UPDATE STRATEGIES FOR PERTURBED NONSMOOTH EQUATIONS

ROLAND GRIESSE, THOMAS GRUND, AND DANIEL WACHSMUTH

Abstract. Nonsmooth operator equations in function spaces are considered, which depend on perturbation parameters. The nonsmoothness arises from a projection onto an admissible interval. Lipschitz stability in L^∞ and Bouligand differentiability in L^p of the parameter-to-solution map are derived. An adjoint problem is introduced for which Lipschitz stability and Bouligand differentiability in L^∞ are obtained. Three different update strategies, which recover a perturbed from an unperturbed solution, are analyzed. They are based on Taylor expansions of the primal and adjoint variables, where the latter admits error estimates in L^∞. Numerical results are provided.

1. Introduction

In this work we consider nonsmooth operator equations of the form

$$u = \Pi_{[a,b]}(g(\theta) - G(\theta)u), \qquad (\mathcal{O}_\theta)$$

where the unknown $u \in L^2(D)$ is defined on some bounded domain $D \subset \mathbb{R}^N$, and $\Pi_{[a,b]}$ denotes the pointwise projection onto the set

$$U_{\text{ad}} = \{u \in L^2(D) : a(x) \le u(x) \le b(x) \text{ a.e. on } D\}.$$

Such nonsmooth equations appear as a reformulation of the variational inequality

$$\text{Find } u \in U_{\text{ad}} \text{ s.t. } \langle u + G(\theta)u - g(\theta), v - u\rangle \ge 0 \quad \text{for all } v \in U_{\text{ad}}. \qquad (\mathcal{VI}_\theta)$$

Applications of $(\mathcal{VI}_\theta)$ abound, and we mention in particular control-constrained optimal control problems.

Throughout, $G(\theta) : L^2(D) \to L^{2+\delta}(D)$ is a bounded and monotone linear operator with smoothing properties, such as a solution operator to a differential equation, and $g(\theta) \in L^\infty(D)$. Both G and g may depend nonlinearly and also in a nonsmooth way on a parameter θ in some normed linear space Θ. Under conditions made precise in Section 2, $(\mathcal{O}_\theta)$ has a unique solution $u[\theta]$ for any given θ. We are concerned here with the behavior of $u[\theta]$ under perturbations of the parameter. In particular, we establish the directional differentiability of the nonsmooth map $u[\cdot]$ with uniformly vanishing remainder, a concept called Bouligand differentiability (B-differentiability for short). We prove B-differentiability of $u[\cdot] : \Theta \to L^p(D)$ for $p \in [1, \infty)$, which is a sharp result and allows a Taylor expansion of $u[\cdot]$ around a reference parameter θ_0 with error estimates in $L^p(D)$.

Date: June 19, 2006.

2000 *Mathematics Subject Classification.* 46G05, 46T20, 49K20, 49K40, 58E35 .

Key words and phrases. variational inequality, nonsmooth equation, Bouligand derivative, optimal control, Taylor expansion.

Based on this Taylor expansion, we analyze three update strategies

$$\begin{aligned}\mathcal{C}_1(\theta) &:= u_0 + u'[\theta_0](\theta - \theta_0)\\ \mathcal{C}_2(\theta) &:= \Pi_{[a,b]}\big(u_0 + u'[\theta_0](\theta - \theta_0)\big)\\ \mathcal{C}_3(\theta) &:= \Pi_{[a,b]}\big(\phi_0 + \phi'[\theta_0](\theta - \theta_0)\big)\end{aligned}$$

which allow to recover approximations of the perturbed solution $u[\theta]$ from the reference solution $u_0 = u[\theta_0]$ and derivative information. Our main result is that $(\mathcal{C}_3)$, which involves a dual (adjoint) variable satisfying

$$\phi = g(\theta) - G(\theta)\Pi_{[a,b]}\phi,$$

allows error estimates in $L^\infty(D)$ while the other strategies do not. We therefore advocate to use update strategy $(\mathcal{C}_3)$.

As an important application, our setting accomodates linear–quadratic optimal control problems, where u is the control variable, $\mathcal{S}$ represents the control–to–state map associated to a linear elliptic or parabolic partial differential equation and $G = \mathcal{S}^\star\mathcal{S}$. Then $(\mathcal{O}_\theta)$ are necessary and sufficient optimality conditions. We shall elaborate on this case later on.

In the context of optimal control, B-differentiability of optimal solutions for semilinear problems has been investigated in [4, 6]. We provide here a simplified proof in the linear case.

The outline of the paper is as follows: In Section 2, we specify the problem setting and recall the concept of B-differentiability. In Sections 3 and 4, we prove the Lipschitz stability of the solution map $u[\cdot]$ into $L^\infty(D)$ and its B-differentiability into $L^p(D)$, $p < \infty$. Section 5 is devoted to the analysis of the adjoint problem, for which we prove B-differentiability into $L^\infty(D)$. In Section 6, we discuss the application of the semismooth Newton method to the original problem and the problem associated with the derivative. We analyze the three update strategies $(\mathcal{C}_1)$–$(\mathcal{C}_3)$ in Section 7 and prove error estimates. In Section 8 we apply our results to the optimal control of a linear elliptic partial differential equation and report on numerical results confirming the superiority of the adjoint-based strategy $(\mathcal{C}_3)$.

Throughout, c and L denote generic positive constants which take different values in different locations.

2. Problem Setting

Let us specify the standing assumptions for problem $(\mathcal{O}_\theta)$ taken to hold throughout the paper. We assume that $D \subset \mathbb{R}^N$ is a bounded and measurable domain, $N \geq 1$. By $L^p(D)$, $1 \leq p \leq \infty$, we denote the usual Sobolev spaces on D. We write $\langle u, v\rangle$ to denote the scalar product of two functions $u, v \in L^2(D)$. The norm in $L^p(D)$ is denoted by $\|\cdot\|_p$ or simply $\|\cdot\|$ in the case $p = 2$. The space of bounded linear operators from $L^p(D)$ to $L^q(D)$ is denoted by $\mathcal{L}(L^p(D), L^q(D))$ and its norm by $\|\cdot\|_{p\to q}$.

The lower and upper bounds $a, b : D \to [-\infty, \infty]$ for the admissible set are functions satisfying $a(x) \leq b(x)$ a.e. on D. We assume the existence of an admissible function $u_\infty \in L^\infty(D) \cap U_{\mathrm{ad}}$. Hence, the admissible set

$$U_{\mathrm{ad}} = \{u \in L^2(D) : a(x) \leq u(x) \leq b(x) \text{ a.e. on } D\}$$

is nonempty, convex and closed but not necessarily bounded in $L^2(D)$. $\Pi_{[a,b]}$ denotes the pointwise projection of a function on D onto U_{ad}, i.e.,

$$\Pi_{[a,b]}u = \max\{a, \min\{u, b\}\}$$

pointwise on D. Note that $\Pi_{[a,b]} : L^p(D) \to L^p(D)$ is Lipschitz continuous with Lipschitz constant 1 for all $p \in [1, \infty]$.

Finally, let Θ be the normed linear space of parameters with norm $\|\cdot\|$ and let $\theta_0 \in \Theta$ be a given reference parameter. We recall two definitions:

Definition 2.1. *A function $f : X \to Y$ is said to be locally Lipschitz continuous at $x_0 \in X$ if there exists an open neighborhood of x_0 and $L > 0$ such that*

$$\|f(x) - f(y)\|_Y \leq L\|x - y\|_X$$

holds for all x, y in the said neighborhood of x_0. In addition, f is said to be locally Lipschitz continuous if it is locally Lipschitz continuous at all $x_0 \in X$.

Definition 2.2. *A function $f : X \to Y$ between normed linear spaces X and Y is said to be B-differentiable at $x_0 \in X$ if there exists $\varepsilon > 0$ and a positively homogeneous operator $f'(x_0) : X \to Y$ such that*

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + r(x_0; x - x_0)$$

holds for all $x \in X$, where the remainder satisfies $\|r(x_0; x - x_0)\|_Y / \|x - x_0\|_X \to 0$ as $\|x - x_0\|_X \to 0$. In addition, f is said to be B-differentiable if it is B-differentiable at all $x_0 \in X$.

The B-derivative is also called a directional Fréchet derivative, see [1]. Recall that an operator $A : X \to Y$ is said to be positively homogeneous if $A(\lambda x) = \lambda A(x)$ holds for all $\lambda \geq 0$ and all $x \in X$.

Let us specify the standing assumptions for the function g:

(1) g is locally Lipschitz continuous from Θ to $L^\infty(D)$
(2) g is B-differentiable from Θ to $L^\infty(D)$.

Moreover, we assume that $G : \Theta \to \mathcal{L}(L^2(D), L^2(D))$ satisfies the following smoothing properties with some $\delta > 0$:

(3) $G(\theta)$ is bounded from $L^p(D)$ to $L^{p+\delta}(D)$ for all $p \in [2, \infty)$ and all $\theta \in \Theta$
(4) $G(\theta)$ is bounded from $L^p(D)$ to $L^\infty(D)$ for all $p > p_0$ and all $\theta \in \Theta$.

In addition, we demand that $G(\theta) : L^2(D) \to L^2(D)$ is monotone for all $\theta \in \Theta$:

$$\langle G(\theta)(u - v), u - v\rangle \geq 0 \quad \text{for all } u, v \in L^2(D),$$

and that

(5) G is locally Lipschitz continuous from Θ to $\mathcal{L}(L^2(D), L^2(D))$
(6) G is locally Lipschitz continuous from Θ to $\mathcal{L}(L^\infty(D), L^\infty(D))$.

Finally, we assume that

(7) G is B-differentiable from Θ to $\mathcal{L}(L^{p_0+\delta}(D), L^\infty(D))$.

Remark 2.3. *For control-constrained optimal control problems, $G = \mathcal{S}^\star\mathcal{S}$ where $\mathcal{S}$ is the solution operator of the differential equation involved. An example is presented in Section 8. If assumptions (1)–(2) and (5)–(7) hold only at a specified parameter θ_0 and (3)–(4) hold only in a neighborhood of θ_0, the subsequent analysis remains valid locally.*

In the sequel, we will need the B-derivative of a composite function.

