A SENSITIVITY-BASED EXTRAPOLATION TECHNIQUE FOR THE NUMERICAL SOLUTION OF STATE-CONSTRAINED OPTIMAL CONTROL PROBLEMS

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Abstract. Sensitivity analysis (with respect to the regularization parameter) of the solution of a class of regularized state constrained optimal control problems is performed. The theoretical results are then used to establish an extrapolation-based numerical scheme for solving the regularized problem for vanishing regularization parameter. In this context, the extrapolation technique provides excellent initializations along the sequence of reducing regularization parameters. Finally, the favorable numerical behavior of the new method is demonstrated and a comparison to classical continuation methods is provided.

Key words. extrapolation, mixed control-state constraints, PDE-constrained optimization, semismooth Newton algorithm, sensitivity, state constraints.

AMS subject classifications. 49M15, 49M37, 65K05, 90C33

1. Introduction. The numerical treatment of optimal control problems for partial differential equations (PDEs) with pointwise state inequality constraints is challenging due to the measure-valuedness of the Lagrange multiplier associated with the state constraints; see [1] for an analytical assessment. A typical instance of such a problem is given by

$$(P) \qquad \begin{cases} \text{minimize } J(u,y) := \frac{1}{2}\|y-y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)} \\ \text{over } (u,y) \in L^2(\Omega) \times H^1_0(\Omega) \cap H^2(\Omega) \\ \text{subject to } Ay = u \quad \text{in } \Omega,\ y = 0 \quad \text{on } \Gamma, \\ \qquad\qquad y_a \le y \le y_b \quad \text{a.e. in } \Omega, \end{cases}$$

where $\Omega \subset \mathbb{R}^N$ is a bounded and sufficiently regular domain, A is a second order elliptic partial differential operator, and y_d, α, y_a, y_b are given data which will be specified shortly.

In order to have a numerical technique at hand for solving (P) with stable iteration numbers as the mesh size of discretization is reduced, one can use an approach based on mixed control-state constraints as investigated in [10]. In fact, in order to overcome the measure-valuedness of the Lagrange multiplier associated with the pointwise inequality constraints in (P) one adds ϵu to y in the set of pointwise inequality constraints and then uses the result in [10] which yields an L^2-property of the Lagrange multiplier associated with the modified set of constraints. The regular multiplier therefore represents a smooth approximation of the measure-valued quantity. Using this

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technique, (P) becomes

$$(P_\epsilon) \qquad \begin{cases} \text{minimize } J(u,y) := \frac{1}{2}\|y-y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)} \\ \text{over } (u,y) \in L^2(\Omega)\times H^1_0(\Omega) \\ \text{subject to } Ay = u \quad \text{in } \Omega,\ y = 0 \quad \text{on } \Gamma, \\ \qquad\qquad y_a \le \epsilon u + y \le y_b \quad \text{a.e. in } \Omega, \end{cases}$$

Let $(\bar{y}_\epsilon, \bar{u}_\epsilon)$ denote the solution of (P_ϵ). For solving (P_ϵ) efficiently, in [3, 7] a semismooth Newton method (SSN) was proposed on a function space as well as on a discrete level. Besides the locally superlinear convergence, the mesh-independence of SSN for $\epsilon > 0$ was established.

In view of (P) one is interested in studying the behavior of the solution algorithm as $\epsilon \to 0$. For the numerics in the case of vanishing regularization parameter, however, in [3, 7] it turned out to be crucial to suitably tune ϵ as it tends to zero and, even more importantly, to initialize the algorithm for solving (P_ϵ) appropriately along the sequence. Ignoring these issues typically makes the numerical algorithm suffer from ill-conditioning which is usually reflected by large iteration numbers and reduced numerical solution accuracy.

In this note we focus on this latter point and propose an numerical approach based on an extrapolation technique in order to overcome the aforementioned problems. For this, we first need to study the quality of the dependence of $(\bar{y}_\epsilon, \bar{u}_\epsilon)$ on ϵ. For instance, under a strict complementarity assumption we prove differentiability of the solution to (P_ϵ) with respect to ϵ. Let $(\dot{y}_\epsilon, \dot{u}_\epsilon)$ denote the corresponding derivative. We then establish a system of sensitivity equations which characterize $(\dot{y}_\epsilon, \dot{u}_\epsilon)$ uniquely. Subsequently, the theoretical findings are employed in our numerical approach.

The remainder of the paper is organized as follows: In the rest of this section we detail the problem under investigation and settle the notation (subsection 1.1), and we recall some results on (P_ϵ) (subsection 1.2). The subsequent section 2 is devoted to Lipschitz and differentiability properties of the solution to (P_ϵ) with respect to $\epsilon > 0$. Then, in section 3 we define our semismooth Newton-type solver based on extrapolation in ϵ. We end this paper by a report on the numerical behavior including a comparison to a technique without extrapolation in section 4. It turns out that our new method compares favorably to classical continuation methods without extrapolation.

1.1. General assumptions and notation. In connection with our model problem (P), throughout this paper we assume that Ω is an open bounded domain in $\mathbb{R}^N$, $N \in \{2,3\}$, with sufficiently smooth boundary Γ. The upper and lower bounds $y_a, y_b \in \mathcal{C}(\overline{\Omega})$ on the state variable y satisfy $y_a(x) < y_b(x)$ for all $x \in \overline{\Omega}$ and guarantee that the feasible set of (P) is non-empty. Moreover, the desired state $y_d \in L^2(\Omega)$ and $\alpha > 0$ are assumed to be fixed. By u we denote the control variable. The second-order elliptic partial differential operator A is defined by

$$Ay(x) = -\sum_{i,j=1}^{N} D_i(a_{ij}(x)D_j y(x)),$$

where the coefficient functions $a_{ij} \in C^{0,1}(\bar{\Omega})$ satisfy the ellipticity condition

$$\sum_{i,j=1}^{N} a_{ij}(x)\xi_i\xi_j \ge \theta\|\xi\|^2_{\mathbb{R}^N} \quad \forall\ (\xi,x) \in \mathbb{R}^N \times \overline{\Omega}$$

for some constant $\theta > 0$. Furthermore, $A^\star$ stands for the associated adjoint operator. By G we denote the solution operator $G : L^2(\Omega) \to H^1_0(\Omega) \cap H^2(\Omega)$ that assigns to every $u \in L^2(\Omega)$ the

solution $y = y(u) \in H_0^1(\Omega) \cap H^2(\Omega)$ of the state equation

$$Ay = u \text{ in } \Omega, \quad y = 0 \text{ on } \Gamma.$$

We set $S = \imath_0 G$, where $\imath_0$ denotes the compact embedding operator from $H^1(\Omega)$ to $L^2(\Omega)$.

Using the above notation and assumptions, the regularized problem (P_ϵ) can be expressed as follows:

$$(P_\epsilon) \qquad \begin{cases} \text{minimize } f(u) := \frac{1}{2}\|Su - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)} & \text{over } u \in L^2(\Omega) \\ \text{subject to } y_a \le (S + \epsilon I)u \le y_b \quad \text{a.e. in } \Omega, \end{cases}$$

where I denotes the identity operator in $L^2(\Omega)$. In [9] the name Lavrentiev regularized problem was coined for (P_ϵ).

