FEASIBLE AND NONINTERIOR PATH-FOLLOWING IN CONSTRAINED MINIMIZATION WITH LOW MULTIPLIER REGULARITY[*]

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Abstract. Primal-dual path-following methods for constrained minimization problems in function space with low multiplier regularity are introduced and analyzed. Regularity properties of the path are proved. The path structure allows us to define approximating models, which are used for controlling the path parameter in an iterative process for computing a solution of the original problem. The Moreau–Yosida regularized subproblems of the new path-following technique are solved efficiently by semismooth Newton methods. The overall algorithmic concept is provided, and numerical tests (including a comparison with primal-dual path-following interior point methods) for state constrained optimal control problems show the efficiency of the new concept.

1. Introduction. The efficient numerical solution of inequality constrained minimization problems in function space with low Lagrange multiplier regularity is still a significant challenge. Prototype problems include optimal control problems with pointwise state constraints, boundary control problems in which the control has to satisfy pointwise constraints on the boundary, and classes of control problems with "solutions très faibles" (that is, "very weak solutions" in the sense of Lions). The common feature is low regularity of the Lagrange multipliers associated with the pointwise constraints. This has an immediate effect when characterizing optimality of solutions. Indeed, in the presence of inequality constraints, first order optimality conditions typically involve a so-called *complementarity system* (see, e.g., [10]), which in turn is influenced by the regularity of the Lagrange multiplier associated with the inequality constraint. To be specific, let us assume that $x_1 \in X_1$ has to satisfy the pointwise (almost everywhere) constraint

$$(1.1) \qquad x_1 \leq \psi,$$

where X_1 denotes a Hilbert space continuously embedded into $L^2(\omega)$ and $\omega \subset \mathbb{R}^m$ is a bounded domain. Further $\psi \in L^2(\omega)$, and $\leq$ represents the natural ordering in $L^2(\omega)$. Let $\lambda \in X_1^*$ denote the Lagrange multiplier associated with constraint (1.1), where X_1^* is the topological dual space of X_1. First order optimality characterizations include the complementarity condition

$$(1.2) \qquad x_1 \leq \psi, \quad \langle \lambda, x_1 - \xi \rangle_{X_1^*, X_1} \geq 0 \quad \text{for all } \xi \leq \psi, \, \xi \in X_1$$

at an optimal solution x_1 with associated Lagrange multiplier λ. Without additional regularity, system (1.2) does not admit a pointwise interpretation, which is frequently crucial for numerical algorithms.

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In fact, solution techniques and their (local) convergence behavior often hinge on the multiplier regularity. Classical active set methods, for instance, require a pointwise (almost everywhere) interpretation of λ for the active set estimation. In the case of pointwise constraints, techniques like the projected gradient methods will not work without modification since the sum of the iteration variable and the gradient of the objective, which coincides with the negative multiplier, is needed for the update. Since the iteration variable and the gradient have different regularity properties, this is not feasible in general. An analogous comment applies for projected Newton techniques. Recently it was found that semi smooth Newton methods are highly efficient in solving certain classes of constrained optimization problems in function space [4, 5, 9, 10, 11, 21]. These methods rely on a pointwise almost everywhere interpretation of the complementarity system (1.2) and smoothing properties of the control-to-adjoint-state mapping. In fact, the pointwise interpretation allows us to express (1.2) equivalently as

$$(1.3) \qquad \lambda - \max\left(0, \lambda + c(x_1 - \psi)\right) = 0,$$

for some arbitrarily fixed $c > 0$, and the smoothing of the control-to-adjoint-state operator typically implies that the mapping

$$\theta : x_1 \mapsto \lambda(x_1) + c(x_1 - \psi)$$

can be considered as $\theta : X_1 \to L^q(\omega)$ with $q > 2$. The norm gap between $L^q(\omega)$ and the space $L^2(\omega)$, in which inequality (1.1) is posed, is crucial in proving generalized differentiability of

$$x_1 \mapsto \max(0, \theta(x_1)),$$

and in arguing well-definedness and locally superlinear convergence of the generalized (semismooth) Newton method for solving the underlying nonsmooth first order optimality system; see [10] for details. Again, the low multiplier regularity may prevent the pointwise interpretation and/or the smoothing of the control-to-adjoint-state mapping.

An approach for solving state constrained optimal control problems that does not rely on the use of multipliers was introduced in [13]. This method operates with the interface (boundary) between the active set $\{x_1 = \psi\}$ and the inactive set $\{x_1 < \psi\}$ as the optimization variable, and the constrained minimization problem is transformed into a shape optimization problem. Since the interface allows for a unique identification of the inactive region, the multiplier itself is not an issue. While this technique is appealing due to its favorable analytical properties, the implementation is rather technical.

Based on recent work [12], in this paper we propose a primal-dual path-following concept for solving the aforementioned constrained minimization problems. It relies on a (generalized) Moreau–Yosida-type regularization of the max-operation involving a scalar parameter. The resulting regular subproblems can be solved efficiently by, e.g., semismooth Newton methods. The relaxation parameter induces a primal-dual path and a path value functional, for which good low-parametric models can be found based on the structure of the relaxation term. These models are subsequently used for driving the path parameter to its limit, i.e., to find a solution of the original (less regular) problem. This procedure has several analytical as well as numerical benefits as follows:

- sufficiently regular subproblems for which standard methods (like semismooth Newton algorithms) converge rapidly in function space setting;

- simple path structure such that one can find good approximating models for the primal-dual path value functional;
- controlled path-parameter updates based on model functions to avoid ill-conditioning;
- wide applicability.

Compared to other path-following concepts, like primal-dual path-following interior point methods (see, e.g., [6, 22, 25, 26] for finite dimensional versions and [20, 23] for function space treatments), the numerical implementation of our technique is rather user-friendly. In fact, in many cases (see, e.g., [1, 25]) competitive primal-dual path-following interior point methods require the addition of slack variables, which increases the problem size, and then appropriate pivot choices for reducing the indefinite system, which has to be solved in every iteration, in order to make the method feasible for large scale optimization. Additionally, within our path-following framework existing subproblem solvers can readily be used. In contrast to our approach, the successful analysis of interior point methods in function space [20, 23, 24] requires sufficient regularity of the multipliers, which prevents an immediate application of these concepts to the problem class considered in this paper. For an alternative regularization concept for state constrained optimal control problems, we refer to [19].

In the case of regular Lagrange multipliers, our earlier work [1, 10] indicates that semismooth Newton and primal-dual active set methods are superior to path-following strategies. This includes a wide class of pointwise control constraints in the optimal control of partial differential equations.

The rest of the paper is organized as follows. In the next section we introduce the problem class under consideration, specify the relaxed path-problems, and analyze properties of the primal-dual path. In section 3 we discuss several constrained optimal control problems which are covered by our model problem. Among these we consider state constrained optimal control problems and Dirichlet boundary control problems. The primal-dual path value function, its differentiability properties, and the definition of approximating models are the contents of section 4. The algorithm is introduced in section 5. A report on test runs, including a comparison of the new method with primal-dual path-following interior point and primal-dual active set techniques, is also given.

2. Problem formulation and properties of the path. Let X_1, X_2, and W be real Hilbert spaces with

$$X_1 \hookrightarrow L^2(\omega) \hookrightarrow X_1^*,$$

where X_1^* denotes the dual of X_1 and ω a bounded domain in $\mathbb{R}^m$. Further set $X = X_1 \times X_2$ and let $x = (x_1, x_2)$ denote a generic element in X.

Let $E \in \mathcal{L}(X, W)$, $f \in W$, and $\psi \in X_1$. Further let $J : X \to \mathbb{R}$ denote a quadratic functional satisfying the following assumption.

ASSUMPTION 2.1. *There exists a constant $\alpha > 0$ such that*

$$(2.1) \qquad\qquad \langle J'(x) - J'(y), x - y \rangle_{X^*, X} \geq \alpha |x - y|_X^2$$

whenever $E(x - y) = 0$ for $x, y \in X$.

Here $\langle \cdot, \cdot \rangle_{X^*, X}$, at times denoted by $\langle \cdot, \cdot \rangle$, stands for the duality pairing between X and X^*. We set

$$C := \begin{pmatrix} E \\ (I, 0) \end{pmatrix} : X \to W \times X_1$$

and assume that

(2.2) $\qquad\qquad\qquad\qquad C$ is surjective.

The problem under consideration is

(P) $\qquad$
$$\begin{aligned} &\text{minimize } J(x) \text{ over } x \in X \\ &\text{subject to } Ex = f, \\ &\qquad\qquad x_1 \leq \psi, \end{aligned}$$

where $\leq$ denotes the ordering in $L^2(\omega)$. By Assumption 2.1 and (2.2) there exists a unique solution $x^* \in X$ to (P). Further by (2.2) there exists [17] a unique Lagrange multiplier pair $(p^*, \lambda^*) \in W^* \times X_1^*$ such that

(2.3)
$$\begin{aligned} &J'(x^*) + E^* p^* + (\lambda^*, 0) = 0 \text{ in } X^*, \\ &\lambda^* \geq 0, \quad x_1^* - \psi \leq 0, \quad \langle \lambda^*, x_1^* - \psi \rangle_{X_1^*, X_1} = 0, \end{aligned}$$

where $\lambda^* \geq 0$ stands for $\langle \lambda^*, \phi \rangle_{X_1^*, X_1} \geq 0$ for all $\phi \in X_1$ with $\phi \geq 0$. In section 3 we give examples from optimal control with control or state constraints which are covered by our general framework.

We also consider the following problem without inequality constraints:

($\tilde{\text{P}}$) $\qquad$
$$\begin{aligned} &\text{minimize } J(x) \text{ over } x \in X \\ &\text{subject to } Ex = f, \end{aligned}$$

as well as the regularized problems

(P_γ) $\qquad$
$$\begin{aligned} &\text{minimize } J(x, \gamma) := J(x) + \frac{1}{2\gamma} \int_\omega | \left(\bar{\lambda} + \gamma(x_1 - \psi) \right)^+ |^2 dw \text{ over } x \in X \\ &\text{subject to } Ex = f, \end{aligned}$$

where $\gamma > 0$ represents a relaxation (or regularization) parameter and $\bar{\lambda} \in L^2(\omega)$ is an optional shift-parameter. For every $\gamma > 0$ there exists a unique solution $x_\gamma = (x_{1,\gamma}, x_{2,\gamma})$ to (P_γ) satisfying

(2.4)
$$\begin{aligned} &Ex_\gamma = f, \\ &J'(x_\gamma) + E^* p_\gamma + (\lambda_\gamma, 0) = 0 \text{ in } X^*, \\ &\lambda_\gamma = \left(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi) \right)^+ \text{ in } L^2(\omega). \end{aligned}$$

In view of (1.3), the last equation in (2.4) suggests that $\bar{\lambda}$ acts as a regular approximation of the Lagrange multiplier corresponding to $x_1 \leq \psi$. Further, in section 3 we find that in some cases, $\bar{\lambda}$ can be chosen such that $x_{1,\gamma} \leq \psi$ for γ sufficiently large.

