Optimization Techniques for Solving Elliptic Control Problems with Control and State Constraints: Part 1. Boundary Control

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Abstract. We study optimal control problems for semilinear elliptic equations subject to control and state inequality constraints. In a first part we consider boundary control problems with either Dirichlet or Neumann conditions. By introducing suitable discretization schemes, the control problem is transcribed into a nonlinear programming problem. It is shown that a recently developed interior point method is able to solve these problems even for high discretizations. Several numerical examples with Dirichlet and Neumann boundary conditions are provided that illustrate the performance of the algorithm for different types of controls including bang-bang and singular controls. The necessary conditions of optimality are checked numerically in the presence of active control and state constraints.

Keywords: elliptic control problems, boundary control, control and state constraints, discretization techniques, interior point optimization methods

1. Introduction

This is the first part of two papers in which we develop nonlinear programming techniques for solving elliptic control problems under general control and state inequality constraints. In the first part, we study boundary control problems with boundary conditions of either Dirichlet or Neumann type. The second part is devoted to elliptic problems with distributed control.

There are several recent papers on both the theoretical treatment and numerical solution methods for elliptic control problems. First order necessary and second order sufficient optimality conditions for Neumann boundary conditions have been given in Casas [9] and Casas et al. [10, 11]. First order necessary conditions for linear operators and Dirichlet or Neumann boundary conditions are obtained in Bergounioux, Kunisch [3], Ito, Kunisch [16], Kunisch, Volkwein [18]. These authors have demonstrated that an augmented Lagrangian techniques combined with a SQP approach lead to first order conditions and provide an efficient numerical algorithm.

Despite this work on elliptic problems, we feel it worthwhile to consider these problems from a more systematic numerical point of view. We treat semilinear elliptic operators
and concentrate on handling possibly nonlinear control and state constraints jointly. Our numerical approach will be able to capture also controls of bang-bang or singular type for which the Legendre condition is not satisfied. This type of control is well studied for ODE control problems, but we are not aware of any numerical example for elliptic problems although Hettich et al. [14, 15] present some theoretical work on the subject. Moreover, we analyze adjoint variables corresponding to equality and inequality constraints in the discretized problem. This enables us to check first order necessary conditions explicitly in the presence of active control and state constraints. As a byproduct, we give an informal form of first order necessary conditions for problems with Dirichlet boundary control. Such conditions have not been given in the literature to full extent so far.

In the application of NLP-techniques to optimal control, there are two components that have been extensively worked out for ODE control problems; cf., e.g., Barclay et al. [1], Betts [4], Betts, Huffmann [5], Büskens [7], Büskens, Maurer [8], Grachev, Evtushenko [13], Teo et al. [22]. The first aspect concerns the suitable choice of a discretization scheme while the other is the selection of the NLP-method. One has two options for the discretization scheme. The first one is to discretize both the control and state variables and to incorporate the integration method as an explicit equality constraint at each gridpoint. This approach leads to a high-dimensional NLP-problem with a sparse structure of the Jacobian; cf. Barclay et al. [1]. The other discretization approach consists in treating the discretized control variables as the only optimization variables while the state variable is expressed and computed as a function of the control variable. This leads to a lower-dimensional NLP with a rather dense Jacobian. However, in this approach derivatives usually can not be calculated explicitly but only through a numerical differentiation scheme.

In this paper, we formulate NLP-problems using a full discretization scheme where the optimization variables comprise both the control and state variables. The resulting NLP-problems may contain up to 40,000 variables. To solve such a high-dimensional and sparse NLP-problem, the interior point method developed by Vanderbei, Shanno [23] has turned out to be particularly efficient and reliable.

The organization of the first part is the following. In Section 2 we discuss necessary optimality conditions for elliptic problems with Neumann boundary control. Necessary optimality conditions for problems with Dirichlet boundary conditions have not yet been developed in the literature for the general problem considered here. In Section 3 we state an informal form of such necessary conditions. Section 4 formulates NLP-problems associated with discretized versions of the elliptic problems. Necessary conditions of Kuhn-Tucker type are discussed both for Dirichlet and Neumann boundary conditions. Finally, in Section 5 we present several numerical examples for both types of boundary conditions. Example 5.2 exhibits a singular control while Examples 5.4, 5.6 and 5.8 present bang-bang controls.

2. Elliptic control problems with Neumann boundary conditions

The following elliptic control problem with control and state constraints constitutes a generalization of elliptic problems considered in Casas [9], Casas et al. [10, 11], Ito, Kunisch [16], Kunisch, Volkwein [18]. The problem is to determine a control \( u \in L^\infty(\Gamma) \) that minimizes
the functional
\[ F(y, u) = \int_{\Omega} f(x, y(x)) \, dx + \int_{\Gamma} g(x, y(x), u(x)) \, dx \] (2.1)

subject to the state equation
\[ -\Delta y(x) + d(x, y(x)) = 0, \quad \text{for } x \in \Omega, \]
\[ \partial_n y(x) = b(x, y(x), u(x)), \quad \text{for } x \in \Gamma, \] (2.2)

and the inequality constraints on control and state
\[ C(x, y(x), u(x)) \leq 0, \quad \text{for } x \in \Gamma, \]
\[ S(x, y(x)) \leq 0, \quad \text{for } x \in \bar{\Omega}. \] (2.3)

In this setting, \( \Omega \subset \mathbb{R}^2 \) is a bounded domain with piecewise smooth boundary \( \Gamma = \partial \bar{\Omega} \). The derivative in the direction of the outward unit normal \( \partial_n \) in (2.2). Note that the state inequality constraints (2.4) are supposed to hold on the closure of \( \Omega \).

The Laplacian \(-\Delta\) in (2.2) can be replaced by an elliptic operator
\[ Ay(x) = -\sum_{k,j=1}^2 \partial_{x_j} \left( a_{ij}(\cdot) \partial_{x_j} y \right)(x), \]

where the coefficients \( a_{ij} \in C^2(\bar{\Omega}) \) satisfy the following coercivity condition with some \( c > 0 \):
\[ \sum_{k,j=1}^2 a_{ij}(x) v_k v_j \geq c \left( v_1^2 + v_2^2 \right), \quad \forall x \in \bar{\Omega}, \quad v \in \mathbb{R}^2. \]

However, in the sequel we restrict the discussion to the operator \( A = -\Delta \) which simplifies the form of the necessary conditions and the presentation of the numerical approach in Section 4. The functions \( f : \Omega \times \mathbb{R} \to \mathbb{R}, \ g : \Gamma \times \mathbb{R}^2 \to \mathbb{R}, \ d : \Omega \times \mathbb{R} \to \mathbb{R}, \ b : \Gamma \times \mathbb{R}^2 \to \mathbb{R}, \ C : \Gamma \times \mathbb{R}^2 \to \mathbb{R} \) and \( S : \bar{\Omega} \times \mathbb{R} \to \mathbb{R} \) are assumed to be \( C^2 \)-functions. It is straightforward to include more than one inequality constraint into (2.3) or (2.4). However, since both the state and control variable are scalar variables, the active sets for different inequality constraints are disjoint and hence can be treated separately.

