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# On an Elliptic Optimal Control Problem with Pointwise Mixed Control-State Constraints <sup>\*</sup>

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**Summary.** A nonlinear elliptic control problem with pointwise control-state constraints is considered. Existence of regular Lagrange multipliers, first-order necessary and second-order sufficient optimality conditions are derived. The theory is verified by numerical examples.

**Key words:** Semilinear elliptic equation, pointwise state-constraints, necessary conditions, sufficient conditions, SQP method

**AMS subject classifications.** 49K20, 49M15, 49M29

## 1 Introduction

In this paper, we consider the following semilinear elliptic optimal control problem with distributed control and pointwise mixed control-state constraints

$$(P) \left\{ \begin{array}{l} \text{minimize } J(y, u) := \frac{1}{2} \int_{\Omega} (y - y_d)^2 dx + \frac{\kappa}{2} \int_{\Omega} u^2(x) dx \\ \text{subject to } \begin{array}{ll} -\Delta y(x) + d(y(x)) = u(x) & \text{in } \Omega \\ \partial_{\nu} y(x) + y(x) = 0 & \text{on } \Gamma \end{array} \\ \text{and } y_a(x) \leq \lambda u(x) + y(x) \leq y_b(x) \quad \text{a.e. in } \Omega, \end{array} \right. \quad (1)$$
$$(2)$$

where  $\Omega \subset \mathbb{R}^N$ ,  $N = \{2, 3\}$ , is a bounded domain with  $C^{0,1}$ -boundary  $\Gamma$  and  $\nu$  denotes the outward unit normal. The function  $d : \mathbb{R} \rightarrow \mathbb{R}$  is twice

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<sup>\*</sup> Supported by the DFG Research Center "Mathematics for key technologies" (FZT 86) in Berlin.

continuously differentiable and monotonic increasing. Furthermore, the second derivative  $d''$  is assumed to be locally Lipschitz-continuous. Moreover,  $\kappa > 0$  and  $\lambda \neq 0$  are real numbers, and the bounds  $y_a$  and  $y_b$  are fixed functions in  $L^\infty(\Omega)$  with  $y_a(x) \leq y_b(x)$  a.e. in  $\Omega$ .

This paper is a contribution to the theory of distributed optimal control problems with pointwise state-constraints. The associated numerical analysis is known to be quite complicated, since the Lagrange multipliers for the state-constraints are in general regular Borel measures. We refer, for instance, to Casas [4] for first-order necessary optimality conditions, Casas, Tröltzsch and Unger [7] for second-order sufficient conditions and to Bergounioux, Ito and Kunisch [1] or Bergounioux and Kunisch [3] for associated numerical methods.

The analysis is often simpler for problems with mixed pointwise control-state constraints, since Lagrange multipliers are more regular there. For the elliptic case with quadratic objective and linear equation, this has been shown in the recent paper [10]. However, the corresponding proofs are quite technical.

Here, we consider a particular class of constraints, where the analysis can be developed by a simple trick: Locally, the problem (P) is converted to one with pointwise box-constraints, where the analysis is easy to perform. We will show that problem (P) has regular Lagrange multipliers in  $L^\infty(\Omega)$ . In view of this, we are able to derive first- and second-order optimality conditions for (P). Moreover, we report on associated numerical tests.

It should be underlined that we investigate the problem for a fixed parameter  $\lambda \neq 0$ . Though  $\lambda$  is used as a small regularization parameter in the numerical tests, we do not study here the complicated question of convergence of optimal solutions and multipliers as  $\lambda \rightarrow 0$ . The problem (P) is interesting in itself for  $\lambda$  fixed.

*Remark 1.* The theory below also works for  $-\Delta y(x) + y(x) + d(y(x)) = u(x)$  in  $\Omega$ ,  $\partial_\nu y(x) = 0$  on  $\Gamma$  instead of (1). This is the case studied in the numerical tests in Section 5.

## 2 Standard results

In this section, we recall some well-known results on (P). We consider  $y$  in the state space  $Y = H^1(\Omega) \cap C(\bar{\Omega})$  and the control  $u$  in  $L^2(\Omega)$ . Moreover, we introduce the control-to-state operator  $G : L^2(\Omega) \rightarrow Y$  that assigns  $y$  to  $u$ . The following result is well known, [4]:

**Theorem 1.** *Under the assumptions on  $d$  and  $\Omega$  stated in Section 1, the state equation (1) admits for all  $u \in L^2(\Omega)$  exactly one solution  $y = G(u) \in Y$ , and the estimate*

$$\|y\|_{H^1(\Omega)} + \|y\|_{C(\bar{\Omega})} \leq c_\infty \|u\|_{L^2(\Omega)} \quad (3)$$

*holds true with a constant  $c_\infty$  that only depends on  $\Omega$ .*

Due to  $\dim \Omega \leq 3$ , we obtain the following results for the derivatives of  $G$  (cf.[6]):

**Lemma 1.** *Under the assumptions on  $d$ ,  $G$  is twice continuously Fréchet differentiable from  $L^2(\Omega)$  to  $Y$ . Its first derivative, denoted by  $w = G'(u)h$ ,  $h \in L^2(\Omega)$ , is given by the solution of the linearized equation*

$$\begin{aligned} -\Delta w + d'(y)w &= h && \text{in } \Omega \\ \partial_\nu w + w &= 0 && \text{on } \Gamma \end{aligned} \quad (4)$$

with  $y = G(u)$ . Moreover, the second derivative  $z = G''(u)[u_1, u_2]$  solves the equation

$$\begin{aligned} -\Delta z + d'(y)z &= -d''(y)y_1y_2 && \text{in } \Omega \\ \partial_\nu z + z &= 0 && \text{on } \Gamma \end{aligned} \quad (5)$$

with  $y$  as defined above, and  $y_i = G'(u)u_i$ ,  $i = 1, 2$ .

The next theorem states the existence of an optimal solution for (P).

**Theorem 2.** *If the admissible set is not empty, then (P) admits at least one global solution.*

*Proof:* The proof is more or less standard: In all what follows, we denote the global solution by  $(\bar{y}, \bar{u})$ , where  $\bar{y} = G(\bar{u})$  and  $\bar{u}$  is said to be an optimal control. By  $\kappa > 0$ , we find a bounded minimizing sequence  $\{u_n\} \subset L^2(\Omega)$  and we can assume without loss of generality  $u_n \rightharpoonup \bar{u}$ ,  $n \rightarrow \infty$ . By Theorem 1, the associated sequence  $\{y_n\}$  is bounded in  $H^1(\Omega)$ , hence we are justified to assume  $y_n \rightarrow \bar{y}$  in  $L^2(\Omega)$ . Together with the boundedness in  $C(\bar{\Omega})$  that follows from (3), this yields  $d(y_n) \rightarrow d(\bar{y})$  in  $L^2(\Omega)$ ,  $\bar{y} = G(\bar{u})$ . The optimality of  $\bar{u}$  is a standard conclusion.  $\square$

We should mention that our theory does not rely on this existence result. It is also applicable to any *local* solution  $\bar{u}$ .