We refer to

$$\mathcal{C} = \{(x_\gamma, p_\gamma, \lambda_\gamma) \in X \times W^* \times X_1^* : \gamma \in (0, \infty)\}$$

as the *primal-dual path* associated with (P). For $r > 0$ we further set

$$\mathcal{C}_r = \{(x_\gamma, p_\gamma, \lambda_\gamma) : \gamma \in [r, \infty)\}.$$

PROPOSITION 2.1. *For every $r > 0$, the path $\mathcal{C}_r$ is bounded and, as $\gamma \to \infty$, we have $(x_\gamma, p_\gamma, \lambda_\gamma) \rightharpoonup (x^*, p^*, \lambda^*)$ in $X \times W^* \times X_1^*$. Moreover $x_\gamma \to x^*$ in X.*

Proof. From (2.4) we have

$$\langle J'(x_\gamma) - J'(x^*), x_\gamma - x^* \rangle_{X^*,X} + (\lambda_\gamma, x_{1,\gamma} - x_1^*)_{L^2} = \langle J'(x^*), x^* - x_\gamma \rangle_{X^*,X},$$

and by (2.1),

(2.5) $$\alpha |x_\gamma - x^*|_X^2 + (\lambda_\gamma, x_{1,\gamma} - x_1^*)_{L^2} \leq \langle J'(x^*), x^* - x_\gamma \rangle_{X^*,X}.$$

As in [14],

(2.6) $$(\lambda_\gamma, x_{1,\gamma} - x_1^*)_{L^2} \geq \frac{1}{\gamma}|\lambda_\gamma|_{L^2}^2 - \frac{1}{\gamma}(\lambda_\gamma, \bar{\lambda})_{L^2},$$

and hence,

(2.7) $$\alpha |x_\gamma - x^*|_X^2 + \frac{1}{2\gamma}|\lambda_\gamma|_{L^2}^2 \leq |J'(x^*)|_{X^*}|x^* - x_\gamma|_X + \frac{1}{2\gamma}|\bar{\lambda}|_{L^2}^2.$$

In particular we have that $\{x_\gamma\}_{\gamma \geq r}$ is bounded for every $r > 0$. By (2.2),

$$C^*(p_\gamma, \lambda_\gamma) = -J'(x_\gamma),$$

and since C is surjective it follows that $\{(p_\gamma, \lambda_\gamma)\}$ is bounded in $W^* \times X_1^*$. Hence, there exists $(\hat{x}, \hat{p}, \hat{\lambda})$ such that for a subsequence, $(x_\gamma, p_\gamma, \lambda_\gamma) \rightharpoonup (\hat{x}, \hat{p}, \hat{\lambda})$. Since $\lambda_\gamma \geq 0$ for all $\gamma > 0$, we find $\langle \hat{\lambda}, \phi \rangle_{X_1^*, X_1} \geq 0$ for all $\phi \in X_1$ with $\phi \geq 0$. As in [14, section 3], one argues that $\hat{x} \leq \psi$. By (2.3) and (2.4),

(2.8) $$\langle J'(x_\gamma) - J'(x^*), x_\gamma - x^* \rangle_{X^*,X} + \langle \lambda_\gamma - \lambda^*, x_{1,\gamma} - x_1^* \rangle_{X_1^*, X_1} = 0,$$

and from (2.6) we have $(\lambda_\gamma, x_{1,\gamma} - x_1^*) \geq -\frac{1}{2\gamma}|\bar{\lambda}|_{L^2}^2$. Further, from (2.8) with Assumption 2.1 holding we arrive at

$$0 \leq \alpha |x_\gamma - x^*|_X^2 \leq \frac{1}{2\gamma}|\bar{\lambda}|_{L^2}^2 + \langle \lambda^*, x_{1,\gamma} - x^* \rangle_{X_1^*, X_1}.$$

Passing to the limit as $\gamma \to \infty$ yields

$$0 \leq \alpha \limsup_{\gamma \to \infty} |x_\gamma - x^*|_X^2 = \langle \lambda^*, \hat{x}_1 - x_1^* \rangle_{X_1^*, X_1} = \langle \lambda^*, \hat{x}_1 - \psi \rangle_{X_1^*, X_1} \leq 0,$$

and therefore $\lim_{\gamma \to \infty} x_\gamma = x^*$. Taking the limit in (2.4), we find

$$\langle J'(x^*), \phi \rangle_{X^*,X} + \langle E^*\hat{p}, \phi \rangle_{X^*,X} + \langle \hat{\lambda}, \phi_1 \rangle_{X_1^*, X_1} = 0$$

for all $\phi = (\phi_1, \phi_2) \in X$. This equation also holds with $(\hat{p}, \hat{\lambda})$ replaced by (p^*, λ^*). Since C^* is injective, we have $(\hat{p}, \hat{\lambda}) = (p^*, \lambda^*)$. Since the accumulation point of every weakly convergent subsequence of $\{(x_\gamma, p_\gamma, \lambda_\gamma)\}$ is (x^*, p^*, λ^*), the whole sequence converges weakly.   □

We point out that condition (2.2) is a convenient sufficient condition, which is used for the existence of a Lagrange multiplier and for the a priori estimate just below (2.7). It holds for a reasonably wide class of interesting applications, as will be shown in section 3. In more involved applications, these two consequences of (2.2) must be argued by utilizing the specific properties of the underlying problem.

Next we treat the case $\bar{\lambda} = 0$ and $\gamma \to 0^+$, i.e., convergence towards the problem without inequality constraints.

PROPOSITION 2.2. *If $\bar{\lambda} = 0$, then the path $\mathcal{C}_0$ is bounded in $X \times W^* \times X_1^*$ and $\lim_{\gamma \to 0^+}(x_\gamma, p_\gamma, \lambda_\gamma) = (\tilde{x}, \tilde{p}, 0)$, where $\tilde{x}$ is the solution to $(\tilde{P})$ with Lagrange multiplier $\tilde{p}$ associated with the constraint $Ex = f$.*

Proof. By (2.4) and (2.7), the family $\{(x_\gamma, p_\gamma, \lambda_\gamma)\}_{\gamma > 0}$ is bounded. Moreover $\lim_{\gamma \to 0^+} \lambda_\gamma = 0$ in $L^2(\omega)$ by (2.7). Taking the limit $\gamma \to 0^+$ in (2.4), we find that each accumulation point of $\{(x_\gamma, p_\gamma, \lambda_\gamma)\}_{\gamma > 0}$ must satisfy

$$J'(\tilde{x}) + E^* \tilde{p} = 0, \quad E\tilde{x} = f.$$

This implies the claim.   □

Now we study smoothness properties of the primal-dual path.

PROPOSITION 2.3. *The primal-dual path $\mathcal{C}_r$ is globally Lipschitz continuous for every $r > 0$, and $\gamma \mapsto \lambda_\gamma$ is locally Lipschitz continuous in $L^2(\omega)$. If $\bar{\lambda} = 0$, then $\mathcal{C}_0$ is globally Lipschitz continuous.*

Proof. Let $\gamma, \bar{\gamma} \in [r, \infty)$. Then

(2.9)
$$J'(x_\gamma) - J'(x_{\bar{\gamma}}) + E^*(p_\gamma - p_{\bar{\gamma}}) + \left(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi)\right)^+ - \left(\bar{\lambda} + \bar{\gamma}(x_{1,\bar{\gamma}} - \psi)\right)^+ = 0,$$

and hence with Assumption 2.1 holding,

$$\alpha|x_\gamma - \bar{x}_\gamma|_X^2 + \left(\left(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi)\right)^+ - \left(\bar{\lambda} + \bar{\gamma}(x_{1,\gamma} - \psi)\right)^+ \right.$$
$$\left. + \left(\bar{\lambda} + \bar{\gamma}(x_{1,\gamma} - \psi)\right)^+ - \left(\bar{\lambda} + \bar{\gamma}(x_{1,\bar{\gamma}} - \psi)\right)^+, x_{1,\gamma} - x_{1,\bar{\gamma}}\right)_{L^2} \leq 0.$$

Since $x \mapsto (z + x)^+$ is monotone, we have

$$\alpha|x_\gamma - x_{\bar{\gamma}}|_X^2 \leq |\gamma - \bar{\gamma}|\,|x_{1,\gamma} - \psi|_{L^2}|x_{1,\gamma} - x_{1,\bar{\gamma}}|_{L^2}.$$

Boundedness of $\{x_{1,\gamma}\}_{\gamma \geq r}$ implies Lipschitz continuity of $\gamma \mapsto x_\gamma$ for $\gamma \geq r$.

From (2.9) we deduce that

$$C^*(p_\gamma - p_{\bar{\gamma}}, \lambda_\gamma - \lambda_{\bar{\gamma}}) = J'(x_{\bar{\gamma}}) - J'(x_\gamma).$$

Therefore surjectivity of C implies that $\gamma \mapsto (p_\gamma, \lambda_\gamma)$ is Lipschitz continuous on $[r, \infty)$. For $\bar{\lambda} = 0$ we have that $\{x_\gamma\}_{\gamma > 0}$ is bounded, and global Lipschitz continuity of $\mathcal{C}_0$ follows as before.

Local Lipschitz continuity of $\gamma \mapsto \lambda_\gamma$ in $L^2(\omega)$ results from

$$|\lambda_\gamma - \lambda_{\bar{\gamma}}|_{L^2} = \left| \left(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi)\right)^+ - \left(\bar{\lambda} + \bar{\gamma}(x_{1,\bar{\gamma}} - \psi)\right)^+ \right|_{L^2}$$
$$\leq |(\gamma - \bar{\gamma})x_{1,\gamma}|_{L^2} + |\bar{\gamma}(x_{1,\gamma} - x_{1,\bar{\gamma}})|_{L^2} + |\gamma - \bar{\gamma}||\psi|_{L^2}.   □$$

Henceforth we set for $\gamma > 0$

$$S_\gamma = \{z \in \omega : \bar{\lambda}(z) + \gamma(x_{1,\gamma} - \psi)(z) > 0\}$$

and

$$g(\gamma) = \bar{\lambda} + \gamma(x_{1,\gamma} - \psi).$$

Below we shall assume that X_1 embeds compactly into $L^2(\omega)$. Since $\gamma \mapsto (x_\gamma, p_\gamma)$ is Lipschitz continuous,

$$\left(\frac{1}{\bar\gamma - \gamma}(x_{\bar\gamma} - x_\gamma), \frac{1}{\bar\gamma - \gamma}(p_{\bar\gamma} - p_\gamma) \right)$$

admits a weak accumulation point $(\dot x_\gamma^+, \dot p_\gamma^+)$ in $X \times W^*$ as $\bar\gamma \to \gamma$. Further,

$$\frac{1}{\bar\gamma - \gamma}\left(g(\bar\gamma) - g(\gamma) \right)$$

has $\dot g(\gamma) = x_{1,\gamma} - \psi + \gamma \dot x_{1,\gamma}^+$ as a strong accumulation point in $L^2(\omega)$.

Since J is quadratic, $J''(x_\gamma)$ is independent of x_γ and we henceforth simply use J'' for the bounded linear operator from X to X^*.

PROPOSITION 2.4. *Assume that $X_1 \hookrightarrow L^2(\omega)$ is compact, and set*

$$S_\gamma^+ = S_\gamma \cup \{z : \bar\lambda(z) + \gamma(x_{1,\gamma} - \psi)(z) = 0 \wedge \dot g(\gamma)(z) \geq 0\}.$$

Then $(\dot x_\gamma, \dot p_\gamma)$ satisfies

$$\langle J''(\dot x_\gamma), v \rangle_{X^*,X} + \langle E^* \dot p_\gamma, v \rangle_{X^*,X} + \left((x_{1,\gamma} - \psi + \gamma \dot x_{1,\gamma}^+)\chi_{S_\gamma^+}, v_1 \right) = 0$$

for all $v = (v_1, v_2) \in X$.