Then under appropriate assumptions on the function \( d \) it can be shown that the state Eq. (2.2) admits for each \( u \in L^\infty(\Gamma) \) a weak solution \( y \in Y = C(\bar{\Omega}) \cap H^1(\Omega) \) (cf. Casas et al. [10]), i.e., it holds
\[ \int_{\Omega} [\Delta y(x) \Delta v(x) + d(x, y(x)) v(x)] \, dx = \int_{\Gamma} b(x, y(x), u(x)) v(x) \, dx \]

for all \( v \in H^1(\Omega) \). An optimal solution of problem (2.1)–(2.4) will be denoted by \( \bar{u} \) and \( \bar{y} \). From [10] we infer the further assumption that the function \( b \) in the Neumann condition
(2.2) is sufficiently smooth and satisfies the following inequality with suitable \( \epsilon > 0 \),

\[
  b_{\gamma}(x, y, u) \leq 0 \quad \text{for all } x \in \Gamma, \ |y - \bar{y}(x)| < \epsilon, \ |u - \bar{u}(x)| < \epsilon. \tag{2.5}
\]

Questions of existence of optimal solutions will not be discussed here. The active sets for the inequality constraints (2.3) and (2.4) are defined by

\[
  J(C) := \{ x \in \Gamma \mid C(x, y(x), \bar{u}(x)) = 0 \}, \quad J(S) := \{ x \in \Omega \mid S(x, y(x)) = 0 \}.
\]

It is required that the following regularity conditions hold:

\[
  C_u(x, y(x), \bar{u}(x)) \neq 0 \quad \forall x \in J(C), \quad S_u(x, y(x)) \neq 0 \quad \forall x \in J(S). \tag{2.6}
\]

Here and in the following, partial derivatives are denoted by subscripts.

First order optimality conditions for a local optimal solution \( \bar{u} \) and \( \bar{y} \) can be derived by generalizing the line of proof in Casas [9], Casas et al. [10, 11]. Problem (2.1)–(2.4) is considered as a mathematical programming problem in Banach spaces to which the first order Kuhn-Tucker conditions are applicable. In particular, this approach requires that the complementarity condition given in Zowe, Kurcyusz [24] is satisfied; cf. Casas et al. [11]. We do not discuss this regularity condition in detail although condition (2.6) forms part of it. The first order necessary conditions imply that there exist an adjoint state \( \bar{q} \in W^{1,1}(\Omega) \), a multiplier \( \bar{\lambda} \in L^\infty(\Gamma) \), and a bounded Borel measure \( \bar{\mu} \) on \( \Omega \) such that the following three conditions hold,

1. \textit{adjoint equation:}

\[
  -\Delta \bar{q}(x) + \bar{q}(x)d_{\gamma}(x, y(x)) + f_{\gamma}(x, y(x)) + S_{\gamma}(x, y(x)) \bar{\mu} = 0 \quad \text{on } \Omega, \tag{2.7}
\]

\[
  \partial_{\gamma} \bar{q}(x) - \bar{q}(x)b_{\gamma}(x, y(x), \bar{u}(x)) + g_{\gamma}(x, y(x), \bar{u}(x)) \\
  + \bar{\lambda}(x)C_{\gamma}(x, y(x), \bar{u}(x)) + S_{\gamma}(x, y(x)) \bar{\mu} = 0 \quad \text{on } \Gamma, \tag{2.8}
\]

2. \textit{minimum condition on } \Gamma:

\[
  g_u(x, y(x), \bar{u}(x)) - \bar{q}(x)b_u(x, y(x), \bar{u}(x)) + \bar{\lambda}(x)C_u(x, y(x), \bar{u}(x)) = 0, \tag{2.9}
\]

3. \textit{complementarity condition:}

\[
  \bar{\lambda}(x) \geq 0 \quad \text{on } J(C), \quad \bar{\lambda}(x) = 0 \quad \text{on } \Gamma \setminus J(C), \\
  d\bar{\mu} \geq 0 \quad \text{on } J(S), \quad d\bar{\mu} = 0 \quad \text{on } \Omega \setminus J(S). \tag{2.10}
\]

The adjoint Eqs. (2.7), (2.8) are understood in the weak sense, cf. Casas et al. [11]. According to Bourbaki [6], Chapter 9, the bounded Borel measure \( \bar{\mu} \) appearing in the adjoint Eqs. (2.7), (2.8) has the decomposition

\[
  \bar{\mu} = \bar{v} \cdot dx + \bar{v}_s \cdot \bar{\mu}_s, \tag{2.11}
\]
where \( dx \) represents the Lebesgue measure and \( \bar{\mu} \) is singular with respect to \( dx \); the functions \( \bar{v}, \bar{v}_t \) are measurable on \( \tilde{\Omega} \). The problem of obtaining the decomposition (2.11) explicitly is related to the difficulty of determining the structure of the active set \( J(S) \). To our knowledge, the literature does not contain any numerical examples where the decomposition (2.11) has actually been computed. In Section 4, we shall make an attempt to approximate the measure by the multipliers of the discretized problem.

In later applications, we shall mostly deal with cost functionals of tracking type (cf. Ito, Kunisch [16]),

\[
F(y, u) = \frac{1}{2} \int_{\Omega} (y(x) - y_d(x))^2 \, dx + \frac{\alpha}{2} \int_{\Gamma} (u(x) - u_d(x))^2 \, dx
\]  

(2.12)

with given functions \( y_d \in C(\tilde{\Omega}), u_d \in L^\infty(\Gamma) \), and a nonnegative weight \( \alpha \geq 0 \). The control and state constraints (2.3) and (2.4) are supposed to be box constraints of the simple type

\[
y(x) \leq \psi(x) \quad \text{on} \quad \Omega, \quad u_1(x) \leq u(x) \leq u_2(x) \quad \text{on} \quad \Gamma,
\]  

(2.13)

with functions \( \psi \in C(\tilde{\Omega}) \) and \( u_1, u_2 \in L^\infty(\Gamma) \). For these data the adjoint Eqs. (2.7), (2.8) become

\[
\begin{align*}
-\Delta \bar{q}(x) + \bar{q}(x)d_y(x, \bar{y}(x)) + \bar{y}(x) - y_d(x) + \bar{\mu} &= 0 \quad \text{on} \quad \Omega, \\
\partial_y \bar{q}(x) - \bar{q}(x)b_y(x, \bar{y}(x), \bar{u}(x)) + \bar{\lambda}(x)C_y(x, \bar{y}(x), \bar{u}(x)) &= 0 \quad \text{on} \quad \Gamma.
\end{align*}
\]  

(2.14)

If the function \( b \) in (2.2) has the form \( b(x, y, u) = u + b_0(x, y), \) i.e., if \( b_u \equiv 1 \) holds, then the minimum condition (2.9) reduces to

\[
[u(\bar{u}(x) - u_d(x)) - \bar{q}(x)][u - \bar{u}(x)] \geq 0 \quad \forall x \in \Gamma, u \in [u_1(x), u_2(x)].
\]  

(2.15)

Case \( \alpha > 0 \): condition (2.15) shows that the control \( u(x) \) is given by the projection of \( u_d(x) + \bar{q}(x)/\alpha \) on the interval \([u_1(x), u_2(x)]\) which can be stated more explicitly as

\[
\bar{u}(x) = \begin{cases} 
  u_d(x) + \bar{q}(x)/\alpha, & \text{if } u_d(x) + \bar{q}(x)/\alpha \in (u_1(x), u_2(x)), \\
  u_1(x), & \text{if } u_d(x) + \bar{q}(x)/\alpha \leq u_1(x), \\
  u_2(x), & \text{if } u_d(x) + \bar{q}(x)/\alpha \geq u_2(x).
\end{cases}
\]  

(2.16)

Case \( \alpha = 0 \): we obtain an optimal control of bang-bang or singular type:

\[
\bar{u}(x) = \begin{cases} 
  u_1(x), & \text{if } \bar{q}(x) < 0, \\
  u_2(x), & \text{if } \bar{q}(x) > 0, \\
  \text{singular}, & \text{if } \bar{q}(x) = 0 \quad \text{on} \quad \Gamma_s \subset \Gamma, \, \text{meas}(\Gamma_s) > 0.
\end{cases}
\]  

(2.17)

Thus, for \( \alpha = 0 \) the adjoint function \( \bar{q}(x) \) on the boundary plays the role of a switching function. The isolated zeros of \( \bar{q}(x)|_\Gamma \) are the switching points of a bang-bang control.
3. Elliptic control problems with Dirichlet boundary conditions