Lemma 2.4. *Consider normed linear spaces X, Y, Z and mappings $F : Y \to Z$, $G : X \to Y$. Assume that the mapping G is B-differentiable at $\theta_0 \in X$ and that F is B-differentiable at $G(\theta_0)$. Furthermore assume that G is locally Lipschitz continuous at θ_0 and that $F'(G(\theta_0))$ is locally Lipschitz continuous at 0. Then the mapping $H : X \to Z$ defined by $H = F \circ G$ is B-differentiable at θ_0 with the derivative*

$$H'(\theta_0) = F'(G(\theta_0)) \circ G'(\theta_0).$$

Proof. Applying B-differentiability of F and G we obtain

$$\begin{aligned} F(G(\theta)) - F(G(\theta_0)) &= F'(G(\theta_0))\,(G(\theta) - G(\theta_0)) + r_F, \\ &= F'(G(\theta_0))\,(G'(\theta_0)(\theta - \theta_0) + r_G) + r_F \end{aligned} \tag{2.1}$$

with the remainder terms r_F and r_G satisfying

$$\frac{\|r_F\|_Z}{\|G(\theta) - G(\theta_0)\|_Y} \to 0 \text{ as } \|G(\theta) - G(\theta_0)\|_Y \to 0$$

and

$$\frac{\|r_G\|_Y}{\|\theta - \theta_0\|_X} \to 0 \text{ as } \|\theta - \theta_0\|_X \to 0$$

respectively. Now let us write

$$\begin{aligned} F'(G(\theta_0))\,(G'(\theta_0)(\theta - \theta_0) + r_G) &= F'(G(\theta_0))G'(\theta_0)(\theta - \theta_0) \\ &+ F'(G(\theta_0))\,(G'(\theta_0)(\theta - \theta_0) + r_G) - F'(G(\theta_0))G'(\theta_0)(\theta - \theta_0). \end{aligned} \tag{2.2}$$

Putting (2.1) and (2.2) together, we get an expression for the remainder term

$$\begin{aligned} &F(G(\theta)) - F(G(\theta_0)) - F'(G(\theta_0))G'(\theta_0)(\theta - \theta_0) \\ &\quad = r_F + F'(G(\theta_0))\,(G'(\theta_0)(\theta - \theta_0) + r_G) - F'(G(\theta_0))G'(\theta_0)(\theta - \theta_0) \end{aligned} \tag{2.3}$$

Note that $G'(\theta_0)(\theta - \theta_0)$ and r_G are small in the norm of Y whenever $\theta - \theta_0$ is small in the norm of X. Since $F'(G(\theta_0))$ is locally Lipschitz continuous at 0, we can estimate

$$\|F(G(\theta)) - F(G(\theta_0)) - F'(G(\theta_0))G'(\theta_0)(\theta - \theta_0)\|_Z \le \|r_F\|_Z + c_{F'}\|r_G\|_Y.$$

It remains to prove that the right-hand side, divided by $\|\theta - \theta_0\|_X$, vanishes for $\|\theta - \theta_0\|_X \to 0$. This is true for $\|r_G\|_Y$. So we have to investigate $\|r_F\|_Z$:

$$\frac{\|r_F\|_Z}{\|\theta - \theta_0\|_X} = \frac{\|r_F\|_Z}{\|G(\theta) - G(\theta_0)\|_Y}\frac{\|G(\theta) - G(\theta_0)\|_Y}{\|\theta - \theta_0\|_X} \le c_G \frac{\|r_F\|_Z}{\|G(\theta) - G(\theta_0)\|_Y}$$

by the local Lipschitz continuity of G at θ_0. For $\|\theta - \theta_0\|_X \to 0$ it follows $\|G(\theta) - G(\theta_0)\|_Y \to 0$. Hence, the right-hand side vanishes for $\|\theta - \theta_0\|_X \to 0$. And the proof is complete. ☐

Combining locally Lipschitz continuity and B-differentiability, we can prove a useful continuity result for the B-derivative.

Lemma 2.5. *Consider normed linear spaces X, Y and the mapping $G : X \to Y$. Let G be B-differentiable and locally Lipschitz continuous at $\theta_0 \in X$. Then it holds $\|G'(\theta_0)(\theta - \theta_0)\|_Y \to 0$ for $\|\theta - \theta_0\|_X \to 0$, i.e. the B-derivative is continuous in the origin with respect to the direction.*

Proof. By local Lipschitz continuity of G at θ_0, there exist $\epsilon > 0$ and $L > 0$ such that

$$\|G(\theta) - G(\theta_0)\|_Y \le L\|\theta - \theta_0\|_X \quad \forall \theta \in X : \|\theta - \theta_0\|_X < \epsilon.$$

Let us write

$$G(\theta) = G(\theta_0) + G'(\theta_0)(\theta - \theta_0) + r_G$$

with the remainder r_G satisfying

$$\frac{\|r_G\|_Y}{\|\theta - \theta_0\|_X} \to 0 \text{ as } \|\theta - \theta_0\|_X \to 0.$$

Then, we have

$$\|G'(\theta_0)(\theta - \theta_0)\|_Y \le L\|\theta - \theta_0\|_X + \|r_G\|_Y,$$

and it follows that the right-hand side tends to zero as $\|\theta - \theta_0\|_X \to 0$. □

3. Lipschitz Stability of the Solution Map

In this section we draw some simple conclusions from the assumptions made in Section 2. We recall that our problem $(\mathcal{O}_\theta)$ is equivalent to the following variational inequality:

$$\text{Find } u \in U_{\text{ad}} \text{ s.t. } \langle u + G(\theta)u - g(\theta), v - u\rangle \ge 0 \quad \text{for all } v \in U_{\text{ad}}. \qquad (\mathcal{VI}_\theta)$$

We begin by proving the Lipschitz stability of solutions $u[\theta]$ with respect to the $L^2(D)$ norm.

Lemma 3.1. *For any given $\theta \in \Theta$, $(\mathcal{O}_\theta)$ has a unique solution $u[\theta] \in L^2(D)$. The solution map $u[\cdot]$ is locally Lipschitz continuous from Θ to $L^2(D)$.*

Proof. Let $\theta \in \Theta$ be given and let $F(u) = u + G(\theta)u - g(\theta)$. By monotonicity of $G(\theta)$ it follows that $\langle F(u_1) - F(u_2), u_1 - u_2\rangle \ge \|u_1 - u_2\|^2$, hence F is strongly monotone. This implies the unique solvability of $(\mathcal{VI}_\theta)$ and thus of $(\mathcal{O}_\theta)$, see, for instance, [3].

If $\theta' \in \Theta$ is another parameter, then we obtain from $(\mathcal{VI}_\theta)$

$$\langle u + G(\theta)u - g(\theta), u' - u\rangle + \langle u' + G(\theta')u' - g(\theta'), u - u'\rangle \ge 0.$$

Inserting the term $G(\theta')u - G(\theta')u$ and using the monotonicity of $G(\theta')$, we obtain

$$\|u' - u\|^2 \le \left(\|G(\theta) - G(\theta')\|_{2\to2}\|u\| + \|g(\theta) - g(\theta')\|\right)\|u' - u\|.$$

This proves the local Lipschitz continuity of $u[\cdot]$ at any given parameter θ: Suppose that θ and θ' are in some ball of radius ε around θ_0 such that, by Assumption (5), $\|G(\theta) - G(\theta')\|_{2\to2} \le L\|\theta - \theta'\|$. If we set $u_0 = u[\theta_0]$, then $\|u - u_0\| \le L\|\theta - \theta_0\|\|u_0\| \le \varepsilon L\|u_0\|$ and thus $\|u\| \le \varepsilon L\|u_0\| + \|u_0\|$. Hence $\|u' - u\| \le L\|\theta - \theta'\|(1 + \varepsilon L)\|u_0\|$. □

By exploiting the smoothing properties of $G(\theta)$, this result can be strenghtened:

Proposition 3.2. *The solution map $u[\cdot]$ is locally Lipschitz continuous from Θ to $L^\infty(D)$.*

Proof. We use a bootstrapping argument to show that the solution $u[\theta]$ lies in $L^\infty(D)$. The fact that $g(\theta) \in L^\infty(D)$ and the smoothing property (3) of $G(\theta)$ yield $g(\theta) - G(\theta)u[\theta] \in L^{2+\delta}(D)$. By the properties of the projection, it follows from $(\mathcal{O}_\theta)$ that $u[\theta] \in L^{2+\delta}(D)$. Repeating this argument until $2 + n\delta > p_0$, we find $u[\theta] \in L^\infty(D)$ by Assumption (4).

We prove without loss of generality the local Lipschitz continuity of $u[\cdot]$ at the reference parameter θ_0. Let θ and θ' be any two parameters in a ball of radius ε around θ_0 such that $\|G(\theta) - G(\theta')\|_{\infty\to\infty} \le L\|\theta - \theta'\|$ and $\|g(\theta) - g(\theta')\|_\infty \le L\|\theta - \theta'\|$ hold. Using the Lipschitz continuity of the projection, we obtain

$$\begin{aligned}\|u - u'\|_{2+\delta} &\le \|g(\theta) - g(\theta')\|_{2+\delta} + \|G(\theta)u - G(\theta')u'\|_{2+\delta}\\ &\le c\,\|g(\theta) - g(\theta')\|_\infty + \|G(\theta)(u - u')\|_{2+\delta} + \|(G(\theta) - G(\theta'))u'\|_{2+\delta}\\ &\le c\,L\,\|\theta - \theta'\| + c\,\|u - u'\| + c\,L\,\|\theta - \theta'\|\|u'\|_\infty\end{aligned}$$

for some $c > 0$ and hence the local Lipschitz stability for $u[\cdot]$ in $L^{2+\delta}(D)$ follows. Repeating this argument until $2 + n\delta > p_0$, we obtain the local Lipschitz stability for $u[\cdot]$ in $L^\infty(D)$. □

4. B-Differentiability of the Solution Map

In this section we study the differentiability properties of the solution map $u[\cdot]$, which depend on the properties of the projection. We extend the results of [5]. Let us define a set $I[a, b, u_0]$ by

$$I[a,b,u_0] = \left\{ u \in L^2(D) : \begin{array}{lll} u(x) = 0 & & u_0(x) \notin [a(x), b(x)] \\ u(x) = 0 & \text{if} & u_0(x) = a(x) = b(x) \\ u(x) \geq 0 & & u_0(x) = a(x) \\ u(x) \leq 0 & & u_0(x) = b(x) \end{array} \right\}.$$

The pointwise projection on this set is denoted by $\Pi_{I[a,b,u_0]}$. By construction it holds for $u_0, u, a, b \in L^2(D)$, $a \leq b$

$$\begin{aligned} \Pi_{I[a,b,u_0]}(u) &= -\Pi_{I[-b,-a,-u_0]}(-u), \\ \Pi_{I[a,+\infty,u_0]}(u) &= \Pi_{I[0,+\infty,u_0-a]}(u), \\ \Pi_{I[a,b,u_0]}(u) &= \Pi_{I[a,+\infty,u_0]}\left(\Pi_{I[-\infty,b,u_0]}(u)\right). \end{aligned} \tag{4.1}$$

It turns out that $\Pi_{I[a,b,u_0]}$ is the B-derivative of the projection onto the admissible set $\Pi_{[a,b]}$. We start with the proof of B-differentiability of the projection on the cone of non-negative functions.