*Remark 2.* Obviously, all admissible controls must be bounded and measurable, since  $y_a, y_b \in L^\infty(\Omega)$  and  $y \in C(\bar{\Omega})$  imply  $u \in L^\infty(\Omega)$  because of the constraint (2).

### 3 First-order conditions - regular multipliers

We start by introducing the reduced objective functional by

$$J(y, u) = J(G(u), u) =: f(u).$$

Thus, (P) is equivalent to minimizing  $f(u)$  subject to

$$y_a(x) \leq \lambda u(x) + (G(u))(x) \leq y_b(x) \quad \text{a.e. in } \Omega. \quad (6)$$

Since  $J$  is of tracking type, it is twice continuously differentiable. Together with the differentiability of  $G$  (cf. Lemma 1), this yields the following lemma.

**Lemma 2.** *Under the assumptions of Lemma 1,  $f$  is twice continuously Fréchet differentiable from  $L^2(\Omega)$  to  $\mathbb{R}$ . Its first derivative is given by*

$$f'(u)h = (\kappa u + q, h)_{L^2(\Omega)}, \quad (7)$$

where  $q$  solves the adjoint equation

$$\begin{aligned} -\Delta q + d'(y)q &= y - y_d && \text{in } \Omega \\ \partial_\nu q + q &= 0 && \text{on } \Gamma, \end{aligned} \quad (8)$$

with  $y = G(u)$ . For the second derivative, we obtain

$$f''(u)[u_1, u_2] = (y_1, y_2)_{L^2(\Omega)} + \kappa(u_1, u_2)_{L^2(\Omega)} - \int_{\Omega} d''(y) y_1 y_2 q \, dx, \quad (9)$$

where  $y$  and  $q$  are as defined above, and  $y_i = G'(u)u_i$ ,  $i = 1, 2$ .

*Proof:* Although the arguments are standard, we recall the main ideas for convenience of the reader. From  $f(u) = J(G(u), u) = 1/2 \|G(u) - y_d\|_{L^2(\Omega)}^2 + \kappa/2 \|u\|_{L^2(\Omega)}^2$ , we get

$$f'(u)h = (y - y_d, w)_{L^2(\Omega)} + \kappa(u, h)_{L^2(\Omega)},$$

where  $y = G(u)$  and  $w = G'(u)h$  denotes the weak solution of the linearized equation (4) with the right hand side  $h$ . Now, choosing  $q$  as test function in the weak formulation of (4), we obtain

$$\int_{\Omega} \nabla w \cdot \nabla q \, dx + \int_{\Omega} d'(y) w q \, dx + \int_{\Gamma} w q \, ds = \int_{\Omega} h q \, dx.$$

On the other hand, we insert  $w$  in the weak formulation of equation (8):

$$\int_{\Omega} \nabla q \cdot \nabla w \, dx + \int_{\Omega} d'(y) q w \, dx + \int_{\Gamma} q w \, ds = \int_{\Omega} (y - y_d) w \, dx.$$

Subtracting one equation from the other finally yields  $(y - y_d, w)_{L^2(\Omega)} = (h, q)_{L^2(\Omega)}$ . Applying again the chain rule, we arrive at

$$\begin{aligned} f''(u)[u_1, u_2] &= (G'(u)u_1, G'(u)u_2)_{L^2(\Omega)} + (G(u) - y_d, G''(u)[u_1, u_2])_{L^2(\Omega)} \\ &\quad + \kappa(u_1, u_2)_{L^2(\Omega)}. \end{aligned}$$

A similar discussion as above, where  $z = G''(u)[u_1, u_2]$  denotes the weak solution of (5), then gives  $(y - y_d, z)_{L^2(\Omega)} = -(d''(y) y_1 y_2, q)_{L^2(\Omega)}$ .  $\square$

*Remark 3.* Notice that, for a given right hand side in  $L^2(\Omega)$ , equation (8) admits a solution  $q$  in  $Y$ , since the differential operator in (8) has the same form as the one in (4).

Next, we substitute  $\lambda u + G(u) = v$  and consider the associated nonlinear equation

$$\lambda u + G(u) = v \quad (10)$$

for a given  $v$  in a neighborhood of  $\bar{v} = \lambda \bar{u} + G(\bar{u})$ . This substitution will be used for the transformation of (P) into a purely control-constrained problem. By the implicit function theorem, we show under a suitable regularity assumption that (10) admits a unique solution in a neighborhood of the optimal solution  $\bar{u}$  for all given  $v \in L^2(\Omega)$  in a neighborhood of  $\bar{v}$ . To this aim, we introduce an auxiliary operator  $T : L^2(\Omega) \times L^2(\Omega) \rightarrow L^2(\Omega)$  by  $T(u, v) = \lambda u + G(u) - v$ . Associated with  $T$  is a mapping  $K : v \mapsto u$  that is implicitly defined by  $T(K(v), v) = 0$ . To apply the implicit function theorem, we need that

$$\frac{\partial T}{\partial u}(\bar{u}, \bar{v})u = \lambda u + G'(\bar{u})u,$$

is invertible, where  $\bar{v} = \lambda \bar{u} + G(\bar{u})$ . Due to Lemma 1,  $G'(\bar{u})$  is continuous from  $L^2(\Omega)$  to  $H^1(\Omega) \cap C(\bar{\Omega})$ . Let us consider  $G'(\bar{u})$  with range in  $L^2(\Omega)$  and denote this operator by  $\mathbf{G}$ . Because of the compact embedding of  $H^1(\Omega)$  in  $L^2(\Omega)$ ,  $\mathbf{G}$  is compact, and hence  $\mathbf{G}$  represents a Fredholm operator that has only countably many eigenvalues accumulating at 0. Here and in the following,  $I : L^2(\Omega) \rightarrow L^2(\Omega)$  denotes the identity.

We rely on the following REGULARITY ASSUMPTION:

(R) The prescribed  $\lambda \neq 0$  is not an eigenvalue of  $-\mathbf{G}$ , i.e. the equation  $\lambda u + G'(\bar{u})u = 0$  admits only the trivial solution.

Note that this is fulfilled for all  $\lambda > 0$ .

From the theory of Fredholm operators, it is known that the equation

$$\frac{\partial T}{\partial u}(\bar{u}, \bar{v})u = \lambda u + G'(\bar{u})u = f$$

is uniquely solvable for given  $f \in L^2(\Omega)$ , provided that (R) is satisfied. Thus,  $\frac{\partial T}{\partial u}(\bar{u}, \bar{v})$  is continuously invertible by the Banach theorem, and hence the implicit function theorem gives the existence of open balls  $B_{r_1}(\bar{u})$ ,  $B_{\rho_1}(\bar{v})$  in  $L^2(\Omega)$  such that for all  $v \in B_{\rho_1}(\bar{v})$ , there is exactly one  $u \in B_{r_1}(\bar{u})$  with  $T(u, v) = 0$ . Therefore, by the definition of  $T$ , equation (10) has exactly one solution  $u \in B_{r_1}(\bar{u})$  for all  $v \in B_{\rho_1}(\bar{v})$ . Notice that  $K$  is of class  $C^2$  since  $T$  is twice continuously Fréchet differentiable in  $L^2(\Omega)$  with respect to  $u$ .