1.2. Standard results. For every $\epsilon > 0$ standard arguments guarantee the existence of a unique solution of (P_ϵ). Throughout the paper we denote this solution by $\bar{u}_\epsilon$ with associated state $\bar{y}_\epsilon$. As in [9], first order optimality of $(\bar{y}_\epsilon, \bar{u}_\epsilon)$ can be characterized as follows:

THEOREM 1.1 (First-order optimal conditions for (P_ϵ)). *The pair $(\bar{y}_\epsilon, \bar{u}_\epsilon)$ is optimal for (P_ϵ) if and only if there exist an adjoint state $p_\epsilon \in H_0^1(\Omega) \cap H^2(\Omega)$ and Lagrange multipliers $\mu_\epsilon^a, \mu_\epsilon^b \in L^2(\Omega)$ such that*

$$A\bar{y}_\epsilon = \bar{u}_\epsilon \quad \text{in } \Omega, \quad \bar{y}_\epsilon = 0 \quad \text{on } \Gamma, \tag{1.1}$$

$$A^\star p_\epsilon = \bar{y}_\epsilon - y_d + \mu_\epsilon^b - \mu_\epsilon^a \quad \text{in } \Omega, \quad p_\epsilon = 0 \quad \text{on } \Gamma, \tag{1.2}$$

$$p_\epsilon + \alpha\bar{u}_\epsilon - \epsilon(\mu_\epsilon^a - \mu_\epsilon^b) = 0, \tag{1.3}$$

$$\epsilon\bar{u}_\epsilon + \bar{y}_\epsilon \ge y_a, \quad \mu_\epsilon^a \ge 0, \quad (\mu_\epsilon^a, \epsilon\bar{u}_\epsilon + \bar{y}_\epsilon - y_a)_{L^2(\Omega)} = 0, \tag{1.4}$$

$$\epsilon\bar{u}_\epsilon + \bar{y}_\epsilon \le y_b, \quad \mu_\epsilon^b \ge 0, \quad (\mu_\epsilon^b, \epsilon\bar{u}_\epsilon + \bar{y}_\epsilon - y_b)_{L^2(\Omega)} = 0. \tag{1.5}$$

Using the maximum operator, the complementarity system (1.4)–(1.5) can be equivalently expressed as

$$\mu_\epsilon^a = \max(0, \mu_\epsilon^a - \mu_\epsilon^b + \gamma(y_a - \epsilon\bar{u}_\epsilon - \bar{y}_\epsilon)), \tag{1.6}$$

$$\mu_\epsilon^b = \max(0, \mu_\epsilon^b - \mu_\epsilon^a + \gamma(\epsilon\bar{u}_\epsilon + \bar{y}_\epsilon - y_b)), \tag{1.7}$$

with an arbitrarily fixed $\gamma > 0$, cf. [4, 11]. For the choice $\gamma := \alpha/\epsilon^2$ in (1.6)–(1.7) and using (1.3), a short computation yields

$$\mu_\epsilon^a = \max(0, \frac{1}{\epsilon}p_\epsilon + \frac{\alpha}{\epsilon^2}(y_a - \bar{y}_\epsilon)), \tag{1.8}$$

$$\mu_\epsilon^b = \max(0, -\frac{1}{\epsilon}p_\epsilon + \frac{\alpha}{\epsilon^2}(\bar{y}_\epsilon - y_b)). \tag{1.9}$$

This latter system will be useful in our subsequent analysis.

Finally, we mention that in [8, Theorem 3.3] the strong convergence in $L^2(\Omega)$ of $\bar{u}_\epsilon$ to $\bar{u}$, the optimal control of (P), is proved. Further, in [3] the Hölder continuity (with exponent $\frac{1}{2}$) of $\bar{u}_\epsilon$ with respect to $\epsilon > 0$ is established.

2. Regularity of solutions to (P_ϵ). As pointed out in the introduction, one of our main goals is to establish Lipschitz continuity and differentiability of the mapping $\epsilon \mapsto \bar{y}_\epsilon$. For this purpose the transformation of (P_ϵ) into an associated minimization problem with pure control constraints will be useful.

We start our investigation by considering the operator $(\epsilon I + S)$. It is well known that the linear operator $S = \imath_0 G : L^2(\Omega) \to L^2(\Omega)$ is positive-definite. For this reason, the equation

$$(\epsilon I + S)z = 0$$

admits only the trivial solution $z = 0$. Thus, by the Fredholm alternative, the compactness property of S ensures the existence of the inverse operator $(\epsilon I + S)^{-1}$. Setting $(\epsilon I + S)^{-1} v = u$, or equivalently $u = \frac{1}{\epsilon}(v - \imath_0 y(u))$ in (P_ϵ), we transform (P_ϵ) into the following optimal control problem with (pointwise) box constraints imposed on the new control variable v:

$$(P_\epsilon^v) \qquad \begin{cases} \text{minimize } f_\epsilon(v) := \frac{1}{2}\|S_\epsilon v - y_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2\epsilon^2}\|v - S_\epsilon v\|^2_{L^2(\Omega)} & \text{over } v \in L^2(\Omega) \\ \text{subject to } y_a \le v \le y_b \quad \text{a.e. in } \Omega. \end{cases}$$

Here we use $S_\epsilon = \imath_0 G_\epsilon$, where the operator G_ϵ assigns to each $v \in L^2(\Omega)$ the solution $y_\epsilon(v) = y_\epsilon \in H_0^1(\Omega) \cap H^2(\Omega)$ of the following elliptic equation:

$$(E_\epsilon) \qquad Ay_\epsilon + \frac{1}{\epsilon} y_\epsilon = \frac{1}{\epsilon} v \quad \text{in } \Omega, \quad y_\epsilon = 0 \quad \text{on } \Gamma.$$

In what follows, we denote the unique solution of (P_ϵ^v) by $\bar{v}_\epsilon$ with associated optimal state $\bar{y}_\epsilon$. Obviously, (P_ϵ^v) and (P_ϵ) are equivalent, i.e., $\bar{v}_\epsilon$ solves (P_ϵ^v) if and only if $\bar{u}_\epsilon = (\epsilon I + S)^{-1}\bar{v}_\epsilon$ is the optimal solution of (P_ϵ). We use the auxiliary problem (P_ϵ^v) in the following analysis.

The first derivative of f_ϵ at v in an arbitrary direction $s \in L^2(\Omega)$ is given by

$$f'_\epsilon(v)s = (S_\epsilon v - y_d + \frac{\alpha}{\epsilon^2}(S_\epsilon v - v), S_\epsilon s)_{L^2(\Omega)} + \frac{\alpha}{\epsilon^2}(v - S_\epsilon v, s)_{L^2(\Omega)}.$$

By standard arguments, this can be equivalently expressed as

$$f'_\epsilon(v) = q_\epsilon(v) - \frac{\alpha}{\epsilon^2} y_\epsilon(v) + \frac{\alpha}{\epsilon^2} v, \tag{2.1}$$

where the adjoint state $q_\epsilon = q_\epsilon(v) \in H_0^1(\Omega) \cap H^2(\Omega)$ is defined as the solution of the following adjoint equation:

$$A^\star q_\epsilon + \frac{1}{\epsilon} q_\epsilon = \frac{1}{\epsilon}(y_\epsilon(v) - y_d + \frac{\alpha}{\epsilon^2}(y_\epsilon(v) - v)) \quad \text{in } \Omega, \quad q_\epsilon = 0 \quad \text{on } \Gamma. \tag{2.2}$$

2.1. Lipschitz continuity. Next we establish a Lipschitz property of y_ϵ and various other quantities. Since one might by interested in (P_ϵ) independently of (P), we reduce the regularity requirements on, e.g., Ω, as we do not assume to have $H^2(\Omega)$-regularity of the states and adjoints pertinent to (P_ϵ).

For this purpose, let $\mathcal{D} = (\epsilon_l, \epsilon_u) \subset \mathbb{R}_{++}$ with $0 < \epsilon_l < \epsilon_u$.