Theorem 4.1. *The projection $\Pi_{[0,+\infty]}$ is B-differentiable from $L^p(D)$ to $L^q(D)$ for $1 \leq q < p \leq \infty$. And it holds*

$$\Pi_{[0,+\infty]}(u) = \Pi_{[0,+\infty]}(u_0) + \Pi_{I[0,+\infty,u_0]}(u - u_0) + r_1 \tag{4.2a}$$

where

$$\frac{\|r_1\|_q}{\|u - u_0\|_p} \to 0 \text{ as } \|u - u_0\|_p \to 0. \tag{4.2b}$$

Remark 4.2. *The claim for the case $p = \infty$ was proven in* [5]. *A counterexample was given there, which shows that the projection is not B-differentiable from $L^\infty(D)$ to $L^\infty(D)$.*

Proof of Theorem 4.1. Clearly, the function $\Pi_{I[0,+\infty,u_0]}$ is positively homogeneous. Let us define the function r as the remainder term

$$r = \Pi_{[0,+\infty]}(u) - \Pi_{[0,+\infty]}(u_0) - \Pi_{I[0,+\infty,u_0]}(u - u_0). \tag{4.3}$$

A short calculation shows that

$$r(x) = \begin{cases} |u(x)| & \text{if } u(x)u_0(x) < 0 \\ 0 & \text{otherwise} \end{cases} \tag{4.4}$$

holds, see also the discussion in [5]. It implies the estimate $r(x) \leq |u(x) - u_0(x)|$. Now suppose that $1 \leq q < p \leq \infty$. It remains to prove

$$\frac{\|r\|_q}{\|u - u_0\|_p} \to 0 \text{ as } \|u - u_0\|_p \to 0. \tag{4.5}$$

We will argue by contradiction. Assume that (4.5) does not hold. Then there exists $\epsilon > 0$ such that for all $\delta > 0$ there is a function u_δ with $\|u_\delta - u_0\|_p < \delta$ and satisfying

$$\frac{\|r_\delta\|_q}{\|u_\delta - u_0\|_p} \geq \epsilon. \tag{4.6}$$

Here, r_δ is the remainder term defined as in (4.3). Let us choose a sequence $\{\delta_k\}$ with $\lim_{k\to\infty}\delta_k = 0$, $u_k = u_{\delta_k}$, and $r_k := r_{\delta_k}$. By Egoroff's Theorem, for each $\sigma > 0$ there exists a set $D_\sigma \subset D$ with $\text{meas}(D \setminus D_\sigma) < \sigma$ such that the convergence $u_k \to u_0$ is uniform on D_σ. It allows us to estimate

$$\begin{aligned}\|r_k\|_q &\le \left(\int_{D\setminus D_\sigma} |u_k(x) - u_0(x)|^q dx\right)^{1/q} + \left(\int_{D_\sigma} |r_k(x)|^q dx\right)^{1/q} \\ &\le \sigma^{\frac{1}{q}-\frac{1}{p}} \|u_k - u_0\|_p + \left(\int_{D_\sigma} |r_k(x)|^q dx\right)^{1/q}.\end{aligned}$$

Here, the second addend needs more investigation. Let us define a subset $D_{\sigma,k}$ of D_σ by

$$D_{\sigma,k} = \left\{ x \in D_\sigma : 0 < |u_0(x)| < \sup_{x'\in D_\sigma} |u_k(x') - u_0(x')| \right\}.$$

Then by construction it holds $r_k(x) = 0$ on $D_\sigma \setminus D_{\sigma,k}$, compare (4.4). Observe that $\text{meas}(D_{\sigma,k}) \to 0$ as $k \to \infty$ due to the uniform convergence of u_k to u_0 on D_σ. And we can proceed with

$$\begin{aligned}\|r_k\|_q &\le \sigma^{\frac{1}{q}-\frac{1}{p}} \|u_k - u_0\|_p + \left(\int_{D_\sigma} |r_k(x)|^q dx\right)^{1/q} \\ &= \sigma^{\frac{1}{q}-\frac{1}{p}} \|u_k - u_0\|_p + \left(\int_{D_{\sigma,k}} |r_k(x)|^q dx\right)^{1/q} \\ &\le \sigma^{\frac{1}{q}-\frac{1}{p}} \|u_k - u_0\|_p + \text{meas}(D_{\sigma,k})^{\frac{1}{q}-\frac{1}{p}} \|u_k - u_0\|_p,\end{aligned}$$

which is a contradiction to (4.6). □

Now, we calculate the B-derivative of $\Pi_{[a,b]}$ using the chain rule developed in Lemma 2.4.

Theorem 4.3. *The projection $\Pi_{[a,b]}$ is B-differentiable from $L^p(D)$ to $L^q(D)$ for $1 \le q < p \le \infty$. And it holds*

$$\Pi_{[a,b]}(u) = \Pi_{[a,b]}(u_0) + \Pi_{I[a,b,u_0]}(u - u_0) + r_1 \tag{4.7a}$$

where

$$\frac{\|r_1\|_q}{\|u - u_0\|_p} \to 0 \text{ as } \|u - u_0\|_p \to 0. \tag{4.7b}$$

Proof. The projection $\Pi_{[a,b]}$ can be written as a composition of two projections on the set of non-negative functions as

$$\Pi_{[a,b]}(u) = \Pi_{[0,+\infty]}\left(b - \Pi_{[0,+\infty]}(b - u) - a\right) + a.$$

The projection $\Pi_{[0,+\infty]}$ and its B-derivative $\Pi_{I[0,+\infty,u_0]}$ are Lipschitz continuous. Thus, the B-differentiability of $\Pi_{[a,b]}$ follows by Lemma 2.4.

The chain rule yields the derivative

$$\begin{aligned}\Pi'_{[a,b]}(u_0)(u - u_0) &= \Pi_{I[0,+\infty,b-\Pi_{[0,+\infty]}(b-u_0)-a]}\left(-\Pi_{I[0,+\infty,b-u_0]}(-(u - u_0))\right) \\ &= \Pi_{I[0,+\infty,b-\Pi_{[0,+\infty]}(b-u_0)-a]}\left(\Pi_{I[-\infty,b,u_0]}(u - u_0)\right) \\ &= \Pi_{I\left[a,+\infty,\Pi_{[-\infty,b]}(u_0)\right]}\left(\Pi_{I[-\infty,b,u_0]}(u - u_0)\right).\end{aligned}$$

Here, we used the properties (4.1) of the projection Π_I. It remains to prove that the right-hand side is equal to $\Pi_{I[a,b,u_0]}(u - u_0)$. To this end, let us introduce the following disjoint subsets of D:

$$D_1 := \{x \in D : u_0(x) \le b(x)\},$$
$$D_2 := \{x \in D : b(x) < u_0(x)\}.$$

Let us denote by χ_{D_i} the characteristic function of the set D_i. The projection Π_I is additive with respect to functions with disjoint support, i.e.

$$\Pi_{I[a,b,u_0]}(v) = \Pi_{I[a,b,u_0]}(\chi_{D_1} v) + \Pi_{I[a,b,u_0]}(\chi_{D_2} v)$$

holds for all a, b, u_0, v. Since $\Pi'_{[a,b]}(u_0)(u-u_0)$ is a composition of such projections, we can split

$$\Pi'_{[a,b]}(u_0)(u-u_0) = \Pi'_{[a,b]}(u_0)(\chi_{D_1}(u-u_0)) + \Pi'_{[a,b]}(u_0)(\chi_{D_2}(u-u_0)).$$

Furthermore, it holds $\Pi_{I[a,b,u_0]}(\chi_{D_i} v) = \Pi_{I[a,b,\chi_{D_i} u_0]}(\chi_{D_i} v)$. At first, we have $\chi_{D_1}\Pi_{[-\infty,b]}(\chi_{D_1} u_0) = \chi_{D_1} u_0$.

$$\begin{aligned}\Pi'_{[a,b]}(u_0)(\chi_{D_1}(u-u_0)) &= \Pi_{I\left[a,+\infty,\Pi_{[-\infty,b]}(u_0)\right]}\left(\Pi_{I[-\infty,b,u_0]}(\chi_{D_1}(u-u_0))\right)\\ &= \Pi_{I[a,+\infty,u_0]}\left(\Pi_{I[-\infty,b,u_0]}(\chi_{D_1}(u-u_0))\right)\\ &= \Pi_{I[a,b,u_0]}(\chi_{D_1}(u-u_0)).\end{aligned}$$

The last equality follows from the third property of Π_I in (4.1).

For the second set D_2, we have

$$\Pi_{I[-\infty,b,u_0]}(\chi_{D_2}(u-u_0)) = 0,$$

since $u_0(x)$ is not admissible for $x \in D_2$. For the same reason, we get also

$$\Pi_{I[a,b,u_0]}(\chi_{D_2}(u-u_0)) = 0,$$

which gives

$$\Pi'_{[a,b]}(u_0)(\chi_{D_2}(u-u_0)) = 0 = \Pi_{I[a,b,u_0]}(\chi_{D_2}(u-u_0)).$$

Consequently, we obtain

$$\begin{aligned}\Pi'_{[a,b]}(u_0)(u-u_0) &= \Pi'_{[a,b]}(u_0)(\chi_{D_1}(u-u_0)) + \Pi'_{[a,b]}(u_0)(\chi_{D_2}(u-u_0))\\ &= \Pi_{I[a,b,u_0]}(\chi_{D_1}(u-u_0)) + \Pi_{I[a,b,u_0]}(\chi_{D_2}(u-u_0))\\ &= \Pi_{I[a,b,u_0]}(u-u_0),\end{aligned}$$

and the claim is proven. □

Let us remark that the result of the last two Theorems is sharp with respect to the choice of function spaces:

Remark 4.4. *The projection is not B-differentiable from $L^p(D)$ to $L^p(D)$ for any p, as the following example shows. Take $a = 0$, $b = +\infty$, $D = (0,1)$. We choose $u_0(x) = -1$ and*

$$u_k(x) = \begin{cases} 1 & \text{if } x \in (0, 1/k) \\ -1 & \text{otherwise.} \end{cases}$$

In this case, the remainder term given by (4.4) is $r_{1,k} = (u_k - u_0)/2$. Therefore it holds

$$\frac{\|r_{1,k}\|_p}{\|u_k - u_0\|_p} = \frac{1}{2} \not\to 0 \text{ for } k \to \infty.$$

As a side result of the previous theorem, however, we get for $\alpha \in (-\infty, 1)$

$$\frac{\|r_{1,k}\|_p}{\|u_k - u_0\|_p^\alpha} \to 0 \text{ for } k \to \infty.$$

We are now in the position to prove B-differentiability of the solution mapping $u[\theta]$ of our non-smooth equation $(\mathcal{O}_\theta)$.

Theorem 4.5. *The solution mapping $u[\theta]$ of problem $(\mathcal{O}_\theta)$ is B-differentiable from Θ to $L^p(D)$, $2 \le p < \infty$. The Bouligand derivative of $u[\cdot]$ at θ_0 in direction θ, henceforth called $u'[\theta_0]\theta$, is the unique solution of the non-smooth equation*

$$u = \Pi_{I[a,b,\phi_0]}(g'(\theta_0)\theta - G(\theta_0)u - (G'(\theta_0)\theta)u_0) \qquad (\mathcal{O}'_{\theta_0;\theta})$$

where $u_0 = u[\theta_0]$ and $\phi_0 = g(\theta_0) - G(\theta_0)u_0$.

