$$f(x, v) = \frac{1}{2\alpha} |v - y^d(x)|^2 + \iota_{(-\infty, c]}(v)$$

is a proper, convex, and normal integrand, and hence we can proceed by pointwise computation.

Let $x \in \Omega$ be arbitrary. For the Fenchel conjugate with respect to y ,

$$f^*(x, z) = \sup_{v \leq c} vz - \frac{1}{2\alpha} |v - y^d(x)|^2,$$

we consider the first-order necessary conditions for the maximizer

$$\bar{v} = \text{proj}_{(-\infty, c]}(\alpha z + y^d(x)).$$

Inserting this into the definition and making the case distinction whether $\alpha v + y^d(x) \leq c$ yields

$$f^*(x, z) = \begin{cases} cz - \frac{1}{2\alpha} |c - y^d(x)|^2 & z > \alpha^{-1}(c - y^d(x)), \\ \frac{\alpha}{2} |z|^2 + zy^d(x) & z \leq \alpha^{-1}(c - y^d(x)). \end{cases}$$

The subdifferential (with respect to z) is given by

$$(3.8) \quad \partial f^*(x, z) = \begin{cases} \{c\} & z > \alpha^{-1}(c - y^d(x)), \\ \{\alpha z + y^d(x)\} & z \leq \alpha^{-1}(c - y^d(x)). \end{cases}$$

(Note that the cases agree for $z = \alpha^{-1}(c - y^d(x))$, i.e., $z \mapsto \partial f^*(x, z)$ is single-valued and hence $z \mapsto f^*(x, z)$ is continuously differentiable for almost every $x \in \Omega$.)

To compute the pointwise proximal mapping $\text{prox}_{\sigma f^*(x, \cdot)}(v)$ for given $x \in \Omega$, we use the resolvent formula

$$\text{prox}_{\sigma f^*(x, \cdot)}(v) = (\text{Id} + \sigma \partial f^*(x, \cdot))^{-1}(v) =: w,$$

i.e., $v \in \{w\} + \sigma \partial f^*(x, w)$, together with (3.8) and distinguish the two cases

- (i) $v = w + \sigma c$, i.e., $w = v - \sigma c$, if $w > \alpha^{-1}(c - y^d(x))$, i.e., if $v > \alpha^{-1}(c - y^d(x)) + \sigma c$;
- (ii) $v = w + \sigma(\alpha w + y^d(x))$, i.e., $w = (1 + \sigma\alpha)^{-1}(v - \sigma y^d(x))$, if $w \leq \alpha^{-1}(c - y^d(x))$, i.e., if

$$v \leq \frac{1 + \sigma\alpha}{\alpha} (c - y^d(x)) + \sigma z = \alpha^{-1}(c - y^d(x)) + \sigma c.$$

Together we obtain

$$[\text{prox}_{\sigma F^*}(v)](x) = \begin{cases} v(x) - \sigma c & v(x) > \frac{1}{\alpha}(c - y^d(x)) + \sigma c, \\ (1 + \sigma\alpha)^{-1}(v(x) - \sigma y^d(x)) & v(x) \leq \frac{1}{\alpha}(c - y^d(x)) + \sigma c. \end{cases}$$

For the Moreau–Yosida regularization $f_\gamma^*(x, v) = f^*(x, v) + \frac{\gamma}{2} |v|^2$, we similarly obtain

$$[\text{prox}_{\sigma F_\gamma^*}(v)](x) = \begin{cases} (1 + \sigma\gamma)^{-1}(v(x) - \sigma c) & v(x) > \frac{1 + \sigma\gamma}{\alpha}(c - y^d(x)) + \sigma c, \\ (1 + \sigma(\alpha + \gamma))^{-1}(v(x) - \sigma y^d(x)) & v(x) \leq \frac{1 + \sigma\gamma}{\alpha}(c - y^d(x)) + \sigma c. \end{cases}$$

Again, we use the acceleration scheme (2.12) for $\mu < \gamma_G = 1$. Algorithm 2 now has the following explicit form, where $\llbracket P \rrbracket$ for a logical proposition P depending on $x \in \Omega$, denotes the pointwise Iverson bracket, i.e., $\llbracket P \rrbracket(x) = 1$ if $P(x)$ is true and 0 else.