LEMMA 2.1. *There exists a positive real number $c_s(\epsilon_l)$ such that*

$$\|y_{\epsilon_1}(v) - y_{\epsilon_2}(v)\|_{H_0^1(\Omega)} \le c_s(\epsilon_l)\|v\|_{L^2(\Omega)}|\epsilon_1 - \epsilon_2|$$

for all $v \in L^2(\Omega)$ *and* $\epsilon_i \in \mathcal{D}$, $i = 1, 2$.

Proof. We note that standard elliptic regularity estimates yield a constant $c > 0$ independent of ϵ and v such that

$$\|y_\epsilon(v)\|_{H_0^1(\Omega)} \leq c\|\frac{1}{\epsilon}v\|_{L^2(\Omega)} \tag{2.3}$$

for all $v \in L^2(\Omega)$ and $\epsilon \in \mathcal{D}$. Now, let $\epsilon_i \in \mathcal{D}$, $i = 1, 2$, and $v \in L^2(\Omega)$. By definition, for $i = 1, 2$ the states $y_{\epsilon_i}(v) = y_{\epsilon_i}$ satisfy

$$Ay_{\epsilon_i} + \frac{1}{\epsilon_i}y_{\epsilon_i} = \frac{1}{\epsilon_i}v \quad \text{in } \Omega, \quad y_{\epsilon_i} = 0 \quad \text{on } \Gamma.$$

From this we infer

$$A(y_{\epsilon_1} - y_{\epsilon_2}) + \frac{1}{\epsilon_1}(y_{\epsilon_1} - y_{\epsilon_2}) = (\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2})(v - y_{\epsilon_2}) \quad \text{in } \Omega, \quad y_{\epsilon_1} - y_{\epsilon_2} = 0 \quad \text{on } \Gamma,$$

and hence due to (2.3)

$$\begin{aligned}
\|y_{\epsilon_1}(v) - y_{\epsilon_2}(v)\|_{H_0^1(\Omega)} &\leq |\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2}|\, c\, \|v - y_{\epsilon_2}(v)\|_{L^2(\Omega)} \\
&\leq |\epsilon_1 - \epsilon_2|\frac{c}{{\epsilon_l}^2}(\|v\|_{L^2(\Omega)} + \|y_{\epsilon_2}(v)\|_{L^2(\Omega)}) \\
&\leq |\epsilon_1 - \epsilon_2|\frac{c}{\epsilon_l^2}(1 + \frac{c}{\epsilon_l})\|v\|_{L^2(\Omega)}.
\end{aligned}$$

Setting $c_s(\epsilon_l) := \frac{c}{\epsilon_l^2}(1 + \frac{c}{\epsilon_l})$ yields the assertion. □

We proceed by proving the Lipschitz continuity of the adjoint states q_ϵ.

LEMMA 2.2. *There exists a positive real number* $c_q(\mathcal{D})$ *such that*

$$\|q_{\epsilon_1}(v) - q_{\epsilon_2}(v)\|_{H_0^1(\Omega)} \leq c_q(\mathcal{D})(\|v\|_{L^2(\Omega)} + 1)|\epsilon_1 - \epsilon_2|,$$

for all $v \in L^2(\Omega)$ *and* $\epsilon_1, \epsilon_2 \in \mathcal{D}$.

Proof. An argument analogous to the one in the proof of Lemma 2.1 implies that there exists a constant $c(\mathcal{D}) > 0$ independent of ϵ and v such that

$$\|q_\epsilon(v)\|_{H_0^1(\Omega)} \leq c(\mathcal{D})(\|v\|_{L^2(\Omega)} + 1) \tag{2.4}$$

for all $\epsilon \in \mathcal{D}$ and $v \in L^2(\Omega)$. Let $\epsilon_1, \epsilon_2 \in \mathcal{D}$. By definition $q_{\epsilon_1}(v) = q_{\epsilon_1}$ and $q_{\epsilon_2}(v) = q_{\epsilon_2}$ solve, for $i = 1, 2$,

$$A^\star q_{\epsilon_i} + \frac{1}{\epsilon_i}q_{\epsilon_i} = \frac{1}{\epsilon_i}(y_{\epsilon_i}(v) - y_d + \frac{\alpha}{\epsilon_i^2}(y_{\epsilon_i}(v) - v)) \quad \text{in } \Omega, \quad q_{\epsilon_i} = 0 \quad \text{on } \Gamma.$$

Hence, the difference $q_{\epsilon_1} - q_{\epsilon_2}$ satisfies

$$A^\star(q_{\epsilon_1} - q_{\epsilon_2}) + \frac{1}{\epsilon_1}(q_{\epsilon_1} - q_{\epsilon_2}) = r \quad \text{in } \Omega, \quad q_{\epsilon_1} - q_{\epsilon_2} = 0 \text{ on } \Gamma,$$

where

$$r = \frac{1}{\epsilon_1}(y_{\epsilon_1}(v) - y_{\epsilon_2}(v)) + (\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2})(y_{\epsilon_2}(v) - y_d) + \frac{\alpha}{\epsilon_1^3}(y_{\epsilon_1}(v) - y_{\epsilon_2}(v)) + (\frac{\alpha}{\epsilon_1^3} - \frac{\alpha}{\epsilon_2^3})(y_{\epsilon_2}(v) - v) + (\frac{1}{\epsilon_2} - \frac{1}{\epsilon_1})q_{\epsilon_2}.$$

Since $|\epsilon_2^3 - \epsilon_1^3| = |(\epsilon_2^2 + \epsilon_1^2 + \epsilon_2\epsilon_1)(\epsilon_2 - \epsilon_1)| \leq 3\epsilon_u^2|\epsilon_2 - \epsilon_1|$, Lemma 2.1 and (2.4) yield a constant $c_q(\mathcal{D}) > 0$ independent of ϵ_1, ϵ_2 such that

$$\|q_{\epsilon_1}(v) - q_{\epsilon_2}(v)\|_{H_0^1(\Omega)} \leq \|r\|_{L^2(\Omega)} \leq c_q(\mathcal{D})|\epsilon_1 - \epsilon_2|(\|v\|_{L^2(\Omega)} + 1),$$

which ends the proof. □

For arguing the Lipschitz continuity of the controls, we require uniform positive definiteness of f_ϵ'', which we establish next.

LEMMA 2.3. *There exists a positive real number $\delta(\mathcal{D})$ such that for all $\epsilon \in \mathcal{D}$, we have*

$$f_\epsilon''(v)s^2 \geq \delta(\mathcal{D})\|s\|_{L^2(\Omega)}^2 \quad \forall v, s \in L^2(\Omega). \tag{2.5}$$

Proof. Let $v \in L^2(\Omega)$ and $\epsilon \in \mathcal{D}$ be arbitrarily fixed. Then, it holds by definition that $f_\epsilon(v) = f((S + \epsilon I)^{-1}v)$. Hence, for an arbitrary direction $s \in L^2(\Omega)$, the chain rule implies

$$\begin{aligned} f_\epsilon''(v)s^2 &= f''((S+\epsilon I)^{-1}v)((S+\epsilon I)^{-1}s)^2 \\ &= (S(S+\epsilon I)^{-1}s, S(S+\epsilon I)^{-1}s)_{L^2(\Omega)} + \alpha((S+\epsilon I)^{-1}s, (S+\epsilon I)^{-1}s)_{L^2(\Omega)} \\ &\geq \alpha((S+\epsilon I)^{-1}s, (S+\epsilon I)^{-1}s)_{L^2(\Omega)} \\ &= \alpha\|(S+\epsilon I)^{-1}s\|_{L^2(\Omega)}^2 \\ &\geq \frac{\alpha}{\|S+\epsilon I\|_{L^2,L^2}^2}\|s\|_{L^2(\Omega)}^2 \\ &\geq \frac{\alpha}{(\|S\|_{L^2,L^2} + \epsilon_u)^2}\|s\|_{L^2(\Omega)}^2. \end{aligned}$$