Proof. The problem $(\mathcal{O}'_{\theta_0;\theta})$ is equivalent to finding a solution $u \in I[a,b,\phi_0]$ of the variational inequality

$$\langle u + G(\theta_0)u + (G'(\theta_0)\theta)u_0 - g'(\theta_0)\theta,\, v - u\rangle \ge 0 \quad \forall v \in I[a,b,\phi_0].$$

By monotonicity of $G(\theta_0)$ this variational inequality is uniquely solvable, compare Lemma 3.1. Moreover, the projection $\Pi_{I[a,b,\phi_0]}$ is positively homogeneous. So the mapping $\theta \mapsto u'[\theta_0]\theta$ is positively homogeneous as well.

Now, let us take $\theta_1 \in \Theta$ and $u_1 := u[\theta_1]$. Let $p \in [2,\infty)$ be fixed. Further, let u^d be the solution of $(\mathcal{O}'_{\theta_0;\theta})$ for $\theta = \theta_1 - \theta_0$, i.e.

$$u^d = \Pi_{I[a,b,\phi_0]}(g'(\theta_0)(\theta_1-\theta_0) - G(\theta_0)u^d - G'(\theta_0)(\theta_1-\theta_0)u_0). \tag{4.8}$$

Let us investigate the difference $u_1 - u_0$. We obtain by B-differentiability of the projection from $L^{p+\delta}(D)$ to $L^p(D)$

$$\begin{aligned} u_1 - u_0 &= \Pi_{[a,b]}(g(\theta_1) - G(\theta_1)u_1) - \Pi_{[a,b]}(g(\theta_0) - G(\theta_0)u_0) \\ &= \Pi_{I[a,b,g(\theta_0)-G(\theta_0)u_0]}(g(\theta_1) - G(\theta_1)u_1 - g(\theta_0) + G(\theta_0)u_0) + r_1 \\ &= \Pi_{I[a,b,\phi_0]}(g(\theta_1) - G(\theta_1)u_1 - g(\theta_0) + G(\theta_0)u_0) + r_1. \end{aligned} \tag{4.9}$$

The remainder term r_1 satisfies

$$\frac{\|r_1\|_p}{\|g(\theta_1) - G(\theta_1)u_1 - g(\theta_0) + G(\theta_0)u_0\|_{p+\delta}} \to 0$$

as $\|g(\theta_1) - G(\theta_1)u_1 - g(\theta_0) + G(\theta_0)u_0\|_{p+\delta} \to 0$. Applying Lipschitz continuity of $u[\cdot]$, G, and g, we get

$$\begin{aligned} \|g(\theta_1) - G(\theta_1)u_1 - g(\theta_0) + G(\theta_0)u_0\|_{p+\delta} &\le c\,(\|\theta_1-\theta_0\| + \|u_1-u_0\|_p) \\ &\le c\,\|\theta_1-\theta_0\|. \end{aligned}$$

Hence, we find for the remainder term

$$\frac{\|r_1\|_p}{\|\theta_1-\theta_0\|} \to 0 \text{ as } \|\theta_1-\theta_0\| \to 0. \tag{4.10}$$

Let us rewrite (4.9) as

$$\begin{aligned} u_1 - u_0 - r_1 &= \Pi_{I[a,b,\phi_0]}\big(g(\theta_1) - g(\theta_0) - G(\theta_0)(u_1-u_0) - (G(\theta_1)-G(\theta_0))u_1\big) \\ &= \Pi_{I[a,b,\phi_0]}\big(g'(\theta_0)(\theta_1-\theta_0) + r_1^g - G(\theta_0)(u_1-u_0) \\ &\qquad - (G'(\theta_0)(\theta_1-\theta_0) + r_1^G)u_1\big) \\ &= \Pi_{I[a,b,\phi_0]}\big(g'(\theta_0)(\theta_1-\theta_0) - G(\theta_0)(u_1-u_0-r_1) \\ &\qquad - G'(\theta_0)(\theta_1-\theta_0)u_1 + r_1^g + r_1^G u_1 - G(\theta_0)r_1\big) \\ &= \Pi_{I[a,b,\phi_0]}\big(g'(\theta_0)(\theta_1-\theta_0) - G(\theta_0)(u_1-u_0-r_1) \\ &\qquad - G'(\theta_0)(\theta_1-\theta_0)u_1 + r_1^*\big) \end{aligned}$$

with a remainder term $r_1^* = r_1^g + r_1^G u_1 - G(\theta_0) r_1$ satisfying

$$\frac{\|r_1^*\|_p}{\|\theta_1 - \theta_0\|} \to 0 \text{ as } \|\theta_1 - \theta_0\| \to 0. \tag{4.11}$$

We can interpret $u^r := u_1 - u_0 - r_1$ as the solution of the non-smooth equation

$$u^r = \Pi_{I[a,b,\phi_0]}\big(g'(\theta_0)(\theta_1 - \theta_0) - G(\theta_0)u^r - G'(\theta_0)(\theta_1 - \theta_0)u_1 + r_1^*\big),$$

which is similar to (4.8) but perturbed by $-G'(\theta_0)(\theta_1 - \theta_0)(u_1 - u_0) + r_1^*$. Analogously as in Section 3, it can be shown that the solution mapping of that equation is Lipschitz continuous in the data, i.e., the map $r \ni L^p(D) \mapsto u \in L^p(D)$, where $u = \Pi_{I[a,b,\phi_0]}(-G(\theta_0)u + r)$, is Lipschitz continuous.

So we can estimate

$$\begin{aligned} \|u_1 - u_0 - r_1 - u^d\|_p = \|u^r - u^d\|_p &\le c\,\|G'(\theta_0)(\theta_1 - \theta_0)(u_1 - u_0)\|_p + c\,\|r_1^*\|_p \\ &\le c\,\|G'(\theta_0)(\theta_1 - \theta_0)(u_1 - u_0)\|_\infty + c\,\|r_1^*\|_p. \end{aligned} \tag{4.12}$$

Using the assumptions on G, we obtain by Lemma 2.5

$$\|G'(\theta_0)(\theta_1 - \theta_0)\|_{\infty\to\infty} \to 0 \text{ as } \|\theta_1 - \theta_0\| \to 0.$$

The mapping $\theta \mapsto u[\theta]$ is locally Lipschitz continuous from Θ to $L^\infty(D)$, see Proposition 3.2. Both properties imply

$$\frac{\|G'(\theta_0)(\theta_1 - \theta_0)(u_1 - u_0)\|_\infty}{\|\theta_1 - \theta_0\|} \to 0 \text{ as } \|\theta_1 - \theta_0\| \to 0. \tag{4.13}$$

Combining (4.11)–(4.13) yields in turn

$$\frac{\|u_1 - u_0 - r_1 - u^d\|_p}{\|\theta_1 - \theta_0\|} \to 0 \text{ as } \|\theta_1 - \theta_0\| \to 0. \tag{4.14}$$

Finally, we have

$$\|u_1 - (u_0 + u^d)\|_p \le \|u_1 - u_0 - r_1 - u^d\|_p + \|r_1\|_p$$

and consequently by (4.10) and (4.14)

$$\frac{\|u_1 - (u_0 + u^d)\|_p}{\|\theta_1 - \theta_0\|} \to 0 \text{ as } \|\theta_1 - \theta_0\| \to 0. \tag{4.15}$$

Hence, u^d is the Bouligand derivative of $u[\cdot]$ at θ_0 in the direction $\theta_1 - \theta_0$. □

Remark 4.6. *This result cannot be strengthened. The map $u[\theta]$ cannot be Bouligand from Θ to $L^\infty(D)$. To see this, consider the case $G = 0$. It trivially fulfills all requirements of Section 2. Then $u[\theta] = \Pi_{[a,b]}(g(\theta))$ holds, but the projection $\Pi_{[a,b]}$ is not B-differentiable from $L^\infty(D)$ to $L^\infty(D)$, see Remark 4.4.*

Lemma 4.7. *The B-derivative $u'[\theta_0]$ satisfies for all $\alpha \in (-\infty, 1)$*

$$\frac{\|u[\theta_0] + u'[\theta_0](\theta_1 - \theta_0) - u[\theta_1]\|_\infty}{\|\theta_1 - \theta_0\|^\alpha} \to 0 \text{ as } \|\theta_1 - \theta_0\| \to 0.$$

Proof. Here, we will follow the steps of the proof of the previous theorem. Let α be less than 1. The limiting factors in the proof are the remainder terms r_1 and r_1^*. We obtain for r_1 and r_1^* due to Remark 4.4 the property

$$\frac{\|r_1\|_\infty}{\|\theta_1 - \theta_0\|^\alpha} \to 0 \text{ and } \frac{\|r_1^*\|_\infty}{\|\theta_1 - \theta_0\|^\alpha} \to 0 \text{ as } \|\theta_1 - \theta_0\| \to 0.$$

Combining these with estimates (4.12)–(4.15) completes the proof. □

5. Properties of the Adjoint Problem

In this section we investigate an adjoint problem defined by

$$\phi = g(\theta) - G(\theta)\Pi_{[a,b]}(\phi). \tag{$\mathcal{D}_\theta$}$$

If we interpret ($\mathcal{O}_\theta$) as an optimal control problem with control constraints, see Section 8, then problem ($\mathcal{D}_\theta$) is an equation for the adjoint state. The primal and adjoint formulations are closely connected: If $u[\theta]$ is the unique solution of ($\mathcal{O}_\theta$) then

$$\phi := g(\theta) - G(\theta)u[\theta] \tag{5.1}$$

is a solution of ($\mathcal{D}_\theta$), which means that ($\mathcal{D}_\theta$) admits at least one solution. And if ϕ is a solution of the dual (adjoint) equation ($\mathcal{D}_\theta$) then the projection $u = \Pi_{[a,b]}(\phi[\theta])$ is the unique solution of the original problem ($\mathcal{O}_\theta$).

Now, let us briefly answer the question of uniqueness of adjoint solutions. If ϕ_1 and ϕ_2 are two solutions of ($\mathcal{D}_\theta$), then both $\Pi_{[a,b]}(\phi_1)$ and $\Pi_{[a,b]}(\phi_2)$ are solutions of ($\mathcal{O}_\theta$). By Lemma 3.1 this problem has a unique solution, hence $\Pi_{[a,b]}(\phi_1) = \Pi_{[a,b]}(\phi_2)$. For the difference $\phi_1 - \phi_2$ we have

$$\begin{aligned} \phi_1 - \phi_2 &= g(\theta) - G(\theta)\Pi_{[a,b]}(\phi_1) - \big(g(\theta) - G(\theta)\Pi_{[a,b]}(\phi_2)\big) \\ &= -G(\theta)(\Pi_{[a,b]}(\phi_1) - \Pi_{[a,b]}(\phi_2)) = 0, \end{aligned}$$

which implies in fact the unique solvability of ($\mathcal{D}_\theta$). In the following, we denote this unique solution by $\phi[\theta]$. An immediate conclusion of the considerations in Section 3 is the Lipschitz property of $\phi[\cdot]$.