The following elliptic control problem with control and state constraints generalizes the elliptic problems considered in Bergounioux, Kunisch [3], Ito, Kunisch [16]. When admitting Dirichlet boundary conditions, the functions \( g \) in the cost functional (2.1), \( b \) in the boundary conditions (2.2), and \( C \) in the constraints (2.3) do not depend on the state variable \( y \). This leads to the problem of finding a control \( u \in L^\infty \) that minimizes the functional

\[
F(y, u) = \int_{\Omega} f(x, y(x)) \, dx + \int_{\Gamma} g(x, u(x)) \, dx
\]  

subject to the state equation

\[
-\Delta y(x) + d(x, y(x)) = 0, \quad \text{for } x \in \Omega,
\]

\[
y(x) = b(x, u(x)), \quad \text{for } x \in \Gamma,
\]  

and the inequality constraints on control and state

\[
C(x, u(x)) \leq 0, \quad \text{for } x \in \Gamma, \tag{3.3}
\]

\[
S(x, y(x)) \leq 0, \quad \text{for } x \in \Omega. \tag{3.4}
\]

When treating Dirichlet boundary conditions, an intrinsic difficulty arises from the fact that the solution operator \( u(\cdot)\big|_{\Gamma} \to y(\cdot) \) for (3.2) is not sufficiently smooth as to give an appropriate form of first order necessary conditions: cf., Lions [19], Lions, Magenes [20], Chapter 2. A weak formulation of first order necessary conditions for linear elliptic equations may be found in Bergounioux, Kunisch [3]. Instead of trying to prove first order necessary conditions under strong assumptions we content ourselves with deriving first order necessary conditions in a purely formal way. This form of the necessary conditions will be justified by its analogy in the first order necessary conditions for the discretized version of the elliptic problem; cf. Section 4.2.

Denote an optimal solution of problem (3.1)–(3.4) by \( \bar{u} \) and \( \bar{y} \). The active sets of inequality constraints (3.3) and (3.4) are

\[
J(C) := \{ x \in \Gamma \mid C(x, \bar{u}(x)) = 0 \}, \quad J(S) := \{ x \in \Omega \mid S(x, \bar{y}(x)) = 0 \}.
\]

We require the following regularity conditions:

\[
C_u(x, \bar{u}(x)) \neq 0 \quad \text{on } J(C), \quad S_y(x, \bar{y}(x)) \neq 0 \quad \text{on } J(S). \tag{3.5}
\]

Let \( q \) and \( p \) be multipliers associated with the elliptic equation and the Dirichlet boundary condition in (3.2), and let \( \lambda \) resp. \( \mu \) be the multiplier resp. the Borel measure associated with the control and state inequality constraints (3.3) and (3.4). Then the Lagrangian for
problem (3.1)–(3.4) becomes

\[
\mathcal{L}(y, u, q, p, \lambda, \mu) := \int_{\Omega} f(x, y(x)) \, dx + \int_{\Gamma} g(x, u(x)) \, dx \\
+ \int_{\Omega} \left[-\Delta y(x) + d(x, y(x))q(x)\right] \, dx + \int_{\Omega} S(x, y(x)) \, d\mu(x) \\
+ \int_{\Gamma} [y(x) - b(x, u(x))]p(x) \, dx + \int_{\Gamma} \lambda(x)C(x, u(x)) \, dx.
\]

The first order necessary condition with respect to the state variable gives

\[
\mathcal{L}_y(y, \bar{u}, \bar{q}, \bar{p}, \bar{\lambda}, \bar{\mu})y = 0 \quad \text{for all } y.
\]

Function evaluation along a stationary solution \((\bar{y}, \bar{u}, \bar{q}, \bar{p}, \bar{\lambda}, \bar{\mu})\) will be denoted henceforth by a bar, e.g., \(\bar{f} = f(x, \bar{y})\), etc. Using partial integration (Green’s theorem),

\[
\int_{\Omega} (-\Delta yq + y\Delta q) \, dx = \int_{\Gamma} (-q\partial_y y + y\partial_q q) \, dx,
\]

we rewrite \(\tilde{\mathcal{L}}_y y = 0\) as

\[
\tilde{\mathcal{L}}_y y = \int_{\Omega} \left[-\Delta \tilde{q} + \tilde{q}\tilde{d}_t + \tilde{f}_y + \tilde{S}_y \tilde{\lambda}\right] y \, dx + \int_{\Gamma} \left[\partial_y \tilde{q} - \tilde{p}\right] y \, dx - \int_{\Gamma} \tilde{q} \partial_y y \, dx = 0
\]

which holds for all functions \(y\). From this we obtain the adjoint equations:

\[
-\Delta \tilde{q}(x) + \tilde{q}(x)d_t(x, \tilde{y}(x)) + f_y(x, \tilde{y}(x)) + S_y(x, \tilde{y}(x))\tilde{\lambda} = 0 \quad \text{on } \Omega, \quad (3.6)
\]
\[
\tilde{q}(x) = 0 \quad \text{on } \Gamma. \quad (3.7)
\]

Moreover, we find the multiplier \(p = -\partial_y q\) on \(\Gamma\). Then the optimality condition for the control variable is evaluated as

\[
\tilde{L}_u u = [\tilde{g}_u + (\partial_q \tilde{q})\tilde{b}_u + \tilde{\lambda}\tilde{C}_u]u = 0 \quad \text{for all } u,
\]

which yields the minimum condition:

\[
g_u(x, \tilde{u}(x)) + \partial_q \tilde{q}(x)b_u(x, \tilde{u}(x)) + \tilde{\lambda}(x)C_u(x, \tilde{u}(x)) = 0 \quad \text{on } \Gamma. \quad (3.8)
\]

The complementarity condition is similar to (2.10):

\[
\tilde{\lambda}(x) \geq 0 \quad \text{on } J(C), \quad \tilde{\lambda}(x) = 0 \quad \text{on } \Gamma \setminus J(C), \\
d\tilde{\mu} \geq 0 \quad \text{on } J(S), \quad d\tilde{\mu} = 0 \quad \text{on } \Omega \setminus J(S). \quad (3.9)
\]

The Borel measure \(\tilde{\mu}\) has a decomposition similar to the one in (2.11).
Note that the minimum condition (3.8) agrees with the condition (2.9) if we replace \( q \) formally by \(-\partial_\nu \tilde{q}\). Hence, assuming functionals of tracking type (2.12), box constraints (2.13) for control and state and the property \( b_u \equiv 1 \), we obtain the counterparts of the control laws (2.16), (2.17).

**Case \( \alpha > 0 \):** the control is determined by

\[
\bar{u}(x) = \begin{cases} 
    u_d(x) - \partial_\nu \tilde{q}(x)/\alpha, & \text{if } u_d(x) - \partial_\nu \tilde{q}(x)/\alpha \in (u_1(x), u_2(x)), \\
    u_1(x), & \text{if } u_d(x) - \partial_\nu \tilde{q}(x)/\alpha \leq u_1(x), \\
    u_2(x), & \text{if } u_d(x) - \partial_\nu \tilde{q}(x)/\alpha \geq u_2(x).
\end{cases}
\]

(3.10)

**Case \( \alpha = 0 \):** the optimal control is of bang-bang or singular type

\[
\bar{u}(x) = \begin{cases} 
    u_1(x), & \text{if } \partial_\nu \tilde{q}(x) < 0, \\
    u_2(x), & \text{if } \partial_\nu \tilde{q}(x) > 0, \\
    \text{singular, if } \partial_\nu \tilde{q}(x) = 0 \text{ on } \Gamma_s \subset \Gamma, \text{ meas}(\Gamma_s) > 0.
\end{cases}
\]

(3.11)

Thus, for \( \alpha = 0 \) the outward normal derivative \( \partial_\nu \tilde{q}(x) \) on the boundary plays the role of a switching function. The isolated zeros of \( \partial_\nu \tilde{q}(x) \) are the switching points of a bang-bang control.