**Lemma 3.** *The first- and second-order derivatives of  $K : L^2(\Omega) \rightarrow L^2(\Omega)$  are given by*

$$K'(v) = \left( \lambda I + G'(K(v)) \right)^{-1}, \quad (11)$$

$$K''(v)[v_1, v_2] = - \left( \lambda I + G'(K(v)) \right)^{-1} G''(K(v))[K'(v)v_1, K'(v)v_2]. \quad (12)$$

*Proof:* As  $K$  is implicitly defined by  $T(K(v), v) = 0$ , the equation  $\lambda K(v) + G(K(v)) = v$  holds true for all  $v$  in a neighborhood of  $\bar{v}$ . Differentiating on both sides yields

$$\lambda K'(v) + G'(K(v))K'(v) = I, \quad (13)$$

which implies (11). Next, we apply both sides of (13) to  $v_1$  and differentiate in the direction  $v_2$ . One obtains

$$\lambda K''(v)[v_1, v_2] + G''(K(v))[K'(v)v_1, K'(v)v_2] + G'(K(v))K''(v)[v_1, v_2] = 0.$$

Resolving for  $K''(v)[v_1, v_2]$  immediately gives (12).  $\square$

With these results at hand, we can convert (P), at least locally around  $\bar{u}$ , into an optimization problem in the variable  $v$  by substituting  $\lambda u + G(u) = v$ . For the objective functional, we obtain

$$J(y, u) = f(u) = f(K(v)) =: F(v),$$

where  $F$  is defined at least on  $B_{\rho_1}(\bar{v})$ . Local optimality of  $\bar{u}$  implies the existence of an open ball  $B_{r_2}(\bar{u})$  in  $L^2(\Omega)$  such that  $f(\bar{u}) \leq f(u)$  for all  $u \in B_{r_2}(\bar{u})$  with  $y_a(x) \leq \lambda u(x) + y(x) \leq y_b(x)$ . This yields

$$F(\bar{v}) \leq F(v) \quad (14)$$

for all  $v \in L^2(\Omega)$  satisfying  $y_a(x) \leq v(x) \leq y_b(x)$  a.e. in  $\Omega$  and  $\|v - \bar{v}\|_{L^2(\Omega)} < \rho_2$  with a sufficiently small  $\rho_2 > 0$ . This  $\rho_2$  is taken so small so that  $\rho_2 \leq \rho_1$  and  $u = K(v) \in B_{r_2}(\bar{u})$ . Thus,  $\bar{v}$  is the optimal solution of

$$(PV) \begin{cases} \text{minimize} & F(v) \\ \text{subject to} & v \in V_{ad}, v \in B_{\rho_2}(\bar{v}) \end{cases}$$

with an admissible set defined by

$$V_{ad} := \{v \in L^2(\Omega) \mid y_a(x) \leq v(x) \leq y_b(x) \text{ a.e. in } \Omega\}.$$

Now, we are able to derive the following standard result.

**Lemma 4.** *Assume that (R) is fulfilled. Then the variational inequality*

$$F'(\bar{v})(v - \bar{v}) \geq 0 \quad (15)$$

*holds true for all  $v \in V_{ad}$ .*

*Proof:* Since  $V_{ad}$  is convex, we have for arbitrary  $v \in V_{ad}$  that  $v_t = \bar{v} + t(v - \bar{v}) \in V_{ad} \forall t \in [0, 1]$ . Moreover, we find  $\|v_t - \bar{v}\|_{L^2(\Omega)} < \rho_2$  if  $t$  is sufficiently small. Thus, (14) yields

$$\frac{F(\bar{v} + t(v - \bar{v})) - F(\bar{v})}{t} \geq 0.$$

Since  $f$  and  $K$  are Fréchet differentiable, the same holds for  $F$ . Thus, passing to the limit  $t \downarrow 0$  implies (15).  $\square$

By the Riesz theorem, the functional  $F'(\bar{v}) \in L^2(\Omega)^*$  can be identified with a function from  $L^2(\Omega)$ . Let us denote this function by  $\mu$ , i.e.

$$F'(\bar{v})v = \int_{\Omega} \mu(x) v(x) dx. \quad (16)$$

Furthermore, we define nonnegative functions  $\mu_a, \mu_b \in L^2(\Omega)$  by

$$\begin{aligned} \mu_a(x) &= \mu(x)_+ = \frac{1}{2}(\mu(x) + |\mu(x)|), \\ \mu_b(x) &= \mu(x)_- = \frac{1}{2}(-\mu(x) + |\mu(x)|). \end{aligned} \quad (17)$$

Then,  $\mu(x) = \mu_a(x) - \mu_b(x)$  and identifying  $F'(\bar{v})$  with  $\mu$  implies

$$F'(\bar{v}) + \mu_b - \mu_a = 0. \quad (18)$$

We show that the functions  $\mu_a, \mu_b$ , that have been defined by (17), are Lagrange multipliers for the control-state constraints (2). To see this, let us first set up the optimality system that should be satisfied at  $(\bar{y}, \bar{u})$ . We derive it in a formal way by the following Lagrange function  $\mathcal{L} : Y \times L^2(\Omega) \times H^1(\Omega) \times L^2(\Omega)^2 \rightarrow \mathbb{R}$ :

$$\begin{aligned} \mathcal{L}(y, u, p, \omega) &= J(y, u) - \int_{\Omega} \nabla y \cdot \nabla p dx - \int_{\Omega} d(y) p dx - \int_{\Gamma} y p ds + \int_{\Omega} u p dx \\ &\quad + \int_{\Omega} (\mu_b(\lambda u + y - y_b) + \mu_a(y_a - \lambda u - y)) dx \end{aligned} \quad (19)$$

with  $\omega := (\mu_a, \mu_b)$ . Note that the last integral is well defined because of  $\mu_a, \mu_b \in L^2(\Omega)$ . The optimality system consists of  $\partial \mathcal{L} / \partial y = 0$ ,  $\partial \mathcal{L} / \partial u = 0$  and the complementary slackness conditions. We show that this is the expected optimality system for  $(\bar{y}, \bar{u})$  following from the variational inequality (15) for  $\bar{v}$ . Straightforward computations give that  $\partial \mathcal{L} / \partial y(\bar{y}, \bar{u}, p, \omega)y = 0$  for all  $y \in H^1(\Omega)$  is equivalent to the adjoint equation

$$\begin{aligned} -\Delta p + d'(\bar{y})p &= \bar{y} - y_d + \mu_b - \mu_a && \text{in } \Omega \\ \partial_\nu p + p &= 0 && \text{on } \Gamma. \end{aligned} \quad (20)$$

Analogously,  $\partial \mathcal{L} / \partial u(\bar{y}, \bar{u}, p, \omega)u = 0$  for all  $u \in L^2(\Omega)$  corresponds to

$$\kappa \bar{u} + p + \lambda(\mu_b - \mu_a) = 0. \quad (21)$$

In the following, we will show that (20) and (21), together with the complementary slackness condition

$$(\mu_a, y_a - \lambda \bar{u} - \bar{y})_{L^2(\Omega)} = (\mu_b, \lambda \bar{u} + \bar{y} - y_b)_{L^2(\Omega)} = 0, \quad (22)$$

indeed follow from the variational inequality (15).