Corollary 5.1. *The mapping $\phi[\theta]$ is locally Lipschitz from Θ to $L^\infty(D)$.*

Thus, we found that $\phi[\cdot]$ inherits Lipschitz continuity from $u[\cdot]$. However, in contrast to the primal map $u[\cdot]$, the adjoint map $\phi[\cdot]$ is B-differentiable into $L^\infty(D)$. The property which allows us to prove this result is that in ($\mathcal{D}_\theta$), the smoothing operator $G(\theta)$ is applied *after* the projection $\Pi_{[a,b]}$.

Theorem 5.2. *The mapping $\phi[\theta]$ is B-differentiable from Θ to $L^\infty(D)$. The B-derivative of $\phi[\cdot]$ at θ_0 in direction θ, henceforth called $\phi'[\theta_0]\theta$, is the solution of the non-smooth equation*

$$\phi = g'(\theta_0)\theta - G(\theta_0)\Pi_{I[a,b,\phi_0]}(\phi) - (G'(\theta_0)\theta)\Pi_{[a,b]}(\phi_0), \tag{5.2}$$

where $\phi_0 = \phi[\theta_0] = g(\theta_0) - G(\theta_0)u[\theta_0]$.

Proof. Due to the linearity of G, the B-derivative of $H(\theta) := G(\theta)u[\theta]$ at θ_0, in the direction of θ, can be written as

$$H'(\theta_0)\theta = G(\theta_0)u'[\theta_0]\theta + (G'(\theta_0)\theta)u_0,$$

where $u_0 = u[\theta_0]$. By Theorem 4.5, $u[\cdot]$ is B-differentiable from Θ to $L^{p_0+\delta}(D)$. Together with the B-differentiability of $G(\cdot)$ from Θ to $\mathcal{L}(L^{p_0+\delta}(D), L^\infty(D))$, the relationship $\phi[\theta] = g(\theta) - G(\theta)u[\theta]$ implies B-differentiability of $\phi[\cdot]$ from Θ to $L^\infty(D)$. The formula (5.2) is obtained by differentiating equation ($\mathcal{D}_\theta$). □

We now discuss the use of the derivative of $\phi[\theta]$ to obtain an update rule for the primal variable $u[\theta]$. Suppose that $u_0 = u[\theta_0]$ and $\phi_0 = \phi[\theta_0]$ are the solutions of the primal and dual problems at the reference parameter θ_0. We use the following construction as a first-order approximation of $u[\theta]$:

$$\tilde{u}[\theta_0, \theta - \theta_0] := \mathcal{C}_3(\theta) = \Pi_{[a,b]}\big(\phi_0 + \phi'[\theta_0](\theta - \theta_0)\big). \tag{5.3}$$

We can prove that the L^∞-norm of the remainder $u[\theta] - \tilde{u}[\theta_0, \theta - \theta_0]$, divided by $\|\theta - \theta_0\|$, vanishes as $\theta \to \theta_0$. This is a stronger result than can be obtained using merely the B-differentiability. There, the remainder $u[\theta] - u[\theta_0] - u'[\theta_0](\theta - \theta_0)$, divided by $\|\theta - \theta_0\|$, vanishes only in weaker L^p-norms. We refer to Section 7 for a comparison of this advanced update rule with the conventional rules $(\mathcal{C}_1)$ and $(\mathcal{C}_2)$.

Corollary 5.3. *Let* $\tilde{u}[\theta_0, \theta - \theta_0]$ *be given by* (5.3). *Then*

$$\frac{\|u[\theta] - \tilde{u}[\theta_0,\, \theta - \theta_0]\|_\infty}{\|\theta - \theta_0\|} \to 0 \text{ as } \theta \to \theta_0.$$

Proof. By construction, we have

$$u[\theta] - \tilde{u}[\theta_0,\, \theta - \theta_0] = \Pi_{[a,b]}(\phi[\theta]) - \Pi_{[a,b]}\big(\phi[\theta_0] + \phi'[\theta_0](\theta - \theta_0)\big).$$

The projection is Lipschitz from $L^\infty(D)$ to $L^\infty(D)$, hence we can estimate

$$\|u[\theta] - \tilde{u}[\theta_0,\, \theta - \theta_0]\|_\infty \le \|\phi[\theta] - \phi[\theta_0] - \phi'[\theta_0](\theta - \theta_0)\|_\infty.$$

We know already by Theorem 5.2 that $\phi[\theta]$ is B-differentiable at θ_0 from Θ to $L^\infty(D)$. Thus, it holds for $\|\theta - \theta_0\| \to 0$

$$\frac{\|\phi[\theta] - \phi[\theta_0] + \phi'[\theta_0](\theta - \theta_0)\|_\infty}{\|\theta - \theta_0\|} \to 0.$$

for $\theta - \theta_0 \to 0$. Consequently, we get the same behavior for the remainder $u[\theta] - \tilde{u}[\theta_0,\, \theta - \theta_0]$, which proves the claim. ☐

In the next section we discuss how the quantities $u[\theta_0]$, $\phi[\theta_0]$ and the required directional derivatives of these quantities can be computed. It turns out that the derivative $\phi'[\theta_0](\theta - \theta_0)$ is available at no additional cost when evaluating $u'[\theta_0](\theta - \theta_0)$, so the new update rule $(\mathcal{C}_3)$ incurs no additional cost.

On the other hand, it is also easily possible to obtain $\phi'[\theta_0](\theta - \theta_0)$ a posteriori from $u'[\theta_0](\theta - \theta_0)$. Once $u'[\theta_0](\theta - \theta_0)$ is known, $\phi'[\theta_0](\theta - \theta_0)$ can be computed from

$$\phi'[\theta_0](\theta - \theta_0) = g'(\theta_0)(\theta - \theta_0) - G(\theta_0)u'[\theta_0](\theta - \theta_0) - (G'(\theta_0)(\theta - \theta_0))u_0.$$

Hence the a posteriori computation of ϕ' involves only the application of G and G' and it is not necessary to solve any additional non-smooth equations. For optimal control problems the quantity $\phi'[\theta_0](\theta - \theta_0)$ is closely related to the adjoint state of the problem belonging to $u'[\theta_0](\theta - \theta_0)$.

6. Computation of the Solution and its Derivative

In this section we address the question how to solve problem $(\mathcal{O}_\theta)$ for the nominal parameter θ_0 and the derivative problem $(\mathcal{O}'_{\theta_0;\theta})$ algorithmically. In the recent past, generalized Newton methods in function spaces have been developed [2, 9], where a generalized set-valued derivative plays the role of the Fréchet derivative in the classical Newton method. The semismooth Newton concept can be applied here, in view of the smoothing properties of the operator $G(\theta_0)$.

Let us consider the following nonsmooth equation:

$$F(u) := -u + g(\theta_0) - G(\theta_0)u - \max\{0, g(\theta_0) - G(\theta_0)u - b\} \\ - \min\{0, g(\theta_0) - G(\theta_0)u - a\} = 0. \quad (6.1)$$

It is easy to check that (6.1) holds if and only if u solves $(\mathcal{O}_\theta)$ at θ_0.

Following [2], we infer that F is Newton differentiable as a map from $L^p(D)$ to $L^p(D)$ for any $p \in [2, \infty]$. The usual norm gap in the min and max functions is compensated by the smoothing properties of $G(\theta_0)$. The generalized derivative of F is set-valued, and we take

$$F'(u)\,\delta u = -G(\theta_0)\,\delta u - \delta u + \chi_{\mathcal{A}^+(u)} G(\theta_0)\,\delta u + \chi_{\mathcal{A}^-(u)} G(\theta_0)\,\delta u$$

as a particular choice. Here,

$$\begin{aligned} \mathcal{A}^+(u) &= \{x \in D : g(\theta_0) - G(\theta_0)u - b \geq 0\} \qquad & \mathcal{A}(u) &= \mathcal{A}^+(u) \cup \mathcal{A}^-(u) \\ \mathcal{A}^-(u) &= \{x \in D : g(\theta_0) - G(\theta_0)u - a \leq 0\} \qquad & \mathcal{I}(u) &= D \setminus \mathcal{A}(u) \end{aligned}$$

are the so-called active and inactive sets, and χ_A is the characteristic function of a measurable set A. A generalized Newton step $F'(u)\,\delta u = -F(u)$ can be computed by splitting the unknown δu into its parts supported on the active and inactive sets. Then a simple calculation shows that

$$\begin{aligned} \text{on } \mathcal{A}^+(u):&\quad \delta u_{|\mathcal{A}^+(u)} = b - u \\ \text{on } \mathcal{A}^-(u):&\quad \delta u_{|\mathcal{A}^-(u)} = a - u \\ \text{on } \mathcal{I}(u):&\quad (G(\theta_0) + I)\,\delta u_{|\mathcal{I}(u)} = g(\theta_0) - G(\theta_0)u - u - G(\theta_0)\,\delta u_{|\mathcal{A}(u)}. \end{aligned}$$

Lemma 6.1. *For given $u \in L^p(D)$ where $2 \leq p \leq \infty$, the generalized Newton step $F'(u)\,\delta u = -F(u)$ has a unique solution $\delta u \in L^p(D)$.*

Proof. We only need to verify that the step on the inactive set $\mathcal{I}(u)$ is indeed uniquely solvable. This follows from the strong monotonicity of $G(\theta_0) + I$, considered as an operator from $L^2(\mathcal{I}(u))$ to itself, compare the proof of Lemma 3.1. Hence the unique solution has an a priori regularity $\delta u \in L^2(D)$. The terms of lowest regularity on the right hand sides are the terms $-u$. Hence δu inherits the $L^p(D)$ regularity of u. Note that in case b or a are equal to $\pm\infty$ on a subset of D, this subset can not intersect $\mathcal{A}^+(u)$ or $\mathcal{A}^-(u)$ and thus the update δu lies in $L^\infty(D)$, provided that $u \in L^\infty(D)$, even if the bounds take on infinite values. ☐

By the previous lemma, the generalized Newton iteration is well-defined. For a convergence analysis, we refer to [2, 9]. For completeness, we state the semismooth Newton method for problem $(\mathcal{O}_\theta)$ below (Algorithm 1). Note that the dual variable

Algorithm 1 Semismooth Newton algorithm to compute u_0 and ϕ_0.

```
1:  Choose u_0 ∈ L^∞(D) and set n := 0
2:  Set φ_n := g(θ_0) − G(θ_0)u_n
3:  Set r_n := F(u_n) = φ_n − u_n − max{0, φ_n − b} − min{0, φ_n − a}
4:  while ‖r_n‖_∞ > tol do
5:      Set δu_{|A+(u_n)} := b − u_n on A+(u_n)
6:      Set δu_{|A−(u_n)} := a − u_n on A−(u_n)
7:      Solve (G(θ_0) + I) δu_{|I(u_n)} = φ_n − u_n − G(θ_0)δu_{|A(u_n)} on I(u_n)
8:      Set u_{n+1} := u_n + δu
9:      Set φ_{n+1} := g(θ_0) − G(θ_0)u_{n+1}
10:     Set r_{n+1} := F(u_{n+1}) = φ_{n+1} − u_{n+1} − max{0, φ_{n+1} − b} − min{0, φ_{n+1} − a}
11:     Set n := n + 1
12: end while
13: Set u_0 := u_n and φ_0 := φ_n
```