Algorithm 5 Accelerated primal-dual algorithm for state constraints

- 1: choose u^0, p^0
 - 2: **for** $i = 0, \dots, N$ **do**
 - 3: $u^{i+1} = \frac{1}{1+\tau_i}(u^i - \tau_i S'(u^i)^* p^i)$
 - 4: $\omega_i = 1/\sqrt{1+2\mu\tau^i}, \quad \tau^{i+1} = \omega_i \tau^i, \quad \sigma_{i+1} = \sigma_i/\omega_i$
 - 5: $\bar{u}^{i+1} = u^{i+1} + \omega_i(u^{i+1} - u^i)$
 - 6: $r^{i+1} = p^i + \sigma_{i+1} S(\bar{u}^{i+1})$
 - 7: $\chi^{i+1} = \llbracket r^{i+1} > \frac{1+\sigma_{i+1}\gamma}{\alpha}(c - y^d) + \sigma_{i+1}c \rrbracket$
 - 8: $p^{i+1} = \frac{1}{1+\sigma_{i+1}\gamma} \chi^{i+1} (r^{i+1} - \sigma_{i+1}c) + \frac{1}{1+\sigma_{i+1}(\alpha+\gamma)} (1 - \chi^{i+1}) (r^{i+1} - \sigma_{i+1}y^d)$
-

Let us assume that strict complementarity holds, i.e., $\alpha v(x) \neq c - y^d(x)$ for a.e. $x \in \Omega$. Then it follows from Corollary B.2 in Appendix B that (2.15) is satisfied for F^* . Furthermore, since $t_v(x) \in \{0, \alpha\}$ for a.e. $x \in \Omega$ and $V_{\partial F^*}(v|\eta) = L^2(\Omega)$ and $V_{\partial F^*}(v|\eta)^\circ = \{0\}$ locally in a neighbourhood of $(\widehat{u}, \widehat{v})$, we deduce that

$$\bar{b}(\widehat{q}|0; H_{\widehat{u}}) = \sup_{t>0} \inf \left\{ \frac{\|S'(\widehat{u})S'(\widehat{u})^* z\|}{\|z\|} \mid 0 \neq z \in L^2(\Omega) \right\}.$$

However, the lower bound

$$\|S'(\widehat{u})^* z\| \geq c\|z\| \quad (z \in L^2(\Omega))$$

does not hold in general. This can be seen by taking any orthonormal basis of $L^2(\Omega)$, which converges weakly but not strongly to zero, and use the fact that $S'(u)$ is a compact operator from $L^2(\Omega)$ to $L^2(\Omega)$ due to the Rellich–Kondrachev embedding theorem. Therefore, also $\bar{b}(\widehat{q}|0; H_{\widehat{u}}) = 0$. By Proposition 2.12, there is thus no metric regularity without regularization ($\gamma > 0$). (Similarly to the L^1 fitting problem, if the state constraints are only prescribed at a finite number of points, it is possible to show metric regularity for $\gamma = 0$ as well.)

The next corollary, which follows similarly to Corollary 3.1, summarizes the convergence results from Theorems 2.6 and 2.11 for the infinite-dimensional state-constrained optimal control problem (3.6).

Corollary 3.4. *Let $\gamma > 0$ and $\mu \in [0, 1)$ be arbitrary (setting $\mu = 0$ after a finite number of iterations). Furthermore, let $(u_\gamma, p_\gamma) \in L^2(\Omega)^2$ be a solution to (3.7), and take $\tau_0, \sigma_0 > 0$ satisfying (2.2b) for $K(u) = S(u) - y^\delta$. Then there exists $\delta > 0$ such that for any initial iterate $(u^1, p^1) \in L^2(\Omega)^2$ with $\|(u^1, p^1) - (u_\gamma, p_\gamma)\| \leq \delta$, the iterates (u^k, p^k) generated by Algorithm 5 converge to a solution (u^*, p^*) to (3.7).*

4 NUMERICAL RESULTS

We now illustrate the convergence behavior of the primal-dual extragradient method for the three model problems in Section 3. Since we are interested in the properties of the algorithm in function spaces, we consider here the case in $d = 1$ dimension to allow for very fine discretizations with reasonable computational effort. We have also tested the model problems in $d = 2$ dimensions and observed very similar behavior.

In each case, the operator S corresponds to the solution of (3.1) for $\Omega = (-1, 1)$ and constant right-hand side $f \equiv 1$. For the implementation, we use a finite element approximation of (3.1) on a uniform grid with $n = 1000$ elements (unless stated otherwise) with a piecewise constant discretization of u and a piecewise linear discretization of y as in [7]. The functional values

$$J_Y(u^i) = F_Y(K(u^i)) + G(u^i)$$

are computed using an approximation of the integrals by mass lumping, which amounts to a proper scaling of the corresponding discrete sums. In this way, the functional values are independent of the mesh size.

The parameters in the primal-dual extragradient method are chosen as follows: The Moreau–Yosida parameter is fixed at $\gamma = 10^{-12}$ unless otherwise stated, and we compare the two cases of $\mu = 0$ (no acceleration) and $\mu = 1 - 10^{-16} < 1 = \gamma_G$ (full acceleration). We point out that this value of γ is significantly smaller than those for which semismooth Newton methods tend to converge even with continuation; cf. [6, 7]. As a starting value, we take in each case $u^0 \equiv 1$ and $p^0 \equiv 0$. The (initial) step sizes are set to $\sigma_0 = \tilde{L}^{-1}$ and $\tau_0 = 0.99\tilde{L}^{-1}$, where $\tilde{L} = \max\{1, \|S''(u^0)u^0\|/\|u^0\|\}$ is a very simple estimate of the Lipschitz constant of $K' = S'$. The algorithm (and the acceleration) is terminated after a prescribed number N of iterations. The MATLAB implementation used to generate the results in this section can be downloaded from <https://github.com/clason/nlpdegm>.