**Theorem 3.** *If  $\bar{u}$  is locally optimal with associated state  $\bar{y}$ , then there exist nonnegative Lagrange multipliers  $\mu_a \in L^\infty(\Omega)$  and  $\mu_b \in L^\infty(\Omega)$  and an associated adjoint state  $p \in H^1(\Omega) \cap C(\bar{\Omega})$  such that the adjoint equation (20), the condition (21), and the complementary slackness conditions (22) are satisfied.*

*Proof:* We show that  $\mu_a, \mu_b$  defined by (17) do this. Moreover, we verify  $\mu_a, \mu_b \in L^\infty(\Omega)$ . To this end, we first have to transfer all expressions in terms of  $v$  to such in terms of  $(y, u)$ .

(i) *Adjoint equation and condition (21):*

We start with equation (18) where we express  $F'$  in terms of  $f$  and  $u$ . We recall  $F(v) = f(K(v))$ . By the chain rule, it holds  $F'(\bar{v})v = f'(K(\bar{v}))K'(\bar{v})v$ . Hence, (18) is equivalent to

$$f'(K(\bar{v}))K'(\bar{v})v + (\mu_b - \mu_a, v)_{L^2(\Omega)} = 0 \quad \forall v \in L^2(\Omega).$$

By substituting  $u = K'(\bar{v})v$  and  $\bar{u} = K(\bar{v})$ , one obtains

$$f'(\bar{u})u + (\mu_b - \mu_a, K'(\bar{v})^{-1}u)_{L^2(\Omega)} = 0.$$

Moreover, we insert expression (11) for  $K'(\bar{v})$  and arrive at

$$f'(\bar{u})u + \left( \mu_b - \mu_a, (\lambda I + G'(\bar{u}))u \right)_{L^2(\Omega)} = 0. \quad (23)$$

Lemma 2, equation (7), shows that the first derivative of  $f$  is given by

$$f'(\bar{u})u = (\kappa \bar{u} + q_1, u)_{L^2(\Omega)}, \quad (24)$$

where  $q = q_1$  represents the solution of (8), with  $y = \bar{y}$  in the right hand side. Due to Remark 3, we have  $q_1 \in Y$  because of  $\bar{y} \in Y \subset L^2(\Omega)$ . For the second term in (23), we find

$$\left( \mu_b - \mu_a, (\lambda I + G'(\bar{u}))u \right)_{L^2(\Omega)} = \lambda(\mu_b - \mu_a, u)_{L^2(\Omega)} + (\mu_b - \mu_a, w)_{L^2(\Omega)}, \quad (25)$$

with  $w = G'(\bar{u})u$ , i.e.,  $w$  is the solution of the linearized equation (4) with  $y := \bar{y}$  and  $h := u$ . Arguing as in the proof of Lemma 2, we find



$$(\mu_b - \mu_a, w)_{L^2(\Omega)} = (q_2, u)_{L^2(\Omega)}, \quad (26)$$

where  $q_2$  solves the adjoint equation

$$\begin{aligned} -\Delta q_2 + d'(\bar{y}) q_2 &= \mu_b - \mu_a & \text{in } \Omega \\ \partial_\nu q_2 + q_2 &= 0 & \text{on } \Gamma. \end{aligned} \quad (27)$$

Again, this equation has the same structure as (4). From  $(\mu_b - \mu_a) \in L^2(\Omega)$ , we deduce  $q_2 \in Y$  (cf. Remark 3). Inserting (26), (25) and (24) in (23) yields

$$(\kappa \bar{u} + q_1 + q_2 + \lambda(\mu_b - \mu_a), u)_{L^2(\Omega)} = 0. \quad (28)$$

It is clear that  $p = q_1 + q_2$  solves the adjoint equation (20). Therefore, since  $v$  and hence  $u$  are arbitrary, (28) is equivalent with (21). Moreover, (21) implies

$$\mu_b - \mu_a = -\frac{1}{\lambda}(\kappa \bar{u} + p) \quad (29)$$

with  $p \in Y \subset C(\bar{\Omega})$  and  $\bar{u} \in L^\infty(\Omega)$  due to Remark 2. Thus, since  $\mu_a(x) \cdot \mu_b(x) = 0$  by definition (17), it follows that  $\mu_a, \mu_b \in L^\infty(\Omega)$ , because the right-hand side of (29) is bounded and measurable.

(ii) *Complementary slackness conditions:*

The variational inequality (15) and equation (16) give

$$F'(\bar{v})(v - \bar{v}) = \int_{\Omega} (\mu_a - \mu_b)(v - \bar{v}) dx \geq 0$$

for all  $v \in V_{ad}$  and thus

$$(\mu_a - \mu_b, \bar{v})_{L^2(\Omega)} = \min_{v \in V_{ad}} (\mu_a - \mu_b, v)_{L^2(\Omega)} = (\mu_a, y_a)_{L^2(\Omega)} - (\mu_b, y_b)_{L^2(\Omega)},$$

since  $\mu_a(x) \cdot \mu_b(x) = 0$  and  $\mu_a(x), \mu_b(x) \geq 0$  by definition (17). Therefore, if  $\mu_a(x) > 0$ , we have  $\bar{v}(x) = y_a(x)$ , while  $\mu_b(x) > 0$  implies  $\bar{v}(x) = y_b(x)$ . This immediately yields

$$(\mu_a, y_a - \bar{v})_{L^2(\Omega)} + (\mu_b, \bar{v} - y_b)_{L^2(\Omega)} = 0. \quad (30)$$

However, because of  $\mu_a(x), \mu_b(x) \geq 0$  and  $\bar{v} \in V_{ad}$ , both addends on the right side of (30) are nonpositive and thus we arrive at

$$(\mu_a, y_a - \bar{v})_{L^2(\Omega)} = (\mu_b, \bar{v} - y_b)_{L^2(\Omega)} = 0.$$

Together with  $\bar{v} = \lambda \bar{u} + G(\bar{u}) = \lambda \bar{u} + \bar{y}$ , this implies (22).  $\square$