For the proof we refer to [12]. We now set

$$S_\gamma^0 = \{z \in \omega : \bar\lambda(z) + \gamma(x_{1,\gamma} - \psi)(z) = 0\}.$$

COROLLARY 2.1. *If* $\mathrm{meas}(S_\gamma^0) = 0$, *then $\gamma \mapsto (x_\gamma, p_\gamma) \in X \times W^*$ is weakly differentiable at γ and $(\dot x_\gamma, \dot p_\gamma)$ satisfies*

$$(2.10) \qquad \langle J''(\dot x_\gamma), v \rangle_{X^*,X} + \langle E^* \dot p_\gamma, v \rangle_{X^*,X} + \left((x_{1,\gamma} - \psi + \gamma \dot x_{1,\gamma})\chi_{S_\gamma}, v_1 \right) = 0$$

for all $v = (v_1, v_2) \in X$. Moreover $\gamma \mapsto x_\gamma$ is strongly differentiable at γ.

Proof. Every accumulation point $(\dot x_\gamma, \dot p_\gamma)$ of

$$\left(\frac{1}{\bar\gamma - \gamma}(x_{\bar\gamma} - x_\gamma), \frac{1}{\bar\gamma - \gamma}(p_{\bar\gamma} - p_\gamma) \right)$$

as $\bar\gamma \to \gamma$ satisfies the conclusion of Proposition 2.4. If there are two weak accumulation points, then their difference $(\bar x_\gamma, \bar p_\gamma)$ satisfies $E \bar x_\gamma = 0$ and

$$(2.11) \qquad \langle J''(\bar x_\gamma), v \rangle_{X^*,X} + \langle \bar p_\gamma, Ev \rangle_{X^*,X} + \gamma(\bar x_{1,\gamma} \chi_{S_\gamma}, v_1)_{L^2} = 0$$

for all $v = (v_1, v_2) \in X$. Setting $v = \bar x_\gamma$ in (2.11), we have

$$\langle J''(\bar x_\gamma), \bar x_\gamma \rangle_{X^*,X} + \gamma(\bar x_{1,\gamma} \chi_{S_\gamma}, \bar x_{1,\gamma}) = 0,$$

which implies that $\bar x_\gamma = 0$ by Assumption 2.1. Due to (2.2) and (2.11) we have $\bar p_\gamma = 0$, and weak differentiability follows. From (2.4) and (2.11) we have

$$\left\langle J''(\dot x_\gamma) - \frac{1}{\bar\gamma - \gamma}\left(J'(x_{\bar\gamma}) - J'(x_\gamma) \right), \dot x_\gamma - \frac{1}{\bar\gamma - \gamma}(x_{\bar\gamma} - x_\gamma) \right\rangle_{X^*,X} + \epsilon(\bar\gamma, \gamma) = 0,$$

where

$$\epsilon(\bar{\gamma},\gamma) = \Big((x_{1,\gamma} - \psi + \gamma \dot{x}_{1,\gamma})\chi_{S_\gamma}$$
$$-\frac{1}{\bar{\gamma}-\gamma}\Big[\big(\bar{\lambda} + \bar{\gamma}(x_{1,\bar{\gamma}} - \psi)\big)^+$$
$$- \big(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi)\big)^+\Big], \dot{x}_{1,\gamma} - \frac{1}{\bar{\gamma}-\gamma}(x_{1,\bar{\gamma}} - x_{1,\gamma})\Big)_{L^2}.$$

Since

$$\lim_{\bar{\gamma}\to\gamma} \epsilon(\bar{\gamma},\gamma) = 0,$$

strong differentiability of $\gamma \mapsto x_\gamma$ at γ follows from Assumption 2.1.   □

3. Applications. In this section we discuss several classes of constrained optimal control problems which are special instances of the general problem (P).

3.1. State constraints. The optimal control problem with state constraints,

$$\text{minimize } J(x) = \frac{1}{2}|y - y_d|^2_{L^2(L^2)} + \frac{\beta}{2}|u|^2_{L^2(L^2)} \text{ over } x \in X$$
$$\text{subject to } y_t - \Delta y = u \text{ in } (0,T) \times \Omega,$$
$$y(0,\cdot) = 0, \quad y = 0 \text{ on } (0,T) \times \Gamma,$$
$$y \le \psi \text{ a.e. in } (0,T) \times \Omega,$$

with $\Gamma = \partial\Omega$ and $x = (y,u)$ is a special case of (P), where

$$X_1 = \{y \in L^2(0,T; H_0^1(\Omega) \cap H^2(\Omega)) : y_t \in L^2(0,T; L^2(\Omega))\},$$
$$X_2 = W = L^2(0,T; L^2(\Omega)),$$
$$\omega = (0,T) \times \Omega,$$
$$E(y,u) = y_t - \Delta y - u,$$

$\beta > 0$, $T > 0$, $y_d \in W$, $\psi \in X_1$, and Ω a bounded domain in $\mathbb{R}^n$, is a special case of (P) with Assumption 2.1 and (2.2) satisfied. The general framework of section 2 provides dual variables $(p^*, \lambda^*) \in W \times X_1^*$. Additional regularity can be obtained by using the optimality conditions; see, e.g., [2, 3].

3.2. Dirichlet control with control constraints. Consider that

$$\text{minimize } J(x) = \frac{1}{2}|y - y_d|^2_{L^2(\Omega)} + \frac{\beta}{2}|u|^2_{H^1(\Gamma)} \text{ over } x \in X$$
(3.1)
$$\text{subject to } -\Delta y = f \text{ in } \Omega,$$
$$y = u \text{ on } \Gamma,$$
$$u \le \psi \text{ a.e. in } \Gamma,$$

is a special case of (P) with $x = (u,y)$,

$$X = H^1(\Gamma) \times H^1(\Omega), \quad W = H^{1/2}(\Gamma) \times H^{-1}(\Omega),$$
$$E(y,u) = (y - u, -\Delta y - f),$$

$\beta > 0$, $y_d \in H^2(\Omega)$, $\psi \in C^2(\Gamma)$, and Ω a bounded domain in $\mathbb{R}^n$, $n \le 4$, with smooth boundary Γ. Since the variational solution $y = y(u)$ to

$$-\Delta y = f \text{ in } \Omega, \quad y = u \text{ on } \Gamma,$$

satisfies

$$|y(u)|_{H^1} \leq K(|u|_{H^{1/2}} + |f|_{H^{-1}})$$

for some constant K independent of $u \in H^{1/2}(\Gamma)$ and $f \in H^{-1}(\Omega)$, it follows that Assumption 2.1 is satisfied. To verify (2.2) let $(\tilde{u}_1, \tilde{y}, \tilde{u}_2) \in H^{1/2}(\Gamma) \times H^{-1}(\Omega) \times H^1(\Gamma)$. Choose $u = \tilde{u}_2$ and let $y \in H^1(\Omega)$ be the unique variational solution to

$$-\Delta y = \tilde{y} \text{ in } \Omega, \quad y = \tilde{u}_1 + u \text{ on } \Gamma.$$

Then

$$C(y,u) = \begin{pmatrix} y - u \\ -\Delta y \\ u \end{pmatrix} = \begin{pmatrix} \tilde{u}_1 \\ \tilde{y} \\ \tilde{u}_2 \end{pmatrix} \in H^{1/2}(\Gamma) \times H^{-1}(\Omega) \times H^1(\Gamma),$$

and thus C is surjective.

In this case the Lagrange multiplier associated with the inequality constraint $u \leq \psi$ is in $H^{-1}(\Gamma)$ and, hence, the primal-dual active set strategy without regularization cannot be defined.

The regularized problem is given by

$$(3.2) \quad \begin{aligned} &\text{minimize } \frac{1}{2}|y - y_d|^2_{L^2(\Omega)} + \frac{\beta}{2}|u|^2_{H^1(\Gamma)} + \frac{1}{2\gamma}|\left(\bar{\lambda} + \gamma(u - \psi)\right)^+|^2_{L^2(\Gamma)} \\ &\text{subject to } -\Delta y = f \text{ in } \Omega, \\ &\qquad\qquad y = u \text{ on } \Gamma, \end{aligned}$$

with $\bar{\lambda} \in C(\Gamma)$, $\bar{\lambda} \geq 0$. The optimality system for this problem is given by

$$(3.3) \quad \begin{aligned} &-\Delta y = f \text{ in } \Omega, \quad y = u \text{ on } \Gamma, \\ &-\Delta p = y_d - y \text{ in } \Omega, \quad p = 0 \text{ on } \Gamma, \\ &\beta(-\Delta_\Gamma + I)u + \frac{\partial p}{\partial n} + \left(\bar{\lambda} + \gamma(u - \psi)\right)^+ = 0 \text{ in } H^{-1}(\Gamma), \end{aligned}$$

where Δ_Γ denotes the Laplace–Beltrami operator on Γ; see [8]. Let $(y^*, u^*) = (y^*(u^*), u^*)$ denote the solution to (3.1). Then

$$\begin{aligned} &\frac{1}{2}|y_\gamma - y_d|^2_{L^2(\Omega)} + \frac{\beta}{2}|u_\gamma|^2_{H^1(\Gamma)} + \frac{1}{2\gamma}|\left(\bar{\lambda} + \gamma(u_\gamma - \psi)\right)^+|^2_{L^2(\Gamma)} \\ &\leq \frac{1}{2}|y^* - y_d|^2_{L^2(\Omega)} + \frac{\beta}{2}|u^*|^2_{H^1(\Gamma)} + \frac{1}{2\gamma}|\bar{\lambda}|^2_{L^2(\Gamma)}, \end{aligned}$$

and hence,

$$(3.4) \quad |u_\gamma|_{H^1} \leq K\left(1 + \frac{1}{\sqrt{\gamma}}|\bar{\lambda}|\right)_{L^2(\Gamma)}.$$

Here and below, K denotes a constant independent of $|\bar{\lambda}|_{L^2(\Gamma)}$ and γ. From well-known estimates [16, p. 188] for elliptic equations (3.3) and (3.4), we deduce that

$$|y_\gamma|_{H^{3/2}(\Omega)} \leq K\left(1 + \frac{1}{\sqrt{\gamma}}|\bar{\lambda}|_{L^2(\Gamma)}\right),$$

$$|p_\gamma|_{H^{7/2}(\Omega)} \leq K\left(1 + \frac{1}{\sqrt{\gamma}}|\bar{\lambda}|_{L^2(\Gamma)}\right),$$

$$\left|\frac{\partial p_\gamma}{\partial n}\right|_{H^2(\Gamma)} \leq K\left(1 + \frac{1}{\sqrt{\gamma}}|\bar{\lambda}|_{L^2(\Gamma)}\right),$$

and hence,

$$(3.5) \qquad \left| \frac{\partial p_\gamma}{\partial n} \right|_{L^\infty(\Gamma)} \leq K \left(1 + \frac{1}{\sqrt{\gamma}} |\bar{\lambda}|_{L^2(\Gamma)} \right),$$

if $n \leq 4$. From the last equation in (3.3), we deduce that

$$\beta \left\langle (-\Delta_\Gamma + I)\, (u_\gamma - \psi), (u_\gamma - \psi)^+ \right\rangle_{X_1^*, X_1} + \left(\frac{\partial p_\gamma}{\partial n} + \bar{\lambda} + \gamma(u_\gamma - \psi), (u_\gamma - \psi)^+ \right)_{L^2(\Gamma)}$$
$$+ \beta \left((-\Delta_\Gamma + I)\psi, (u_\gamma - \psi)^+ \right)_{L^2(\Gamma)} = 0,$$

and thus,

$$\beta |(u_\gamma - \psi)^+|^2_{H^1(\Gamma)} + \gamma |(u_\gamma - \psi)^+|^2_{L^2(\Gamma)} + \left(\bar{\lambda} + \beta(-\Delta_\Gamma + I)\psi + \frac{\partial p_\gamma}{\partial n}, (u_\gamma - \psi)^+ \right)_{L^2(\Gamma)} \leq 0.$$

From (3.5) it follows that

$$\beta |(u_\gamma - \psi)^+|^2_{H^1(\Gamma)} + \gamma |(u_\gamma - \psi)^+|^2_{L^2(\Gamma)}$$
$$+ \left(\bar{\lambda} + \beta(-\Delta_\Gamma + I)\psi - K \left(1 + \frac{|\bar{\lambda}|}{\sqrt{\gamma}} \right), (u_\gamma - \psi)^+ \right)_{L^2(\Gamma)} \leq 0.$$

Hence, if $\bar{\lambda}$ is sufficiently large such that

$$\bar{\lambda}(x) > \beta(\Delta_\Gamma - I)\psi(x) + 2K \quad \text{for all } x \in \Gamma,$$

then there exists $\bar{\gamma}$ such that

$$u_\gamma \leq \psi \text{ a.e. on } \Gamma \text{ for all } \gamma \geq \bar{\gamma},$$

and thus u_γ is feasible for $\gamma \geq \bar{\gamma}$.