Defining $\delta(\mathcal{D}) := \alpha/(\|S\|_{L^2,L^2} + \epsilon_u)^2$, the lemma is verified. □

THEOREM 2.1. *The mapping $\mathbf{v} : \mathcal{D} \to L^2(\Omega)$, $\epsilon \mapsto \bar{v}_\epsilon$, is Lipschitz-continuous.*

Proof. Suppose that $\epsilon_1, \epsilon_2 \in \mathcal{D}$. By definition $\mathbf{v}(\epsilon_1) = \bar{v}_{\epsilon_1}$ and $\mathbf{v}(\epsilon_2) = \bar{v}_{\epsilon_2}$ solve $(P_{\epsilon_1}^v)$ and $(P_{\epsilon_2}^v)$, respectively. Hence, first order optimality yields

$$\begin{aligned} f_{\epsilon_1}'(\bar{v}_{\epsilon_1})(v - \bar{v}_{\epsilon_1}) \geq 0 \quad \forall v \in V_{ad}, \\ f_{\epsilon_2}'(\bar{v}_{\epsilon_2})(v - \bar{v}_{\epsilon_2}) \geq 0 \quad \forall v \in V_{ad}, \end{aligned}$$

where $V_{ad} = \{v \in L^2(\Omega) \mid y_a \leq v \leq y_b\}$. Since $\bar{v}_{\epsilon_1}$ and $\bar{v}_{\epsilon_2}$ are feasible, i.e., $\bar{v}_{\epsilon_1}, \bar{v}_{\epsilon_2} \in V_{ad}$, the inequalities above imply

$$(f_{\epsilon_1}'(\bar{v}_{\epsilon_1}) - f_{\epsilon_2}'(\bar{v}_{\epsilon_2}))(\bar{v}_{\epsilon_2} - \bar{v}_{\epsilon_1}) \geq 0, \tag{2.6}$$

which is equivalent to

$$(f_{\epsilon_1}'(\bar{v}_{\epsilon_1}) - f_{\epsilon_1}'(\bar{v}_{\epsilon_2}) + f_{\epsilon_1}'(\bar{v}_{\epsilon_2}) - f_{\epsilon_2}'(\bar{v}_{\epsilon_2}))(\bar{v}_{\epsilon_2} - \bar{v}_{\epsilon_1}) \geq 0. \tag{2.7}$$

Since f'_{ϵ_1} is Fréchet-differentiable, there exists $\tilde{v} \in L^2(\Omega)$ such that

$$(f'_{\epsilon_1}(\bar{v}_{\epsilon_1}) - f'_{\epsilon_1}(\bar{v}_{\epsilon_2}))(\bar{v}_{\epsilon_2} - \bar{v}_{\epsilon_1}) = -f''_{\epsilon_1}(\tilde{v})(\bar{v}_{\epsilon_2} - \bar{v}_{\epsilon_1})^2.$$

Then (2.7) yields

$$(f'_{\epsilon_1}(\bar{v}_{\epsilon_2}) - f'_{\epsilon_2}(\bar{v}_{\epsilon_2}))(\bar{v}_{\epsilon_2} - \bar{v}_{\epsilon_1}) \geq f''_{\epsilon_1}(\tilde{v})(\bar{v}_{\epsilon_2} - \bar{v}_{\epsilon_1})^2 \tag{2.8}$$

and further

$$\begin{gathered}\big(\|q_{\epsilon_1}(\bar{v}_{\epsilon_2}) - q_{\epsilon_2}(\bar{v}_{\epsilon_2})\|_{L^2(\Omega)} + \tfrac{\alpha}{\epsilon_1^2}\|y_{\epsilon_1}(\bar{v}_{\epsilon_2}) - y_{\epsilon_2}(\bar{v}_{\epsilon_2})\|_{L^2(\Omega)} + \\ \tfrac{\alpha}{\epsilon_1^2\epsilon_2^2}|\epsilon_1 - \epsilon_2| \cdot |\epsilon_1 + \epsilon_2|(\|y_{\epsilon_2}(\bar{v}_{\epsilon_2})\|_{L^2(\Omega)} + \|\bar{v}_{\epsilon_2}\|_{L^2(\Omega)})\big)\|\bar{v}_{\epsilon_2} - \bar{v}_{\epsilon_1}\|_{L^2(\Omega)} \geq f''_{\epsilon_1}(\tilde{v})(\bar{v}_{\epsilon_2} - \bar{v}_{\epsilon_1})^2,\end{gathered}$$

where we used (2.1). Due to Lemma 2.1, Lemma 2.2 and Lemma 2.3, there exists a constant $c(\mathcal{D}) > 0$ independent of ϵ_1, ϵ_2 such that

$$c(\mathcal{D})|\epsilon_2 - \epsilon_1|(\|\bar{v}_{\epsilon_2}\|_{L^2(\Omega)} + 1) \geq \|\bar{v}_{\epsilon_2} - \bar{v}_{\epsilon_1}\|_{L^2(\Omega)}. \tag{2.9}$$

Notice that the operator $\mathbf{v}(\cdot)$ is uniformly bounded in $L^\infty(\Omega)$, as $\bar{v}_\epsilon \in V_{ad}$ for all $\epsilon \in \mathbb{R}_{++}$. This together with (2.9) proves the assertion. □

We have the following immediate corollaries establishing the Lipschitz continuity of $\bar{y}_\epsilon$ and $\bar{u}_\epsilon$.

COROLLARY 2.1. *The mapping $\epsilon \mapsto \bar{y}_\epsilon$ is Lipschitz-continuous from $\mathcal{D}$ to $H_0^1(\Omega)$.*

Proof. Theorem 2.1 and Lemma 2.1 guarantee the existence of a constant $c(\mathcal{D}) > 0$ independent of $\epsilon_1, \epsilon_2 \in \mathcal{D}$ such that

$$\|\bar{y}_{\epsilon_1} - \bar{y}_{\epsilon_2}\|_{H_0^1(\Omega)} \leq \|y_{\epsilon_1}(\bar{v}_{\epsilon_1}) - y_{\epsilon_2}(\bar{v}_{\epsilon_1})\|_{H_0^1(\Omega)} + \|y_{\epsilon_2}(\bar{v}_{\epsilon_1} - \bar{v}_{\epsilon_2})\|_{H_0^1(\Omega)} \leq c(\mathcal{D})|\epsilon_1 - \epsilon_2|,$$

for all $\epsilon_1, \epsilon_2 \in \mathcal{D}$. □

COROLLARY 2.2. *The mapping $\epsilon \mapsto \bar{u}_\epsilon$ is Lipschitz-continuous from $\mathcal{D}$ to $L^2(\Omega)$.*

Proof. The assertion is immediate since, by construction, $\bar{u}_\epsilon = \frac{1}{\epsilon}(\bar{v}_\epsilon - \bar{y}_\epsilon)$ for all $\epsilon > 0$. □

Clearly, the corollaries 2.1 and 2.2 further imply the following result.