### 4. Discretization and optimization techniques

The discussion of discretization schemes is restricted to the standard situation where the elliptic operator is the Laplacian \( A = -\Delta \) and the domain is the unit square \( \Omega = (0, 1) \times (0, 1) \). The generalization to a general elliptic operator is straightforward. However, the modifications for an arbitrary domain \( \Omega \) depend essentially on the geometry of the boundary \( \Gamma \).

The purpose of this section is to develop discretization techniques by which the problem (2.1)–(2.4) with Neumann boundary conditions resp. problem (3.1)–(3.4) with Dirichlet boundary conditions is transformed into a nonlinear programming problem (NLP-problem) of the form

\[
\text{Minimize } F^h(z) \quad \text{subject to } G^h(z) = 0, \quad H(z) \leq 0.
\]

(4.1)

The functions \( F^h, G^h \) and \( H \) are sufficiently smooth and of appropriate dimension. The upper subscript \( h \) denotes the dependence on the stepsize. The optimization variable \( z \) will comprise both the state and the control variables.

The form (4.1) will be achieved by solving the elliptic Eq. (2.2) with the standard five-point-star discretization scheme. Choose a number \( N \in \mathbb{N}_+ \) and the stepsize \( h := 1/(N+1) \). Consider the mesh points

\[
x_{ij} = (ih, jh), \quad 0 \leq i, j \leq N + 1,
\]
and consider the following sets of indices \((i, j)\) residing either in the domain \(\Omega\) or on the four edges of the boundary \(\Gamma\):

\[
\begin{align*}
I(\Omega) & := \{(i, j) \mid 1 \leq i, j \leq N\}, \\
I(\Gamma) & := \{(i, j) \mid i = 1, \ldots, N, j = 0 \text{ or } j = N + 1, \\
& \quad j = 1, \ldots, N, i = 0 \text{ or } i = N + 1\}, \\
I(\tilde{\Omega}) & := I(\Omega) \cup I(\Gamma).
\end{align*}
\]

(4.2)

We have \(#I(\Omega) = N^2\) and \(#I(\Gamma) = 4 \cdot N\). Denote approximations for the values \(y(x_{ij})\) of the state variables by \(y_{ij}\) for \((i, j) \in I(\tilde{\Omega})\) and denote approximations of the values \(u(x_{ij})\) of the control variables by \(u_{ij}\) for \((i, j) \in I(\Gamma)\).

Now we shall specify the functions \(F^h, G^h, H\) for the optimization problem (4.1) both for Neumann and Dirichlet boundary conditions.

### 4.1. Neumann boundary conditions

The optimization variable \(z\) in (4.1) is taken as the vector

\[
z := \left((y_{ij}), (u_{ij})_{(i,j) \in I(\Gamma)}\right) \in \mathbb{R}^{N^2 + 4N + 4N}.
\]

Equality constraints are obtained by applying the five-point-star to the elliptic equation \(-\Delta y(x) + d(x, y(x)) = 0\) in (2.2) in all points \(x_{ij}\) with \((i, j) \in I(\Omega)\):

\[
G^h_{ij}(z) := 4y_{ij} - y_{i+1,j} - y_{i-1,j} - y_{i,j+1} - y_{i,j-1} + h^2d(x_{ij}, y_{ij}) = 0.
\]

(4.3)

The derivative \(\partial_y y(x_{ij})\) in the direction of the outward normal is approximated by the expression \(y_{ij}^n/h\) where

\[
y_{ij}^n := \begin{cases} 
    y_0 - y_{i,1}, & \text{for } j = 0, \\
    y_{i,0} - y_{1,j}, & \text{for } i = 0, \\
    y_{i+1,j} - y_{i,j+1} - y_{i,j-1} - y_{i-1,j} + h^2d(x_{ij}, y_{ij}) = 0. & \text{for } i = 1, \ldots, N \\
    y_{i,j+1} - y_{i,j}, & \text{for } j = 1, \ldots, N, \\
    y_{i,N+1} - y_{i,N}, & \text{for } j = N + 1, \\
    y_{i,N+1} - y_{i,N} & \text{for } j = N + 1, \text{ and } i = 1, \ldots, N.
\end{cases}
\]

(4.4)

Then the discrete form of the Neumann boundary condition in (2.2) leads to the equality constraints

\[
B^h(z) := y_{ij}^n - hb(x_{ij}, y_{ij}, u_{ij}) = 0 \quad \text{for } (i, j) \in I(\Gamma).
\]

(4.5)

The control and state inequality constraints (2.3) and (2.4) yield the inequality constraints

\[
S(x_{ij}, y_{ij}) \leq 0, \quad (i, j) \in I(\tilde{\Omega}),
\]

(4.6)

\[
C(x_{ij}, y_{ij}, u_{ij}) \leq 0, \quad (i, j) \in I(\Gamma).
\]

(4.7)
Observe that these inequality constraints do not depend on the meshsize \( h \). Later on, this fact will require a scaling of the Lagrange multipliers. The discretized form of the cost function (2.1) is

\[
F^h(z) := h^2 \sum_{(i,j) \in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j) \in I(\Gamma)} g(x_{ij}, y_{ij}, u_{ij}).
\]

Then the relations (4.3)–(4.8) define an NLP-problem of the form (4.1). The Lagrangian function for this NLP-problem becomes

\[
L(z, q, \mu, \lambda) := h^2 \sum_{(i,j) \in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i,j) \in I(\Gamma)} g(x_{ij}, y_{ij}, u_{ij})
\]

\[
+ \sum_{(i,j) \in I(\Omega)} q_{ij} G^h_{ij}(z) + \sum_{(i,j) \in I(\Gamma)} \mu_{ij} S(x_{ij}, y_{ij})
\]

\[
+ \sum_{(i,j) \in I(\Gamma)} [q_{ij} B^h(z) + \lambda_{ij} C(x_{ij}, y_{ij}, u_{ij})].
\]

The Lagrange multipliers \( q = (q_{ij})_{(i,j) \in I(\Omega)}, \mu = (\mu_{ij})_{(i,j) \in I(\Omega)} \) resp. \( \lambda = (\lambda_{ij})_{(i,j) \in I(\Gamma)} \) are associated with the equality constraints (4.3) and (4.5), the inequality constraints (4.6), resp. the inequality constraints (4.7). The multipliers \( \lambda \) and \( \mu \) satisfy complementarity conditions corresponding to (2.10):

\[
\lambda_{ij} \geq 0 \quad \text{and} \quad \lambda_{ij} C(x_{ij}, y_{ij}, u_{ij}) = 0 \quad \text{for all } (i, j) \in I(\Gamma),
\]

\[
\mu_{ij} \geq 0 \quad \text{and} \quad \mu_{ij} S(x_{ij}, y_{ij}) = 0 \quad \text{for all } (i, j) \in I(\Omega).
\]

The discussion of the necessary conditions of optimality

\[
0 = L_z = \left( L_{y_{ij}} (i,j) \in I(\Omega), L_{u_{ij}} (i,j) \in I(\Gamma) \right)
\]

will be performed for different combinations of indices \( (i, j) \). For indices \( (i, j) \in I(\Omega) \) we obtain the relations

\[
0 = L_{y_{ij}} = 4q_{ij} - q_{i+1,j} - q_{i-1,j} - q_{i,j+1} - q_{i,j-1} + h^2 q_{ij} d_y(x_{ij}, y_{ij})
\]

\[
+ h^2 f_y(x_{ij}, y_{ij}) + \mu_{ij} S_y(x_{ij}, y_{ij}).
\]

Hence, the Lagrange multipliers \( q = (q_{ij}) \) satisfy the five-point-star difference equations for the adjoint equation \(-\Delta \tilde{q} + \tilde{q}d_x + f_x S \tilde{\mu} = 0\) in (2.7) if we make the following identification for the Borel measure \( \tilde{\mu} \). Let \( sq(h^2) \) denote a square centered at \( x_{ij} \) with area \( h^2 \). Then we have the approximation

\[
\int_{sq(h^2)} d\tilde{\mu} \sim \mu_{ij}.
\]