ϕ_0 appears naturally as an auxiliary quantity in the iteration, so it is available at no extra cost. With minor modifications, the same routine solves the derivative problems $(\mathcal{O}'_{\theta_0;\theta})$ for $u'[\theta_0](\theta)$ and (5.2) for $\phi'[\theta_0](\theta)$ simultaneously. Similarly as before, we consider the nonsmooth equation

$$\begin{aligned}\widehat{F}(\widehat{u}) := -\widehat{u} + g'(\theta_0)\theta - G(\theta_0)\widehat{u} - (G'(\theta_0)\theta)u_0 \\ - \max\{0, g'(\theta_0)\theta - G(\theta_0)\widehat{u} - (G'(\theta_0)\theta)u_0 - \widehat{b}\} \\ - \min\{0, g'(\theta_0)\theta - G(\theta_0)\widehat{u} - (G'(\theta_0)\theta)u_0 - \widehat{a}\} = 0. \quad (6.2)\end{aligned}$$

Hats indicate variables that are associated with derivatives. The new bounds $\widehat{a}$ and $\widehat{b}$ depend on the solution and adjoint solution u_0 and ϕ_0 of the reference problem, through the definition of $I[a, b, \phi_0]$ in Section 4:

$$\widehat{a} = \begin{cases} 0 & \text{where } u_0 = a \text{ or } \phi_0 \notin [a, b] \\ -\infty & \text{elsewhere} \end{cases} \qquad \widehat{b} = \begin{cases} 0 & \text{where } u_0 = b \text{ or } \phi_0 \notin [a, b] \\ \infty & \text{elsewhere.} \end{cases} \quad (6.3)$$

The active and inactive sets $\widehat{\mathcal{A}}^+(\widehat{u})$ etc. for the derivative problem are taken with respect to the bounds $\widehat{a}$ and $\widehat{b}$. For the ease of reference, we also state the semismooth Newton method for the derivative problems $\widehat{u} = u'[\theta_0]\theta$ and $\widehat{\phi} = \phi'[\theta_0]\theta$, see Algorithm 2. Note that these quantities satisfy

$$\begin{aligned} u'[\theta_0](\theta) &= \Pi_{I[a,b,\phi_0]}\phi'[\theta_0]\theta \\ \phi'[\theta_0](\theta) &= g'(\theta_0)\theta - G(\theta_0)u'[\theta_0]\theta - (G'(\theta_0)\theta)u_0, \end{aligned}$$

so each can be computed from the other.

Algorithm 2 Semismooth Newton algorithm to compute $u'[\theta_0]\theta$ and $\phi'[\theta_0]\theta$.

Choose $\widehat{u}_0 \in L^\infty(D)$ and set $n := 0$
Set the bounds $\widehat{a}$ and $\widehat{b}$ according to (6.3)
Set $\widehat{\phi}_n := g'(\theta_0)\theta - G(\theta_0)\widehat{u}_n - (G'(\theta_0)\theta)u_0$
Set $\widehat{r}_n := \widehat{F}(\widehat{u}_n) = \widehat{\phi}_n - \widehat{u}_n - \max\{0, \widehat{\phi}_n - \widehat{b}\} - \min\{0, \widehat{\phi}_n - \widehat{a}\}$
while $\|\widehat{r}_n\|_\infty > tol$ **do**
    Set $\delta u_{|\widehat{\mathcal{A}}^+(\widehat{u}_n)} := \widehat{b} - \widehat{u}_n$ on $\widehat{\mathcal{A}}^+(\widehat{u}_n)$
    Set $\delta u_{|\widehat{\mathcal{A}}^-(\widehat{u}_n)} := \widehat{a} - \widehat{u}_n$ on $\widehat{\mathcal{A}}^-(\widehat{u}_n)$
    Solve $(G(\theta_0) + I)\,\delta u_{|\widehat{\mathcal{I}}(\widehat{u}_n)} = \widehat{\phi}_n - \widehat{u}_n - G(\theta_0)\delta u_{|\widehat{\mathcal{A}}(\widehat{u}_n)}$ on $\widehat{\mathcal{I}}(\widehat{u}_n)$
    Set $\widehat{u}_{n+1} := \widehat{u}_n + \delta u$
    Set $\widehat{\phi}_{n+1} := g'(\theta_0)\theta - G(\theta_0)\widehat{u}_{n+1} - (G'(\theta_0)\theta)u_0$
    Set $\widehat{r}_{n+1} := \widehat{F}(\widehat{u}_{n+1}) = \widehat{\phi}_{n+1} - \widehat{u}_{n+1} - \max\{0, \widehat{\phi}_{n+1} - \widehat{b}\} - \min\{0, \widehat{\phi}_{n+1} - \widehat{a}\}$
    Set $n := n + 1$
end while
Set $u'[\theta_0]\theta := \widehat{u}_n$ and $\phi'[\theta_0]\theta := \widehat{\phi}_n$

7. Update Strategies and Error Estimates

In this section, we analyze three different update strategies for the solution of $(\mathcal{O}_\theta)$. Suppose that $\theta_0 \in \Theta$ is a given reference parameter, and that $u_0 = u[\theta_0]$ is the unique solution of $(\mathcal{O}_\theta)$ associated to this parameter. Our goal is to analyze strategies to approximate the perturbed solution $u[\theta]$ using the known reference solution u_0 and derivative information $u'[\theta_0]$ or $\phi'[\theta_0]$. Such strategies are particularly useful if they provide a reasonable approximation of the perturbed solution at lower numerical effort than is required by the repeated solution of the perturbed problem. We will see below that our strategies fulfill this condition to some degree. However, the full potential of these update schemes can only be revealed in nonlinear applications, where the solution of the derivative problem is significantly less expensive then the solution of the original problem. This deserves further investigation.

The three strategies we are considering are:

$$\mathcal{C}_1(\theta) := u_0 + u'[\theta_0](\theta - \theta_0) \tag{$\mathcal{C}_1$}$$

$$\mathcal{C}_2(\theta) := \Pi_{[a,b]}\big(u_0 + u'[\theta_0](\theta - \theta_0)\big) \tag{$\mathcal{C}_2$}$$

$$\mathcal{C}_3(\theta) := \Pi_{[a,b]}\big(\phi_0 + \phi'[\theta_0](\theta - \theta_0)\big). \tag{$\mathcal{C}_3$}$$

Apparently, all of the above yield approximations of $u[\theta]$ in the vicinity of θ_0. Our main result is:

Theorem 7.1. *The update strategies* ($\mathcal{C}_1$)–($\mathcal{C}_3$) *admit the following approximation properties:*

$$\frac{\|\mathcal{C}_1(\theta) - u[\theta]\|_p}{\|\theta - \theta_0\|} \to 0 \text{ as } \|\theta - \theta_0\| \to 0 \quad \text{for all } p \in [2, \infty) \tag{7.1}$$

$$\frac{\|\mathcal{C}_2(\theta) - u[\theta]\|_p}{\|\theta - \theta_0\|} \to 0 \text{ as } \|\theta - \theta_0\| \to 0 \quad \text{for all } p \in [2, \infty) \tag{7.2}$$

$$\frac{\|\mathcal{C}_3(\theta) - u[\theta]\|_p}{\|\theta - \theta_0\|} \to 0 \text{ as } \|\theta - \theta_0\| \to 0 \quad \text{for all } p \in [2, \infty]. \tag{7.3}$$

Strategies ($\mathcal{C}_2$) *and* ($\mathcal{C}_3$) *yield feasible approximations, i.e.,* $\mathcal{C}_i(\theta) \in U_{ad}$ *for* $i = 2, 3$. *The error term for* ($\mathcal{C}_2$) *is not larger than the term for* ($\mathcal{C}_1$).

Proof. Equation (7.1) follows immediately from the B-differentiability result for $u[\cdot]$, Theorem 4.5. For the second strategy, we have

$$\begin{aligned} \|\mathcal{C}_2(\theta) - u[\theta]\|_p &= \|\Pi_{[a,b]}\big(u_0 + u'[\theta_0](\theta - \theta_0)\big) - u[\theta]\|_p \\ &= \|\Pi_{[a,b]}\big(u_0 + u'[\theta_0](\theta - \theta_0)\big) - \Pi_{[a,b]}(u[\theta])\|_p \\ &\le \|u_0 + u'[\theta_0](\theta - \theta_0) - u[\theta]\|_p \\ &= \|\mathcal{C}_1(\theta) - u[\theta]\|_p, \end{aligned}$$

by the Lipschitz property of the projection, and the result follows as before. Finally, (7.3) was proven in Corollary 5.3. □

Corollary 7.2. *Strategies* ($\mathcal{C}_1$)–($\mathcal{C}_3$) *admit the following approximation property:*

$$\|\mathcal{C}_i(\theta) - u[\theta]\|_\infty \to 0 \text{ as } \|\theta - \theta_0\| \to 0, \quad \text{for } i = 1, 2, 3.$$

Proof. For strategy ($\mathcal{C}_1$), the claim was proven in Lemma 4.7 with $\alpha = 0$. For ($\mathcal{C}_2$), we estimate as in the proof of Theorem 7.1 and obtain

$$\begin{aligned} \|\mathcal{C}_2(\theta) - u[\theta]\|_\infty &= \|\Pi_{[a,b]}\big(u_0 + u'[\theta_0](\theta - \theta_0)\big) - u[\theta]\|_\infty \\ &= \|\Pi_{[a,b]}\big(u_0 + u'[\theta_0](\theta - \theta_0)\big) - \Pi_{[a,b]}(u[\theta])\|_\infty \\ &\le \|u_0 + u'[\theta_0](\theta - \theta_0) - u[\theta]\|_\infty \\ &= \|\mathcal{C}_1(\theta) - u[\theta]\|_\infty \end{aligned}$$

The claim for ($\mathcal{C}_3$) follows directly from (7.3). □

Remark 7.3. *All three update strategies come at practically the same numerical cost, namely the solution of one derivative problem. Note that both* $u'[\theta_0](\theta - \theta_0)$ *and* $\phi'[\theta_0](\theta - \theta_0)$ *are computed simultaneously by Algorithm 2. The additional projection in* ($\mathcal{C}_2$) *and* ($\mathcal{C}_3$) *is inexpensive. However, only* ($\mathcal{C}_2$) *and* ($\mathcal{C}_3$) *yield feasible approximations of the perturbed solution, and only* ($\mathcal{C}_3$) *has a remainder quotient* (7.3) *which vanishes uniformly on the domain* D. *Therefore, we advocate* *the use of the* $(\mathcal{C}_3)$ *strategy to compute corrections of the nominal solution* u_0 *in the presence of perturbations.*

In the next section, our findings are supported by numerical experiments.