COROLLARY 2.3. *The mapping $\epsilon \mapsto p_\epsilon$ is Lipschitz-continuous from $\mathcal{D}$ to $H_0^1(\Omega)$.*

Proof. Utilizing (1.3) in (1.2) and exploiting the Lipschitz continuity of $\bar{u}_\epsilon$ and $\bar{y}_\epsilon$, respectively, yields the assertion. □

2.2. Parameter sensitivity. We define the functions $g_a, g_b : \mathcal{D} \to L^2(\Omega)$ by

$$g_a(\epsilon) = \frac{1}{\epsilon}p_\epsilon - \frac{\alpha}{\epsilon^2}\bar{y}_\epsilon + \frac{\alpha}{\epsilon^2}y_a, \tag{2.10}$$

$$g_b(\epsilon) = -\frac{1}{\epsilon}p_\epsilon + \frac{\alpha}{\epsilon^2}\bar{y}_\epsilon - \frac{\alpha}{\epsilon^2}y_b, \tag{2.11}$$

Suppose that $\epsilon \in \mathcal{D}$ is arbitrarily fixed. Then the Lipschitz-continuity of the mapping $\epsilon \mapsto (\bar{u}_\epsilon, \bar{y}_\epsilon, p_\epsilon)$ from $\mathcal{D}$ to $L^2(\Omega) \times H_0^1(\Omega) \times H_0^1(\Omega)$ ensures the existence of a weak accumulation point $(\dot{u}_\epsilon, \dot{y}_\epsilon, \dot{p}_\epsilon) \in L^2(\Omega) \times H_0^1(\Omega) \times H_0^1(\Omega)$ of

$$\left(\frac{\bar{u}_{\epsilon_n} - \bar{u}_\epsilon}{\epsilon_n - \epsilon}, \frac{\bar{y}_{\epsilon_n} - \bar{y}_\epsilon}{\epsilon_n - \epsilon}, \frac{p_{\epsilon_n} - p_\epsilon}{\epsilon_n - \epsilon}\right) \tag{2.12}$$

as $\epsilon_n \to \epsilon \in \mathcal{D}$ for $n \to \infty$. Further,

$$\begin{aligned}\frac{1}{\epsilon_n - \epsilon}(g_a(\epsilon_n) - g_a(\epsilon)) &= \frac{1}{\epsilon_n - \epsilon}(\frac{1}{\epsilon_n}p_{\epsilon_n} - \frac{\alpha}{\epsilon_n^2}\bar{y}_{\epsilon_n} + \frac{\alpha}{\epsilon_n^2}y_a - \frac{1}{\epsilon}p_\epsilon + \frac{\alpha}{\epsilon^2}\bar{y}_\epsilon - \frac{\alpha}{\epsilon^2}y_a)\\ &= \frac{1}{\epsilon_n - \epsilon}(\frac{1}{\epsilon}(p_{\epsilon_n} - p_\epsilon) - (\frac{1}{\epsilon} - \frac{1}{\epsilon_n})p_{\epsilon_n} + (\frac{\alpha}{\epsilon^2} - \frac{\alpha}{\epsilon_n^2})\bar{y}_{\epsilon_n}\\ &\qquad -\frac{\alpha}{\epsilon^2}(\bar{y}_{\epsilon_n} - \bar{y}_\epsilon) - (\frac{\alpha}{\epsilon^2} - \frac{\alpha}{\epsilon_n^2})y_a)\\ &= \frac{1}{\epsilon}\frac{p_{\epsilon_n} - p_\epsilon}{\epsilon_n - \epsilon} - \frac{1}{\epsilon\epsilon_n}p_{\epsilon_n} + \frac{\alpha(\epsilon_n + \epsilon)}{\epsilon^2\epsilon_n^2}\bar{y}_{\epsilon_n} - \frac{\alpha}{\epsilon^2}\frac{\bar{y}_{\epsilon_n} - \bar{y}_\epsilon}{\epsilon_n - \epsilon} - \frac{\alpha(\epsilon_n + \epsilon)}{\epsilon^2\epsilon_n^2}y_a\end{aligned}$$

has a weak accumulation

$$\dot{g_a}(\epsilon) = \frac{1}{\epsilon}\dot{p}_\epsilon - \frac{1}{\epsilon^2}p_\epsilon + \frac{2\alpha}{\epsilon^3}\bar{y}_\epsilon - \frac{\alpha}{\epsilon^2}\dot{y}_\epsilon - \frac{2\alpha}{\epsilon^3}y_a$$

in $H_0^1(\Omega)$ as $\epsilon_n \to \epsilon$ for $n \to \infty$. Analogously, there exists a weak accumulation point of $\frac{1}{\epsilon_n - \epsilon}(g_b(\epsilon_n) - g_b(\epsilon))$, which is given by

$$\dot{g_b}(\epsilon) = -\frac{1}{\epsilon}\dot{p}_\epsilon + \frac{1}{\epsilon^2}p_\epsilon - \frac{2\alpha}{\epsilon^3}\bar{y}_\epsilon + \frac{\alpha}{\epsilon^2}\dot{y}_\epsilon + \frac{2\alpha}{\epsilon^3}y_b.$$

By the compact embedding $H_0^1(\Omega) \subset L^2(\Omega)$ the accumulation points $\dot{g_a}(\epsilon)$ and $\dot{g_b}(\epsilon)$ are strong in $L^2(\Omega)$.

Without any further assumption, in general there is a need to distinguish between *upper* and *lower* accumulation points depending on whether $\epsilon_n \downarrow \epsilon$ or $\epsilon_n \uparrow \epsilon$, respectively. See [6] for a similar observation in a related context. However, under some type of strict complementarity condition this distinction is not required as all limits over ϵ_n-sequences yield a unique accumulation point. This motivates the following assumption.

ASSUMPTION 2.1. *We assume that the solution of* (P_ϵ) *satisfies the* strict complementarity condition

$$\text{(SC)} \qquad \begin{array}{lcl}\text{meas}\{x \in \Omega \mid g_a(\epsilon)(x) = \ p_\epsilon(x) - \frac{\alpha}{\epsilon}\bar{y}_\epsilon(x) + \frac{\alpha}{\epsilon}y_a(x) \quad = \ 0 \ a.e.\} &=& 0,\\ \text{meas}\{x \in \Omega \mid g_b(\epsilon)(x) = -p_\epsilon(x) + \frac{\alpha}{\epsilon}\bar{y}_\epsilon(x) - \frac{\alpha}{\epsilon}y_b(x) \quad = \ 0 \ a.e.\} &=& 0.\end{array}$$

Notice that by (1.8)–(1.9) the Lagrange multipliers for (P_ϵ) are given by

$$\begin{aligned}\mu_\epsilon^a &= \max(0, \frac{1}{\epsilon}p_\epsilon + \frac{\alpha}{\epsilon^2}(y_a - \bar{y}_\epsilon)) = g_a^+(\epsilon),\\ \mu_\epsilon^b &= \max(0, -\frac{1}{\epsilon}p_\epsilon + \frac{\alpha}{\epsilon^2}(\bar{y}_\epsilon - y_b)) = g_b^+(\epsilon),\end{aligned}$$

where $g_a^+ = \max(0, g_a)$ and analogously for g_b^+. Hence, using (1.3), the condition (SC) requires that

$$\text{meas}\{x \in \Omega : \mu_\epsilon^a(x) + \gamma(y_a - \epsilon\bar{u}_\epsilon - \bar{y}_\epsilon)(x) = 0\} = 0,$$

or equivalently, that the set where the max-operation is non-differentiable is of measure zero; analogously for the set involving μ_ϵ^b and y_b.