4.1 L^1 FITTING

We first consider the L^1 fitting problem (3.2) using the example from [7]: We choose the exact parameter $u^\dagger(x) = 2 - |x|$ and corresponding exact data $y^\dagger = S(u^\dagger)$ and add random-valued impulsive noise by setting

$$y^\delta(x) = \begin{cases} y^\dagger(x) + \|y^\dagger\|\xi(x) & \text{with probability } r, \\ y^\dagger(x) & \text{with probability } 1 - r, \end{cases}$$

where for each $x \in \Omega$, $\xi(x)$ is an independent normally distributed random value with mean 0 and variance δ^2 . For the results shown, we take $r = 0.3$ and $\delta = 0.1$, i.e., 30% of data points are corrupted by 10% noise. We then apply Algorithm 3 with $N = 1000$ iterations and $\alpha = 10^{-2}$ fixed.

Figure 1 compares the convergence behavior of the functional values with $\mu = 0$ and $\mu \approx 1$ (for the same data y^δ). The effect of acceleration can be seen clearly. Note that the convergence is nonmonotone due to the acceleration (and the aggressive choice of step lengths).

The convergence behavior for different mesh sizes is illustrated in Figure 2, which shows the functional values for $n \in \{100, 1000, 1000\}$ (as averages over 10 different realizations of

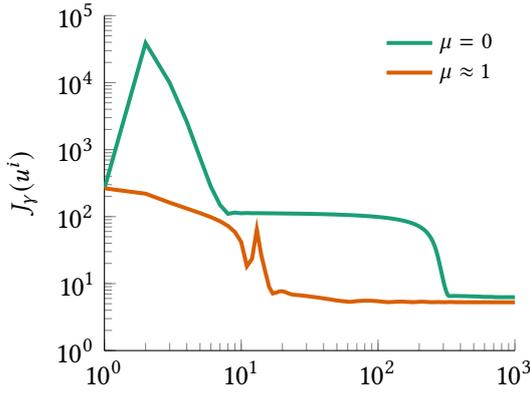


Figure 1: L^1 fitting: convergence without ($\mu = 0$) and with ($\mu \approx 1$) acceleration

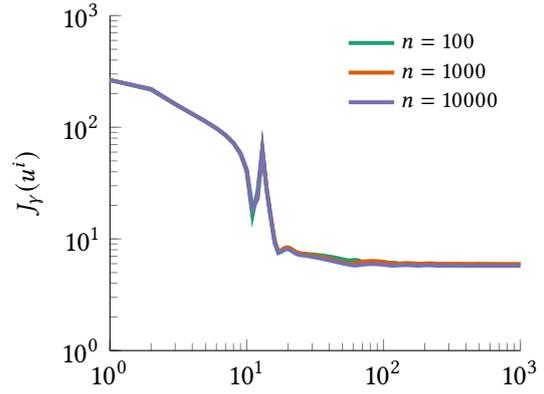
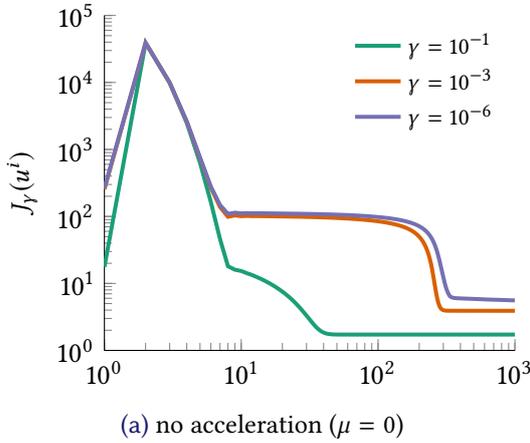
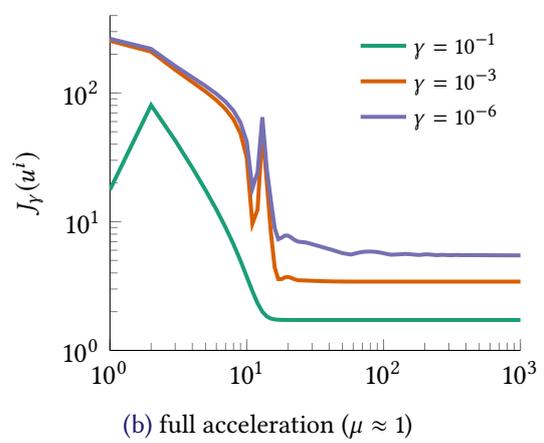


Figure 2: L^1 fitting: convergence for different mesh sizes n (average of 10 realizations)



(a) no acceleration ($\mu = 0$)



(b) full acceleration ($\mu \approx 1$)

Figure 3: L^1 fitting: convergence for different values of Moreau–Yosida regularization parameter γ without and with acceleration

y^δ in order to mitigate the influence of the random data). As can be observed, the number of iterations to reach a given functional value is virtually independent of the mesh size. This property—shared by many function-space algorithms—is often referred to as *mesh independence*.