## 4 Second-order sufficient conditions

As in case of first-order conditions in Section 3, the proof of second-order sufficient conditions for (P) is based on the results for the auxiliary problem (PV), which is an optimization problem with simple box-constraints. For problems of such type, the theory of second-order conditions is well-known. To formulate these conditions for (PV), we introduce the *strongly active set* as follows:

**Definition 1.** *Let  $\tau > 0$  be given. Then the strongly active set  $A_\tau$  is defined by*

$$A_\tau := \{x \in \Omega \mid \mu_a(x) + \mu_b(x) \geq \tau\}.$$

Notice that, according to (17),  $\mu_a$  and  $\mu_b$  cannot be jointly positive. Moreover, the corresponding  $\tau$ -critical cone with respect to  $v$  is defined in a standard way by

$$\hat{C}_\tau := \left\{ v \in L^2(\Omega) \left| \begin{array}{l} v(x) = 0, \text{ a.e. in } A_\tau \\ v(x) \geq 0, \text{ where } \bar{v}(x) = y_a(x) \text{ and } x \notin A_\tau \\ v(x) \leq 0, \text{ where } \bar{v}(x) = y_b(x) \text{ and } x \notin A_\tau \end{array} \right. \right\}, \quad (31)$$

with  $\bar{v} = \lambda \bar{u} + \bar{y}$  as defined above. With these definitions at hand, one can prove by standard arguments the following theorem covering the local optimality of  $\bar{v}$ , cf. eg. [5].

**Theorem 4.** *Suppose that  $\bar{v}$  is feasible for (PV) and satisfies the variational inequality (15). Assume further that the coercivity condition*

$$F''(\bar{v})v^2 \geq \tilde{\delta} \|v\|_{L^2(\Omega)}^2 \quad \forall v \in \hat{C}_\tau \quad (32)$$

*is satisfied with some  $\tilde{\delta} > 0$ . Then there exist  $\tilde{\varepsilon} > 0$  and  $\tilde{\sigma} > 0$  such that*

$$F(v) \geq F(\bar{v}) + \tilde{\sigma} \|v - \bar{v}\|_{L^2(\Omega)}^2 \quad (33)$$

*for all  $v \in V_{ad}$  with  $\|v - \bar{v}\|_{L^\infty(\Omega)} \leq \tilde{\varepsilon}$ .*

Due to (33), (15) and (32) yield local optimality of  $\bar{v}$  for (PV) and hence, (32) is a second-order sufficient optimality condition. It remains to transfer this condition to the original terms  $y$  and  $u$ .

For this reason, we need the following lemma on  $F''(\bar{v})$ .

**Lemma 5.** *Assume that (R) is fulfilled. Then  $F$  is twice continuously Fréchet differentiable at  $\bar{v}$  and its second derivative is given by*

$$F''(\bar{v})v^2 = \mathcal{L}''_{(y,u)}(\bar{y}, \bar{u}, p, \mu)(y, u)^2. \quad (34)$$

*Proof:* Thanks to  $F(v) = f(K(v))$  and (R), it is clear that  $F$  is twice continuously Fréchet differentiable in a neighborhood of  $\bar{v}$ . The chain rule implies

$$F''(v)[v_1, v_2] = f''(K(v))[K'(v)v_1, K'(v)v_2] + f'(K(v))K''(v)[v_1, v_2]. \quad (35)$$

We substitute  $v = \bar{v}$  and thus  $K(\bar{v}) = \bar{u}$ . Moreover, we set  $v_1 = v_2 = v$ , and  $K'(v)v_1 = K'(v)v_2 = K'(\bar{v})v = u$ . Hence, (35) is equivalent to

$$F''(\bar{v})v^2 = f''(\bar{u})u^2 + f'(\bar{u})K''(\bar{v})v^2.$$

In view of (23), we have for the second addend

$$f'(\bar{u})K''(\bar{v})v^2 = -\left(\mu_b - \mu_a, (\lambda I + G'(\bar{u}))K''(\bar{v})v^2\right)_{L^2(\Omega)}.$$

Together with the expression for  $K''(\bar{v})$  in (12), we arrive at

$$\begin{aligned} F''(\bar{v})v^2 &= f''(\bar{u})u^2 + (\mu_b - \mu_a, G''(\bar{u})[K'(\bar{v})v, K'(\bar{v})v])_{L^2(\Omega)} \\ &= f''(\bar{u})u^2 + (\mu_b - \mu_a, G''(\bar{u})u^2)_{L^2(\Omega)}. \end{aligned} \quad (36)$$

Since  $z = G''(\bar{u})u^2$  solves equation (5), similar arguments as in the proof of Lemma 2 give

$$(\mu_b - \mu_a, z)_{L^2(\Omega)} = -(d''(\bar{y})y^2, q_2)_{L^2(\Omega)},$$

where  $q_2$  is the solution of (27) and  $y = G'(\bar{u})u$ , i.e.  $y$  represents the solution of the linearized equation (4). Thus, together with (9) for the second derivative of  $f$  (see Lemma 2), (36) is transformed into

$$F''(\bar{v})v^2 = \|y\|_{L^2(\Omega)}^2 + \kappa \|u\|_{L^2(\Omega)}^2 - \int_{\Omega} d''(\bar{y})y^2 (q_1 + q_2) dx,$$

where  $q_1$  again denotes the solution of (8) with  $y = \bar{y}$  in the right side. As in the proof of Theorem 3, we have  $p = q_1 + q_2$  and hence we obtain

$$\begin{aligned} F''(\bar{v})v^2 &= \|y\|_{L^2(\Omega)}^2 + \kappa \|u\|_{L^2(\Omega)}^2 - \int_{\Omega} d''(\bar{y})y^2 p dx \\ &= J''_{(y,u)}(\bar{y}, \bar{u})(y, u)^2 - \int_{\Omega} d''(\bar{y})y^2 p dx = \mathcal{L}''_{(y,u)}(\bar{y}, \bar{u}, p, \mu)(y, u)^2, \end{aligned}$$

according to the definition of  $\mathcal{L}$  in (19).  $\square$

Based on (31), we define the  $\tau$ -critical cone for the original problem (P), denoted by  $C_\tau$  as follows:

**Definition 2.** (*Critical cone*) Let  $\hat{C}_\tau$  be defined as in (31). The critical cone associated to (P) is given by

$$C_\tau := \{(y, u) \in Y \times L^2(\Omega) \mid y = G'(\bar{u})u \quad \text{and} \quad \lambda u + y \in \hat{C}_\tau\}.$$

Now, we are able to state second-order sufficient conditions for (P).

$$(SSC) \quad \begin{cases} \text{Let } \delta > 0 \text{ exist such that} \\ \mathcal{L}''(\bar{y}, \bar{u}, p, \omega)(y, u)^2 \geq \delta \|u\|_{L^2(\Omega)}^2 \quad \text{for all } (y, u) \in C_\tau. \end{cases}$$

We show that (SSC) is indeed sufficient for local optimality of  $\bar{u}$ .