8. Applications in Optimal Control

In this section, we present some applications of our results in the context of optimal control and report on numerical experiments. As an example, we treat a class of elliptic boundary control problems. The case of distributed control is simpler and therefore omitted. Numerical results are given which illustrate the performance of the update strategies analyzed in Section 7 and support the superiority of scheme $(\mathcal{C}_3)$.

8.1. **Boundary Control of an Elliptic Equation.** Let us suppose that $\Omega \subset \mathbb{R}^N$, $N \in \{2, 3\}$ is a bounded domain with Lipschitz continuous boundary Γ. We define the elliptic differential operator

$$\mathcal{A}y(x) = -\nabla \cdot (A(x)\nabla y(x))$$

where $A(x) = A(x)^\top \in \mathbb{R}^{N\times N}$ has entries in $L^\infty(\Omega)$ such that $\mathcal{A}$ is uniformly elliptic, i.e., $y^\top A(x)y \ge \varrho|y|^2$ holds uniformly in Ω with some $\varrho > 0$. We consider the elliptic partial differential equation with boundary control

$$\begin{aligned} \mathcal{A}y + c_0 y &= 0 \quad \text{on } \Omega \\ \frac{\partial y}{\partial n_A} + \alpha y &= u \quad \text{on } \Gamma \end{aligned} \tag{8.1}$$

where $c_0 \in L^\infty(\Omega)$, $c_0 \ge 0$, $\alpha \in L^\infty(\Gamma)$, $\alpha \ge 0$ such that $\|\alpha\|_{L^2(\Gamma)} + \|c_0\|_{L^2(\Omega)} > 0$. It is well known that (8.1) has a unique solution $y = \mathcal{S}u$ for every $u \in L^2(\Gamma)$. The adjoint operator $\mathcal{S}^\star$ maps a given f to the trace of the unique solution of

$$\begin{aligned} \mathcal{A}p + c_0 p &= f \quad \text{on } \Omega \\ \frac{\partial p}{\partial n_A} + \alpha p &= 0 \quad \text{on } \Gamma. \end{aligned} \tag{8.2}$$

Lemma 8.1 (see [8])**.** *The following are bounded linear operators:*

(1) $\mathcal{S} : L^2(\Gamma) \to L^p(\Omega)$ *for all* $p \in [2, \infty)$.
(2) $\mathcal{S}^\star : L^r(\Omega) \to L^\infty(\Gamma)$ *for all* $r \in (N/2, \infty]$.

We set $D = \Gamma$ and consider the elliptic boundary optimal control problem:

$$\text{Find } u \in U_{\text{ad}} \text{ which minimizes } \frac{1}{2}\|\mathcal{S}u - \theta\|^2_{L^2(\Omega)} + \frac{\gamma}{2}\|u\|^2 \tag{$\mathcal{E}_\theta$}$$

with $\gamma > 0$. For the parameter space, i.e., desired states, it is sufficient to choose $\Theta = L^2(\Omega)$ in order to satisfy the assumptions of Section 2. It is well known that for any given $\theta \in \Theta$, a necessary and sufficient optimality condition for $(\mathcal{E}_\theta)$ is

$$u = \Pi_{[a,b]}\big(-\frac{1}{\gamma}\mathcal{S}^\star(\mathcal{S}u - \theta)\big) \tag{8.3}$$

which fits our setting $(\mathcal{O}_\theta)$ with the choice

$$g(\theta) = \frac{1}{\gamma}\mathcal{S}^\star\theta \qquad\qquad G(\theta) = \frac{1}{\gamma}\mathcal{S}^\star\mathcal{S}.$$

Using Lemma 8.1, one readily verifies the conditions of Section 2. Note that

$$p[\theta] := \gamma\big(g(\theta) - G(\theta)u[\theta]\big) = -\mathcal{S}^\star(\mathcal{S}u[\theta] - \theta) = \gamma\phi[\theta]$$

is the usual adjoint state belonging to problem $(\mathcal{E}_\theta)$, which satisfies (8.2) with $f = -(\mathcal{S}u[\theta] - \theta)$.

8.2. **Numerical Results.** We will verify our analytical results by means of the following example: We consider as a specific choice of (8.1)

$$-\Delta y + y = 0 \quad \text{on } \Omega$$
$$\frac{\partial y}{\partial n} = u \quad \text{on } \Gamma$$

on $\Omega = (0,1) \times (0,1)$. As bounds, we have $a = -10$ and $b = 2$. The control cost factor is $\gamma = 0.1$ and the nominal parameter is $\theta_0(x_1, x_2) = x_1^2 + x_2^2$.

The discretization is carried out with piecewise linear and globally continuous finite elements on a grid with 3121 vertices and 5600 triangles, which is refined near the boundary of Ω, see Figure 8.1. We refer to the corresponding finite element space as $V_h \subset H^1(\Omega)$ and its restriction to the boundary is B_h. During the optimization loop (Algorithm 1), the discretized variables u and ϕ are taken as elements of B_h while the intermediate quantities $\mathcal{S}u$ as well as the adjoint state $-\mathcal{S}^\star(\mathcal{S}u - \theta)$, before restriction to the boundary, are taken in V_h. The computation of the active sets in the generalized Newton's method is done in a simple way, by determining those vertices of the given grid at which $\phi \ge b$ (or $\le a$) are satisfied.

As a caveat, we remark that our convergence results (7.1)–(7.3) for the update strategies $(\mathcal{C}_1)$ through $(\mathcal{C}_3)$ *cannot* be observed when *all* quantities are confined to any *fixed* grid. The reason is that in this entirely static finite-dimensional problem, all L^p-norms are equivalent and hence the numerical results show no difference in the approximation qualities of the different strategies.

In order to obtain more accurate results while keeping a fixed grid for the ease of implementation, we apply three postprocessing steps during the computation, see [7]. The exact procedure used is outlined below as Algorithm 3 and we explain the individual steps. Once the nominal solution $u_0 \in B_h$ is computed as described above (step 1:), the final $\widetilde{u_0} \notin B_h$ is obtained by a postprocessing step, i.e., by a pointwise exact projection of the piecewise linear function $\phi_0 \in B_h$ to the interval $[a, b]$, observing that the intersection of ϕ_0 with the bounds does not usually coincide with boundary vertices of the finite element grid (step 2:). The nominal solution is shown in Figure 8.1 and 8.2.

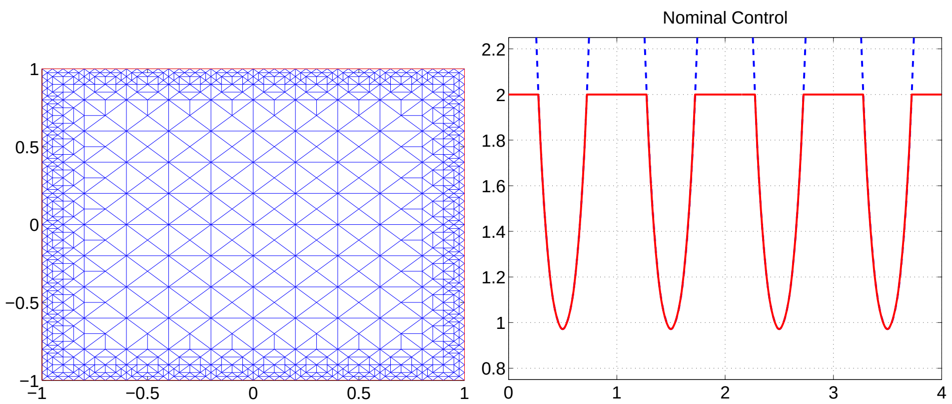

FIGURE 8.1. Mesh refined near the boundary (left). The right figure shows the nominal control u_0 (solid) and dual quantity ϕ_0 (dashed), unrolled from the lower left corner of the domain in counterclockwise direction.

A sequence of perturbed solutions $u[\theta_i]$ corresponding to parameters $\{\theta_i\}_{i=1}^n$ near θ_0 is computed in the same way (step 3:), i.e., with the simple active set strategy on the

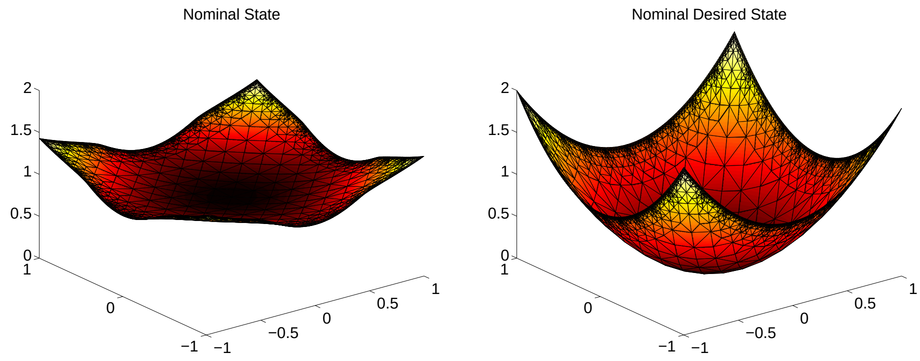

FIGURE 8.2. Nominal state $\mathcal{S}u_0$ (left) and nominal desired state θ_0 (right).

fixed grid and a postprocessing step. In the numerical experiments, every parameter θ_i is obtained by a random perturbation of the finite element coordinates of the desired state θ_0. This allows us to verify that the error estimates of Theorem 7.1 are indeed uniform with respect to the perturbation direction. The perturbations have specified norms, namely

$$\{\|\theta_i - \theta_0\|_2\}_{i=1}^n = \texttt{logspace(0,-2.5,}n\texttt{)} = 10^{-2.5 \cdot \frac{i-1}{n-1}}, \quad i = 1, \ldots, n,$$

where $n = 61$.

The derivative problems for $u'[\theta_0](\theta_i - \theta_0)$ and $\phi'[\theta_0](\theta_i - \theta_0)$ involve bounds which take only the values $\widehat{a}$, $\widehat{b} \in \{0, \pm\infty\}$ and depend on the nominal solution u_0 and adjoint quantity ϕ_0, see (6.3). These bounds are expressed in terms of constant values on the intervals of the boundary grid (step 4:), and again the simple active set strategy on the original grid is used to solve the derivative problems $u'[\theta_0](\theta - \theta_0)$ and $\phi'[\theta_0](\theta - \theta_0)$, see (step 5:), for the various perturbation directions $\theta_i - \theta_0$. Then two postprocessing steps follow. In the first (step 6:), $\widehat{a}$ and $\widehat{b}$ are determined from (6.3) more accurately than before, using the true intersection points of the nominal adjoint variable ϕ_0 with the original bounds a and b. In the second (step 7:), the derivative $u'[\theta_0](\theta - \theta_0)$ is postprocessed and set to the true projection of $\phi'[\theta_0](\theta - \theta_0)$ to the improved bounds $\widehat{a}$ and $\widehat{b}$. The exact procedure used to verify our theoretical results is outlined below as Algorithm 3.