Finally, we report on the effect of the Moreau–Yosida parameter γ on the performance of the algorithm. Figure 3 shows the convergence behavior for $\gamma \in \{10^{-1}, 10^{-3}, 10^{-6}\}$ with and without acceleration. (Note that the regularized functional J_γ depends on γ and hence the absolute function values $J_\gamma(u^i)$ are not directly comparable for different values of γ). Without acceleration ($\mu = 0$), one can observe from Figure 3a that the strong convexity of F_γ^* —with $\gamma_{F_\gamma^*} = \gamma$ —plays a significant role for the performance. In contrast, the case with full acceleration ($\mu \approx 1$, Figure 3b) which exploits the strong convexity of G —where $\gamma_G = 1 \gg \gamma$ —is much less affected by the value of γ , showing equally improved performance for all values of γ .

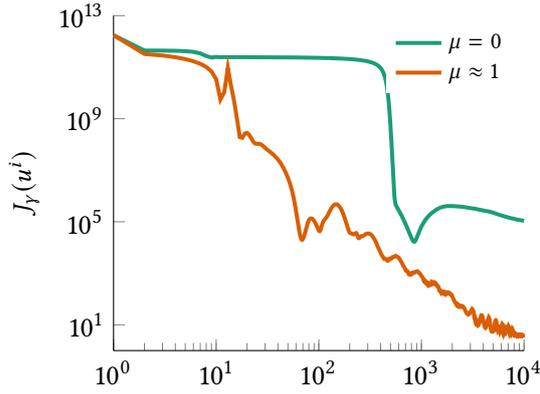


Figure 4: L^∞ fitting: convergence without ($\mu = 0$) and with ($\mu \approx 1$) acceleration

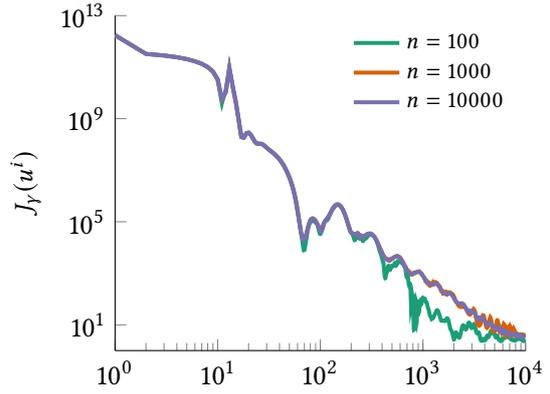


Figure 5: L^∞ fitting: convergence for different mesh sizes n

4.2 L^∞ FITTING

For the L^∞ fitting problem (3.4), we choose a test problem from [6], where y^δ is obtained from $y^\dagger = S(u^\dagger)$ (with u^\dagger as above) by quantization. Specifically, we set

$$y^\delta(x) = y_s \left\lfloor \frac{y^\dagger(x)}{y_s} \right\rfloor, \quad y_s = n_b^{-1} \left(\sup_{x \in \bar{\Omega}} (y^\dagger(x)) - \inf_{x \in \bar{\Omega}} (y^\dagger(x)) \right),$$

where n_b denotes the number of bins and $\lfloor s \rfloor$ denoting the nearest integer to $s \in \mathbb{R}$ (i.e., the data are rounded to n_b discrete equidistant values). Here we take $n_b = 11$ and apply Algorithm 4 for $N = 10000$ iterations.

Again, Figure 4 compares the functional values over the iteration without and with acceleration and demonstrates the significantly better performance of the latter. Similarly, the comparison of different mesh sizes in Figure 5 illustrates the mesh independence of the algorithm (with slightly faster convergence for $n = 100$, which can be explained by the effect of coarse discretization on the rounding procedure). Comparing the effect of γ on the algorithm without (Figure 6a) and with full (Figure 6b) acceleration, one again sees improved robustness with respect to γ for the latter.

4.3 STATE CONSTRAINTS

Finally, we consider the state-constrained optimal control problem (3.6). Here, we choose the desired state $y^d = S(u^\dagger)$ (with u^\dagger again as before) and the constraint $c = 0.68$. The control costs are set to $\alpha = 10^{-12}$, and we again terminate acceleration (and the algorithm) after $N = 10000$ iterations.