If $|u|^2_{H^1(\Gamma)}$ is replaced with $|u|^2_{H^{1/2}(\Gamma)}$ in (3.1) and accordingly $X = H^{1/2}(\Gamma) \times H^1(\Omega)$, then the Lagrange multiplier associated with $u \leq \psi$ is in $H^{-1/2}(\Gamma)$, and again regularization is necessary to employ the primal-dual active set strategy. Following the above arguments, it can be shown that $u_\gamma \leq \psi$ if $\bar{\lambda} \in C^1(\Gamma)$ and if γ is sufficiently large, and that $n \leq 3$.

3.3. Dirichlet control with control constraints, revisited. Here we consider two further alternative formulations for Dirichlet boundary control and their treatment by the primal-dual active set strategy. First, we focus on

$$\text{minimize } \frac{1}{2} |y - y_d|^2_{H^1(\Omega)} + \frac{\beta}{2} |u|^2_{L^2(\Gamma)} \text{ over } (y, u) \in H^1(\Omega) \times L^2(\Gamma)$$

$$(3.6) \qquad \text{subject to } -\Delta y = f \text{ in } \Omega,$$
$$y = u \text{ on } \Gamma,$$
$$u \leq \psi \text{ a.e. on } \Gamma,$$

where $y_d \in H^2(\Omega)$, $\beta > 0$, $f \in L^2(\Omega)$, and $\psi \in H^2(\Gamma)$. Note that (3.6) admits a unique solution $(y^*, u^*) \in H^1(\Omega) \times H^{1/2}(\Gamma)$. The optimality condition for (3.6) is found to be (the variational form of)

$$(3.7) \qquad \begin{aligned} &-\Delta y = f \text{ in } \Omega, \quad y = u \text{ on } \Gamma, \\ &-\Delta p = y_d - y - \Delta y_d - f \text{ in } \Omega, \quad p = 0 \text{ on } \Gamma, \\ &\left(\beta u + \frac{\partial p}{\partial n} - \frac{\partial y_d}{\partial n}, h \right)_{L^2(\Gamma)} \geq 0 \quad \text{for all } h \in \mathcal{C}(u^*), \end{aligned}$$

where $(y, p) \in H^1(\Omega) \times H^1(\Omega)$, and

$$\mathcal{C}(u^*) = \{h = u - u^* : u \in L^2(\Gamma),\ u \leq \psi\}.$$

Next consider p as a function of $u \in L^2(\Gamma)$ defined via the first four equations in (3.7). Note that the mapping $u \mapsto y(u)$ is continuous from $L^2(\Gamma)$ to $L^2(\Omega)$ (see [16]) and further that $u \mapsto \frac{\partial p(u)}{\partial n}$ is continuous from $L^2(\Gamma)$ to $H^{1/2}(\Gamma)$. Hence, the inequality in (3.7) can be equivalently expressed as

$$\beta u + \lambda = \frac{\partial}{\partial n}(y_d - p),$$
$$\lambda = (\lambda + c(u - \psi))^+$$

for any $c > 0$. Choosing $c = \beta$, this in turn is equivalent to

(3.8) $$\beta u + \frac{\partial}{\partial n}(y_d - p) + \left(\frac{\partial}{\partial n}(y_d - p) - \beta\psi\right)^+ = 0.$$

As observed above, $u \mapsto \frac{\partial p(u)}{\partial n}$ is continuous from $L^2(\Gamma)$ to $H^{1/2}(\Gamma)$. Hence, for each n there exists $q > 2$ such that $u \mapsto \frac{\partial p(u)}{\partial n}$ is continuous from $L^2(\Gamma)$ to $L^q(\Gamma)$. Now standard techniques [10] can be applied to argue that the primal-dual active set strategy applied to (3.8) is locally superlinearly convergent in $L^2(\Gamma)$.

3.4. Optimal control problem with "solutions très faibles." Finally, we turn to the boundary control problem with solutions in the sense of "solutions très faibles"; e.g. [15, p.76],

$$\text{minimize } \frac{1}{2}\left|\frac{\partial y}{\partial n} - y_d\right|^2_{H^{-1}(\Gamma)} + \frac{\beta}{2}|u|^2_{L^2(\Gamma)} \text{ over } (u, y) \in L^2(\Gamma) \times L^2(\Omega)$$

(3.9) $$\text{subject to } -(y, \Delta v)_{L^2(\Omega)} - (f, v)_{L^2(\Omega)} + \left(u, \frac{\partial v}{\partial n}\right)_{L^2(\Gamma)} = 0$$

$$\text{for all } v \in H^2(\Omega) \cap H_0^1(\Omega),$$
$$u \leq \psi,$$

where $y_d \in H^{-1}(\Gamma)$, $f \in L^2(\Omega)$, $\psi \in L^2(\Gamma)$. We recall that $u \mapsto \frac{\partial y}{\partial n}$ is a continuous mapping from $L^2(\Gamma)$ to $H^{-1}(\Gamma)$; see [15, p. 78]. The adjoint equation for the optimal control problem (3.9) is given by

(3.10) $$-\Delta p = 0 \text{ in } \Omega, \quad p = (-\Delta_\Gamma)^{-1}\left(y_d - \frac{\partial y}{\partial n}\right) \text{ on } \Gamma,$$

and it is known (see [15, p. 77] and [16]) that $p \in H^{3/2}(\Omega)$ and $\frac{\partial p}{\partial n} \in L^2(\Gamma)$. The optimality system for (3.9) consists of the variational equation in (3.9), the adjoint equation (3.10), and the optimality condition

(3.11) $$\beta u + \lambda + \frac{\partial p}{\partial n} = 0,$$
$$\lambda = (\lambda + c(u - \psi))^+$$

for any $c > 0$. Choosing $c = \beta$ we find, as above, that (3.11) is equivalent to

(3.12) $$\beta u + \frac{\partial p}{\partial n} + \left(\frac{\partial p}{\partial n} - \beta\psi\right)^+ = 0.$$

Note that $u \mapsto \frac{\partial p}{\partial n}$ is a continuous mapping from $L^2(\Gamma)$ into itself, which is not smoothing. Thus, the max-operation in (3.12) is not generalized differentiable in the sense of [10]. The latter property, however, is essential for a superlinear convergence of the primal-dual active set strategy, which we, hence, cannot expect in connection with (3.12).

Turning to the regularized version, we consider, for $\gamma > 0$,

$$
\text{minimize } \frac{1}{2} \left| \frac{\partial y}{\partial n} - y_d \right|^2_{H^{-1}(\Gamma)} + \frac{\beta}{2} |u|^2_{L^2(\Gamma)} + \frac{1}{2\gamma} \int_\Gamma \left| \left(\bar{\lambda} + \gamma(u - \psi) \right)^+ \right|^2
$$

(3.13)
$$
\text{over } (u, y) \in L^2(\Gamma) \times L^2(\Omega)
$$
$$
\text{subject to } - (y, \Delta v)_{L^2(\Omega)} - (f, v)_{L^2(\Omega)} + \left(u, \frac{\partial v}{\partial n} \right)_{L^2(\Gamma)} = 0
$$
$$
\text{for all } v \in H^2(\Omega) \cap H^1_0(\Omega).
$$

The optimality system consists of the primal equation, the adjoint equation (3.10), and the optimality condition

$$
\beta u + \frac{\partial p}{\partial n} + \left(\bar{\lambda} + \gamma(u - \psi) \right)^+ = 0.
$$

Consequently the solution u_γ to (3.13) is still in only $L^2(\Gamma)$, in general, and the primal-dual active set strategy for (3.13) may not be (superlinearly) convergent.

4. The value functional and its model. Next we introduce the optimal value functional of (P_γ), study its smoothness properties, and approximate it by low-parametric families of model functions. These model functions will be used in section 5, where we develop a path-following algorithm operating with a reliable γ-update strategy.

DEFINITION 4.1. *The functional*

$$
\gamma \mapsto V(\gamma) = J(x_\gamma) + \frac{1}{2\gamma} \int_\omega |(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+|^2 dw
$$

defined on $(0, \infty)$ *is called the* primal-dual-path value functional.

The smoothness and monotonicity properties of V provide useful information for tuning γ in an iterative procedure.