Figure 8.3 (left) shows the behavior of the approximation errors

$$\|\text{approximation error}_i\|_p = \|\mathcal{C}_1(\theta_i - \theta_0) - u[\theta_i]\|_p,$$

while Figure 8.3 (right) shows the behavior of the error quotients

$$\frac{\|\text{approximation error}_i\|_p}{\|\text{size of perturbation}\|_{L^2(\Omega)}} = \frac{\|\mathcal{C}_i(\theta_i - \theta_0) - u[\theta_i]\|_p}{\|\theta_i - \theta_0\|_{L^2(\Omega)}}$$

as in (7.1)–(7.3). In the enumerator, the $L^p(\Gamma)$ norms for $p \in \{2, \infty\}$ are used. The scales in Figure 8.3 are doubly logarithmic and they are the same for each of the plots.

Using the procedure for the discretized problems outlined in Algorithm 3, we observe the following results:

(1) The approximation error for strategy $(\mathcal{C}_2)$ is indeed smaller (approximately by a factor of 2) than the error using strategy $(\mathcal{C}_1)$, see Figure 8.3 (first and second row), as expected from Theorem 7.1.

Algorithm 3 The discretized procedure used to obtain the numerical results.

1: Run Algorithm 1 on the fixed grid (Figure 8.1). Active sets are determined by boundary mesh points. The results u_0 and ϕ_0 are elements of B_h. The state $\mathcal{S}u_0$ and adjoint state $-\mathcal{S}^\star(\mathcal{S}u_0 - \theta_0)$ are elements of V_h.
2: Obtain an improved solution $\widetilde{u_0} = \Pi_{[a,b]}(\phi_0)$ by carrying out the exact projection (postprocessing) of the adjoint quantity $\phi_0 \in B_h$ to the bounds a and b. $\widetilde{u_0}$ is no longer in B_h.
3: Repeat steps 1: and 2: for a sequence of perturbations $\{\theta_i\}_{i=1}^n$ near θ_0 to obtain solutions u_i and, by postprocessing, improved solutions $\widetilde{u}_i$, $i = 1, \dots, n$. (This is to form the difference quotients (7.1)–(7.3) later.)
4: Compute the bounds $\widehat{a}$ and $\widehat{b}$ by (6.3) as functions which are constant (possibly $\pm\infty$) on the intervals of the boundary grid.
5: Run Algorithm 2 on the fixed grid (Figure 8.1), for the given sequence of perturbation directions $\theta_i - \theta_0$, $i = 1. \dots, n$. One obtains the derivatives $u'[\theta_0](\theta_i - \theta_0)$ and dual derivatives $\phi'[\theta_0](\theta_i - \theta_0)$, both elements of B_h.
6: Obtain an improved choice for the bounds $\widehat{a}$ and $\widehat{b}$ by determining the exact transition points in (6.3).
7: Obtain an improved derivative $\widetilde{u}'[\theta_0](\theta_i - \theta_0)$ by carrying out the exact projection (postprocessing) of the dual derivative $\phi'[\theta_0](\theta - \theta_0)$ to the improved bounds $\widehat{a}$ and $\widehat{b}$.

(2) The approximation error for strategy ($\mathcal{C}_3$) is in turn smaller (approximately by a factor of 7) than the error using strategy ($\mathcal{C}_2$), see Figure 8.3 (second and third row).
(3) As predicted by Theorem 7.1, the error quotient in the $L^\infty(\Gamma)$ norm does not tend to zero for strategies ($\mathcal{C}_1$) and ($\mathcal{C}_2$), see Figure 8.3 (top right and middle right).
(4) Theorem 7.1 predicts the approximation error and its quotient for strategy ($\mathcal{C}_3$) to tend to zero in particular in the $L^\infty(\Gamma)$-norm. In the experiments, we observe that the approximation error tends to a constant (approximately $6.3 \cdot 10^{-14}$, see Figure 8.3 (bottom left)). This is to be expected as we reach the discretization limit on the given grid.

To summarize, Theorem 7.1 is confirmed by the numerical results. The update strategy ($\mathcal{C}_3$), which involves the dual variable ϕ, performs significantly better than the strategies based on the primal variable u. We can also offer a geometric interpretation for this: The derivative $u'[\theta_0]$ of the primal variable u_0 is given by a projection and it is zero on the so-called strongly active sets, i.e., where $\phi_0 \notin [a, b]$, compare Theorem 4.5 and (6.3). Consequently, the primal-based strategies ($\mathcal{C}_1$) and ($\mathcal{C}_2$) can only predict a possible growth of the active sets from u_0 to $u[\theta]$, and not their shrinking. On the other hand, the derivative of the dual variable $\phi'[\theta_0]$ (Theorem 5.2) has a different structure and it can capture the change of active sets more accurately. Since $u'[\theta_0]$ and $\phi'[\theta_0]$ are available simultaneously, see Algorithm 2, we advocate the use of strategy ($\mathcal{C}_3$) to recover a perturbed from an unperturbed solution.

References

[1] F. Bonnans and A. Shapiro. *Perturbation Analysis of Optimization Problems*. Springer, Berlin, 2000.
[2] M. Hintermüller, K. Ito, and K. Kunisch. The primal-dual active set strategy as a semismooth Newton method. *SIAM Journal on Optimization*, 13(3):865–888, 2002.

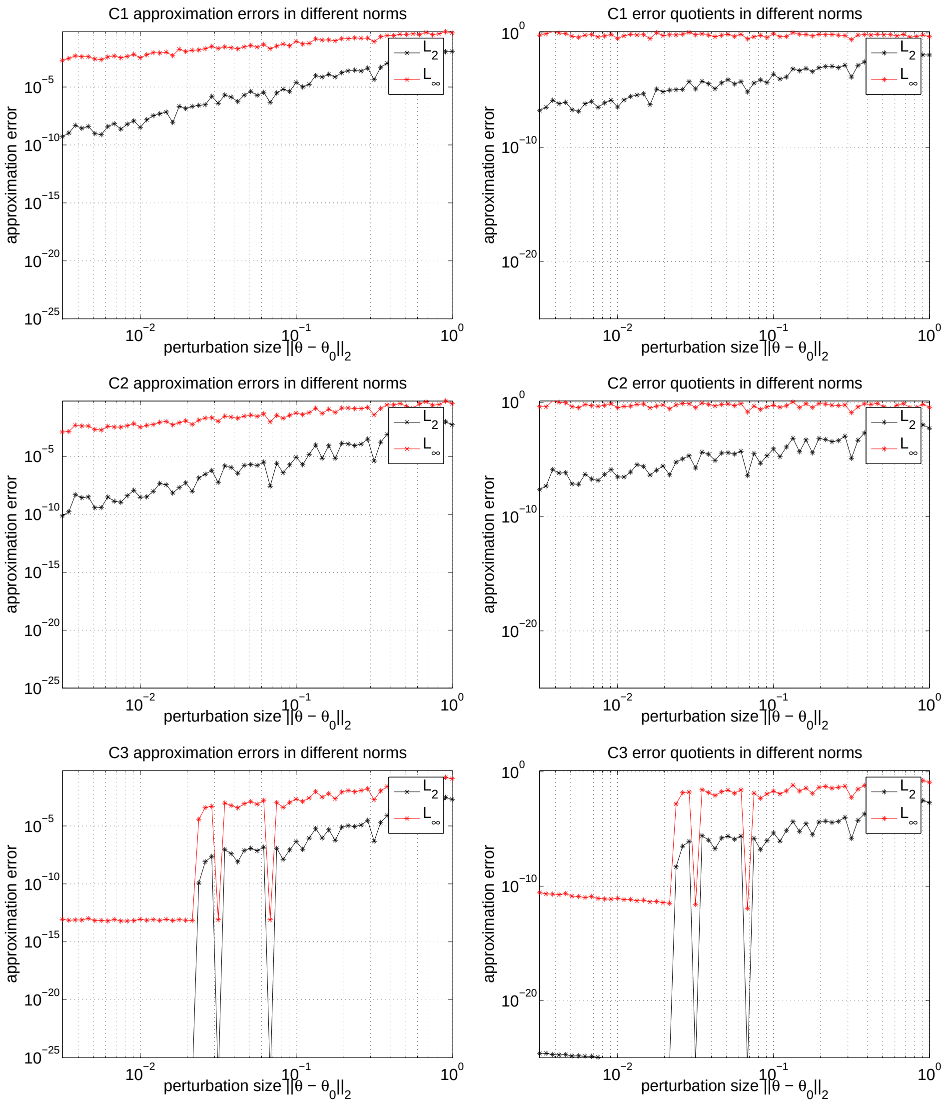

FIGURE 8.3. Approximation errors $\|\mathcal{C}_i(\theta) - u[\theta]\|_p$ (left) and error quotients (7.1)–(7.3) (right) in different $L^p(\Gamma)$ norms, plotted against the size of the perturbation $\|\theta_i - \theta_0\|_2$ in a double logarithmic scale. Top row refers to strategy $(\mathcal{C}_1)$, middle row to $(\mathcal{C}_2)$, bottom row to $(\mathcal{C}_3)$. In each plot, the upper line corresponds to $p = \infty$, the lower to $p = 2$.

[3] D. Kinderlehrer and G. Stampacchia. *An Introduction to Variational Inequalities and their Applications*. Academic Press, New York, 1980.

[4] K. Malanowski. Sensitivity analysis for parametric optimal control of semilinear parabolic equations. *Journal of Convex Analysis*, 9(2):543–561, 2002.

[5] K. Malanowski. Remarks on differentiability of metric projections onto cones of nonnegative functions. *Journal of Convex Analysis*, 10(1):285–294, 2003.

[6] K. Malanowski. Solutions differentiability of parametric optimal control for elliptic equations. In *System modeling and optimization, Proceedings of the IFIP TC7 Conference*, volume 130, pages 271–285. Kluwer, 2003.

[7] C. Meyer and A. Rösch. Superconvergence properties of optimal control problems. *SIAM Journal on Control and Optimization*, 43(3):970–985, 2004.

[8] F. Tröltzsch. *Optimale Steuerung partieller Differentialgleichungen*. Vieweg, Wiesbaden, 2005.
[9] M. Ulbrich. Semismooth Newton methods for operator equations in function spaces. *SIAM Journal on Optimization*, 13:805–842, 2003.

Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austrian Academy of Sciences, Altenbergerstrasse 69, A–4040 Linz, Austria

E-mail address: roland.griesse@oeaw.ac.at

URL: http://www.ricam.oeaw.ac.at/people/page/griesse

Institute of Mechatronics, Reichenhainer Strasse 88, D–09126 Chemnitz, Germany

E-mail address: thomas.grund@mail.com

Technische Universität Berlin, Sekretariat MA 4-5, Strasse des 17. Juni 136, D–10623 Berlin, Germany

E-mail address: wachsmut@math.tu-berlin.de

URL: http://www.math.tu-berlin.de/~wachsmut/