As before, Figures 7 and 8 illustrate the benefit of acceleration and the mesh independence of the algorithm, respectively. Since in this example, the solution only becomes feasible for very small values of γ , the visual comparison of the effect of γ on the performance is more

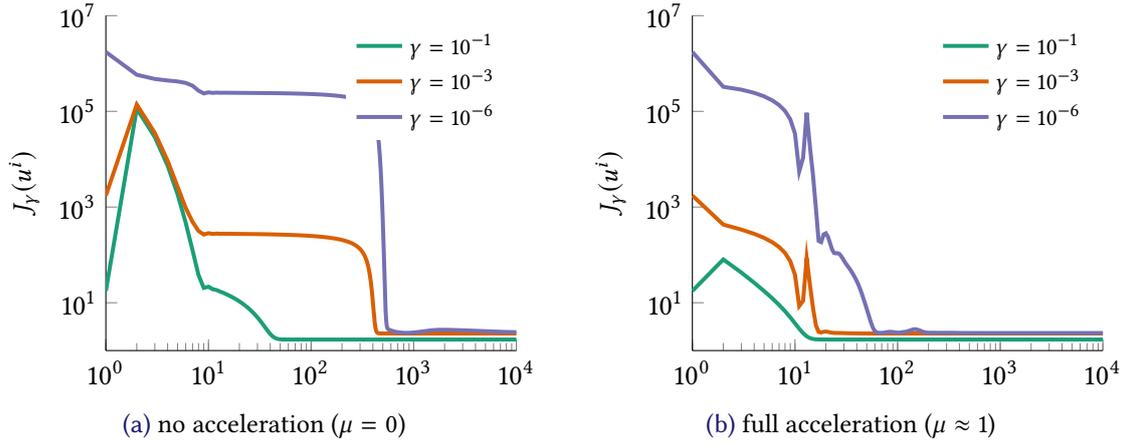


Figure 6: L^∞ fitting: convergence for different values of Moreau–Yosida regularization parameter γ without and with acceleration

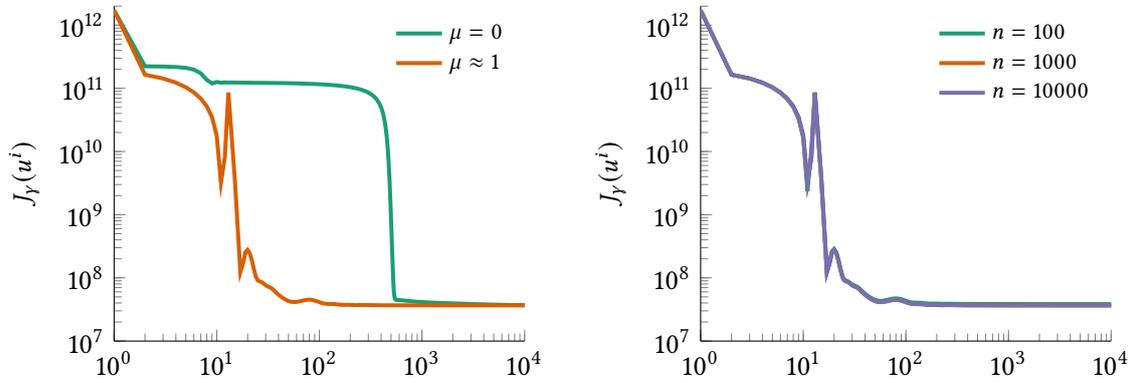


Figure 7: State constraints: convergence without ($\mu = 0$) and with ($\mu \approx 1$) acceleration

Figure 8: State constraints: convergence for different mesh sizes n

difficult. Nevertheless, comparing Figure 9 with Figure 7 shows again that acceleration reduces the influence of γ on the performance, although the effect is much less pronounced in this example.

5 CONCLUSION

Accelerated primal-dual extragradient methods with nonlinear operators can be formulated and analyzed in function space. Their convergence rests on metric regularity of the corresponding saddle-point inclusion, which can be verified for the class of PDE-constrained optimization problems considered here after introducing a Moreau–Yosida regularization. Unlike semismooth Newton methods (which also require Moreau–Yosida regularization in function space, cf., e.g.,

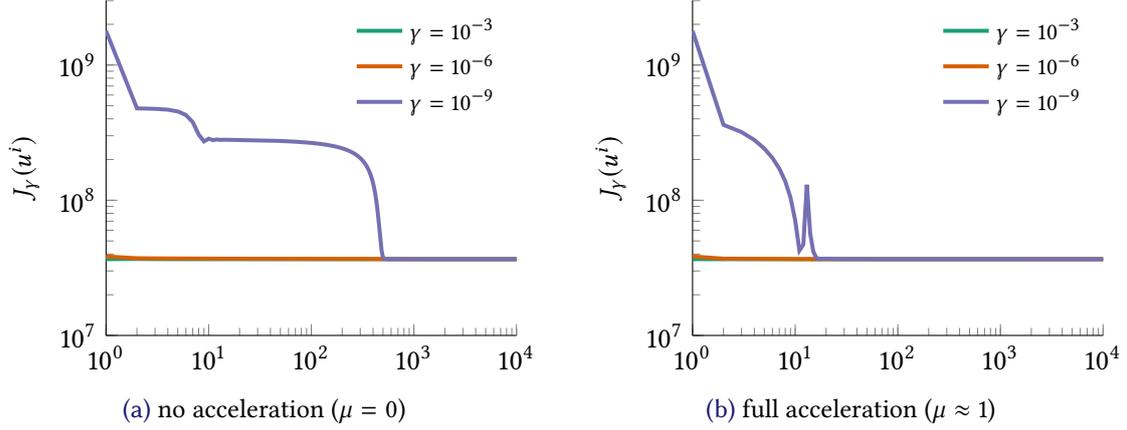


Figure 9: State constraints: convergence for different values of Moreau–Yosida regularization parameter γ without and with acceleration