**Theorem 5.** Let  $(\bar{y}, \bar{u})$  satisfy the first-order necessary optimality conditions for Problem (P) and assume that condition (SSC) is fulfilled with some  $\delta > 0$ ,  $\tau > 0$ . Then there exist  $\varepsilon > 0$  and  $\sigma > 0$  such that

$$J(y, u) \geq J(\bar{y}, \bar{u}) + \sigma \|u - \bar{u}\|_{L^2(\Omega)}^2 \quad (37)$$

for all  $(y, u) \in Y \times L^2(\Omega)$  with  $y = G(u)$ ,  $y_a(x) \leq \lambda u(x) + y(x) \leq y_b(x)$ , and  $\|u - \bar{u}\|_{L^\infty(\Omega)} \leq \varepsilon$ .

*Proof:* First, we choose an arbitrary pair  $(\eta, h) \in C_\tau$  and define  $v := \lambda h + \eta$ . Notice that  $\eta = G'(\bar{u})h$  holds according to the definition of  $C_\tau$ . Due to Lemma 5, one obtains

$$F''(\bar{v})v^2 = L''_{(y,u)}(\bar{y}, \bar{u}, p, \mu)(\eta, h)^2 \geq \delta \|h\|_{L^2(\Omega)}^2, \quad (38)$$

where we used condition (SSC) for the last estimate. Due to  $h = (\lambda I + G'(\bar{u}))^{-1}v$ , (38) is equivalent to

$$\begin{aligned} F''(\bar{v})v^2 &\geq \delta \|(\lambda I + G'(\bar{u}))^{-1}v\|_{L^2(\Omega)}^2 \\ &\geq \delta \left( \frac{1}{\|\lambda I + G'(\bar{u})\|_{\mathcal{L}(L^2(\Omega))}} \|v\|_{L^2(\Omega)} \right)^2 \\ &\geq \delta \|\lambda I + G'(\bar{u})\|_{\mathcal{L}(L^2(\Omega))}^{-2} \|v\|_{L^2(\Omega)}^2 \\ &= \tilde{\delta} \|v\|_{L^2(\Omega)}^2, \end{aligned} \quad (39)$$

with  $\tilde{\delta} > 0$ . Because of  $(\eta, h) \in C_\tau$ , clearly  $v \in \hat{C}_\tau$  holds true. Moreover, thanks to (R), every  $v \in \hat{C}_\tau$  can be expressed by some  $(\eta, h) \in C_\tau$ , and hence (39) holds true for all  $v \in \hat{C}_\tau$ . In this way,  $F''$  satisfies a coercivity condition and thus, Theorem 4 yields

$$F(v) \geq F(\bar{v}) + \tilde{\sigma} \|v - \bar{v}\|_{L^2(\Omega)}^2 \quad (40)$$

for all  $v \in V_{ad}$  with  $\|v - \bar{v}\|_{L^\infty(\Omega)} \leq \tilde{\varepsilon}$ . In particular, we may take

$$v = \lambda u + G(u),$$

where  $u$  is taken arbitrary with  $y_a(x) \leq \lambda u(x) + G(u)(x) \leq y_b(x)$  and  $\|u - \bar{u}\|_{L^\infty(\Omega)} \leq \varepsilon$  such that  $\|v - \bar{v}\|_{L^\infty(\Omega)} \leq \tilde{\varepsilon}$  and  $\|v - \bar{v}\|_{L^2(\Omega)} \leq \rho_1$ . Notice that, because of (R), to every  $v \in V_{ad}$  with  $\|v - \bar{v}\|_{L^2(\Omega)} \leq \rho_1$  a function  $u$  exists with  $u = K(v)$  and  $\|u - \bar{u}\|_{L^2(\Omega)} \leq r_1$ . On the other hand, the continuity of the mapping  $\lambda I + G$  from  $L^\infty(\Omega)$  to  $L^\infty(\Omega)$  ensures that  $\|u - \bar{u}\|_{L^\infty(\Omega)} \leq \varepsilon$  implies  $\|v - \bar{v}\|_{L^\infty} \leq r$ . If we take  $\varepsilon$  sufficiently small, then it follows that  $r \leq \tilde{\varepsilon}$  and  $\|v - \bar{v}\|_{L^2(\Omega)} \leq c \|v - \bar{v}\|_{L^\infty(\Omega)} \leq \rho_1$ . Hence, for all  $u$  with  $\|u - \bar{u}\|_{L^\infty(\Omega)} \leq \varepsilon$ , there exists a  $v$  with  $\lambda u + G(u) = v$  and with  $\|v - \bar{v}\|_{L^\infty(\Omega)} \leq \tilde{\varepsilon}$ . Then, with  $F(v) = f(u)$  and  $F(\bar{v}) = f(\bar{u})$ , (40) gives

$$f(u) \geq f(\bar{u}) + \tilde{\sigma} \|\lambda u + G(u) - (\lambda \bar{u} + G(\bar{u}))\|_{L^2(\Omega)}^2 \quad (41)$$

for all  $u$  with  $\lambda u + G(u) \in V_{ad}$  and  $\|u - \bar{u}\|_{L^\infty(\Omega)} \leq \varepsilon$ . This already implies the local optimality of  $\bar{u}$ . It remains to show the quadratic growth condition (37). A Taylor expansion for the last term in (41) yields

$$\lambda u + G(u) - (\lambda \bar{u} + G(\bar{u})) = \lambda(u - \bar{u}) + G'(\bar{u})(u - \bar{u}) + r_1^G(\bar{u}, u - \bar{u}),$$

and, since  $G$  is continuously Fréchet differentiable from  $L^2(\Omega)$  to  $Y$  (see Lemma 1), the remainder term satisfies

$$\frac{\|r_1^G\|_{L^2(\Omega)}}{\|u - \bar{u}\|_{L^2(\Omega)}} \rightarrow 0, \quad \text{as } \|u - \bar{u}\|_{L^2(\Omega)} \rightarrow 0. \quad (42)$$

Therefore, we obtain

$$\begin{aligned} & \|\lambda u + G(u) - (\lambda \bar{u} + G(\bar{u}))\|_{L^2(\Omega)} \\ &= \|(\lambda I + G'(\bar{u}))(u - \bar{u}) + r_1^G\|_{L^2(\Omega)} \\ &\geq \|(\lambda I + G'(\bar{u}))(u - \bar{u})\|_{L^2(\Omega)} - \|r_1^G\|_{L^2(\Omega)} \\ &\geq \left( \frac{1}{\|(\lambda I + G'(\bar{u}))^{-1}\|_{\mathcal{L}(L^2(\Omega))}} - \frac{\|r_1^G\|_{L^2(\Omega)}}{\|u - \bar{u}\|_{L^2(\Omega)}} \right) \|u - \bar{u}\|_{L^2(\Omega)} \\ &\geq \tilde{c} \|u - \bar{u}\|_{L^2(\Omega)}. \end{aligned}$$

Since  $(\lambda I + G'(\bar{u}))$  is continuously invertible because of (R), (42) yields  $\tilde{c} > 0$  if  $\|u - \bar{u}\|_{L^2(\Omega)}$  is sufficiently small. Thus (41) implies

$$f(u) \geq f(\bar{u}) + \tilde{\sigma} \tilde{c}^2 \|u - \bar{u}\|_{L^2(\Omega)}^2 = f(\bar{u}) + \sigma \|u - \bar{u}\|_{L^2(\Omega)}^2. \quad \square$$

*Remark 4.* Clearly, due to (37),  $\bar{u}$  is a strict optimal solution.