Recall the decomposition (2.11) of the measure \( \tilde{\mu} = \bar{\nu} \cdot dx + \bar{v}_x \cdot \tilde{\mu}_x \). If the singular part of the measure vanishes, i.e. \( \bar{v}_x \cdot \tilde{\mu}_x = 0 \), then (4.10) yields the approximation for the
density \( \tilde{v} \):

\[
\tilde{v}(x_{ij}) \sim \mu_{ij}/h^2.
\] (4.11)

In case that the measure \( \tilde{\mu} = \tilde{v} \cdot \delta(x - x_{ij}) \) is a delta distribution, we obtain from (4.10) the relation

\[
\tilde{v}_i \sim \mu_{ij}.
\] (4.12)

For indices \((i, j) \in I(\Gamma)\) on the boundary we get, e.g., for \( j = 0, i = 1, \ldots, N \):

\[
0 = L_{y_{i0}} = -q_{i1} + q_{i0} - q_{i0}h \beta_j(x_{i0}, y_{i0}, u_{i0}) + h \beta_j(x_{i0}, y_{i0}, u_{i0})
+ \lambda_{i0} C_j(x_{i0}, y_{i0}, u_{i0}) + \mu_{i0} S_j(x_{i0}, y_{i0})
\]

This is just the discrete version of the Neumann boundary condition (2.8) if we identify

\[
h \tilde{\lambda}(x_{i0}) \sim \lambda_{i0}, \quad \int_{s(h)} d\tilde{\mu} \sim \mu_{i0},
\] (4.13)

where \( s(h) \) is a line segment on \( \Gamma \) of length \( h \) centered at \( x_{i0} \). For the special decomposition \( \tilde{\mu} = \tilde{v} \cdot dx \) this leads to the identifications

\[
\tilde{\lambda}(x_{i0}) \sim \lambda_{i0}/h, \quad \tilde{v}(x_{i0}) \sim \mu_{i0}/h.
\] (4.14)

Similar relations hold for other indices \((i, j) \in I(\Gamma)\). Finally, necessary conditions with respect to the control variables \( u_{ij}, (i, j) \in I(\Gamma) \) are determined, e.g., for indices \( j = 0, i = 1, \ldots, N \), by

\[
0 = L_{u_{i0}} = h g_a(x_{i0}, y_{i0}, u_{i0}) - q_{i0}h b_a(x_{i0}, y_{i0}, u_{i0}) + \lambda_{i0} C_a(x_{i0}, y_{i0}, u_{i0}) + \mu_{i0} S_a(x_{i0}, y_{i0}, u_{i0})
\]

This is the discrete version of the optimality condition (2.9) for the control, if we use again the identification \( h \tilde{\lambda}(x_{i0}) \sim \lambda_{i0} \).

4.2. Dirichlet boundary conditions

The Dirichlet boundary conditions in (3.2) are incorporated by the relations

\[
y_{ij} = b(x_{ij}, u_{ij}) \quad \text{for all } (i, j) \in I(\Gamma).
\] (4.15)

Hence it suffices to work with a reduced number of optimization variables in (4.1), namely we can take

\[
z := (y_{ij})_{(i,j) \in I(\Omega)}, (u_{ij})_{(i,j) \in I(\Gamma)} \in \mathbb{R}^{N^2 + 4N}.
\]
The *equality constraints* agree with those from (4.3),

\[ G^h_{ij}(z) := 4y_{ij} - y_{i+1,j} = y_{i,j+1} - y_{i,j-1} = h^2d(x_{ij}, y_{ij}) = 0 \]  

(4.16)

for all indices \((i, j) \in I(\Omega)\) where the values \(y_{ij}\) on the boundary are substituted from the relations (4.15). The control and state inequality constraints (3.3) resp. (3.4) give rise to the *inequality constraints*:

\begin{align*}
S(x_{ij}, y_{ij}) & \leq 0, \quad (i, j) \in I(\Omega), \\
C(x_{ij}, u_{ij}) & \leq 0, \quad (i, j) \in I(\Gamma).
\end{align*}

(4.17) (4.18)

Finally, the cost function is derived from (3.1) as

\[ F^h(z) := h^2 \sum_{(i, j) \in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i, j) \in I(\Gamma)} g(x_{ij}, u_{ij}). \]

(4.19)

By means of (4.16)–(4.19) we have obtained an NLP-problem of the form (4.1).

Let us evaluate the first order optimality conditions of Kuhn-Tucker type for problem (4.16)–(4.19). The Lagrangian function becomes

\[ L(z, q, \mu, \lambda) := h^2 \sum_{(i, j) \in I(\Omega)} f(x_{ij}, y_{ij}) + h \sum_{(i, j) \in I(\Gamma)} g(x_{ij}, u_{ij}) \\
+ \sum_{(i, j) \in I(\Omega)} [q_{ij}G^h_{ij}(z) + \mu_{ij}S(x_{ij}, y_{ij})] + \sum_{(i, j) \in I(\Gamma)} \lambda_{ij}C(x_{ij}, u_{ij}), \]

(4.20)

where the Lagrange multipliers \(q = (q_{ij})_{(i, j) \in I(\Omega)}, \mu = (\mu_{ij})_{(i, j) \in I(\Omega)}\) and \(\lambda = (\lambda_{ij})_{(i, j) \in I(\Gamma)}\) are associated with the equality constraints (4.16), the inequality constraints (4.17), and the inequality constraints (4.18). The multipliers \(\lambda\) and \(\mu\) satisfy the complementarity conditions corresponding to (3.9):

\[ \lambda_{ij} \geq 0 \quad \text{and} \quad \lambda_{ij}C(x_{ij}, u_{ij}) = 0 \quad \text{for all } (i, j) \in I(\Gamma), \]
\[ \mu_{ij} \geq 0 \quad \text{and} \quad \mu_{ij}S(x_{ij}, y_{ij}) = 0 \quad \text{for all } (i, j) \in I(\Omega). \]

In the next step we discuss the necessary conditions of optimality

\[ 0 = L_z = \left( L_{y_{ij}} \right)_{(i, j) \in I(\Omega)}, \left( L_{u_{ij}} \right)_{(i, j) \in I(\Gamma)} \]

for different combinations of indices \((i, j)\). For indices \(2 \leq i, j \leq N - 1\) we obtain the relations

\[ 0 = L_{y_{ij}} = 4q_{ij} - q_{i+1,j} = q_{i,j+1} - q_{i,j-1} + h^2d(x_{ij}, y_{ij}) + h^2f_y(x_{ij}, y_{ij}) + \mu_{ij}S_y(x_{ij}, y_{ij}). \]
Hence, for this set of indices we see that the Lagrange multipliers $q = (q_{ij})$ satisfy the five-point-star difference equations for the adjoint equation $-\Delta \bar{q} + \bar{q}d_y + f_y + S_y \bar{\mu} = 0$ in (3.6) if we use the same identification for the Borel measure $\bar{\mu}$ as in (4.10),

$$\int_{\partial (\Omega)} d\bar{\mu} \sim \mu_{ij}. \quad (4.21)$$

from which we also get the special cases (4.11) and (4.12). The situation is different for indices with either $i = 1; j = 1; i = N$ or $j = N$. E.g., for indices $j = 1; i = 2, \ldots, N - 1$, we get

$$0 = L_{yi} = 4q_{11} - q_{i+1,1} - q_{i-1,1} - q_{i2} + h^2 q_{11} d_y(x_{i1}, y_{i1}) + h^2 f_y(x_{i1}, y_{i1}) + \mu_{i1} S_y(x_{i1}, y_{i1}).$$

Note that this equation does not involve the variable $q_{10}$ on the boundary. Defining $q_{10} = 0$ we arrive again at the discretized form of the adjoint Eq. (3.6) using approximations as in (4.10)–(4.12). Similar relations hold for index combinations $i = 1; j = 2, \ldots, N - 1$, or $i = N; j = 2, \ldots, N - 1$, or $j = N; i = 2, \ldots, N - 1$. For the remaining indices we find, e.g. for $i = j = 1$:

$$0 = L_{y1} = 4q_{11} - q_{21} - q_{12} + h^2 q_{11} d_y(x_{11}, y_{11}) + h^2 f_y(x_{11}, y_{11}) + \mu_{11} S_y(x_{11}, y_{11}).$$

These relations do not involve the boundary variables $q_{10}$ and $q_{01}$. Again, defining $q_{10} = 0$ and $q_{01} = 0$ we recover the adjoint equations. In summary, by requiring the Dirichlet boundary condition for the adjoint variables,

$$q_{ij} = 0 \quad \text{for } (i, j) \in I(\Gamma),$$

we see that the adjoint equation holds for all indices $(i, j) \in I(\Omega)$.