[6, 7, 11]), however, in practice it is not necessary for convergence to choose γ sufficiently large. Hence, no continuation or warm starts are required. In addition, formulating and analyzing the algorithm in function space leads to mesh independence. These properties are observed in our numerical examples.

This work can be extended in a number of directions. We plan to investigate the possibility of obtaining convergence estimates on the primal variable alone under lesser assumptions. An alternative would be to exploit the uniform stability with respect to regularization for fixed discretization, and with respect to discretization for fixed regularization, to obtain a combined convergence for a suitably chosen net $(\gamma, h) \rightarrow (0, 0)$. This is related to the adaptive regularization and discretization of inverse problems [8, 14]. Furthermore, it would be of interest to extend our analysis to include nonsmooth regularizers G , which were excluded in the current work for the sake of the presentation.

APPENDIX A A SLIGHTLY IMPROVED VERSION OF [9, LEM. 4.1]

Here we improve the sufficient condition [9, Lem. 4.1 (i)] to allow for a more general linear operator \bar{F} than $\bar{F} = \gamma I$ as well as for a more general cone $V_{\bar{G}}$ than $V_{\bar{G}} = X$ arising from the graphical derivative of ∂F_γ^* and ∂G , respectively. These modifications are necessary for the treatment of state constraints; the latter is also the basis for extending the analysis in [9] to cover pointwise constraints on the primal variable as mentioned in Remark 3.2.

Lemma A.1. *Let $V = V_{\bar{G}} \times V_{\bar{F}} \subset X \times Y$ be a cone, and let $\bar{G} : X \rightarrow X$, $\bar{F} : Y \rightarrow Y$, and $\bar{K} : X \rightarrow Y$ be bounded linear operators with \bar{G} and \bar{F} self-adjoint. Define*

$$T := \begin{pmatrix} \bar{G} & \bar{K}^* \\ -\bar{K} & \bar{F} \end{pmatrix}.$$

Suppose both $\bar{G} \geq_{V_{\bar{G}}} c_G^2 I$ and $\bar{F} \geq_{V_{\bar{F}}} c_F^2 I$ for some $c_G, c_F > 0$, i.e.,

$$\langle \bar{G}\xi, \xi \rangle \geq c_G^2 \|\xi\|^2 \quad (\xi \in V_{\bar{G}}) \quad \text{and} \quad \langle \bar{F}\eta, \eta \rangle \geq c_F^2 \|\eta\|^2 \quad (\eta \in V_{\bar{F}}).$$

Then there exists $c > 0$ with

$$\inf_{z \in V^\circ} \|T^*w - z\|^2 \geq c\|w\|^2 \quad (w \in V).$$

Proof. With $w = (\xi, \eta) \in V = V_{\bar{G}} \times V_{\bar{F}}$, and $z = (\mu, \nu) \in V^\circ$, we expand

$$\begin{aligned} \text{(A.1)} \quad \|T^*w - z\|^2 &= \|\bar{G}\xi - \bar{K}^*\eta - \mu\|^2 + \|\bar{K}\xi + \bar{F}\eta - \nu\|^2 \\ &= \|\bar{G}\xi\|^2 + \|\bar{K}^*\eta + \mu\|^2 - 2\langle (\bar{K}\bar{G} - \bar{F}\bar{K})\xi, \eta \rangle \\ &\quad + \|\bar{K}\xi - \nu\|^2 + \|\bar{F}\eta\|^2 - 2\langle \bar{F}\eta, \nu \rangle - 2\langle \bar{G}\xi, \mu \rangle. \end{aligned}$$

Let $\lambda, \beta > 0$ be arbitrary. We can insert $0 = \langle (\Lambda\bar{K} - \bar{K}\bar{M})\xi, \eta \rangle$ and $0 = \langle (\bar{K}M - \bar{K}M)\xi, \eta \rangle$ into (A.1). We can also use $\langle \eta, (\Lambda - \bar{F})\nu \rangle \geq 0$ for all $\nu \in V_{\bar{F}}^\circ$ and $\eta \in V_{\bar{F}}$ and similarly $\langle \xi, (M - \bar{G})\mu \rangle \geq 0$ for all $\mu \in V_{\bar{G}}^\circ$ and $\xi \in V_{\bar{G}}$. Thus