## 5 Numerical tests

For our numerical tests, we consider an optimal control problem that differs slightly from (P), as already mentioned in Remark 1. Instead of (1), the state equation is now given by

$$\begin{aligned} -\Delta y(x) + y(x) + d(y(x)) &= u(x) && \text{in } \Omega \\ \partial_\nu y(x) &= 0 && \text{on } \Gamma. \end{aligned} \quad (43)$$

One can easily verify that the theory presented above is also valid with the new state equation (43).

We investigated two examples with different nonlinearities  $d(y)$ . In both cases, the desired state was given by

$$y_d(x_1, x_2) = 8 \sin(\pi x_1) \sin(\pi x_2) - 4$$

and the bounds were fixed at  $y_a(x_1, x_2) \equiv -1$  and  $y_b(x_1, x_2) \equiv 1$ . The Tikhonov regularization parameter was set to  $\kappa = 0.5 \cdot 10^{-5}$ . Moreover, to approximate a purely state constrained problem, we fixed  $\lambda = 0.5 \cdot 10^{-5}$ . In the first example, the nonlinearity was defined by

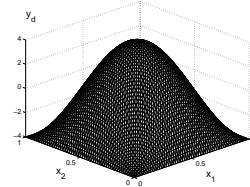
$$d(y) = y^3, \quad (44)$$

whereas we took

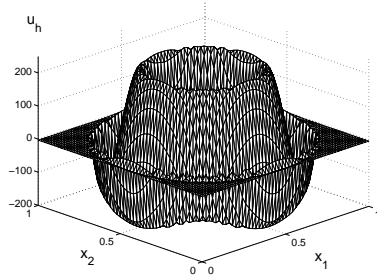
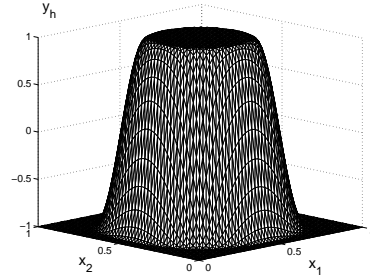
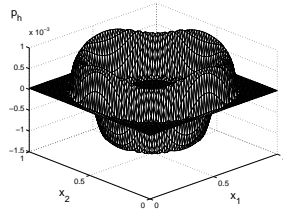
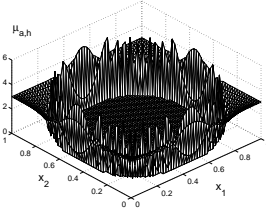
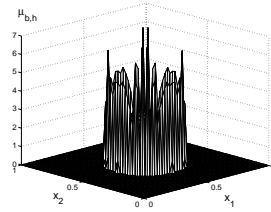
$$d(y) = e^{5y} \quad (45)$$

in the second one. Thus, the assumptions on  $d$  mentioned in Section 1, are fulfilled in both cases.

The optimization problems were solved numerically by a SQP method that is described in detail for instance in [8] or [9]. To solve the arising linear quadratic problems, a primal-dual active set strategy was applied, see for instance [1] or [3]. We used a conforming finite element method with linear ansatz functions to solve the state equation and the adjoint equation. For all computations, uniform meshes were used. The number of intervals in one dimension, denoted by  $N$ , is related to the mesh-size, i.e. the diameter of the triangles, by  $h = \sqrt{2}N^{-1}$ . The following figures show the numerical solution for the first example. This computation was performed with a mesh size  $N=50$ . Here and in the following, the numerical solutions are denoted by the subscript  $h$ .



**Fig. 1.** Desired state  $y_d$ .

Fig. 2. Control  $u_h$  in the first example.Fig. 3. State  $y_h$  in the first example.Fig. 4. Adjoint state  $p_h$ .Fig. 5. Lagrange multiplier  $\mu_{a,h}$ .Fig. 6. Lagrange multiplier  $\mu_{b,h}$ .

As one can see in the Figures 5 and 6, the Lagrange multipliers tend to be irregular on the boundaries of the active sets. This might indicate that the Lagrange multipliers associated with the state constraints for  $\lambda = 0$  should be measures. This verifies the known theory, see for instance Casas [4] or Bergounioux and Kunisch [2]. However, in view of (21) with  $p = G'(\bar{u})^*(G(\bar{u}) - y_d + \mu)$ , the equation for  $\mu = \mu_a - \mu_b$  is given by

$$\lambda \mu + G'(\bar{u})^* \mu = G'(\bar{u})^*(y_d - G(\bar{u})) - \kappa \bar{u}$$

with a compact operator  $G'(\bar{u})^* : L^2(\Omega) \rightarrow L^2(\Omega)$ . This equation is ill-posed for  $\lambda = 0$ . Therefore, as  $\lambda = 0.5 \cdot 10^{-5}$  is chosen quite small, we are faced with the characteristic difficulties of ill-posed problems. In view of this, the computed Lagrange multipliers are certainly overlaid by rounding errors that are difficult to quantify.

To describe the convergence behaviour of the algorithm, the values of the discrete objective functional  $J_h = 1/2 \|y_h - y_d\|_{L^2(\Omega)}^2 + \kappa/2 \|u_h\|_{L^2(\Omega)}^2$  are displayed in the following Tables 1-3 for each step of the SQP-iteration, denoted by  $its_{SQP}$ . As a further convergence indicator, the error in the semilinear state

equation is approximated by

$$e_y = \frac{\|G_h^{-1}(y_h) - u_h\|_{L^2(\Omega)}}{\|y_h\|_{L^2(\Omega)}},$$

where  $G_h$  denotes the discrete control-to-state operator  $G_h : u_h \mapsto y_h$ . Thus,  $e_y$  quantifies the relative error of the discrete analogon of  $-\Delta y + c y + d(y) - u$ , i.e. the error in the semilinear state equation. Similarly the error in the adjoint equation is measured by

$$e_p = \frac{\|(G'_h(y_h)^{-1})^* p_h - (y_h - y_d + \mu_{b,h} - \mu_{a,h})\|_{L^2(\Omega)}}{\|p_h\|_{L^2(\Omega)}},$$

where  $(G'_h(y_h)^{-1})^*$  is associated with  $-\Delta p + c p + d'(y) p$ . Furthermore, the error in the necessary condition (21) is approximated by

$$e_{opt} = \|\kappa u_h + p_h + \lambda(\mu_{b,h} - \mu_{a,h})\|_{L^2(\Omega)}.$$