Next we study the behavior of

$$\frac{g_a^+(\epsilon_n) - g_a^+(\epsilon)}{\epsilon_n - \epsilon} \quad \text{and} \quad \frac{g_b^+(\epsilon_n) - g_b^+(\epsilon)}{\epsilon_n - \epsilon}$$

as $\epsilon_n \to \epsilon$ for $n \to \infty$. For this purpose we introduce

$$S_{a,\epsilon} := \{x \in \Omega : g_a(\epsilon)(x) > 0\}$$

and analogously $S_{b,\epsilon}$. By $S_{a,\epsilon}^c$ and $S_{b,\epsilon}^c$ we denote the complement of $S_{a,\epsilon}$ and $S_{b,\epsilon}$ in Ω, respectively. Note that due to Assumption 2.1, we have

$$\operatorname{meas} S_{a,\epsilon} = \operatorname{meas}\{x \in \Omega : g_a(\epsilon)(x) \geq 0\}$$

and analogously for $S_{b,\epsilon}$. Hence, for $v \in L^2(\Omega)$ we infer

$$\begin{aligned}\int_\Omega \left(\frac{g_a^+(\epsilon_n) - g_a^+(\epsilon)}{\epsilon_n - \epsilon}\right) v\,dx &= \frac{1}{\epsilon_n - \epsilon}\int_{S_{a,\epsilon}^c} (g_a^+(\epsilon_n) - g_a^+(\epsilon))v\,dx \\ &+ \frac{1}{\epsilon_n - \epsilon}\int_{S_{a,\epsilon}} (g_a^+(\epsilon_n) - g_a(\epsilon_n))v\,dx + \frac{1}{\epsilon_n - \epsilon}\int_{S_{a,\epsilon}} (g_a(\epsilon_n) - g_a(\epsilon))v\,dx\end{aligned}$$

For $n \to \infty$, Lebesgue's bounded convergence theorem and Assumption 2.1 yield

$$\begin{aligned}&\frac{1}{\epsilon_n - \epsilon}\int_{S_{a,\epsilon}^c} (g_a^+(\epsilon_n) - g_a^+(\epsilon))v\,dx \to 0,\\ &\frac{1}{\epsilon_n - \epsilon}\int_{S_{a,\epsilon}} (g_a^+(\epsilon_n) - g_a(\epsilon_n))v\,dx \to 0,\\ &\frac{1}{\epsilon_n - \epsilon}\int_{S_{a,\epsilon}} (g_a(\epsilon_n) - g_a(\epsilon))v\,dx \to \int_\Omega \dot{g}_a(\epsilon)\chi_{S_{a,\epsilon}} v\,dx,\end{aligned}$$

where $\chi_{S_{a,\epsilon}}$ is the characteristic function of $S_{a,\epsilon}$. The analogous result holds true for g_b^+. These properties of g_a^+, g_b^+ are important for the proof of the following theorem.

THEOREM 2.2. *Suppose that the solution of (P_ϵ) satisfies Assumption 2.1. Then the mappings $\mathbf{y} : \mathcal{D} \to L^2(\Omega)$, $\epsilon \mapsto \bar{y}_\epsilon$, and $\mathbf{p} : \mathcal{D} \to L^2(\Omega)$, $\epsilon \mapsto p_\epsilon$, are strongly differentiable at $\epsilon \in \mathcal{D}$.*

Proof. Let $(\delta u, \delta y, \delta p)$ be the difference of two weak accumulation points of

$$\left(\frac{\bar{u}_{\epsilon_n} - \bar{u}_\epsilon}{\epsilon_n - \epsilon}, \frac{\bar{y}_{\epsilon_n} - \bar{y}_\epsilon}{\epsilon_n - \epsilon}, \frac{p_{\epsilon_n} - p_\epsilon}{\epsilon_n - \epsilon}\right),$$

as $\epsilon_n \to \epsilon$. By $\delta\mu_a$ and $\delta\mu_b$ we denote the difference of the associated weak accumulation points of $\frac{g_a^+(\epsilon_n) - g_a^+(\epsilon)}{\epsilon_n - \epsilon}$ and $\frac{g_b^+(\epsilon_n) - g_b^+(\epsilon)}{\epsilon_n - \epsilon}$. Due to first order optimality, $(\delta u, \delta y, \delta p, \delta\mu^a, \delta\mu^b)$ is characterized by

$$A\delta y = \delta u \quad \text{in } \Omega, \quad \delta y = 0 \quad \text{on } \Gamma, \tag{2.13}$$

$$A^\star \delta p = \delta y + \delta\mu^b - \delta\mu^a \quad \text{in } \Omega, \quad \delta p = 0 \quad \text{on } \Gamma, \tag{2.14}$$

$$\delta p + \alpha\delta u + \epsilon(\delta\mu^b - \delta\mu^a) = 0, \tag{2.15}$$

$$\delta\mu^a = \left(\frac{1}{\epsilon}\delta p - \frac{\alpha}{\epsilon^2}\delta y\right)\chi_{S_{a,\epsilon}}, \tag{2.16}$$

$$\delta\mu^b = \left(-\frac{1}{\epsilon}\delta p + \frac{\alpha}{\epsilon^2}\delta y\right)\chi_{S_{b,\epsilon}}. \tag{2.17}$$

Inserting equations (2.15)–(2.17) in (2.13) and (2.14) and then rearranging terms, we obtain

$$A\delta y + \frac{1}{\epsilon}(\chi_{S_{a,\epsilon}} + \chi_{S_{b,\epsilon}})\delta y = \frac{1}{\alpha}(-I + \chi_{S_{a,\epsilon}} + \chi_{S_{b,\epsilon}})\delta p \quad \text{in } \Omega, \quad \delta y = 0 \quad \text{on } \Gamma,$$
$$A^\star \delta p + \frac{1}{\epsilon}(\chi_{S_{a,\epsilon}} + \chi_{S_{b,\epsilon}})\delta p = (I + \frac{\alpha}{\epsilon^2}\chi_{S_{a,\epsilon}} + \frac{\alpha}{\epsilon^2}\chi_{S_{b,\epsilon}})\delta y \quad \text{in } \Omega, \quad \delta p = 0 \quad \text{on } \Gamma.$$

The latter system implies

$$\begin{aligned} 0 \geq (\frac{1}{\alpha}(-I + \chi_{S_{a,\epsilon}} + \chi_{S_{b,\epsilon}})\delta p, \delta p)_{L^2} &= (A\delta y + \frac{1}{\epsilon}(\chi_{S_{a,\epsilon}} + \chi_{S_{b,\epsilon}})\delta y, \delta p)_{L^2} \\ &= (\delta y, A^\star \delta p + \frac{1}{\epsilon}(\chi_{S_{a,\epsilon}} + \chi_{S_{b,\epsilon}})\delta p)_{L^2} \\ &= (\delta y, (I + \frac{\alpha}{\epsilon^2}\chi_{S_{a,\epsilon}} + \frac{\alpha}{\epsilon^2}\chi_{S_{b,\epsilon}})\delta y)_{L^2} \\ &\geq \|\delta y\|^2_{L^2(\Omega)} \geq 0. \end{aligned}$$

From this we infer $\delta y = \delta p = 0$, and hence by (2.15)–(2.16) $\delta u = \delta \mu_a = \delta \mu_b = 0$. Thus, as $\epsilon_n \to \epsilon$, $(\frac{\bar{y}_{\epsilon_n} - \bar{y}_\epsilon}{\epsilon_n - \epsilon}, \frac{p_{\epsilon_n} - p_\epsilon}{\epsilon_n - \epsilon})$ has a unique weak accumulation point in $H^1_0(\Omega) \times H^1_0(\Omega)$, and, by the compact-embedding of $H^1_0(\Omega)$ in $L^2(\Omega)$, the assertion is shown. □