PROPOSITION 4.1. *The value functional V is differentiable with*

$$
\dot{V}(\gamma) = -\frac{1}{2\gamma^2} \int_\omega |(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+|^2 + \frac{1}{\gamma} \int_\omega (\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+ (x_{1,\gamma} - \psi).
$$

Proof. For $\bar{\gamma}, \gamma \in (0, \infty)$ we have from (4),

$$
\langle J'(x_{\bar{\gamma}} + x_\gamma), x_{\bar{\gamma}} - x_\gamma \rangle_{X^*, X} + (\lambda_{\bar{\gamma}} + \lambda_\gamma, x_{1,\bar{\gamma}} - x_{1,\gamma})_{L^2} = 0,
$$

and therefore

$$V(\bar{\gamma}) - V(\gamma) = J(x_{\bar{\gamma}}) - J(x_{\gamma}) + \frac{1}{2\bar{\gamma}} \int_{\omega} |(\bar{\lambda} + \bar{\gamma}(x_{1,\bar{\gamma}} - \psi))^+|^2$$

$$- \frac{1}{2\gamma} \int_{\omega} |(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+|^2$$

$$= \langle J'(x_{\bar{\gamma}} + x_{\gamma}), x_{\bar{\gamma}} - x_{\gamma} \rangle_{\mathrm{X}^*,\mathrm{X}} + \frac{1}{2\bar{\gamma}} \int_{\omega} |(\bar{\lambda} + \bar{\gamma}(x_{1,\bar{\gamma}} - \psi))^+|^2$$

$$- \frac{1}{2\bar{\gamma}} \int_{\omega} |(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+|^2$$

$$= \frac{1}{2\bar{\gamma}} \int_{\omega} |(\bar{\lambda} + \bar{\gamma}(x_{1,\bar{\gamma}} - \psi))^+|^2 - \frac{1}{2\gamma} \int_{\omega} |(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+|^2$$

$$- \frac{1}{2} \int_{\omega} ((\bar{\lambda} + \bar{\gamma}(x_{1,\bar{\gamma}} - \psi))^+ + (\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+)(x_{1,\bar{\gamma}} - x_{1,\gamma})$$

$$= \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3.$$

It can now be argued just as in the proof of Proposition 4.1 of [12] that

$$\lim_{\bar{\gamma} \to \gamma} \frac{1}{\bar{\gamma} - \gamma} |\mathcal{I}_2| = \lim_{\bar{\gamma} \to \gamma} \frac{1}{\bar{\gamma} - \gamma} |\mathcal{I}_3| = 0$$

and further,

$$\lim_{\bar{\gamma} \to \gamma} \frac{1}{\bar{\gamma} - \gamma} \mathcal{I}_1 = - \frac{1}{2\gamma^2} \int_{\omega} ((\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+)^2$$

$$+ \frac{1}{\gamma} \int_{\omega} (\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+ (x_{1,\gamma} - \psi),$$

as desired. □

It turns out that the monotonicity properties of V may depend on the choice of $\bar{\lambda}$. For the following discussion we assume that the solution $\tilde{x}$ to $(\tilde{\mathrm{P}})$ does not satisfy $\tilde{x}_1 \le \psi$. Let us start by first considering the case $\bar{\lambda} = 0$. We have

(4.1) $$\dot{V}(\gamma) = \frac{1}{2} \int_{\omega} |(x_{1,\gamma} - \psi)^+|^2 > 0.$$

Indeed, if $\dot{V}(\gamma) = 0$ for some $\gamma > 0$, then $x_{1,\gamma} \le \psi$, i.e., $x_{1,\gamma}$ is feasible. Thus, $\lambda_{\gamma} = 0$ and, from (2.3) and (2.4), we find that $(x_{\gamma}, \lambda_{\gamma}) = (\tilde{x}, 0)$ is the solution to (2.3) with $\tilde{x}_1 \le \psi$ which was ruled out by assumption. In case there exist $\bar{\lambda}$ and $\bar{\gamma} > 0$ such that

(4.2) $$x_{1,\gamma} \le \psi \quad \text{for all} \quad \gamma \ge \bar{\gamma},$$

we have by Proposition 4.1 that $\dot{V}(\gamma) \le 0$ for $\gamma \ge \bar{\gamma}$ and, unless the solution $\tilde{x}$ to $(\tilde{\mathrm{P}})$ satisfies $\tilde{x}_1 \le \psi$, we obtain $\dot{V}(\gamma) < 0$ for $\gamma \ge \bar{\gamma}$. In fact, if $\dot{V}(\gamma) = 0$, then

$$0 = \dot{V}(\gamma) \le - \frac{1}{2\gamma^2} \int_{\omega} |(\bar{\lambda} + \gamma(x_{1,\gamma} - \psi))^+|^2 \le 0,$$

and hence $\lambda_{\gamma} = 0$. Therefore $(x_{\gamma}, \lambda_{\gamma}) = (\tilde{x}, 0)$ is the solution of (2.3), which is excluded. Recall that a specific case in which (4.2) holds was given in section 3.2.

Next we study the second order differentiability of V.

PROPOSITION 4.2. *Assume that $X_1 \hookrightarrow L^2(\omega)$ is compact and let $\dot{x}_\gamma$ denote an accumulation point of $\frac{1}{\bar\gamma - \gamma}(x_{1,\bar\gamma} - x_{1,\gamma})$ as $\bar\gamma \to \gamma$. Then for a subsequence γ_n realizing the accumulation point,*

$$
\begin{aligned}
\lim_{\bar\gamma_n \to \gamma} \frac{1}{\bar\gamma_n - \gamma}(\dot V(\bar\gamma_n) - \dot V(\gamma)) = {} & \frac{1}{\gamma^3} \int_\omega |(\bar\lambda + \gamma(x_{1,\gamma} - \psi))^+|^2 \\
& - \frac{2}{\gamma^2} \int_\omega (\bar\lambda + \gamma(x_{1,\gamma} - \psi))^+ (x_{1,\gamma} - \psi) \\
& + \frac{1}{\gamma} \int_\omega (x_{1,\gamma} - \psi)(x_{1,\gamma} - \psi + \gamma \dot x_{1,\gamma}) \chi_{S_\gamma^+}.
\end{aligned}
$$
(4.3)

If $\operatorname{meas}(S_\gamma^\circ) = 0$, then $\gamma \to V(\gamma)$ is twice differentiable at γ, and the second derivative is given by the right-hand side in (4.3) *with $\chi_{S_\gamma^+}$ replaced by χ_{S_γ}.*

Proof. The first claim follows from Proposition 4.1. If meas $(S_\gamma^\circ) = 0$, then accumulation points of $\frac{1}{\bar\gamma - \gamma}(x_{1,\bar\gamma} - x_{1,\gamma})$ as $\bar\gamma \to \gamma$ are unique, and (4.3) with $\chi_{S_\gamma^+}$ replaced by χ_{S_γ}, as well as existence of $\ddot V$ at γ, follow. $\square$

We turn to proposing low-parametric model functions m for V which share some of the qualitative properties of V. Notice that, in general, V is not at our disposal quantitatively. However, we shall see that m can be obtained from solves of the regularized problem for different choices of γ. In the next section, these model functions will then be used as a guideline for updating γ; see (5.2). Throughout the following discussion, we assume that the solution $\tilde x$ to $(\tilde P)$ does not satisfy $\tilde x_1 \le \psi$.

4.1. Case $\bar\lambda = 0$. In this case, $\gamma \to V(\gamma)$ is strictly increasing with $V(0)$ equal to the value of the cost in $(\tilde P)$ and V^∞ the value of the cost in (P).

PROPOSITION 4.3. *The mapping $\gamma \to \dot V(\gamma)$ is monotonically decreasing.*

Proof. For $\bar\gamma > \gamma > 0$ we have

$$
\begin{aligned}
J(x_\gamma) + \frac{\gamma}{2}|(x_{1,\gamma} - \psi)^+|^2 &\le J(x_{\bar\gamma}) + \frac{\gamma}{2}|(x_{1,\bar\gamma} - \psi)^+|^2 \\
&\le J(x_{\bar\gamma}) + \frac{\bar\gamma}{2}|(x_{1,\bar\gamma} - \psi)^+|^2 \le J(x_\gamma) + \frac{\bar\gamma}{2}|(x_{1,\gamma} - \psi)^+|^2,
\end{aligned}
$$

and hence

$$
J(x_\gamma) - J(x_{\bar\gamma}) \le \frac{\gamma}{2}(|(x_{1,\bar\gamma} - \psi)^+|^2 - |(x_{1,\gamma} - \psi)^+|^2),
$$

and further

$$
J(x_{\bar\gamma}) - J(x_\gamma) \le \frac{\bar\gamma}{2}(|(x_{1,\gamma} - \psi)^+|^2 - |(x_{1,\bar\gamma} - \psi)^+|^2),
$$

which implies

$$
0 \le (\bar\gamma - \gamma)(|(x_{1,\gamma} - \psi)^+|^2 - |(x_{1,\bar\gamma} - \psi)^+|^2) = (\bar\gamma - \gamma)(\dot V(\gamma) - \dot V(\bar\gamma)). \quad \square
$$

Note that Proposition 4.3 implies that $\ddot V(\gamma) \le 0$ whenever the second derivative of V exists at γ. This can also be derived from (2.9) and (4.3). A class of functions that satisfies the above properties of V is given by

$$
m(\gamma) = C_1 - \frac{C_2}{(D + \gamma)^r},
$$
(4.4)

with $C_1 \in \mathbb{R}$, $C_2 > 0$, $D > 0$, $r > 0$. In fact, $\dot{m} > 0$, $\ddot{m} < 0$ and $m(0)$, $m(\gamma)$ for $\gamma \to \infty$ are well defined. In our use of m for path-following algorithms, (C_1, C_2, D) will be treated differently from r. While r will be chosen as a fixed number, (C_1, C_2, D) will be updated in an iterative procedure. Let us further note that by a simple rescaling, we can always assume that $D = 1$.

Remark 4.1. To give a second motivation for the choice of the model function, we consider the state constrained problem

$$\text{minimize } J(x) = \frac{1}{2}|y - y_d|_{L^2(\Omega)}^2 + \frac{\beta}{2}|u|_{L^2(\Omega)}^2 \text{ over } x \in X$$

$$\begin{aligned} \text{subject to } -\Delta y &= u && \text{in } \Omega, \\ y &= 0 && \text{on } \partial\Omega, \\ y &\leq \psi && \text{a.e. in } \Omega, \end{aligned}$$

where $\beta > 0$, $x = (y, u) \in X = (H_0^1(\Omega) \cap H^2(\Omega)) \times L^2(\Omega)$, $y_d \in L^2(\Omega)$, $\psi \in L^2(\Omega)$, and Ω is a bounded domain in $\mathbb{R}^n$. We utilize the sensitivity equation with respect to γ and assume that meas $\{z : (y - \psi)(z) = 0\} = \emptyset$. Then from Proposition 2.4 with $S_\gamma = \{z : (y - \psi)(z) > 0\}$, we have

$$-\Delta \dot{y} = \frac{1}{2}\dot{p}, \quad -\Delta \dot{p} + (y_\gamma - \psi)^+ + \gamma \dot{y}\chi_{S_\gamma} = -\dot{y},$$

and hence,

$$\alpha \Delta^2 \dot{y} + \dot{y} + \gamma \dot{y}\chi_{S_\gamma} + (y_\gamma - \psi)^+ = 0.$$

Taking the inner product in $L^2(\Omega)$ with $(y_\gamma - \psi)^+$, we have

$$(\alpha \Delta^2 \dot{y} + \dot{y}, (y_\gamma - \psi)^+) + \gamma(\dot{y}, (y_\gamma - \psi)^+) + |(y_\gamma - \psi)^+|_{L^2}^2 = 0.$$

Replacing $(\alpha \Delta^2 \dot{y}, (y_\gamma - \psi)^+)$ with $(\hat{D}\dot{y}, (y_\gamma - \psi)^+)$, where $\hat{D}$ is a positive constant, we arrive at

(4.5) $$((D + \gamma)\dot{y}, (y_\gamma - \psi)^+) + |(y_\gamma - \psi)^+|_{L^2}^2 = 0,$$

where we set $D = \hat{D} + 1$. Recall from Proposition 4.1 and (4.1) that $|(y_\gamma - \psi)^+|_{L^2}^2 = 2\dot{V}(\gamma)$ and $|(\dot{y}, y_\gamma - \psi)^+| = \ddot{V}(\gamma)$. Since we replaced $\alpha\Delta^2$ with the constant $\hat{D}$, for the purpose of deriving this model, we replace V with its model m and obtain from (4.5)

$$(D + \gamma)\ddot{m}(\gamma) + 2\dot{m}(\gamma) = 0.$$

The solution to this ordinary differential equation is given by (4.4) with $r = 1$.

4.2. Case $\bar{\lambda} \neq 0$. If (4.2) holds, then $\gamma \to V(\gamma)$ is strictly decreasing for $\gamma \geq \bar{\gamma}$, with $\lim_{\gamma \to \infty} V(\gamma)$ equal to the value of the objective of (P), and $\lim_{\gamma \to 0} V(\gamma) = \infty$.