$$\begin{aligned} \|T^*w - z\|^2 &= \|\bar{G}\xi\|^2 + \|\bar{K}^*\eta + \mu\|^2 - 2\langle (\bar{K}\bar{G} - \bar{K}M + \Lambda\bar{K} - \bar{F}\bar{K})\xi, \eta \rangle \\ &\quad + 2\langle \bar{K}\xi, \Lambda\eta \rangle - 2\langle \bar{K}^*\eta, M\xi \rangle + \|\bar{K}\xi - \nu\|^2 + \|\bar{F}\eta\|^2 - 2\langle \bar{F}\eta, \nu \rangle - 2\langle \bar{G}\xi, \mu \rangle \\ &\geq \|\bar{G}\xi\|^2 + \|\bar{K}^*\eta + \mu\|^2 - 2(\beta - \lambda)\langle \xi, \bar{K}^*\eta \rangle \\ &\quad + 2\langle \bar{K}\xi - \nu, \Lambda\eta \rangle - 2\langle \bar{K}^*\eta + \mu, M\xi \rangle + \|\bar{K}\xi - \nu\|^2 + \|\bar{F}\eta\|^2. \end{aligned}$$

This we further estimate using Young's inequality as

$$\|T^*w - z\|^2 \geq (\|\bar{G}\xi\|^2 - \|M\xi\|^2) + (\|\bar{F}\eta\|^2 - \|\Lambda\eta\|^2) - 2(\beta - \lambda)\langle \xi, \bar{K}^*\eta \rangle.$$

Expanding the definitions of M and Λ and using $\bar{G} \geq_{V_{\bar{G}}} c_G^2 I$ and $\bar{F} \geq_{V_{\bar{F}}} c_F^2 I$, we get

$$\|T^*w - z\|^2 \geq (2c_G^2\beta - \beta^2)\|\xi\|^2 + (2c_F^2\lambda - \lambda^2)\|\eta\|^2 - 2(\beta - \lambda)\langle \xi, \bar{K}^*\eta \rangle.$$

Taking $\beta = \lambda$ and $0 < \lambda < 2 \min\{c_G^2, c_F^2\}$, we thus see that (A.1) holds with $c = c(c_F, c_G)$. \square

APPENDIX B SECOND-ORDER GENERALIZED DERIVATIVE FOR STATE CONSTRAINTS

In this appendix we give the the pointwise characterization of the graphical derivative of ∂F^* given by

$$\text{(B.1)} \quad \partial f^*(x, z) = \begin{cases} \{c\} & z > \alpha^{-1}(c - y^d(x)), \\ \{\alpha z + y^d(x)\} & z \leq \alpha^{-1}(c - y^d(x)), \end{cases}$$

required for the verification of (2.15). We begin with the (convexified) graphical derivative of (B.1), where from now on we suppress the dependence on $x \in \Omega$ for the sake of presentation.

Lemma B.1. For ∂f^* as in (B.1), we have

$$(B.2) \quad D(\partial f^*)(v|\zeta)(\Delta v) = \begin{cases} 0, & \alpha v > c - y^d, \zeta = c, \\ \alpha \Delta v, & \alpha v < c - y^d, \zeta = \alpha v + y^d, \\ 0, & \alpha v = c - y^d, \zeta = c, \Delta v \geq 0, \\ \alpha \Delta v, & \alpha v = c - y^d, \zeta = c, \Delta v < 0, \end{cases}$$

and

$$(B.3) \quad \overline{D(\partial f^*)(v|\zeta)(\Delta v)} = \begin{cases} 0, & \alpha v > c - y^d, \zeta = c, \\ \alpha \Delta v, & \alpha v < c - y^d, \zeta = \alpha v + y^d, \\ (-\infty, 0], & \alpha v = c - y^d, \zeta = c, \Delta v \geq 0, \\ \alpha \Delta v + (-\infty, 0], & \alpha v = c - y^d, \zeta = c, \Delta v < 0. \end{cases}$$

Proof. The claim is best seen by inspecting Figure 10; for completeness we however sketch the proof based on casewise inspection of (B.1).

- (i) If $\alpha v \neq c - y^d$, we have $\partial f^*(v) = \{(f^*)'(v)\}$ with $(f^*)'(v)$ differentiable. Computing these differentials yields the first two cases of (B.2), where the constraints on ζ come from $\zeta = (f^*)'(v)$.
- (ii) If $\alpha v = c - y^d$, we have $\partial f^*(v) = \{c\}$, so we need $\zeta = c$. Approaching v with $v^i = v + t^i \Delta v$ with $\Delta v \geq 0$ and $t^i \searrow 0$, we have

$$\limsup_{i \rightarrow \infty} \frac{\partial f^*(v^i) - \zeta}{t^i} = \limsup_{i \rightarrow \infty} \frac{c - c}{t^i} = \{0\}.$$

This gives the third case of (B.2).