The necessary conditions with respect to the control variables $u_i$ are determined for the indices $j = 0, i = 1, \ldots, N$, by

$$0 = L_{u_0} = h g_u(x_{i0}, u_{i0}) - q_{i1} b_u(x_{i0}, u_{i0}) + \lambda_{i0} C_u(x_{i0}, u_{i0})$$

$$= h \left[ g_u(x_{i0}, u_{i0}) - \frac{q_{i1} b_u(x_{i0}, u_{i0})}{h} + \frac{\lambda_{i0}}{h} C_u(x_{i0}, u_{i0}) \right].$$

Observing $q_{10} = 0$ and the approximation of the normal derivative in (4.4), the minimum condition (3.8) holds with the identifications

$$\partial_n \bar{q}(x_{i0}) \sim -q_{i1}/h, \quad \bar{\lambda}(x_{i0}) \sim \lambda_{i0}/h \quad (4.22)$$

Similar identifications hold for the other indices $(i, j) \in I(\Gamma)$. 

OPTIMIZATION TECHNIQUES
4.3. Optimization codes and modeling environment

For the numerical solution of all problems considered in the following section a combination of the AMPL [12] algebraic modeling language and the interior point solver LOQO [23] proved to be both convenient and powerful. In order to make the formulation of mathematical optimization problems generic and independent of both the actual solver used and the programming language it is written in, modeling languages were developed. AMPL provides interfaces to a large number of solvers, both commercial and free-for-research codes. One of the latter ones is LOQO which grew out of an interior point LP optimizer to a convex QP and very recently to a general NLP solver implementing an interior point approach. Although the code is currently still being perfected it proved to be very efficient for the solution of large-scale nonlinear problems in the benchmarks of [21]. It was thus chosen for the following computations; see also the comparison in Example 5.1 below. It should be remarked that LOQO implements an infeasible primal-dual path-following method. The KKT necessary conditions are essentially solved as a system of nonlinear equations with a Newton-like method. Therefore, it causes no problem if iterates are not feasible because it only means that residuals or right-hand sides corresponding to the equality constraints are not zero. At least asymptotically feasibility will be attained. Another feature that makes AMPL attractive and that was exploited is its automatic differentiation capability. Only functions for objective and constraints need to be provided.

5. Numerical examples

We consider elliptic problems with the following specifications: the cost functional is of tracking type (2.13), the elliptic operator in (2.2) is the Laplacian $A = -\Delta$ on the unit square $\Omega = (0, 1) \times (0, 1)$, and the control and state constraints are box constraints given in (2.14). The choice of symmetric functions $y_d(x)$ and $u_d(x)$ in the tracking functional, implies that the optimal control is the same on every edge of $\Gamma = \partial \Omega$. However, we have treated the discretized controls on every edge of $\Gamma$ as independent optimization variables. The symmetry of the optimal control will then be a result of the optimization procedure.

Tests for the following examples were run with different stepsizes and starting values. For convenience, in the sequel we shall report on results obtained for fixed stepsize and starting values:

$$N = 99, \quad h = 1/(N + 1) = 1/100, \quad u_{ij} = 0, \quad y_{ij} = 0.$$  

First, we report on 4 examples with Dirichlet boundary conditions for which partial numerical results are available in the literature.

5.1. Dirichlet boundary conditions

Example 5.1. To enable a comparison, we consider first the example in Bergounioux, Kunisch [3], Section 5.2, with the following data:

$$\text{on } \Omega: \quad -\Delta y(x) = 20, \quad y(x) \leq 3.5, \quad y_d(x) = 3 + 5x_1(x_1 - 1)x_2(x_2 - 1),$$

$$\text{on } \Gamma: \quad y(x) = u(x), \quad 0 \leq u(x) \leq 10, \quad u_d(x) = 0, \quad \alpha = 0.01.$$
The following results were obtained, they are explained below:

Cost functional: $F(\bar{y}, \bar{u}) = 0.196525$, CPU seconds: 96

The optimal control is shown in figure 1. The optimal state and adjoint variable are not shown here, because they are very similar to those in figure 3 where $\alpha = 0.01$ is replaced by $\alpha = 0.0$. It should be noted that the output of Lagrange multipliers is provided by AMPL. It is no difficulty for primal-dual methods to produce multipliers since, in fact they are variables that are computed simultaneously with the primal problem variables. The control constraints are not active while the state variable attains its upper bound only in the center $x_{ij} := (0.5, 0.5)$ of the unit square with dual variable $\mu_{ij} = 0.24602$. This is in agreement with the results in [3]. It can be checked that the adjoint Eq. (3.6) holds in the discretized version with $\Delta_h$ denoting the discretized Laplacian,

$$-\Delta_h \tilde{q}(x) + \tilde{y}(x) - y_d(x) = 0 \quad \text{for } x \neq x_{ij},$$

$$-\Delta_h \tilde{q}(x) + \tilde{y}(x) - y_d(x) + \mu_{ij}/h^2 = 0 \quad \text{for } x = x_{ij}.$$

We verify the second equation in the active gridpoint $x_{ij} = (0.5, 0.5)$ where the following data were obtained: $q_{ij} = -0.21312$, $q_{i-1,j} = -0.15161$, $y_{ij} = 3.5$, $y_{ij} - y_d(x_{ij}) = 0.1875$, $\mu_{ij}/h^2 = 2460.2$. Note that the adjoint function is symmetric around $x_{ij}$. Hence the adjoint equations hold with $-\Delta_h \tilde{q}(x_{ij}) = 4 \cdot (q_{ij} - q_{i-1,j})/h^2 = -2460.40$ and $y_{ij} - y_d(x_{ij}) + \mu_{ij}/h^2 = 2460.39$. The measure $\tilde{\mu}$ in (3.6) is a delta distribution, $\tilde{\mu} = \tilde{v}_s \cdot \delta(x - x_{ij})$, with $\tilde{v}_s \sim \mu_{ij} = 0.24602$ in view of (4.12).

This example will also be used to illustrate the numerical process in more detail.
Table 1. Detailed information on solution of Example 5.1.

<table>
<thead>
<tr>
<th>N + 1</th>
<th>it</th>
<th>AMPL</th>
<th>LOQO</th>
<th>Acc</th>
<th>F(\hat{y}, \hat{u})</th>
<th>y(A, .5)</th>
<th>w(0, .5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>25</td>
<td>1</td>
<td>10</td>
<td>8</td>
<td>.188170</td>
<td>3.449184</td>
<td>1.686801</td>
</tr>
<tr>
<td>100</td>
<td>26</td>
<td>6</td>
<td>96</td>
<td>8</td>
<td>.196525</td>
<td>3.449163</td>
<td>1.690270</td>
</tr>
<tr>
<td>200</td>
<td>29</td>
<td>23</td>
<td>1477</td>
<td>8</td>
<td>.200772</td>
<td>3.449158</td>
<td>1.692029</td>
</tr>
</tbody>
</table>

Table 2. Comparison of different solvers on Example 5.1.