PROPOSITION 4.4. *Assume that $X_1 \hookrightarrow L^2(\omega)$ is compact, that $\text{meas}(S_\gamma^\circ) = 0$, and that (4.2) holds. Then $\ddot{V}(\gamma) \geq 0$.*

Proof. From (4.3) with $S_\gamma^+ = S_\gamma$, we have

$$\ddot{V}(\gamma) = \frac{1}{\gamma^3}\int_{S_\gamma} \bar{\lambda}^2 + \int_{S_\gamma} (x_{1,\gamma} - \psi)\dot{x}_{1,\gamma} \geq \frac{1}{\gamma}\int_{S_\gamma} (x_{1,\gamma} - \psi)^2 + \int_{S_\gamma} (x_{1,\gamma} - \psi)\dot{x}_{1,\gamma}.$$

From Proposition 2.4 and (2.1), we have

$$\gamma|\dot{x}_{1,\gamma}|_{L^2(S_\gamma)} \le |x_{1,\gamma} - \psi|_{L^2(S_\gamma)}.$$

This implies $\ddot{V}(\gamma) \ge 0$.   □

A class of model functions, which satisfy the above properties of V, is given by

$$(4.6) \qquad m(\gamma) = C_1 - \frac{C_2}{(D+\gamma)^r} + \frac{B}{\gamma^r},$$

with $C_1 \in \mathbb{R}$, $B \ge C_2 > 0$, $D > 0$, and $r \in (0,1]$. In fact, $m(0) = \infty$, $\lim_{\gamma \to \infty} m(\gamma) = C_1$, $\dot{m}(\gamma) < 0$, and $\ddot{m}(\gamma) > 0$. A rescaling argument similar to the one for $\bar{\lambda} = 0$ allows us to henceforth assume $D = 1$.

5. Numerics. In this section we specify an inexact path-following method for the numerical solution of (P). In the inner loop, it utilizes a locally superlinearly convergent algorithm for solving the regularized path problem (P_γ). The outer loop employs a γ-update strategy based on our model functions (4.4) (respectively, (4.6)). The section ends with a report on test runs for the solution of some state constrained optimal control problems with distributed control and a linear elliptic PDE as the governing equation. We also compare our new algorithm with a primal-dual path-following interior point method [18, 27] adapted to PDE-constrained minimization as in [1] and with the primal-dual active set strategy [1, 2]. Our test problems include cases when the optimal solution lacks strict complementarity, i.e., when the set $\mathcal{S}^* = \{y^* = \psi \wedge \lambda^* = 0\}$ has positive measure. It is known that lack of strict complementarity may slow the convergence of numerical algorithms. This is due to the difficulty of detecting the correct active (respectively, inactive) set structure in the neighborhood of the solution.

5.1. Inner iteration: An algorithm for solving (P_γ). Here we adopt the primal-dual active set strategy as proposed in [12] for solving problems of the type (P_γ). The method is equivalent to a semismooth Newton algorithm, and, using the techniques in [10], it can be shown to converge locally at a q-superlinear rate.

ALGORITHM PDAS$_\gamma$ (primal-dual active set strategy for γ-regularized problem (P_γ)).

(i) Choose $\bar{\lambda} \ge 0$ and $x^0 \in X$; set $l = 0$.

(ii) Determine the active and inactive sets

$$\mathcal{A}^{l+1} := \{w \in \omega : \bar{\lambda}(w) + \gamma(x_1^l(w) - \psi(w)) > 0\},$$
$$\mathcal{I}^{l+1} := \Omega \setminus \mathcal{A}^{l+1}.$$

(iii) Compute the solution x^{l+1} with associated adjoint state p^{l+1} of

$$\text{minimize } \langle J'(x^l) + \frac{1}{2}\langle J''(x^l)(x - x^l), x - x^l \rangle_{X^*, X}$$
$$+ \frac{1}{2\gamma}|(\bar{\lambda} + \gamma(x_1 - \psi))^+|^2_{L^2(\mathcal{A}^{l+1})} \quad \text{over } x \in X$$

subject to $Ex = f$ in W.

(iv) Compute

$$\lambda^{l+1} = \begin{cases} 0 & \text{on } \mathcal{I}^{l+1}, \\ \bar{\lambda} + \gamma(x_1^{l+1} - \psi) & \text{on } \mathcal{A}^{l+1}, \end{cases}$$

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

The first order optimality system of the minimization problem in step (iii) is given by

$$Ex^{l+1} = f \text{ in } W,$$
$$J''(x^l)x^{l+1} + E^*p^{l+1} + \left(\gamma(x_1^{l+1} - \psi)\chi_{\mathcal{A}^{l+1}}, 0\right)$$
$$= -J'(x^l) + J''(x^l)x^l - \left(\bar{\lambda}\chi_{\mathcal{A}^{l+1}}, 0\right) \text{ in } X^*.$$

Note that this system corresponds to a linearization of (2.4) at x^l. In this context, the max-function

$$x_1 \mapsto \left(\bar{\lambda} + \gamma(x_1 - \psi)\right)^+$$

is linearized separately on the active and inactive sets determined in step (ii). This is equivalent to employing a generalized (or slant) derivative of the max-function in the spirit of [10, 12] in the process of linearization. Consequently, step (iii) is identical to the solution of the linear system within an iteration of a semismooth Newton method for solving (2.4).

5.2. Outer iteration: Inexact solutions and γ-update. For small γ there is no need for highly accurate solutions of the regularized problem (P_γ), since we expect x_γ to be only a coarse approximation of x^*. Rather we propose a procedure requiring approximate solutions of the path problem lying in some neighborhood of the path only. This is similar to the concept considered in [12] and to path-following for log-barrier-functions. For this purpose we introduce the residuals

$$r_x(x) = \|Ex - f\|_W,$$
$$r_p(x, p, \lambda) = \|J'(x) + E^*p + (\lambda, 0)\|_{X^*},$$
$$r_\lambda(x_1, \lambda) = \|\lambda - (\bar{\lambda} + \gamma(x_1 - \psi))^+\|_{X_1^*}$$

and define the neighborhood

$$\mathcal{N}(\gamma, r) = \left\{(x, p, \lambda) \in Z : \max\{r_x(x), r_p(x, p, \lambda), r_\lambda(x_1, \lambda)\} \le \frac{\tau}{\gamma^r}\right\}$$

with $Z = X \times X^* \times L^2(\omega)$ for some fixed $\tau > 0$ and $r > 0$. In our implementation, we typically choose r in accordance with our model (4.4) or (4.6). In the subsequent algorithm, for fixed γ, we stop Algorithm PDAS$_\gamma$ after the first occurrence of $(x^l, p^l, \lambda^l) \in \mathcal{N}(\gamma, r)$ for the first time.

Once an approximate solution of (P_γ) is obtained, we have to update γ. To this end, we introduce the feasibility measure ρ^F and the complementarity measure ρ^C as follows:

$$\rho^F(x_1) := \int_\omega (x_1 - \psi)^+ dz,$$
$$\rho^C(x_1) := \int_{\mathcal{I}(x_1)} (x_1 - \psi)^+ dz + \int_{\mathcal{A}(x_1)} (x_1 - \psi)^- dz,$$

where $\mathcal{A}(x_1) = \{z \in \omega : \bar{\lambda}(z) + \gamma(x_1(z) - \psi(z)) > 0\}$, $\mathcal{I}(x_1) = \omega \setminus \mathcal{A}(x_1)$, and $(\cdot)^- = \min(0, \cdot)$. Whenever $x_1 = x_1^{k+1}$ and $\gamma = \gamma_k$, we write $\mathcal{A}^{k+1}$, $\mathcal{I}^{k+1}$ and ρ_{k+1}^F, ρ_{k+1}^C. For $\max(\rho_{k+1}^F, \rho_{k+1}^C) > 0$, we obtain a candidate γ_{k+1}^+ for γ_{k+1} as

$$(5.1) \qquad \gamma_{k+1}^+ = \max\left(\gamma_k \max\left(\tau_1, \frac{\rho_{k+1}^F}{\rho_{k+1}^C}\right), \frac{1}{\max(\rho_{k+1}^F, \rho_{k+1}^C)^q}\right)$$

with $\tau_1 > 1$ and $q \geq 1$; otherwise we set $\gamma_{k+1}^+ = \tau_1 \gamma_k$. We include the quotient $\rho_{k+1}^F/\rho_{k+1}^C$ in order to significantly increase γ whenever $\rho_{k+1}^F \gg \rho_{k+1}^C$, i.e., when the iterates primarily lack feasibility rather than complementarity. The choice $q > 1$ induces certain growth rates for γ. Similar to [12], we also incorporate the following safeguard based on our model (4.4) (respectively, (4.6)): Unless $\gamma_{k+1} < \tau_2 \gamma_k$, with $\tau_2 > 1$, we reduce γ_{k+1}^+ until

$$(5.2) \qquad |t_k(\gamma_{k+1}) - m_k(\gamma_{k+1})| \leq \tau_3 |J(x^{k+1}, \gamma_k) - J(x^k, \gamma_{k-1})|,$$

where $0 < \tau_3 < 1$ and $t_k(\gamma) = J(x^{k+1}, \gamma_k) + \frac{\partial J(x^k, \gamma_k)}{\partial \gamma}(\gamma - \gamma_k)$. In other words, the linearization of m_k at γ_{k+1} should not be farther away from m_k than the distance of the previous two objective values of the regularized problem. As soon as (5.2) is satisfied, we set $\gamma_{k+1} = \gamma_{k+1}^+$.

Notice that our safeguard involves the model function in iteration k, which we denote by m_k. To determine the parameters in our model, we use the actual approximate information on the value functional and its derivative as well as the value function at some reference point. In what follows, we argue only for the model (4.6). The case (4.4) is treated similarly. Given γ_k in iteration k, for fixing B_k, $C_{1,k}$, and $C_{2,k}$ in the model $m_k(\gamma)$, we use the conditions

$$m_k(\gamma_k) = J(x^k, \gamma_k), \quad \dot{m}_k(\gamma_k) = \frac{\partial J(x^k, \gamma_k)}{\partial \gamma}(x^k, \gamma_k), \quad m_k(\hat{\gamma}) = J(\hat{x}, \hat{\gamma}),$$

where $\hat{x}$ denotes an approximate solution of (P_γ) at a reference value $\gamma = \hat{\gamma}$.

Now we are able to outline our overall algorithm.

ALGORITHM IPF (inexact path-following).

  (i) Initialized $\gamma_0 > 0$, select $r > 0$, and set $k := 0$.
  (ii) Compute $(x^k, p^k, \lambda^k) \in \mathcal{N}(\gamma_k, r)$.
  (iii) Update γ_k by (5.1) with safeguard (5.2) to obtain γ_{k+1}.
  (iv) Set $k = k + 1$ and go to (ii).

In step (ii) we use PDAS$_\gamma$ for performing the inner iteration. The convergence of Algorithm IPF follows immediately from the convergence of Algorithm PDAS$_\gamma$ for every fixed γ and the fact that $\gamma_{k+1} \geq \tau_1 \gamma_k$ with $\tau_1 > 1$ for all k, the property that $\frac{\tau}{\gamma_k^r} \to 0$ for $\gamma_k \to \infty$ in the definition of the neighborhood, and from Proposition 2.1.