The difference between two consecutive iterates, quantified by

$$\delta = \frac{1}{3} \left( \frac{\|u_h^{(n)} - u_h^{(n+1)}\|_{L^2(\Omega)}}{\|u_h^{(n+1)}\|_{L^2(\Omega)}} + \frac{\|y_h^{(n)} - y_h^{(n+1)}\|_{L^2(\Omega)}}{\|y_h^{(n+1)}\|_{L^2(\Omega)}} + \frac{\|p_h^{(n)} - p_h^{(n+1)}\|_{L^2(\Omega)}}{\|p_h^{(n+1)}\|_{L^2(\Omega)}} \right),$$

was used for the termination condition of the SQP method. More precisely, the iteration stopped if  $\delta < 10^{-2}$ . The following table shows the convergence behavior in the first example for a mesh size of  $N=50$ . In addition to the values of  $J_h$  and the error approximations described above, the number of active set iterations denoted by  $it_{AS}$  is shown in the last column.

**Table 1.** Example 1 with  $N=50$

$it_{SQP}$	$J_h$	$e_{opt}$	$e_y$	$e_p$	$\delta$	$\#it_{AS}$
0	3.1099e+00	1.0000e+00	3.5361e-03	9.1101e-04	-	
1	1.3793e+00	4.1930e-20	3.4860e-04	3.7443e-01	5.7686e+02	13
2	1.3757e+00	3.5225e-20	3.7393e-04	4.4817e-05	2.5864e-01	6
3	1.3757e+00	3.3836e-20	3.6347e-04	2.1590e-11	3.3737e-04	1

We observe that  $e_p$  is much smaller than  $e_y$ . A possible explanation for this fact could be that the adjoint equation represents a linear PDE in contrast to the semilinear state equation.

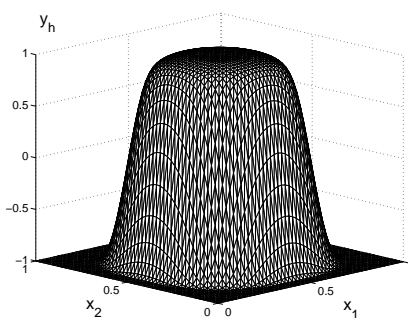
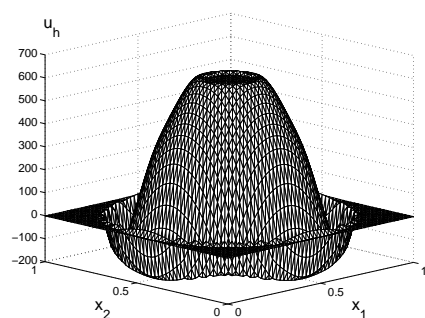
Table 2 illustrates the convergence behaviour in the first example for  $N=100$ . As one can see, the error in the approximation of the PDEs is reduced significantly. However, the value of the discrete objective functional is not decreased noticeably.



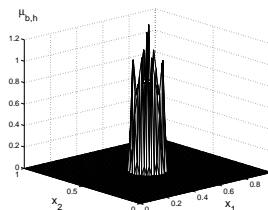
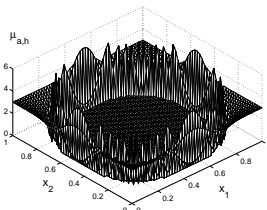
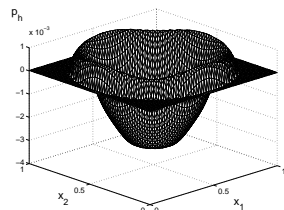
**Table 2.** Example 1 with  $N=100$ 

itsQP	$J_h$	$e_{opt}$	$e_y$	$e_p$	$\delta$	#it <sub>AS</sub>
0	3.1112e+00	1.0000e+00	8.9151e-04	2.3143e-04	-	-
1	1.3800e+00	4.0038e-20	8.8727e-05	9.3948e-02	5.6869e+02	23
2	1.3757e+00	3.3583e-20	9.5252e-05	1.2688e-05	2.6991e-01	8
3	1.3757e+00	3.3876e-20	9.2619e-05	6.4219e-12	3.3493e-04	1

Figures 7–11 show the numerical solution of the second example for  $N=50$ . Again, the Lagrange multipliers are comparatively irregular on the borders of the active sets.



**Fig. 7.** Control  $u_h$  in the second exam- **Fig. 8.** State  $y_h$  in the second example.



**Fig. 9.** Adjoint state  $p_h$ . **Fig. 10.** Lagrange multiplier  $\mu_{a,h}$ . **Fig. 11.** Lagrange multiplier  $\mu_{b,h}$ .

The convergence behavior of the algorithm in this example is illustrated in Table 3. The nonlinearity  $d(y) = e^{5y}$  of this example is much steeper than  $d(y) = y^3$ . Therefore, the number of SQP-iterations is larger than for  $d(y) = y^3$ .

**Table 3.** Example 2 with N=50

it <sub>SQP</sub>	$J_h$	$e_{opt}$	$e_y$	$e_p$	$\delta$	#it <sub>AS</sub>
0	3.1099e+00	1.0000e+00	2.9450e-03	3.4595e-03	-	-
1	3.2742e+00	1.9729e-20	1.9334e-02	3.7889e+00	1.2591e+03	1
2	1.3780e+00	3.6935e-20	2.9660e-02	9.8747e-02	1.1220e+00	13
3	1.5610e+00	8.9187e-20	8.8222e-02	8.0814e-02	5.8821e-01	14
4	1.4711e+00	7.3050e-20	5.4490e-02	6.1055e-03	2.0554e-01	10
5	1.5523e+00	8.6599e-20	8.5751e-02	1.2353e-02	1.8589e-01	10
6	1.5102e+00	8.5926e-20	6.9141e-02	1.2245e-03	8.9151e-02	7
7	1.5449e+00	8.2400e-20	8.2864e-02	1.7494e-03	7.2685e-02	8
8	1.5203e+00	8.3514e-20	7.2910e-02	6.1815e-04	5.2567e-02	5
9	1.5392e+00	8.9509e-20	8.0637e-02	4.7578e-04	3.9750e-02	5
10	1.5248e+00	8.7443e-20	7.4701e-02	2.4842e-04	3.1121e-02	5
11	1.5357e+00	9.0720e-20	7.9241e-02	1.6924e-04	2.3635e-02	4
12	1.5275e+00	8.2449e-20	7.5798e-02	9.1957e-05	1.8277e-02	5
13	1.5337e+00	8.5332e-20	7.8403e-02	5.9436e-05	1.3928e-02	3
14	1.5291e+00	8.6704e-20	7.6457e-02	3.2479e-05	1.0600e-02	3
15	1.5325e+00	8.4110e-20	7.7909e-02	1.9987e-05	8.0250e-03	3

## References

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