<table>
<thead>
<tr>
<th>N + 1</th>
<th>LANCELOT</th>
<th>LOQO</th>
<th>MINOS</th>
<th>SNOPT</th>
<th>BPMPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>7.1</td>
<td>1</td>
<td>5.6</td>
<td>8</td>
<td>.5</td>
</tr>
<tr>
<td>70</td>
<td>15.4</td>
<td>1</td>
<td>10.2</td>
<td>(unbd)</td>
<td>.3</td>
</tr>
<tr>
<td>90</td>
<td>16.2</td>
<td>1</td>
<td>(inf)</td>
<td>(unbd)</td>
<td>.28</td>
</tr>
<tr>
<td>200</td>
<td>–</td>
<td>1</td>
<td>–</td>
<td>–</td>
<td>.14</td>
</tr>
</tbody>
</table>

In Table 1 we summarize the data: size of grid, number of iterations of LOQO, times in seconds for the AMPL compilation and the solution by LOQO, the accuracy as the number of correct significant digits in the objective function value. The primal-dual approach yields upper and lower bounds for this value and thus permits such a statement. In all the following examples this accuracy measure was at least 8 and is therefore not listed. Finally, we list the objective function value and one representative value of both the state and the control variable. While the state variable not far from the active center point has a small error, the control at the midpoints of the edges still varies in the fourth digit. Thus, N + 1 = 100 was chosen for the subsequent calculations. Since the AMPL times were in the range of a few seconds or a few percent of the solution times they will not be given below.

We compare LOQO and other solvers with AMPL interface available to us in Table 2. For N + 1 = 100 not all the codes considered (LANCELOT-A, MINOS-5.5, SNOPT-5.3, BPMPD-2.21; links to all codes in [21]) were successful. Therefore, results are listed for several coarser grids as well as for the finest grid used with LOQO. Given are CPU times on the same platform used above, but scaled to LOQO’s time. MINOS reports one problem as infeasible while SNOPT reports two problems as unbounded. The reason for these messages may also be a “bad starting guess”. All solvers were given the same AMPL file and AMPL initializes variables with zero. For N + 1 = 200 all solvers except LOQO and BPMPD exceeded the available memory (256MB). The convex QP code BPMPD solves with increasing efficiency compared to LOQO but this is only possible, because, in fact, Example 5.1 is a convex QP problem. BPMPD is not applicable to most of the other examples solved below. For another comparison see Example 5.7.

Example 5.2. All data are the same as in Example 5.1 except that we choose α = 0.0 instead of α = 0.01. According to the optimal control law (3.11) we can expect either a bang-bang or a singular control. We find the following results:

Cost functional: \( F(\hat{y}, \hat{u}) = .096695 \), CPU seconds: 78
The optimal control, adjoint variable and optimal state are shown in figures 2 and 3. Both the control and state constraints do not become active. Hence, the optimal control is totally singular on $\Gamma$. This is in accordance with the control law (3.11) since the normal derivative of the adjoint variable satisfies $\partial_\nu \tilde{q} |_{\Gamma} \equiv 0$ which follows from the numerical results $q_{1,1} \equiv 0$ in view of (4.4). In figure 3 as in figures 5 and 7 below the vertical axis is labeled $y/u$ since for these examples both the state and the control are plotted in these figures.
Example 5.3. The data are the same as in Example 5.1 except that we choose more restrictive state and control constraints:

\[
\begin{align*}
\text{on } \Omega: & \quad -\Delta y(x) = 20, \quad y(x) \leq 3.2, \quad y_d(x) = 3 + 5x_1(x_1 - 1)x_2(x_2 - 1), \\
\text{on } \Gamma: & \quad y(x) = u(x), \quad 1.6 \leq u(x) \leq 2.3, \quad u_d(x) \equiv 0, \quad \alpha = 0.01.
\end{align*}
\]

We obtain the following results:

Cost functional: \( F(\tilde{y}, \tilde{u}) = .321010, \) CPU seconds: 103

The optimal control, state and adjoint variable are shown in figures 4 and 5. The optimal control is continuous and has two boundary arcs with \( \tilde{u}(x) = 2.3 \) and one boundary arc with \( \tilde{u}(x) = 1.6 \). The junction points with the boundary are the points \( x_1 = (.02, 0), x_2 = (.18, 0), x_3 = (.23, 0), x_4 = (.77, 0), x_5 = (.82, 0), x_6 = (.98, 0) \) on the bottom edge of \( \Gamma \). By inspecting the switching function in figure 4, we can verify the control law (3.10). The assumption \( b \equiv 1 \) underlying (3.10) obviously holds. Let us check the control condition on the bottom edge of \( \Gamma \) at the points \( x_i \). Observe that \( \partial_b q(x_i) \sim -q_{i1}/h \) according to (4.22) since we have \( q_{i0} = 0 \). Then in view of \( \alpha = h = .01 \) the control law (3.10) takes the form

\[
\tilde{u}(x_0) \sim u_{i0} = \begin{cases} 
q_{i1} \cdot 10^4, & \text{if } q_{i1} \cdot 10^4 \in (1.6, 2.3), \\
1.6, & \text{if } q_{i1} \cdot 10^4 \leq 1.6, \\
2.3, & \text{if } q_{i1} \cdot 10^4 \geq 2.3.
\end{cases}
\]

Figure 4. Optimal control and switching function for Example 5.3.
The active set for the state constraint \(y(x) \leq 3.2\) is the center point \(\bar{x} = x_{ij} = (0.5, 0.5)\). The dual variable for this active inequality constraint is \(\mu_{ij} = .642712\). Again, with these data the validity of the adjoint equation (3.6) can be verified in its discretized form.

**Example 5.4.** The data are those from Example 5.3 but now we choose \(\alpha = 0.0\) expecting to obtain a bang-bang control in contrast to the totally singular control in Example 5.2. This expectation is met with the following results:

Cost functional: \(F(\bar{y}, \bar{u}) = .249178, \text{CPU seconds: } 116\)

The optimal control shown in figure 6 is indeed bang-bang. The switching function on the bottom edge of \(\Gamma\) is \(\partial_u q(x_{i0}) \sim -q_1/h\) according to (4.22). Then figure 6 clearly illustrates the control law (3.11):

\[
\bar{u}(x_{i0}) \sim u_{i0} = \begin{cases} 
1.6, & \text{if } q_1 < 0, \\
2.3, & \text{if } q_1 > 0.
\end{cases}
\]

The switching points on the bottom edge are \(x_1 = (2, 0), \ x_2 = (.8, 0)\). Again, the optimal state displayed in figure 7 is active at the center point \(\bar{x} = x_{ij} = (0.5, 0.5)\). The dual variable for this active inequality constraint is \(\mu_{ij} = .733781\).

### 5.2. Neumann boundary conditions

**Example 5.5.** The first problem has a linear partial differential equation and nonlinear Neumann boundary conditions with data:

on \(\Omega\): \(-\Delta y(x) = 0, \quad y(x) \leq 2.071, \quad y_d(x) = 2 - 2(x_1(x_1 - 1) + x_2(x_2 - 1)),\)

on \(\Gamma\): \(\partial_n y(x) = u(x) - y(x)^2, \quad 3.7 \leq u(x) \leq 4.5, \ u_d(x) \equiv 0, \ \alpha = 0.01.\)
The following results were obtained:

Cost functional: \( F(\bar{y}, \bar{u}) = 0.553324, \) CPU seconds: 494

The optimal control and state are shown in figures 8 and 9. Note that the sign condition (2.5) holds since \( b_y(x, y(x), u(x)) = -2y(x) \leq 0. \) The optimal control is continuous and has two boundary arcs with \( \bar{u}(x) = 3.7 \) and one boundary arc with \( \bar{u}(x) = 4.5. \) The junction points with the boundary are the points \( x_1 = (1.7, 0), x_2 = (3.4, 0), x_3 = (66, 0), x_4 = (83, 0) \) on the bottom edge of \( \Gamma. \) The control law (2.16) was derived under the assumption \( b_u = 1 \) which obviously holds in this example. By looking at the adjoint variable in figure 8, the
The reader may verify that the control law (2.16) is satisfied:

\[
\tilde{u}(x) = \begin{cases} 
\bar{q}(x) \cdot 100, & \text{if } \bar{q}(x) \cdot 100 \in (3.7, 4.5), \\
3.7, & \text{if } \bar{q}(x) \cdot 100 \leq 3.7, \\
4.5, & \text{if } \bar{q}(x) \cdot 100 \geq 4.5. 
\end{cases}
\]