5.3. Numerical tests. In this section we report on numerical results for the solution of the following state constrained optimal control problem:

$$\text{Minimize } J(y, u) = \frac{1}{2}|y - y_d|_{L^2}^2 + \frac{\beta}{2}|u|_{L^2}^2 \text{ over } (y, u) \in X$$
$$\text{subject to } -\Delta y = u \text{ in } \Omega, \quad y = 0 \text{ on } \Gamma,$$
$$y \leq \psi \text{ a.e. in } \Omega.$$

Thus, we have $x = (y, u)$, $X_1 = H_0^1(\Omega)$, $X_2 = L^2(\Omega)$, and $\omega = \Omega = (0, 1)^2$.

For the discretization of the Laplace operator in two dimensions we use a standard regular five-point finite difference stencil with mesh size h. Unless specified otherwise, the subsequent test runs of all algorithms are based on a nested iteration technique. For this purpose we define a grid hierarchy with mesh sizes $\{h_i\}_{i=2}^8$ and $h_i = 2^{-i}$. On every grid, we stop Algorithm IPF as soon as

$$(5.3) \qquad \max(r_x(x^k), r_p(x^k, p^k, \lambda^k), r_d(x_1^k, \lambda^k)) \leq 0.1 \, h_i^2,$$

where $r_d(x_1^k, \lambda^k) = \|\lambda^k - (\lambda^k + x_1^k - \psi)^+\|_{X_1^*}$. For $i = 2$ we initialize the algorithms by choosing $y^0 = \psi_i$, $u_i^0 = -\Delta_i y_i$, and $p_i^0 = \beta u_i^0$. Here and below, subscript i refers to discretized quantities on grid level i. The initial Lagrange multiplier is $\lambda_i^0 = \chi_{\{y_i^0 > \psi_i\}}(\bar{\lambda}_i + \gamma_0(y_i^0 - \psi_i))$ with $\bar{\lambda}_i = \max(y_{d,i} - (\beta\Delta_i^2 + \mathrm{id}_i)\psi_i, 0)$ in the case considered in section 4.2; otherwise $\bar{\lambda}_i = 0$. For $i > 2$, the interpolation of $(x_{i-1}, p_{i-1}, \lambda_{i-1})$, which is the approximate solution for h_{i-1}, is used as the initial value on the grid with mesh size h_i. The interpolation process is as follows. First, we smooth $(u_{i-1}, p_{i-1}, \lambda_{i-1})$ by applying $(-\Delta_{i-1})^{-1}$, the discrete Laplace operator with homogeneous Dirichlet boundary conditions for h_{i-1}, to the respective components. Then a nine-point-interpolation scheme is applied to obtain $(\tilde{u}_i, \tilde{p}_i, \tilde{\lambda}_i)$; see, e.g., [7]. Finally, we compute

$$u_i^0 = -\left(D_{w_1,i}(D_{w_1,i}^0 \tilde{u}_i) + D_{w_2,i}(D_{w_2,i}^0 \tilde{u}_i)\right),$$

where $D_{w_1,i}^0$ stands for symmetric differences with homogeneous Dirichlet boundary conditions in the w_1-direction, and $D_{w_1,i}$ represents symmetric differences with linear extrapolation on the boundary; similar definitions hold for $D_{w_2,i}$ and $D_{w_2,i}^0$. The adjoint state p_i^0 and the multiplier λ_i^0 are computed analogously.

Whenever a nonzero shift $\bar{\lambda}$ is used, then we choose

$$\bar{\lambda} = \max\left(y_d - (\beta\Delta^2 + \mathrm{id})\psi, 0\right).$$

This choice of $\bar{\lambda}$ is inspired by the reduction of the system consisting of state and adjoint equations, by the optimality condition with respect to u, and by setting $x_1 = \psi$.

Problem 1. The problem data are $y_d = 10(\sin(2\pi x_1) + x_2)$, $\psi \equiv 0.01$, $\beta = 0.1$. In Figure 1 we show the optimal state y_h^* (top left plot) and control u_h^* (far right) and the Lagrange multiplier λ_h^* (bottom) on a 128×128 grid. The behavior of λ_h^* along the boundary between the active and inactive sets at the discrete solution clearly suggests the measure-valuedness of λ^*.

For our model of the primal-dual value functional we use (4.6), i.e., we apply the $\bar{\lambda}$-shift, with $r = 0.2$. We use $\gamma_0 = 1E2$ initially. First, we report on the behavior of the algorithms on a fixed grid, i.e., without utilizing the nested iteration concept. In Table 1 we show the iteration numbers for the primal-dual active set method for solving (P) (abbreviated by PDAS), the primal-dual path-following interior point method (PDIP), and our new path-following concept (IPF) for various mesh sizes h. We point out that the stopping rule for each algorithm is given by (5.3). For IPF we also specify the total number of inner iterations, i.e., the total number of iterations of Algorithm PDAS$_\gamma$. In all cases, the algorithms are initialized as in the case of $i = 2$ described above. Further, for Algorithm IPF we use $q = 1.25$ and $\tau_1 = 10$ in (5.1), $\tau_2 = 1.01$ and $\tau_3 = 0.6$ in (5.2), and $\tau = 100$ in $\mathcal{N}(\gamma, r)$. The results in Table 1 indicate that Algorithms IPF and PDIP are superior to PDAS, whereas IPF appears to be more efficient than PDIP. This reflects also our experience from further test runs for additional problems. We also point out that in contrast to PDAS and PDIP our Algorithm IPF admits a function space analysis. As a consequence, the number of (inner) iterations behaves in a rather mesh-independent way. For PDAS a strong dependence of the iteration numbers on the mesh size is observed. The stabilizing iteration numbers for PDIP in the case of mesh refinements suggest that a function space analysis might be possible. However, to the best of our knowledge, no such analysis is yet available for the problem class considered here that includes a regularization parameter tending to zero in the numerical method.
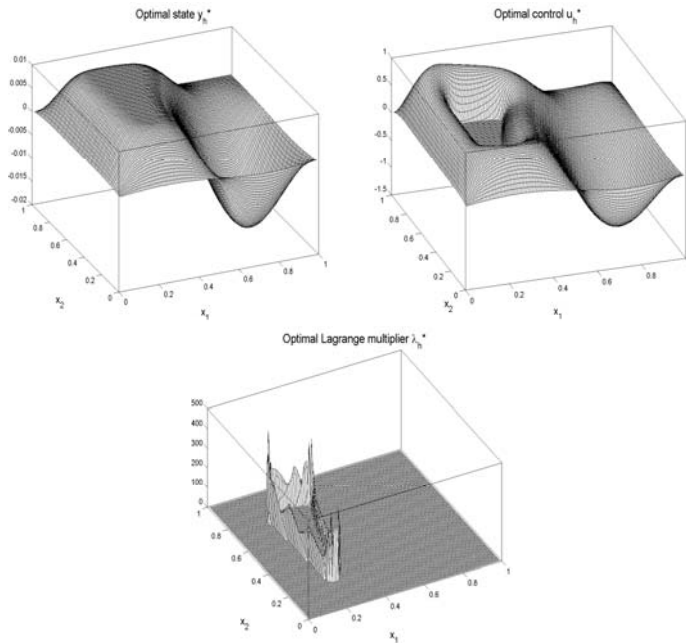
Fig. 1. *Optimal state (top left), optimal control (top right), and optimal multiplier (bottom) for problem 1 with $h = 1/128$.*

TABLE 1
Comparison of iteration numbers for different mesh sizes and methods.

Mesh size h	1/16	1/32	1/64	1/128	1/256
PDAS	14	27	54	113	226
PDIP	12	14	15	19	19
IPF	7(11)	9(15)	9(14)	7(13)	8(15)

Next we report on the outcome of our tests when employing the nested iteration concept and when using the interpolation of the approximate coarse grid solution as the initial point on the next finer grid. The results are summarized in Table 2. Note that for IPF we display only the total number of iterations on the respective grid. First observe that all algorithms experience a speed-up when using the nested iteration concept. PDAS especially, although lacking a function space convergence theory, performs remarkably well in this environment when compared to its variant on fixed grids. With respect to iteration numbers, our path concept is slightly faster than PDIP and PDAS. For a comparison of the CPU-times consumed by the respective algorithm, we define CPU-ratio(*algorithm*) = CPU-time(*algorithm*)/CPU-time(IPF). We have

$$\text{CPU-ratio(PDIP)} \approx 2 \quad \text{and} \quad \text{CPU-ratio(PDAS)} \approx 0.8;$$

i.e., PDIP requires twice as much CPU-time as IPF, while PDAS is slightly faster than IPF. This can be explained by the fact that PDAS performs system solves only on the currently inactive set, whereas IPF has to solve a system on the whole domain. However, we point out that the simple structure of the system matrix of IPF, i.e., $(-\Delta)_i + D_i$, with D_i a positive (semi)definite diagonal matrix on the respective grid

TABLE 2
Problem 1. *Comparison of iteration numbers for different mesh sizes and methods based on nested iteration.*

Mesh size h	1/4	1/8	1/16	1/32	1/64	1/128	1/256	total
PDAS	3	4	4	5	6	6	6	34
PDIP	3	2	4	4	5	6	7	31
IPF	4	3	3	4	5	5	5	29

with mesh size h_i, suggests that one can further speed up the solution process of the linear system in every iteration of Algorithm PDAS$_\gamma$. This, however, is beyond the scope of the present work.

Problem 2 *(lack of strict complementarity).* We construct a test problem for which the active set at the solution contains a subset, where strict complementarity does not hold. For this purpose define $\tilde{p}(w_1, w_2) = -w_1(1 - w_1)w_2(1 - w_2) \in H_0^1(\Omega) \cap C^\infty(\Omega)$ and $\ell(w_1, w_2) = -0.04 + 0.02w_1 - 0.03w_2$. The adjoint state at the solution is given by $p^* = \max(\tilde{p}, \ell)$. Further, we define the active set at the solution as $\mathcal{A}^* = \{\tilde{p} = \ell\}$ and the inactive set as its complement in Ω. We set

$$\tilde{\xi} = \left\{ \begin{array}{l} \Delta\tilde{p} \text{ on } \mathcal{I}^*, \\ 0 \text{ on } \mathcal{A}^*, \end{array} \right.$$

$\xi = \Delta p$, and $\xi_L = \xi - \tilde{\xi}$. Next we decompose the Lagrange multiplier at the solution in a singular part λ_s^* and a regular part λ_r^*. The singular part consists of a line source contribution λ_L^* and an absolutely continuous part λ_a^*:

$$\lambda^* = \lambda_s^* + \lambda_r^* = \lambda_L^* + \lambda_a^* + \lambda_r^*.$$

We define

$$\lambda_L^* = \xi_L, \quad \lambda_a^* = \tilde{\xi}, \quad \lambda_r^*|_{\mathcal{I}^*} = -\tilde{\xi}, \quad \lambda_r^*|_{\mathcal{A}^*} = -100\tilde{p}|_\mathcal{A}.$$

Further, $u^* = p^*/\beta$, with $\beta = 0.01$, and $y^* = (-\Delta)^{-1}p^*/\beta$. The bound is given by $\psi|_{\mathcal{A}^*} = y^*|_{\mathcal{A}^*}$ and $\psi|_{\mathcal{I}^*} = (1/(1 + \text{dist}(\mathcal{A}^*)^{0.1}))y^*|_{\mathcal{I}^*}$. Here $\text{dist}(\mathcal{A}^*)$ denotes the distance function to the active set $\mathcal{A}^*$. The desired state is given by $y_d = y^* + \lambda_r^*$.