REMARK 2.1. *Based on the optimality conditions, the derivatives* $\mathbf{y}'(\epsilon)$ *and* $\mathbf{p}'(\epsilon)$ *satisfy the following system:*

$$A\mathbf{y}'(\epsilon) = \dot{u}_\epsilon \quad \textit{in } \Omega, \quad \mathbf{y}'(\epsilon) = 0 \quad \textit{on } \Gamma, \tag{2.18}$$
$$A^\star \mathbf{p}'(\epsilon) = \mathbf{y}'(\epsilon) + \dot{\mu}_{b,\epsilon} - \dot{\mu}_{a,\epsilon} \quad \textit{in } \Omega, \quad \mathbf{p}'(\epsilon) = 0 \quad \textit{on } \Gamma, \tag{2.19}$$
$$\mathbf{p}'(\epsilon) + \alpha\dot{u}_\epsilon + \epsilon(\dot{\mu}_{b,\epsilon} - \dot{\mu}_{a,\epsilon}) = 0, \tag{2.20}$$
$$\dot{\mu}_{a,\epsilon} = (\frac{1}{\epsilon}\mathbf{p}'(\epsilon) - \frac{1}{\epsilon^2}p_\epsilon + \frac{2\alpha}{\epsilon^3}\bar{y}_\epsilon - \frac{\alpha}{\epsilon^2}\mathbf{y}'(\epsilon) - \frac{2\alpha}{\epsilon^3}y_a)\chi_{\mathcal{S}_{a,\epsilon}}, \tag{2.21}$$
$$\dot{\mu}_{b,\epsilon} = (-\frac{1}{\epsilon}\mathbf{p}'(\epsilon) + \frac{1}{\epsilon^2}p_\epsilon - \frac{2\alpha}{\epsilon^3}\bar{y}_\epsilon + \frac{\alpha}{\epsilon^2}\mathbf{y}'(\epsilon) + \frac{2\alpha}{\epsilon^3}y_b)\chi_{\mathcal{S}_{b,\epsilon}}. \tag{2.22}$$

3. Extrapolation-based algorithm. Next we introduce a semismooth Newton (SSN) algorithm which utilizes the theoretical results of the previous section within an extrapolation framework. Conceptually, we exploit the differentiability property of the solution of (P_ϵ) in order to predict a solution of (P_{ϵ_2}) given an approximate solution of (P_{ϵ_1}) with $\epsilon_1 > \epsilon_2$. Hence, the extrapolation serves the purpose of efficient initializations of the SSN-method for solving (P_ϵ) along a sequence of vanishing regularization parameters.

In section 1.2 we provide an equivalent characterization of first order optimality by using a reformulation based on the max-function; compare (1.6)–(1.7). This reformulation is the starting point for the development of a rapidly convergent algorithm of SSN-type. For this purpose we need a generalized derivative for "linearizing" the max-operations in (1.6)–(1.7). Then we introduce the algorithm which, due to our choice of the generalized derivative, has the flavor of an active set strategy utilizing both the primal and the dual variables for identifying the active sets

$$\bar{\mathcal{A}}^a_\epsilon := \{x \in \Omega : \epsilon\bar{u}_\epsilon(x) + \bar{y}_\epsilon(x) = y_a(x)\}, \tag{3.1}$$
$$\bar{\mathcal{A}}^b_\epsilon := \{x \in \Omega : \epsilon\bar{u}_\epsilon(x) + \bar{y}_\epsilon(x) = y_b(x)\} \tag{3.2}$$

at the optimal solution of (P_ϵ). Subsequently we rely on the following generalized derivative.

DEFINITION 3.1. *Let X, Y be Banach spaces and U be an open set in X. A mapping $F : U \to Y$ is said to be semismooth (or Newton differentiable) in U if there exists a (possibly set-valued) mapping $\partial F : U \rightrightarrows \mathscr{L}(X, Y)$ such that*

$$\sup_{V \in \partial F(x+s)} \|F(x+s) - F(x) - Vs\|_Y = o(\|s\|_X) \quad \text{as } \|s\|_X \to 0 \tag{3.3}$$

is satisfied for all $x \in U$. We call ∂F the Newton differential*, and its elements V are referred to as* Newton maps*.*

As shown in [4], a class of Newton maps for the maximum operator $\mathbb{M}(z) = \max(0, z)$ is given by

$$\partial \mathbb{M}_\xi(z)(x) = \begin{cases} 1 \text{ if } z(x) > 0, \\ 0 \text{ if } z(x) < 0, \\ \xi \text{ if } z(x) = 0, \end{cases} \tag{3.4}$$

with arbitrarily fixed $\xi \in \mathbb{R}$, provided that $\mathbb{M}$ is defined as a mapping from $L^{q_2}(\Omega)$ to $L^{q_1}(\Omega)$ with $1 \le q_1 < q_2$; otherwise, i.e., for $q_1 = q_2$ the mapping $\mathbb{M}$ is not Newton differentiable.

As pointed out earlier, the complementarity system can be equivalently expressed as

$$\begin{array}{rcl} \mu_\epsilon^a & = & \max(0, \frac{1}{\epsilon} p_\epsilon + \frac{\alpha}{\epsilon^2}(y_a - \bar{y}_\epsilon)), \\ \mu_\epsilon^b & = & \max(0, -\frac{1}{\epsilon} p_\epsilon + \frac{\alpha}{\epsilon^2}(\bar{y}_\epsilon - y_b)), \end{array} \tag{3.5}$$

where p_ϵ solves the adjoint equation (1.2). Further note that the equalities in (3.5) have to hold in $L^2(\Omega)$, respectively, and p_ϵ, $\bar{y}_\epsilon \in H_0^1(\Omega) \subset L^q(\Omega)$ with $q > 2$ depending on the spatial dimension due to Sobolev embedding results. Hence, the max-operations are understood as mappings from $L^q(\Omega)$ to $L^2(\Omega)$ with $2 < q$ which guarantees Newton-differentiability. Choosing $\xi = 0$ for the Newton maps of the maximum operators in (3.5), we obtain the following algorithm for solving (P_ϵ); compare also [7].

ALGORITHM 3.1. (Semismooth Newton method)

(i) Initialization: Choose initial data $p^0, y^0 \in L^2(\Omega)$ and set $l = 0$.

(ii) Determine the active and inactive sets:

$$\begin{aligned} \mathcal{A}_a^l &= \{x \in \Omega \ : \ \frac{1}{\epsilon} p^l(x) + \frac{\alpha}{\epsilon^2}(y_a(x) - y^l(x)) > 0 \ \textit{a.e. in } \Omega\}, \\ \mathcal{A}_b^l &= \{x \in \Omega \ : \ -\frac{1}{\epsilon} p^l(x) + \frac{\alpha}{\epsilon^2}(y^l(x) - y_b(x)) > 0 \ \textit{a.e. in } \Omega\}, \\ \mathcal{I}^l &= \Omega \backslash (\mathcal{A}_a^l \cup \mathcal{A}_b^l). \end{aligned}$$

(iii) Find the solution $(y^{l+1}, p^{l+1}, u^{l+1}, \mu_a^{l+1}, \mu_b^{l+1})$ of

$$\begin{array}{rclcl@{\qquad}rclcl} Ay^{l+1} & = & u^{l+1} & \textit{in} & \Omega & A^\star p^{l+1} & = & y^{l+1} - y_d - \mu_a^{l+1} + \mu_b^{l+1} & \textit{in} & \Omega \\ y^{l+1} & = & 0 & \textit{on} & \Gamma, & p^{l+1} & = & 0 & \textit{on} & \Gamma, \end{array}$$

$$\alpha u^{l+1} + p^{l+1} + \epsilon(\mu_b^{l+1} - \mu_a^{l+1}) = 0$$

$$\begin{array}{rclll} \mu_a^{l+1} & = & \frac{1}{\epsilon} p^{l+1} + \frac{\alpha}{\epsilon^2}(y_a - y^{l+1}) & \textit{on} & \mathcal{A}_a^l, \quad \mu_a^{l+1} = 0 \ \textit{on } \mathcal{I}^l \cup \mathcal{A}_b^l \\ \mu_b^{l+1} & = & -\frac{1}{\epsilon} p^{l+1} + \frac{\alpha}{\epsilon^2}(y^{l+1} - y_b) & \textit{on} & \mathcal{A}_b^l, \quad \mu_b^{l+1} = 0 \ \textit{on } \mathcal{I}^l \cup \mathcal{A}_a^l. \end{array}$$

(iv) Stop, or set $l = l + 1$ and go to (ii).