The active set for the state constraint \(y(x) \leq 2.071\) are the midpoints of the edges. The dual variable for this active inequality constraint is \(\mu_{ij} = .00045274\). It can be checked that the adjoint Eqs. (2.7) and (2.8) hold observing the scaling (4.13). As an example, let us
test the Neumann boundary condition (2.8) at the active point $\bar{x} = x_{i0} = (0.5, 0.)$. Hence, we have to verify the relation $q_{i0} - q_{i1} + 2q_{i0} \cdot h \cdot y_{i0} + \mu_{i0} = 0$ which corresponds to the equation $\partial \tilde{q}(\bar{x}) + 2 \cdot \tilde{q}(\bar{x}) \cdot \tilde{y}(\bar{x}) + \bar{\mu} = 0$. We find $q_{i0} = -0.046506$, $q_{i1} = -0.048885$, $y_{i0} = 2.071$, $\mu_{i0} = -0.00045274$ and can check indeed the Neumann condition with $q_{i0} - q_{i1} + 2q_{i0} \cdot h \cdot y_{i0} = 0.0004528$ which agrees with $-\mu_{i0} = 0.00045274$.

**Example 5.6.** The data for the second Neumann problem are:

<table>
<thead>
<tr>
<th>Condition</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>on $\Omega$</td>
<td>$-\Delta y(x) = 0$, $y(x) \leq 2.835$, $y_d(x) = 2 - 2(x_1(x_1 - 1) + x_2(x_2 - 1))$, $6 \leq u(x) \leq 9$, $u_d(x) \equiv 0$, $a = 0$.</td>
</tr>
<tr>
<td>on $\Gamma$</td>
<td>$\partial_y y(x) = u(x) - y(x)^2$, $6 \leq u(x) \leq 9$, $u_d(x) \equiv 0$, $a = 0$.</td>
</tr>
</tbody>
</table>

According to the optimal control law (2.17) we can expect either a bang-bang or a singular control. We get the following results:

Cost functional: $F(\bar{y}, \bar{u}) = 0.015078$, CPU seconds: 864

The optimal control in figure 10 is indeed bang-bang. The switching function $\tilde{q}$ on $\Gamma$ as shown in figure 10 obeys the optimal control law (2.17):

$$\tilde{u}(x) = \begin{cases} 
6, & \text{if } \tilde{q}(x) < 0, \\
9, & \text{if } \tilde{q}(x) > 0.
\end{cases}$$

![Figure 10](image-url) Optimal control and switching function for Example 5.6.
The switching points are approximately $x_1 = (.33, 0)$, $x_2 = (.67, 0)$. Again, the optimal state displayed in figure 11 is active at the midpoints of the edges. The dual variable for this active inequality constraint is $\mu_{ij} = .00002929$.

**Example 5.7.** In this example we choose a nonlinear partial differential equation and linear Neumann boundary conditions:

$$
on \Omega: \quad -\Delta y(x) - y(x) + y(x)^3 = 0, \quad y(x) \leq 2.7,$$

$$y_d(x) = 2 - 2(x_1(x_1 - 1) + x_2(x_2 - 1)), \quad 1.8 \leq u(x) \leq 2.5, \quad u_d(x) \equiv 0, \quad \alpha = 0.01.$$

These equations represent a simplified *Ginzburg-Landau model* for superconductivity in the absence of internal magnetic fields with $y$ the wave function; cf. Ito, Kunisch [16] and Kunisch, Volkwein [18] where tracking functions and control or state constraints have been considered that are different from those used here. LOQO and AMPL provide the results:

Cost functional: $F(\bar{y}, \bar{u}) = .264163$, CPU seconds: 317

The optimal control and state are shown in figures 12 and 13. The optimal control is continuous and has two boundary arcs with $\bar{u}(x) = 1.8$ and one boundary arc with $\bar{u}(x) = 2.5$. The junction points with the boundary are the points $x_1 = (.15, 0)$, $x_2 = (.28, 0)$, $x_3 = (.72, 0)$, $x_4 = (.85, 0)$ on the bottom edge of $\Gamma$. The adjoint variable in figure 12 shows that the control law (2.16) is satisfied:

$$\bar{q}(x) \cdot 100 > 0.1 \quad \text{if} \quad \bar{q}(x) \cdot 100 \in (1.8, 2.5),$$

$$1.8, \quad \text{if} \quad \bar{q}(x) \cdot 100 \leq 1.8,$$

$$2.5, \quad \text{if} \quad \bar{q}(x) \cdot 100 \geq 2.5.$$

The active set for the state constraint $y(x) \leq 2.7$ comprises the points adjacent to the corners of the domain. The dual variable for this active inequality constraint is $\mu_{ij} = .0034574$. 

Figure 11. Optimal state and adjoint variable for Example 5.6.
For this problem the QP-code BPMPD is not applicable. Both MINOS and SNOPT return with error messages as in Example 5.1, while LANCELOT solves the example on grids of \( N + 1 = 50, 70, 90 \) and needs 2 respectively 8.4 respectively 7.2 times as long as LOQO.

**Example 5.8.** The data are those from Example 5.7 but now we choose \( \alpha = 0.0 \) expecting to obtain a bang-bang control. The numerical results are:

Cost functional: \( F(\bar{\bar{y}}, \bar{u}) = .165531 \), CPU seconds: 570
The optimal control shown in figure 14 is indeed bang-bang. The switching function \( q \) on \( \Gamma \) as shown in figure 14 yields the optimal control law (2.17):

\[
\begin{align*}
\bar{u}(x) &= \begin{cases} 
1.8, & \text{if } \tilde{q}(x) < 0, \\
2.5, & \text{if } \tilde{q}(x) > 0.
\end{cases}
\end{align*}
\]

The switching points are approximately \( x_1 = (.21, 0) \), \( x_2 = (.79, 0) \). Again, the optimal state displayed in figure 15 is active at the points adjacent to the corners of the domain. The dual variable for this active inequality constraint is \( \mu_{ij} = .030118 \).
6. Conclusions

Numerical techniques have been developed for solving semilinear elliptic control problems subject to control and state constraints. In the first part of two papers on this subject, boundary control problems with either Dirichlet or Neumann boundary conditions have been treated. We have proposed discretization schemes by which the elliptic control problem is transcribed into a nonlinear programming problem. Since both control and state variables are treated as optimization variables, the resulting NLP-problem is a high-dimensional problem with a sparse structure. Testing different optimization codes, we found that the interior point method LOQO of Vanderbei, Shanno [23] is particularly efficient and reliable. The algorithm provided solution for all types of controls: regular controls, bang-bang controls and singular controls. In each case, we have checked the necessary conditions of optimality for the adjoint variables.

After finishing this paper, we learned about the paper of Bergounioux et al. [2] where interior point methods are compared with methods developed in [3]. We are currently extending our approach to include a test of second order sufficient conditions (SSC). The test of (SSC) can be performed by showing that the projected Hessian of the Lagrangian is positive definite. The importance of (SSC) lies in the fact that it provides a basis for sensitivity analysis and real-time control of perturbed systems; cf., e.g., [7, 8]. Presently, we are carrying over these techniques to elliptic control problems.

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We would like to thank Professor Fredi Tröltzsch for discussions on the necessary conditions for Dirichlet boundary conditions. Helmut Maurer was supported by the Deutsche Forschungsgemeinschaft (DFG) under MA 691/8-2.

References