In Figure 2 we show the optimal state y_h^* (top left) and control u_h^* (top right) and the Lagrange multiplier λ_h^* (bottom) on a 128×128 grid.

Figure 3 provides the bound ψ (top left), the difference $\psi - y^*$ (top right), and the strongly active, weakly active and inactive sets (bottom). For the latter graph note that the weakly active set corresponds to the region where strict complementarity fails to hold (white region). The strongly active set, i.e., the set where $y^* = \psi$ and $\lambda^* > 0$, is displayed in gray. The inactive set is given by the black region.

The parameters in IPF had the values $r = 0.1$, $\tau_1 = 10$, $\tau_2 = 1.01$, $\tau_3 = 0.7$, and $\tau = 100$. We further set $\bar{\lambda} = 0$.

In Table 3 we report the result corresponding to Problem 2. The arrangement of the table is analogous to that of Table 2 for Problem 1. First we note that, compared to the previous problem, the iteration numbers for PDAS increase significantly as the mesh is refined. This is also reflected in the following CPU-time comparison for this example:

$$\text{CPU-ratio(PDIP)} \approx 1.2 \quad \text{and} \quad \text{CPU-ratio(PDAS)} \approx 1.8.$$
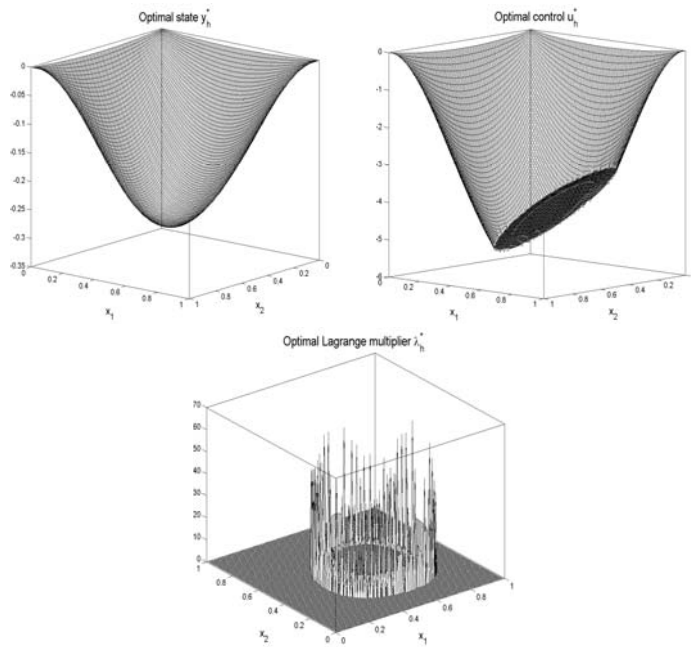
FIG. 2. *Problem* 2. *Optimal state (top left), optimal control (top right), and optimal multiplier (bottom) for* $h = 1/128$.
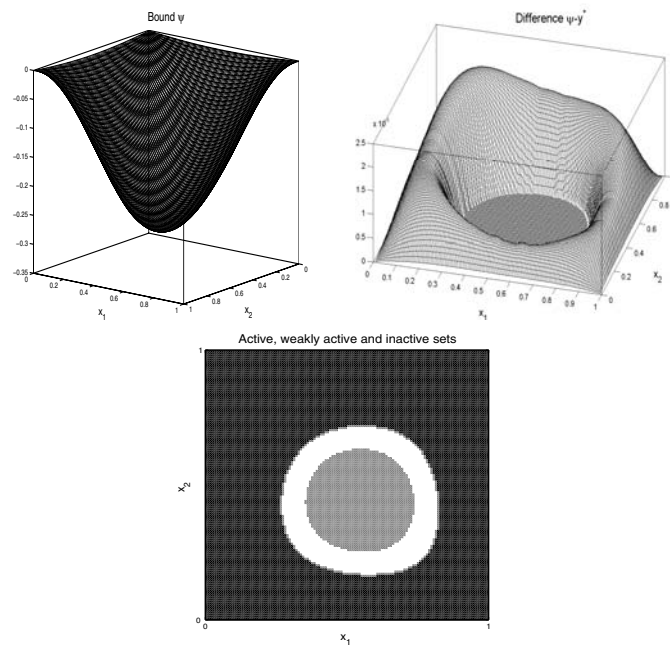

FIG. 3. *Problem* 2. *Bound* ψ *(top left), the difference* $\psi - y^*$ *(top right), and the active and inactive sets (bottom) for* $h = 1/128$.

TABLE 3
Problem 2. *Comparison of iteration numbers for different mesh sizes and methods based on nested iteration.*

Mesh size h	1/4	1/8	1/16	1/32	1/64	1/128	1/256	total
PDAS	2	4	5	9	10	21	40	91
PDIP	3	2	3	3	6	12	11	40
IPF	7	2	4	4	6	8	15	46

Further observe that PDIP needs the lowest total number of iterations, but it requires about 20% more CPU-time than IPF. This can be explained by the fact that interior point approaches typically enlarge the system size by adding slack variables. An a priori system reduction obtained by choosing specific pivots allows us to reduce the large indefinite system occurring in every iteration to a system of the same size as that for IPF. However, in order to compute a solution to the overall system, for PDIP several backward substitutions are required, in contrast to the efforts needed in IPF. Further, we point out that practically relevant versions of primal-dual path-following interior point methods, such as the Mehrotra predictor-corrector algorithm or the Mizuno–Todd–Ye variant (see [1] for an adaptation of these two variants to optimal control of PDEs and for further references), require additional system solves. Depending on the variant, one has either two system solves where the second system has a different right hand side but the same system matrix or two system solves where the second system has a different right hand side *and* a different system matrix as well. The triangular system solves for backward substitution, and the additional system solves mentioned above add significantly to the overall CPU-time. Let us further point out that the reduced systems of PDIP typically have a more involved structure when compared to the systems of IPF; for an account of this fact see, for instance, the systems (4.6) and (4.7) in [1], and the system in Algorithm PDAS$_\gamma$.

REFERENCES

[1] M. BERGOUNIOUX, M. HADDOU, M. HINTERMÜLLER, AND K. KUNISCH, *A comparison of a Moreau–Yosida-based active set strategy and interior point methods for constrained optimal control problems*, SIAM J. Optim., 11 (2000), pp. 495–521.

[2] M. BERGOUNIOUX AND K. KUNISCH, *Primal-Dual Strategy for State-Constrained Optimal Control Problems*, Comput. Optim. Appl., 22 (2002), pp. 193–224.

[3] E. CASAS, *Control of an elliptic problem with pointwise state constraints*, SIAM J. Control Optim., 24 (1986), pp. 1309–1318.

[4] X. CHEN, Z. NASHED, AND L. QI, *Smoothing methods and semismooth methods for nondifferentiable operator equations*, SIAM J. Numer. Anal., 38 (2000), pp. 1200–1216.

[5] J.-C. DE LOS REYES AND K. KUNISCH, *A semi-smooth Newton method for control constrained boundary optimal control of the Navier–Stokes equations*, Nonlinear Anal., 62 (2005), pp. 1289–1316.

[6] A. FORSGREN, P. E. GILL, AND M. H. WRIGHT, *Interior methods for nonlinear optimization*, SIAM Rev., 44 (2002), pp. 525–597.

[7] W. HACKBUSCH, *Multigrid Methods and Applications*, Springer Ser. Computat. Math. 4, Springer-Verlag, Berlin, 1985.

[8] E. HEBEY, *Nonlinear Analysis on Manifolds: Sobolev Spaces and Inequalities*, Courant Lecture Notes in Math. 5, New York University, Courant Institute of Mathematical Sciences, New York, 1999.

[9] M. HINTERMÜLLER AND M. HINZE, *A SQP-semismooth Newton-type algorithm applied to control of the instationary Navier–Stokes system subject to control constraints*, SIAM J. Optim., 16 (2006), pp. 1177–1200.

[10] M. HINTERMÜLLER, K. ITO, AND K. KUNISCH, *The primal-dual active set strategy as a semismooth Newton method*, SIAM J. Optim., 13 (2003), pp. 865–888.

[11] M. HINTERMÜLLER, V. A. KOVTUNENKO, AND K. KUNISCH, *Generalized Newton methods for crack problems with nonpenetration condition*, Numer. Methods Partial Differential Equations, 21 (2005), pp. 586–610.

[12] M. HINTERMÜLLER AND K. KUNISCH, *Path-following methods for a class of constrained minimization problems in function space*, SIAM J. Optim, 17 (2006), pp. 159–187.

[13] M. HINTERMÜLLER AND W. RING, *A level set approach for the solution of a state-constrained optimal control problem*, Numer. Math., 98 (2004), pp. 135–166.

[14] K. ITO AND K. KUNISCH, *Semi-smooth Newton methods for variational inequalities of the first kind*, M2AN Math. Model. Numer. Anal., 37 (2003), pp. 41–62.

[15] J.-L. LIONS, *Optimal Control of Systems Governed by Partial Differential Equations*, Translated from the French by S. K. Mitter. Die Grundlehren der mathematischen Wissenschaften, Band 170. Springer-Verlag, New York, 1971.

[16] J.-L. LIONS AND E. MAGENES, *Problèmes aux limites non homogènes et applications*, Vol. 1, Travaux et Recherches Mathématiques, No. 17, Dunod, Paris, 1968.

[17] H. MAURER AND J. ZOWE, *First and second order necessary and sufficient optimality conditions for infinite-dimensional programming problems*, Math. Programming, 16 (1979), pp. 98–110.

[18] S. MEHROTRA, *On the implementation of a primal-dual interior point method*, SIAM J. Optim., 2 (1992), pp. 575–601.

[19] C. MEYER AND F. TRÖLTZSCH, *On an elliptic optimal control problem with pointwise mixed control-state constraints*, in Recent Advances in Optimization, A. Seeger, ed., Lecture Notes in Econom. Math. Systems 563, Springer, Berlin, 2006, pp. 187–204.

[20] U. PRÜFERT, F. TRÖLTZSCH, AND M. WEISER, *The Convergence of an Interior Point Method for an Elliptic Control Problem with Mixed Control-State Constraints*, Preprint 36-2004, Technische Universität, Berlin, 2004.

[21] M. ULBRICH, *Semismooth Newton methods for operator equations in function spaces*, SIAM J. Optim., 13 (2003), pp. 805–841.

[22] R. J. VANDERBEI, *Linear Programming Foundations and Extensions*, 2nd ed., Internat. Ser. Oper. Res. Sci. 37, Kluwer Academic Publishers, Boston, MA, 2001.

[23] M. WEISER, *Interior Point Methods in Function Space*, ZIB-Report 03-35, Konrad-Zuse Zentrum für Informationstechnik, Berlin, 2003.

[24] M. WEISER AND P. DEUFLHARD, *The Central Path Towards the Numerical Solution of Optimal Control Problems*, ZIB-Report 01-12, Konrad-Zuse Zentrum für Informationstechnik, Berlin, 2001.

[25] S. J. WRIGHT, *Primal-Dual Interior-Point Methods*, SIAM, Philadelphia, 1997.

[26] Y. YE, *Interior Point Algorithms. Theory and Analysis*, John Wiley & Sons Inc., New York, 1997.

[27] Y. ZHANG AND D. T. ZHANG, *On polynomiality of the Mehrotra-type predictor-corrector interior-point algorithms*, Math. Programming, 68 (1995), pp. 303–318.