Typically, we terminate the algorithm by using the stopping rule: $\mathcal{A}_a^n = \mathcal{A}_a^{n-1}$ and $\mathcal{A}_b^n = \mathcal{A}_b^{n-1}$. For a local convergence analysis of SSN-methods of this type we refer to [4].

Fast convergence of the above algorithm hinges on the quality of the initial point. For this purpose, based on Theorem 2.2 we employ an extrapolation strategy with respect to ϵ. We outline our approach next. Let (ϵ_n) be a sequence of regularization parameters given by

$$\epsilon_{n+1} = (1 - \kappa_n)\epsilon_n \quad \text{with } 0 < \kappa_n < 1. \tag{3.6}$$

By Theorem 2.2, the Taylor expansion of $\mathbf{y}$ at ϵ_{n+1} implies

$$\mathbf{y}(\epsilon_{n+1}) \approx \mathbf{y}(\epsilon_n) + \mathbf{y}'(\epsilon_n)(\epsilon_{n+1} - \epsilon_n). \tag{3.7}$$

The derivative $\mathbf{y}'(\epsilon_n)$ may be computed by solving the sensitivity equations (2.18)–(2.22). In order to save CPU-time we propose to use backward differences in ϵ to approximate $\mathbf{y}'(\epsilon_n)$:

$$\mathbf{y}'(\epsilon_n) \approx \frac{\mathbf{y}(\epsilon_n) - \mathbf{y}(\epsilon_{n-1})}{\epsilon_n - \epsilon_{n-1}}. \tag{3.8}$$

Utilizing (3.8) in (3.7), we obtain

$$\mathbf{y}(\epsilon_{n+1}) \approx \mathbf{y}(\epsilon_n) + \frac{\epsilon_{n+1} - \epsilon_n}{\epsilon_n - \epsilon_{n-1}}(\mathbf{y}(\epsilon_n) - \mathbf{y}(\epsilon_{n-1})). \tag{3.9}$$

Using (3.6), the optimal state $\mathbf{y}(\epsilon_{n+1}) = y_{n+1}$ of $(P_{\epsilon_{n+1}})$ is approximated by

$$y_{n+1} \approx y_{n+1}^0 := y_n + \frac{\kappa_n}{\kappa_{n-1}}(1 - \kappa_{n-1})(y_n - y_{n-1}). \tag{3.10}$$

Similarly, the adjoint state $\mathbf{p}(\epsilon_{n+1}) = p_{n+1}$ at ϵ_{n+1} is approximated by

$$p_{n+1} \approx p_{n+1}^0 := p_n + \frac{\kappa_n}{\kappa_{n-1}}(1 - \kappa_{n-1})(p_n - p_{n-1}). \tag{3.11}$$

In this way, we extrapolate the solutions of (P_{ϵ_n}) and $(P_{\epsilon_{n-1}})$ in order to get the initial guess (y_{n+1}^0, p_{n+1}^0) for Algorithm 3.1 to solve the subsequent problem $(P_{\epsilon_{n+1}})$. For ϵ_0 we use $y^0 = p^0 = 0$.

4. Numerical experiments. Our goal in this section is to demonstrate the numerical reliability of our sensitivity-based extrapolation approach. As mentioned before and based on earlier experience [8, 9, 11], due to the high sensitivity of (P_ϵ) with respect to ϵ and the corresponding challenge in its numerical solution for vanishing regularization parameter the initialization along the ϵ-sequence becomes an issue. It turns out that our initialization-by-extrapolation procedure achieves a significant speed up of Algorithm 3.1 compared to classical continuation strategies; compare, e.g., tables 4.2 and 4.3 below.

In our numerical tests we use $\Omega = (0,1) \times (0,1)$ and $A = -\Delta$. The discretization of the problem is based on continuous piecewise linear finite elements on a uniform mesh, and the discrete versions of the active sets $\mathcal{A}_a$ and $\mathcal{A}_b$ are given by

$$\{i : \frac{1}{\epsilon}(p_h)_i + \frac{\alpha}{\epsilon^2}((y_{a,h})_i - (y_h)_i) > 0\},$$
$$\{i : -\frac{1}{\epsilon}(p_h)_i - \frac{\alpha}{\epsilon^2}((y_{b,h})_i - (y_h)_i) > 0\}$$

where the vectors $p_h, y_h, y_{a,h}, y_{b,h} \in \mathbb{R}^{N_h}$ are the values of the corresponding mesh functions at the nodal points of the discretization. Here, h denotes the mesh size of discretization.

The numerical computations were carried out on a PC with a 250-GHz AMD processor and a 16-gigabyte memory.

4.1. Example 1. We choose:

$$y_d = 2\cos(2\pi x_1 x_2),\ y_b = 0,\ y_a = -1,\ \alpha = 10^{-2};$$

see Figure 4.1 for the numerical solution of (P_ϵ) with $\epsilon = 10^{-6}$ and $h = 1/256$.

First, in Table 4.1 we report on the results obtained by Algorithm 3.1 with simple initialization $y^0 = p^0 = 0$, i.e., without the extrapolation strategy, in the case of vanishing regularization parameter. In addition to varying ϵ, we provide the iteration numbers for various mesh sizes h. We clearly detect an unstable behavior of the algorithm with respect to ϵ. Observing each column of Table 4.1, the number of iterations increases considerably as ϵ decreases. We also observe that small mesh sizes catalyze this adverse effect for small ϵ. On the other hand, for large ϵ ($\epsilon > 10^{-4}$ in our case) we even observe a mesh-independent behavior of the algorithm. This property was verified theoretically, also for a nonlinear case, in [7]. We point out that the results of [7] also hold true for small ϵ, but in order to observe the mesh independence effect sufficiently small mesh sizes would be necessary.

Based on our numerical observations, the following reasons are responsible for the unstable behavior of the algorithm: First, the system of linear equations involved in each iteration of the algorithm is severly ill-conditioned for small ϵ. This effect becomes especially apparent on fine meshes. Secondly, the measure structure of the Lagrange multiplier associated with the upper bound complicates the numerical computation considerably. Figure 4.2 demonstrates that the structure of the multiplier becomes more and more singular as $\epsilon \to 0$.

TABLE 4.1
Number of iterations required by Algorithm 3.1 for several choices of the regularization parameter ϵ and mesh sizes h.

	# It. for various h			
ϵ	1/32	1/64	1/128	1/256
10^{-1}	4	4	4	4
10^{-2}	7	6	7	7
10^{-3}	14	14	15	15
10^{-4}	26	40	42	45
10^{-5}	32	59	109	156
10^{-6}	32	62	133	239

The numerical experiments in [12] indicate that a (classical) continuation strategy may accelerate the convergence speed of the algorithm. Utilizing this concept, for our test problem we detect a remarkable speed-up. The basic idea of the continuation method is merely to use the solution of the regularization problem with a slightly larger regularization parameter as the initial data for the subsequent regularized problem (with a smaller parameter). Table 4.2 provides the results for this approach. Compared to the results in Table 4.1, the algorithm converges much faster. However, for the given mesh sizes we still experience the mesh-dependent behavior for fixed parameter $\epsilon \leq 10^{-4}$ as well as the unstable behavior with respect to decreasing ϵ for a fixed mesh size.