- (iii) If $\Delta v < 0$, we obtain

$$\limsup_{i \rightarrow \infty} \frac{\partial f^*(v^i) - \zeta}{t^i} = \limsup_{i \rightarrow \infty} \frac{\alpha(v + t^i \Delta v) + y^d - c}{t^i} = \limsup_{i \rightarrow \infty} \frac{\alpha t^i \Delta v}{t^i} = \{\alpha \Delta v\}.$$

This gives the fourth case of (B.2).

Finally, the first two cases of the convexification (B.3) correspond directly to those of (B.2), while the last two cases come from taking the convex hull of the set

$$A := ([0, \infty) \times \{0\}) \cup \{(\Delta v, \alpha \Delta v) \mid \Delta v < 0\}$$

corresponding to the last two cases of (B.2), which is given by

$$\text{conv } A = ([0, \infty) \times (-\infty, 0]) \cup \{(\Delta v) \times (-\infty, \alpha \Delta v) \mid \Delta v < 0\}.$$

□

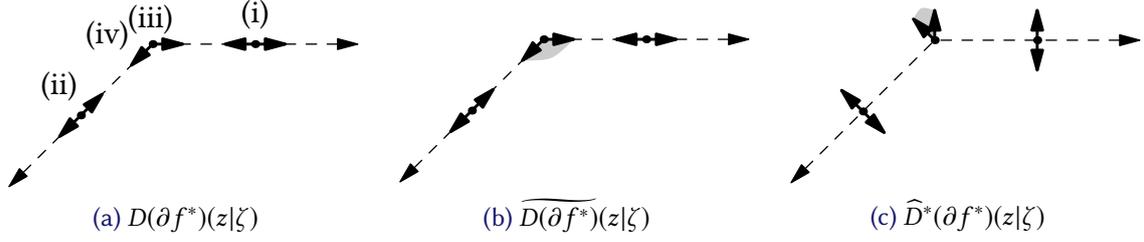


Figure 10: Illustration of the graphical derivative and Fréchet coderivative for ∂f^* as in (B.1). The dashed line is Graph ∂f . The dots indicate the base points (z, ζ) where the graphical derivative or coderivative is calculated, and the thick arrows and gray areas indicate the directions of $(\Delta z, \Delta \zeta)$ relative to the base point. The labels (i) etc. denote the corresponding case of (B.2).

Since f is proper, convex, and normal, so is f^* ; see, e.g., [17, Thm. 14.50] for the former. Furthermore, for almost every $x \in \Omega$, the functional $f^*(x, \cdot)$ is piecewise affine, and hence $\partial f^*(x, \cdot)$ is proto-differentiable; see [17, Prop. 13.9, Thm. 13.40]. We can thus apply [9, Cor. 2.7] to obtain the following pointwise characterization of the second-order generalized derivatives of the corresponding integral functional F^* .

Corollary B.2. *Let ∂f^* be as in (B.1), and*

$$\partial F^*(v) := \{ \eta \in L^2(\Omega) \mid \eta(x) \in \partial f^*(v(x)) \text{ for a.e. } x \in \Omega \}.$$

Suppose $\alpha v(x) \neq c - y^d(x)$ for a.e. $x \in \Omega$. Then

$$(B.4) \quad \widetilde{D}[\partial F^*](v|\eta)(\Delta v) = \begin{cases} T_v \Delta v + V_{\partial F^*}(v|\eta)^\circ, & \Delta v \in V_{\partial F^*}(v|\eta) \text{ and } \eta \in \partial F^*(v), \\ \emptyset, & \text{otherwise,} \end{cases}$$

and

$$(B.5) \quad \widehat{D}^*[\partial F^*](v|\eta)(\Delta \eta) = \begin{cases} T_v^* \Delta \eta + V_{\partial F^*}(v|\eta)^\circ, & -\Delta \eta \in V_{\partial F^*}(v|\eta) \text{ and } \eta \in \partial F^*(v), \\ \emptyset, & \text{otherwise,} \end{cases}$$

for the cone

$$V_{\partial F^*}(v|\eta) = L^2(\Omega),$$

its polar

$$V_{\partial F^*}(v|\eta)^\circ = \{0\} \subset L^2(\Omega),$$

and the linear operator T_v defined by

$$[T_v \Delta v](x) := t_v(x) \Delta v(x), \quad t_v(x) := \begin{cases} 0, & \alpha v(x) > c - y^d(x), \\ \alpha, & \alpha v(x) < c - y^d(x). \end{cases}$$

Remark B.3. We have excluded the case $\alpha v(x) = c - y^d(x)$ —which amounts to a strict complementarity assumption for v —because the calculations of [9] only apply when the polarity relationships in (B.4) and (B.5) regarding V hold. We have verified that the calculations could be improved to handle this non-strictly complementary case. However, since non-strictly complementary solutions can be replaced by strictly complementary solutions by infinitesimal modifications of v , we have decided for concision to simply exclude the case.

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A DATA STATEMENT FOR THE EPSRC

There is no additional data supporting this publication. All source codes used to generate the results in Section 4 are archived at <http://dx.doi.org/10.5281/zenodo.398822>.

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